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Supplemental Material

Differential *in Vitro* Biological Action, Coregulator Interactions, and Molecular Dynamic Analysis of Bisphenol A (BPA), BPAF, and BPC Ligand–ERα Complexes

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Table of Contents

- **Table S1.** qPCR primers used in this study.
- **Table S2.** 74 peptides that positively interact with the E2/ERα complex derived from 32 coregulator.
- **Table S3.** 8 peptides that positively interact with the BPA/ER α complex derived from 7 coregulators.
- **Table S4.** 9 peptides that positively interact with the BPAF/ER α complex derived from 9 coregulators.
- **Table S5.** 25 peptides that positively interact with the BPS/ERα complex derived from 14 coregulators.
- **Table S6.** 35 peptides that negatively interact with the E2/ER α complex derived from 22 coregulators.
- **Table S7.** 44 peptides that negatively interact with the BPA/ERα complex derived from 28 coregulators.
- **Table S8.** 75 peptides that negatively interact with the BPAF/ERα complex derived from 38 coregulators.
- **Table S9.** 31 peptides that negatively interact with the BPS/ER α complex derived from 23 coregulators.

- **Figure S1.** Working model of the MARCoNI assay. Cell lysates ware isolated from the EGFP-tagged full-length human ER α -transfected U2OS cells. For MARCoNI, 25 μL assay mixtures that contain cell lysates, 25 nM of Alexa488-conjugated GFP-antibody (Invitrogen), and 0.2 mM ligand (E2, BPA, BPAF or BPS, pre-diluted in DMSO, final concentration 2%) were prepared on ice. The ligand-modulated coregulator interactions with the EGFP-tagged ER α was assessed using a PamChip® plate which contained the 154 coregulator-derived binding peptides. The positive interaction means that ligand increases peptide binding and negative interaction means that the ligand decreases peptide binding to ER α .
- **Figure S2.** Ligand interactions from the reported X-ray crystal structures. The ligand interactions with ER that were found in the X-ray crystal structures (A) E2, (B) BPA, and (C and D) BPAF in two conformations.
- **Figure S3.** Root mean square deviations (RMSD) of ligand-free ER structures started at agonist (black) and antagonist (red) forms. The X-ray crystal structures were used as the reference structures for RMSD calculations and all backbone heavy atoms of each residue were used to calculate the average RMSD at each time point.
- **Figure S4.** Ligand free conformations of ER α (starting with aqueous agonist form). Starting conformation is in white and the final conformation is in red. The three helices that are involved in creating the coregulator surface are marked.
- **Figure S5.** Ligand free conformations of $ER\alpha$ (starting with antagonist form). Starting conformation is in white and the final conformation is in red.
- **Figure S6.** Root mean square deviations (RMSD) of various ligand bound-ER structures. The X-ray crystal structures were used as the reference structures for these calculations and all backbone heavy atoms of each residue were used to calculate the average RMSD at each time point. For BPA, BPAF, and BPS, the black curve corresponds to the starting ligand in conformation "1" and the red curve to the ligand in conformation "2".
- **Figure S7.** E2-bound conformation of ER α (in which h12 is in agonist conformation). The final conformation of ER α with E2 from the MD simulation.
- **Figure S8.** BPA-bound conformations of ER α . The final conformation of ER α with BPA started in conformation 1 is shown in the blue ribbon; The final conformation of ER α with BPA started in conformation 2 is shown in the red ribbon. BPA is shown in space filling in the ligand binding site of ER α .
- **Figure S9.** BPAF-bound conformations of ER α . The final conformation of ER α with BPAF started in conformation 1 is show in the blue ribbon; The final conformation of ER α with BPAF started in conformation 2 is shown in the red ribbon. BPAF is shown in space filling in the ligand binding site of ER α .
- **Figure S10.** BPS-bound conformations of ER α . The final conformation of ER α with BPS started in conformation 1 is shown in the blue ribbon; The final conformation of ER α with BPS started in conformation 2 is shown in the red ribbon. BPS is shown in space filling in the ligand binding site of ER α .

Figure S11. Root mean square deviations (RMSD) of the ligands in their aqueous environments. Starting structures were used as the reference structures for these calculations and all heavy atoms of the ligand were used to calculate the average RMSD at each time point.

Additional File - Excel Document.

Table S1. qPCR primers used in this study

| Gene symbol and GenBank accession number | Sequence (5'-3') |
|--|----------------------------|
| Human <i>WISP2/CNN5</i> | F: TGAGCGGCACACCGAAGAC |
| (NM_003881) | R: ACAGCCATCCAGCACCAG |
| Human <i>PGR</i> | F: GACGTGGAGGGCGCATAT |
| (NM_000926.4) | R: GCAGTCCGCTGTCCTTTTCT |
| Human <i>GREB1</i> | F: CAAAGAATAACCTGTTGGCCC |
| (NM_014668) | R: GACATGCCTGCGCTCTCATAC |
| Human <i>β-actin</i> | F: GACAGGATGCAGAAGGAGATCAC |
| (NM_001101) | R: GCTGATCCACATCTGCTGGAA |

Table S2. 74 peptides that positively interact a with the E2/ER α complex derived from 32 coregulator

| Peptide | Relative | Coregulator |
|--------------------------|----------------------------|---|
| | binding value ^b | |
| BL1S1_1_11 | 5.8 | BLOC-1: biogenesis of lysosome-related organelles complex-1 |
| | | subunit 1 |
| BRD8_254_276 | 34.3 | TrCP120: thyroid hormone receptor coactivating protein 120kDa |
| CBP_2055_2077 | 1.3 | CBP: CREB-binding protein |
| CBP_57_80 | 24.4 | |
| CENPR_1_18 | 1.5 | CENP-R: centromere protein R |
| EP300_69_91 | 16.5 | P300: histone acetyltransferase p300/E1A-associated protein p300 |
| GNAQ_21_43 | 5.4 | Gαq : guanine nucleotide-binding protein alpha-q |
| HAIR_745_767_C755S/C759S | 18.3 | H: protein hairless |
| IKBB_277_299 | 3.1 | NFkB:NF-kappa-B inhibitor beta |
| ILK_131_153 | 4.5 | ILK-1/p59ILK: Integrin-liked protein kinase |
| JHD2C_2054_2076 | 19.0 | TRIP-8: thyroid receptor-interacting protein 8 |
| LCOR_40_62 | 34.5 | LCoR: ligand-dependent corepressor |
| MED1 591 614 | 11.2 | TRIP-2: thyroid receptor-interacting protein 2 |
| MED1_632_655 | 21.1 | β μ. σ. σ. γ. σ. σ. σ. σ. γ. σ. |
| MLL2 4175 4197 | 2.7 | MLL2/KMT2B: myeloid/lymphoid or mixed-lineage leukemia |
| MLL2_4702_4724 | 3.0 | protein 2 |
| NCOA1_1421_1441 | 5.6 | SRC-1/RIP160: nuclear receptor co-activator 1 |
| NCOA1_620_643 | 45.1 | |
| NCOA1 677 700 | 5.5 | |
| NCOA1_737_759 | 47.5 | |
| NCOA2_628_651 | 12.8 | SRC-2/NCoA-2: nuclear receptor co-activator 2 |
| NCOA2_677_700 | 9.7 | ' ' |
| NCOA2_733_755 | 8.6 | |
| NCOA3_104_123_N-KKK | 2.5 | SRC-3/NCoA-3: nuclear receptor co-activator 3 |
| NCOA3_609_631 | 21.1 | · |
| NCOA3_609_631_C627S | 13.1 | |
| NCOA3_673_695 | 5.8 | |
| NCOA3_725_747 | 6.3 | |
| NCOA6_875_897 | 7.6 | NCoA-6: nuclear receptor co-activator 6 |
| NCOR1_2376_2398 | 2.8 | N-CoR1: nuclear receptor corepressor 1 |
| NELFB_428_450 | 2.2 | NELF-B: negative elongation factor B |
| NELFB 80 102 | 4.9 | |
| NR0B1_1_23 | 7.3 | DAX-1: nuclear receptor subfamily group B member 1 |
| NR0B1_136_159 | 3.9 | |
| NR0B1_68_90_C69S | 6.8 | |
| NR0B2_106_128 | 12.2 | SHP: small heterodimer partner/nuclear receptor subfamily |
| NR0B2_201_223_C207S | 11.1 | member 2 |
| NR0B2_9_31_C9S/C11S | 3.4 | |
| NRBF2_128_150 | 10.4 | NRBF-2: nuclear receptor subfamily 0 group B member 2 |

| NRIP1 1055 1077 | 6.7 | RIP140: receptor-interacting protein 1 |
|--------------------------|------|---|
| NRIP1 120 142 | 15.3 | |
| NRIP1_121_143_P124R | 7.3 | |
| NRIP1_173_195 | 6.6 | |
| NRIP1_173_195_C177S | 4.0 | |
| NRIP1_253_275_C263S | 21.3 | |
| NRIP1_368_390 | 5.1 | |
| NRIP1_488_510 | 8.1 | |
| NRIP1_700_722 | 4.4 | |
| NRIP1_701_723 | 4.4 | |
| NRIP1_805_831 | 4.3 | |
| NRIP1_924_946 | 3.2 | |
| NRIP1_924_946_C945S | 4.5 | |
| NSD1_894_916 | 7.4 | NSDP1: NR-binding SET domain-cotaining protein |
| PELP1_168_190 | 1.2 | PELP1: proline-, glutamic acid-, and leucine-rich protein 1 |
| PELP1_20_42 | 2.0 | |
| PELP1_446_468 | 9.5 | |
| PNRC1_306_327 | 1.7 | PNRC1/B4-2: proline-rich nuclear receptor coactivator 1 |
| PPRC1_151_173 | 6.3 | PRC: PGC-1 related coactivator |
| PR285_1105_1127 | 6.1 | PDIP1: PPAR-gamma DBD-interacting protein 1 |
| PRGC1_130_155 | 5.8 | PGC1α: PPAR-g co-activator 1-alpha |
| PRGC1_134_154 | 5.2 | |
| PRGC2_146_166 | 7.1 | PGC1β: PPAR-g co-activator 1-alpha |
| PRGC2_338_358 | 6.0 | |
| PROX1_57_79 | 12.7 | PROX1: homeobox prospero-like protein |
| RBL2_875_897_C879S/C894S | 1.4 | |
| TIF1A_747_769 | 4.6 | |
| TIP60_476_498 | 12.1 | Tip60: 60 kDa Tat interactive protein |
| TREF1_168_190 | 43.7 | TReP132: transcriptional –regulating factor 1 |
| TRXR1_132_154 | 13.1 | TR: thioredoxinreduactase TR1 |
| UBE3A_649_671 | 2.8 | E6-AP: E6AP ubiquitin protein ligase |
| WIPI1_119_141 | 19.2 | WIPI-1: WD repeat phosphoinositide-interacting protein 1 |
| WIPI1_313_335_C318S | 6.1 | |
| ZNHI3_89_111 | 5.5 | TRIP-3: thyroid receptor interacting protein 3 |
| ZNT9_449_471 | 2.1 | ZnT-9/HUEL: zinc transporter 9/humanembrynic lung protein |

^aPositive interactions defined as: binding value>50, relative binding >1, p-value <0.05 ^bRelative binding value shows each peptide binding relative to the control, 2% DMSO For complete results, see Excel Table S2

Table S3. 8 peptides that positively interact^a with the BPA/ERα complex derived from 7 coregulators

| Peptide | Relative binding value ^b | Coregulator |
|-----------------|-------------------------------------|--|
| NCOA1_620_643 | 2.0 | SRC-1/RIP160: nuclear receptor co-activator 1 |
| NCOA1_737_759 | 2.5 | |
| NCOA2_628_651 | 1.3 | SRC-2/RIP160: nuclear receptor co-activator 1 |
| NCOA6_875_897 | 1.5 | NCoA-6/RAP250: nuclear receptor co-activator 6 |
| NR0B2_106_128 | 1.1 | SHP: small heterodimer partner/nuclear receptor subfamily member 2 |
| NRIP1_1055_1077 | 1.1 | RIP140: receptor-interacting protein 1 |
| PELP1_446_468 | 1.7 | PELP1: proline-, glutamic acid-, and leucine-rich protein 1 |
| PRGC1_134_154 | 1.1 | PGC1α: PPAR-g co-activator 1-alpha |

^aPositive interactions defined as: binding value>50, relative binding >1, p-value <0.05

Table S4. 9 peptides that positively interact^a with the BPAF/ERα complex derived from 9 coregulators

| Peptide | Relative binding value ^b | Coregulator |
|---------------------|-------------------------------------|---|
| KIF11_832_854_C854S | 1.9 | KIF11: kinesin-like protein KIF11 |
| MAPE_356_378 | 1.9 | MAPE: melanoma antigen preferentially express protein |
| NCOA3_104_123_N-KKK | 1.5 | SRC-3/NCoA-2: nuclear receptor co-activator 3 |
| PELP1_446_468 | 1.7 | PELP1: proline-, glutamic acid-, and leucine-rich protein 1 |
| PPRC1_1159_1181 | 1.5 | PRC: PGC-related coactivator |
| PRDM2_948_970 | 1.6 | PRDP2/MTB-ZF: PR domain-containing protein 2 |
| PRGR_102_124 | 3.4 | PR: progesterone receptor |
| TF65_437_459 | 2.2 | TF65: transcription factor p65 |
| ZNT9_449_471 | 1.5 | ZnT-9/HUEL: zinc transporter 9 |

^aPositive interactions defined as: binding value>50, relative binding >1, p-value <0.05

^bRelative binding value shows each peptide binding relative to the control, 2% DMSO For complete results, see Excel Table S2

^bRelative binding value shows each peptide binding relative to the control, 2% DMSO For complete results, see Excel Table S2

Table S5. 25 peptides that positively interact a with the BPS/ER α complex derived from 14 coregulators

| Peptide | Relative binding value ^b | Coregulator |
|---------------------|-------------------------------------|--|
| JHD2C_2054_2076 | 1.5 | TRIP-8: thyroid receptor-interacting protein 8 |
| LCOR_40_62 | 3.1 | LCoR: ligand-dependent corepressor |
| MED1_591_614 | 1.9 | TRIP-2: thyroid receptor-interacting protein 2 |
| NCOA1_1421_1441 | 1.3 | SRC-1/RIP160: nuclear receptor co-activator 1 |
| NCOA1_620_643 | 3.6 | |
| NCOA1_677_700 | 1.6 | |
| NCOA2_628_651 | 1.9 | SRC-2/NCoA-2: nuclear receptor co-activator 2 |
| NCOA2_677_700 | 1.7 | |
| NCOA2_733_755 | 1.4 | |
| NCOA3_609_631 | 2.4 | SRC-3/NCoA-3: nuclear receptor co-activator 3 |
| NCOA3_609_631_C627S | 1.7 | |
| NCOA3_725_747 | 1.2 | |
| NR0B1_1_23 | 1.6 | DAX-1: nuclear receptor subfamily group B member 1 |
| NR0B1_136_159 | 1.2 | |
| NR0B1_68_90_C69S | 1.6 | |
| NR0B2_106_128 | 2.1 | SHP: small heterodimer partner/nuclear receptor subfamily member 2 |
| NRIP1_1055_1077 | 1.9 | RIP140: receptor-interacting protein 1 |
| NRIP1_120_142 | 1.6 | |
| NRIP1_253_275_C263S | 1.9 | |
| NSD1_894_916 | 1.2 | NSDP1: NR-binding SET domain-cotaining protein |
| PELP1_446_468 | 1.6 | PELP1: proline-, glutamic acid-, and leucine-rich protein 1 |
| PRGC1_130_155 | 1.9 | PGC1α: PPAR-g co-activator 1-alpha |
| PRGC1_134_154 | 1.5 | |
| PRGC2_146_166 | 1.5 | PGC1β: PPAR-g co-activator 1-beta |
| TIP60_476_498 | 1.4 | Tip60: 60 kDa Tat interactive protein |

^aPositive interactions defined as: binding value>50, relative binding >1, p-value <0.05 ^bRelative binding value shows each peptide binding relative to the control, 2% DMSO For complete results, see Excel Table S2

Table S6. 35 peptides that negatively interact^a with the E2/ERα complex derived from 22 coregulators

| Peptide | Relative binding value ^b | Coregulator |
|---------------------------|-------------------------------------|--|
| ANDR_10_32 | 0.6 | AR: Androgen receptor |
| CENPR_159_177 | 0.4 | CENP-R: nuclear receptor-interaction factor 3 |
| CHD9_1023_1045 | 0.4 | CHD9: PPAR-alpha-interacting complex protein 320 kDa |
| CHD9_855_877 | 0.4 | |
| CNOT1_140_162 | 0.2 | NOT1H: negative regulator of transcription subunit 1 homolog |
| CNOT1_1626_1648 | 0.3 | |
| CNOT1_1929_1951_C1932S | 0.3 | |
| CNOT1_557_579 | 0.3 | |
| DHX30_49_70 | 0.4 | DHX30: DEAH box protein 30 |
| GELS_376_398 | 0.7 | ADF: actin-depolymerizing factor |
| HAIR_553_575_C567S | 0.4 | H: hairless |
| MAPE_249_271 | 0.7 | OIP4: OPA-interacting protein 4 |
| MAPE_300_322 | 0.3 | |
| MAPE_454_476_C472S | 0.2 | |
| MAPE_91_113 | 0.2 | |
| MEN1_255_277 | 0.6 | MEN1: menin |
| MGMT_86_108 | 0.4 | MGMT: methylated-DNA-protein-cysteine methyltransferase |
| MTA1S_388_410_C393S/C396S | 0.7 | MTA1: metastasis-associated protein |
| NCOR1_2039_2061 | 0.2 | N-CoR1: nuclear receptor corespressor 1 |
| NCOR1_2039_2061_C2056S | 0.2 | |
| NCOR1_2251_2273 | 0.3 | |
| NCOR2_2123_2145 | 0.5 | N-CoR2/SMRT: nuclear receptor corespressor 2 |
| NCOR2_2330_2352 | 0.3 | |
| NCOR2_649_671_C649S | 0.6 | |
| NELFB_328_350 | 0.5 | NELF-B: negative elongation factor B |
| NR0B2_237_257 | 0.3 | SHP: small heterodimer partner/nuclear receptor subfamily member 2 |
| PAK6_248_270 | 0.7 | PAK-6: serine/threonine-protein kinase p21-activated kinase 6 |
| PCAF_178_200 | 0.2 | PCAF: P300/CBP-associated factor |
| PELP1 142 164 | 0.3 | PELP1: proline-, glutamic acid-, and leucine-rich protein 1 |
| PELP1_258_280 | 0.4 | |
| PR285_2216_2238_C2219S | 0.6 | PDIP1: PPAR-gamma DBD-interacting protein 1 |
| TGFI1_325_347_C334S/C346S | 0.5 | TGFI1: transforming growth factor beta-1-induced transcript 1 |
| TGFI1_443_461_C452S/C455S | 0.4 | |
| TIF1A_373_395_C394S | 0.5 | TIF1-a: transcription intermediary factor 1-alpha |
| TREF1_850_872 | 0.5 | TREF1: transcriptional-regulating factor 1 |
| | 1 | |

^aNegative interactions defined as: binding value>50, relative binding <1, p-value <0.05

For complete results, see Excel Table S2

^bRelative binding value shows each peptide binding relative to the control, 2% DMSO

Table S7. 44 peptides that negatively interact^a with the BPA/ERα complex derived from 28 coregulators

| Peptide | Relative binding value ^b | Coregulator |
|---------------------------|-------------------------------------|--|
| ANDR_10_32 | 0.8 | AR: androgen receptor |
| BL1S1_1_11 | 0.8 | BLOC-1: biogenesis of lysosome-related organelles complex-1 subunit 1 |
| CBP_345_368_C367S | 0.6 | CBP: CREB-binding protein |
| CENPR_159_177 | 0.3 | CENP-R: centromere protein R |
| CNOT1_1626_1648 | 0.2 | NOT1H: negative regulator of transcription subunit 1 homolog |
| CNOT1_1929_1951_C1932S | 0.3 | |
| CNOT1_557_579 | 0.4 | |
| DHX30_49_70 | 0.5 | DHX30: DEAH box protein 30 |
| GELS_376_398 | 0.5 | ADF: actin-depolymerizing factor |
| GNAQ_21_43 | 0.7 | Gαq : guanine nucleotide-binding protein alpha-q |
| HAIR_553_575_C567S | 0.4 | H: hairless |
| IKBB_277_299 | 0.7 | NFkB:NF-kappa-B inhibitor beta |
| MAPE_249_271 | 0.6 | OIP4: OPA-interacting protein 4 |
| MAPE_300_322 | 0.8 | |
| MAPE_454_476_C472S | 0.3 | |
| MGMT_86_108 | 0.5 | MGMT: methylated-DNA-protein-cysteine methyltransferase |
| MTA1S_388_410_C393S/C396S | 0.3 | MTA1: metastasis-associated protein |
| NCOR1 1925 1946 | 0.6 | N-CoR1: nuclear receptor corespressor 1 |
| NCOR1 2039 2061 | 0.5 | |
| NCOR1_2039_2061_C2056S | 0.5 | |
| NCOR1_2251_2273 | 0.3 | |
| NCOR2 2123 2145 | 0.5 | N-CoR2/SMRT: nuclear receptor corespressor 2 |
| NCOR2_2330_2352 | 0.2 | 14 Conz/Switt: Hucicul receptor corespicasor 2 |
| NR0B2 9 31 C9S/C11S | 0.6 | SHP: small heterodimer partner/nuclear receptor subfamily member 2 |
| NRIP1 700 722 | 0.8 | RIP140: receptor-interacting protein 1 |
| NRIP1 701 723 | 0.8 | OF THE STATE OF TH |
| NRIP1_924_946 | 0.7 | |
| NSD1_894_916 | 0.6 | NSDP1: NR-binding SET domain-cotaining protein |
| PCAF 178 200 | 0.3 | PCAF: P300/CBP-associated factor |
| PELP1 142 164 | 0.3 | PELP1: proline-, glutamic acid-, and leucine-rich protein 1 |
| PELP1 168 190 | 0.6 | , , |
| PELP1_258_280 | 0.4 | |
| PELP1_496_518_C496S | 0.5 | |
| PELP1_56_78_C71S | 0.6 | |
| PPRC1_1159_1181 | 0.6 | PRC: PGC-related coactivator |
| PR285 1062 1084 | 0.3 | PDIP1: PPAR-gamma DBD-interacting protein 1 |
| PR285_2216_2238_C2219S | 0.4 | J |
| PRDM2 948 970 | 0.6 | PRDP2/MTB-ZF: PR domain-containing protein 2 |
| RAD9A_348_370 | 0.4 | hRAD9: DNA repairexonuclease rad9 homolog A |
| TGFI1 325 347 C334S/C346S | 0.7 | TGFI1: transforming growth factor beta-1-induced transcript 1 |
| TIF1A 373 395 C394S | 0.5 | TIF1-a: transcription intermediary factor 1-alpha |
| TREF1_850_872 | 0.7 | TREF1: transcriptional-regulating factor 1 |
| TRRAP 770 792 | 0.6 | STAF40: transformation/transcription domain-associated protein |
| TRRAP_971_993 | 0.7 | 2. |
| <u> </u> | | |

^aNegative interactions defined as: binding value>50, relative binding <1, p-value <0.05 ^bRelative binding value shows each peptide binding relative to the control, 2% DMSO For complete results, see Excel Table S2

Table S8. 75 peptides that negatively interact a with the BPAF/ER α complex derived from 38 coregulators

| Peptide | Relative binding value ^b | Coregulator |
|------------------------|-------------------------------------|---|
| ANDR_10_32 | 0.4 | AR: androgen receptor |
| BL1S1_1_11 | 0.8 | BLOC-1: biogenesis of lysosome-related organelles complex-1 |
| | | subunit 1 |
| CBP_345_367_C367S | 0.7 | CBP: CREB-binding protein |
| CENPR_159_177 | 0.4 | CENP-R: centromere protein R |
| CHD9_1023_1045 | 0.5 | CHD9: PPAR-alpha-interacting complex protein 320 kDa |
| CNOT1_140_162 | 0.2 | NOT1H: negative regulator of transcription subunit 1 |
| CNOT1_1626_1648 | 0.3 | homolog |
| CNOT1_1929_1951_C1932S | 0.3 | |
| DHX30_49_70 | 0.4 | DHX30: DEAH box protein 30 |
| GNAQ_21_43 | 0.3 | Gαq: guanine nucleotide-binding protein alpha-q |
| HAIR_553_575_C567S | 0.2 | H: hairless |
| IKBB_277_299 | 0.3 | NFkB: NF-kappa-B inhibitor beta |
| MAPE_249_271 | 0.3 | OIP4: OPA-interacting protein 4 |
| MAPE_300_322 | 0.4 | |
| MAPE_454_476_C472S | 0.2 | |
| MAPE_91_113 | 0.4 | |
| MED1_591_614 | 0.5 | TRIP-2: thyroid receptor-interacting protein 2 |
| MED1_632_655 | 0.4 | |
| MLL2_4175_4197 | 0.4 | MLL2/KMT2B: myeloid/lymphoid or mixed-lineage leukemia |
| | | protein 2 |
| NCOA1_1421_1441 | 0.5 | SRC-1/RIP160: nuclear receptor co-activator 1 |
| NCOA1_620_643 | 0.4 | |
| NCOA1_677_700 | 0.4 | |
| NCOA2_628_651 | 0.5 | SRC-2/NCoA-2: nuclear receptor co-activator 2 |
| NCOA2_677_700 | 0.4 | |
| NCOA3_609_631_C627S | 0.3 | SRC-3/NCoA-3: nuclear receptor co-activator 3 |
| NCOA3_673_695 | 0.4 | |
| NCOR1_2039_2061 | 0.3 | N-CoR1: nuclear receptor corespressor 1 |
| NCOR1_2039_2061_C2056S | 0.4 | |
| NCOR1_2376_2398 | 0.5 | |
| NCOR1_662_684_C662S | 0.4 | |
| NCOR2_2330_2352 | 0.3 | N-CoR2/SMRT: nuclear receptor corespressor 2 |
| NCOR2_649_671_C649S | 0.5 | |
| NELFB_328_350 | 0.4 | NELF-B: negative elongation factor B |
| NELFB_428_450 | 0.4 | |
| NR0B1_1_23 | 0.5 | DAX-1: nuclear receptor subfamily member 1 |
| NR0B1_136_159 | 0.5 | |
| NR0B1_68_90_C69S | 0.4 | |
| NR0B2_106_128 | 0.4 | SHP: small heterodimer partner/nuclear receptor subfamily |
| NR0B2_201_223_C207S | 0.4 | member 2 |
| NROB2_9_31_C9S/C11S | 0.2 | |

| NRIP1_120_142 | NRIP1 1055 1077 | 0.5 | RIP140: receptor-interacting protein 1 |
|---|---------------------------|-----|---|
| NRIP1_21_143_P124R 0.4 NRIP1_253_275_C263S 0.5 NRIP1_368_390 0.4 NRIP1_488_510 0.3 NRIP1_700_722 0.4 NRIP1_805_831 0.4 NRIP1_924_946 0.4 NRIP1_924_946_C945S 0.4 NSD1_894_916 0.5 NSDP1: NR-binding SET domain-cotaining protein PAK6_248_270 0.5 PAK 6: serine/threonine –protein kinase PELP1_168_190 0.4 PELP1: proline-, glutamic acid-, and leucine-rich protein 1 PELP1_258_280 0.5 PELP1: proline-, glutamic acid-, and leucine-rich protein 1 PELP1_56_78_C715 0.5 PGC12: proline-, glutamic acid-, and leucine-rich protein 1 PERS5_2216_2238_C2219S 0.2 PDIP1: PPAR-gamma DBD-interacting protein 1 PRGC1_130_155 0.5 PGC1α: PPAR-g co-activator 1-alpha PRGC1_134_154 0.5 PGC1α: PPAR-g co-activator 1-alpha PRGC1_134_154 0.5 PGC1α: PPAR-g co-activator 1-alpha RAD9A_348_370 0.4 PROX1: homeobox prospero-like protein RAPD3_345_345_C346S 0.5 TGF1: transforming growth factor be | | | The Later cooper meet dotting process 2 |
| NRIP1_368_390 | | | |
| NRIP1_488_510 | | | |
| NRIP1_488_510 | | 0.4 | |
| NRIP1_701_723 0.4 NRIP1_805_831 0.4 NRIP1_924_946 0.4 NRIP1_924_946_C945S 0.4 NSD1_894_916 0.5 NSDP1: NR-binding SET domain-cotaining protein PAK6_248_270 0.5 PAK 6: serine/threonine – protein kinase PELP1_168_190 0.4 PELP1: proline-, glutamic acid-, and leucine-rich protein 1 PELP1_258_280 0.5 PELP1: proline-, glutamic acid-, and leucine-rich protein 1 PELP1_56_78_C71S 0.5 PELP1_571_593_C575S/C581S PELP1_571_593_C575S/C581S 0.3 PELP1_571_593_C575S/C581S PR285_2216_2238_C2219S 0.2 PDIP1: PPAR-gamma DBD-interacting protein 1 PRGC1_130_155 0.5 PGC1α: PPAR-g co-activator 1-alpha PRGC1_134_154 0.5 PGC1α: PPAR-g co-activator 1-alpha PROX1_57_79 0.3 PROX1: homeobox prospero-like protein RAD9A_348_370 0.4 hRAD9: DNA repairexonuclease rad9 homolog A TGFI1_325_347_C3345/C346S 0.5 TGFI1: transforming growth factor beta-1-induced transcript TGFI1_443_461_C4525/C455S 0.6 1 TIFIA_377_69 | | 0.3 | |
| NRIP1_805_831 | NRIP1_700_722 | 0.4 | |
| NRIP1_924_946 0.4 NRIP1_924_946_C945S 0.4 NSD1_894_916 0.5 NSDP1: NR-binding SET domain-cotaining protein PAK6_248_270 0.5 PAK 6: serine/threonine – protein kinase PELP1_168_190 0.4 PELP1: proline-, glutamic acid-, and leucine-rich protein 1 PELP1_258_280 0.5 PELP1: proline-, glutamic acid-, and leucine-rich protein 1 PELP1_496_518_C496S 0.4 PELP1: proline-, glutamic acid-, and leucine-rich protein 1 PELP1_571_593_C575S/C581S 0.5 PELP1: proline-, glutamic acid-, and leucine-rich protein 1 PRGC1_130_155 0.5 PELP1: proline-, glutamic acid-, and leucine-rich protein 1 PRGC1_130_155 0.5 PELP1: proline-, glutamic acid-, and leucine-rich protein 1 PRGC1_130_155 0.5 PELP1: proline-, glutamic acid-, and leucine-rich protein 1 PRGC1_130_155 0.5 PELP1: proline-, glutamic acid-, and leucine-rich protein 1 PRGC1_130_155 0.5 PELP1: proline-, glutamic acid-, and leucine-rich protein 1 PRGC1_130_155 0.5 PELP1: proline-, glutamic acid-, and leucine-rich protein 1 PRGC1_130_152 0.5 PDIP1: PPAR-gamma DBD-interacting protein 1 | NRIP1_701_723 | 0.4 | |
| NRIP1_924_946_C945S 0.4 NSD1_894_916 0.5 NSDP1: NR-binding SET domain-cotaining protein PAK6_248_Z70 0.5 PAK 6: serine/threonine –protein kinase PELP1_168_190 0.4 PELP1: proline-, glutamic acid-, and leucine-rich protein 1 PELP1_258_280 0.5 PELP1_19-518_C496S 0.4 PELP1_56_78_C71S 0.5 PELP1_571_593_C575S/C581S 0.3 PELP1_571_593_C575S/C581S 0.3 PDIP1: PPAR-gamma DBD-interacting protein 1 PRGC1_130_155 0.5 PGC1α: PPAR-g co-activator 1-alpha PRGC1_134_154 0.5 PGC1α: PPAR-g co-activator 1-alpha PROX1_57_79 0.3 PROX1: homeobox prospero-like protein RAD9A_348_370 0.4 hRAD9: DNA repairexonuclease rad9 homolog A TGFI1_325_347_C334S/C346S 0.5 TGFI1: transforming growth factor beta-1-induced transcript TGFI1_443_461_C452S/C455S 0.6 1 TIF1a_373_395_C394S 0.2 TIF1-a: transcription intermediary factor 1-alpha TIF1A_747_769 0.4 TIF1-a: transcription intermediary factor 1-alpha TRF1_1850_872 0.7 TREF1: transcriptional-regul | NRIP1_805_831 | 0.4 | |
| NSD1_894_916 0.5 NSDP1: NR-binding SET domain-cotaining protein PAK6_248_270 0.5 PAK 6: serine/threonine – protein kinase PELP1_168_190 0.4 PELP1: proline-, glutamic acid-, and leucine-rich protein 1 PELP1_258_280 0.5 PELP1_96_518_C496S 0.4 PELP1_56_78_C71S 0.5 PELP1_571_593_C575S/C581S 0.3 PR285_2216_2238_C2219S 0.2 PDIP1: PPAR-gamma DBD-interacting protein 1 PRGC1_130_155 0.5 PGC1α: PPAR-g co-activator 1-alpha PRGC1_146_166 0.4 PROX1: homeobox prospero-like protein PROX1_57_79 0.3 PROX1: homeobox prospero-like protein RAD9a_348_370 0.4 hRAD9: DNA repairexonuclease rad9 homolog A TGFI1_443_461_C452S/C455S 0.5 TGFI1: transforming growth factor beta-1-induced transcript TGF11_443_461_C452S/C455S 0.6 1 TIF1A_373_395_C394S 0.2 TIF1-a: transcription intermediary factor 1-alpha TIF1A_747_769 0.4 TREF1: transcriptional-regulating factor 1 TREF1_850_872 0.7 TREF1: transcriptional-regulating factor 1 | NRIP1_924_946 | 0.4 | |
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| PELP1_258_280 0.5 PELP1_496_518_C496S 0.4 PELP1_56_78_C71S 0.5 PELP1_571_593_C575S/C581S 0.3 PR285_2216_2238_C2219S 0.2 PDIP1: PPAR-gamma DBD-interacting protein 1 PRGC1_130_155 0.5 PGC1α: PPAR-g co-activator 1-alpha PRGC1_146_166 0.4 PROX1: homeobox prospero-like protein PROX1_57_79 0.3 PROX1: homeobox prospero-like protein RAD9A_348_370 0.4 hRAD9: DNA repairexonuclease rad9 homolog A TGFI1_325_347_C3345/C346S 0.5 TGFI1: transforming growth factor beta-1-induced transcript TGFI1_443_461_C4525/C455S 0.6 1 TIF1A_373_395_C394S 0.2 TIF1-a: transcription intermediary factor 1-alpha TIF1A_747_769 0.4 Tip60: 60 kDa Tat interactive protein TREF1_850_872 0.7 TREF1: transcriptional-regulating factor 1 TRIP4_149_171_C171S 0.4 ASC-1: activating signal cointegrator 1 TRRAP_770_792 0.6 STAF40: transformation/transcription domain-associated protein TRRAP_971_993 0.5 TR: thioredoxinreduactase TR1 | PAK6_248_270 | 0.5 | PAK 6: serine/threonine –protein kinase |
| PELP1_496_518_C496S 0.4 PELP1_56_78_C71S 0.5 PELP1_571_593_C575S/C581S 0.3 PR285_2216_2238_C2219S 0.2 PDIP1: PPAR-gamma DBD-interacting protein 1 PRGC1_130_155 0.5 PGC1α: PPAR-g co-activator 1-alpha PRGC1_134_154 0.5 PRGC1_166 PROX1_57_79 0.3 PROX1: homeobox prospero-like protein RAD9A_348_370 0.4 hRAD9: DNA repairexonuclease rad9 homolog A TGFI1_325_347_C334S/C346S 0.5 TGFI1: transforming growth factor beta-1-induced transcript TGFI1_443_461_C452S/C455S 0.6 1 TIF1A_373_395_C394S 0.2 TIF1-a: transcription intermediary factor 1-alpha TIF1A_747_769 0.4 TREF1: transcriptional-regulating factor 1 TREF1_850_872 0.7 TREF1: transcriptional-regulating factor 1 TRIP4_149_171_C171S 0.4 ASC-1: activating signal cointegrator 1 TRRAP_770_792 0.6 STAF40: transformation/transcription domain-associated protein TRXR1_132_154 0.2 TR: thioredoxinreduactase TR1 | PELP1_168_190 | 0.4 | PELP1: proline-, glutamic acid-, and leucine-rich protein 1 |
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| PELP1_571_593_C575S/C581S 0.3 PR285_2216_2238_C2219S 0.2 PDIP1: PPAR-gamma DBD-interacting protein 1 PRGC1_130_155 0.5 PGC1α: PPAR-g co-activator 1-alpha PRGC1_134_154 0.5 PRGC2_146_166 PROX1_57_79 0.3 PROX1: homeobox prospero-like protein RAD9A_348_370 0.4 hRAD9: DNA repairexonuclease rad9 homolog A TGFI1_325_347_C334S/C346S 0.5 TGFI1: transforming growth factor beta-1-induced transcript TGFI1_443_461_C452S/C455S 0.6 1 TIF1A_373_395_C394S 0.2 TIF1-a: transcription intermediary factor 1-alpha TIF1A_747_769 0.4 Tip60: 60 kDa Tat interactive protein TREF1_850_872 0.7 TREF1: transcriptional-regulating factor 1 TRIP4_149_171_C171S 0.4 ASC-1: activating signal cointegrator 1 TRRAP_770_792 0.6 STAF40: transformation/transcription domain-associated protein TRXR1_132_154 0.2 TR: thioredoxinreduactase TR1 | PELP1_496_518_C496S | 0.4 | |
| PR285_2216_2238_C2219S 0.2 PDIP1: PPAR-gamma DBD-interacting protein 1 PRGC1_130_155 0.5 PGC1α: PPAR-g co-activator 1-alpha PRGC1_134_154 0.5 PRC1_2 PPAR-g co-activator 1-alpha PRGC2_146_166 0.4 PROX1: homeobox prospero-like protein RAD9A_348_370 0.4 hRAD9: DNA repairexonuclease rad9 homolog A TGF11_325_347_C334S/C346S 0.5 TGF11: transforming growth factor beta-1-induced transcript TGF11_443_461_C452S/C455S 0.6 1 TIF1A_373_395_C394S 0.2 TIF1-a: transcription intermediary factor 1-alpha TIF1A_747_769 0.4 Tip60: 60 kDa Tat interactive protein TREF1_850_872 0.7 TREF1: transcriptional-regulating factor 1 TRIP4_149_171_C171S 0.4 ASC-1: activating signal cointegrator 1 TRRAP_770_792 0.6 STAF40: transformation/transcription domain-associated protein TRXR1_132_154 0.2 TR: thioredoxinreduactase TR1 | PELP1_56_78_C71S | 0.5 | |
| PRGC1_130_155 0.5 PGC1α: PPAR-g co-activator 1-alpha PRGC1_134_154 0.5 PRGC2_146_166 0.4 PROX1_57_79 0.3 PROX1: homeobox prospero-like protein RAD9A_348_370 0.4 hRAD9: DNA repairexonuclease rad9 homolog A TGFI1_325_347_C334\$/C346\$ 0.5 TGFI1: transforming growth factor beta-1-induced transcript TGFI1_443_461_C452\$/C455\$ 0.6 1 TIF1A_373_395_C394\$ 0.2 TIF1-a: transcription intermediary factor 1-alpha TIF1A_747_769 0.4 Tip60: 60 kDa Tat interactive protein TREF1_850_872 0.7 TREF1: transcriptional-regulating factor 1 TRIP4_149_171_C171\$ 0.4 ASC-1: activating signal cointegrator 1 TRRAP_770_792 0.6 STAF40: transformation/transcription domain-associated protein TRXR1_132_154 0.2 TR: thioredoxinreduactase TR1 | PELP1_571_593_C575S/C581S | 0.3 | |
| PRGC1_134_154 0.5 PRGC2_146_166 0.4 PROX1_57_79 0.3 PROX1: homeobox prospero-like protein RAD9A_348_370 0.4 hRAD9: DNA repairexonuclease rad9 homolog A TGFI1_325_347_C334S/C346S 0.5 TGFI1: transforming growth factor beta-1-induced transcript TGFI1_443_461_C452S/C455S 0.6 1 TIF1A_373_395_C394S 0.2 TIF1-a: transcription intermediary factor 1-alpha TIF1A_747_769 0.4 Tip60: 60 kDa Tat interactive protein TREF1_850_872 0.7 TREF1: transcriptional-regulating factor 1 TRIP4_149_171_C171S 0.4 ASC-1: activating signal cointegrator 1 TRRAP_770_792 0.6 STAF40: transformation/transcription domain-associated TRRAP_971_993 0.5 protein TRXR1_132_154 0.2 TR: thioredoxinreduactase TR1 | PR285_2216_2238_C2219S | 0.2 | PDIP1: PPAR-gamma DBD-interacting protein 1 |
| PRGC2_146_166 0.4 PROX1_57_79 0.3 PROX1: homeobox prospero-like protein RAD9A_348_370 0.4 hRAD9: DNA repairexonuclease rad9 homolog A TGFI1_325_347_C334S/C346S 0.5 TGFI1: transforming growth factor beta-1-induced transcript TGFI1_443_461_C452S/C455S 0.6 1 TIF1A_373_395_C394S 0.2 TIF1-a: transcription intermediary factor 1-alpha TIF1A_747_769 0.4 Tip60: 60 kDa Tat interactive protein TREF1_850_872 0.7 TREF1: transcriptional-regulating factor 1 TRIP4_149_171_C171S 0.4 ASC-1: activating signal cointegrator 1 TRRAP_770_792 0.6 STAF40: transformation/transcription domain-associated TRRAP_971_993 0.5 protein TRXR1_132_154 0.2 TR: thioredoxinreduactase TR1 | PRGC1_130_155 | 0.5 | PGC1α: PPAR-g co-activator 1-alpha |
| PROX1_57_79 0.3 PROX1: homeobox prospero-like protein RAD9A_348_370 0.4 hRAD9: DNA repairexonuclease rad9 homolog A TGFI1_325_347_C334S/C346S TGFI1_443_461_C452S/C455S 0.6 1 TIF1A_373_395_C394S TIF1A_747_769 TIF6O_476_498 0.6 Tip60: 60 kDa Tat interactive protein TREF1_850_872 TRIP4_149_171_C171S 0.4 ASC-1: activating signal cointegrator 1 TRRAP_770_792 TRRAP_770_792 TRRAP_971_993 TRXR1_132_154 0.3 PROX1: homeobox prospero-like protein HRAD9: DNA repairexonuclease rad9 homolog A TGFI1: transforming growth factor beta-1-induced transcript TGFI1: transcription intermediary factor 1-alpha TIF1-a: transcription intermediary factor 1-alpha TIP60: 60 kDa Tat interactive protein TREF1: transcriptional-regulating factor 1 STAF40: transformation/transcription domain-associated protein TRXR1_132_154 0.2 TR: thioredoxinreduactase TR1 | PRGC1_134_154 | 0.5 | |
| RAD9A_348_370 O.4 hRAD9: DNA repairexonuclease rad9 homolog A TGFI1_325_347_C334S/C346S O.5 TGFI1: transforming growth factor beta-1-induced transcript TGFI1_443_461_C452S/C455S O.6 1 TIF1A_373_395_C394S TIF1A_747_769 O.4 TIP6O_476_498 O.6 Tip60: 60 kDa Tat interactive protein TREF1_850_872 TRIP4_149_171_C171S O.4 ASC-1: activating signal cointegrator 1 TRRAP_770_792 TRRAP_770_792 O.6 STAF40: transformation/transcription domain-associated protein TRXR1_132_154 O.2 TR: thioredoxinreduactase TR1 | PRGC2_146_166 | 0.4 | |
| TGFI1_325_347_C334S/C346S TGFI1_443_461_C452S/C455S 0.6 TIF1A_373_395_C394S TIF1A_747_769 TIP60_476_498 TREF1_850_872 TRIP4_149_171_C171S TRIP4_149_171_C171S TRRAP_770_792 TRRAP_770_792 TRRAP_770_792 TRRAP_971_993 TRXR1_132_154 0.5 TGFI1: transforming growth factor beta-1-induced transcript 1 TGFI1: transcription intermediary factor 1-alpha 1 TGFI1: transcription intermediary factor 1-alpha 1 TIP60: 60 kDa Tat interactive protein 1 TREF1: transcriptional-regulating factor 1 STAF-1: activating signal cointegrator 1 TRAP_TRAP_TRAP_TRAP_TRAP_TRAP_TRAP_TRAP_ | PROX1_57_79 | 0.3 | PROX1: homeobox prospero-like protein |
| TGFI1_443_461_C452S/C455S 0.6 1 TIF1A_373_395_C394S 0.2 TIF1-a: transcription intermediary factor 1-alpha TIF1A_747_769 0.4 Tip60: 60 kDa Tat interactive protein TREF1_850_872 0.7 TREF1: transcriptional-regulating factor 1 TRIP4_149_171_C171S 0.4 ASC-1: activating signal cointegrator 1 TRRAP_770_792 0.6 STAF40: transformation/transcription domain-associated protein TRXR1_132_154 0.2 TR: thioredoxinreduactase TR1 | RAD9A_348_370 | 0.4 | hRAD9: DNA repairexonuclease rad9 homolog A |
| TIF1A_373_395_C394S TIF1A_747_769 0.4 TIP60_476_498 0.6 Tip60: 60 kDa Tat interactive protein TREF1_850_872 TRIP4_149_171_C171S 0.4 ASC-1: activating signal cointegrator 1 TRRAP_770_792 TRRAP_971_993 0.5 TRXR1_132_154 0.2 TR: thioredoxinreduactase TR1 | TGFI1_325_347_C334S/C346S | 0.5 | TGFI1: transforming growth factor beta-1-induced transcript |
| TIF1A_747_769 0.4 TIP60_476_498 0.6 Tip60: 60 kDa Tat interactive protein TREF1_850_872 0.7 TREF1: transcriptional-regulating factor 1 TRIP4_149_171_C171S 0.4 ASC-1: activating signal cointegrator 1 TRRAP_770_792 0.6 STAF40: transformation/transcription domain-associated protein TRXR1_132_154 0.2 TR: thioredoxinreduactase TR1 | TGFI1_443_461_C452S/C455S | 0.6 | 1 |
| TIP60_476_498 0.6 Tip60: 60 kDa Tat interactive protein TREF1_850_872 0.7 TREF1: transcriptional-regulating factor 1 TRIP4_149_171_C171S 0.4 ASC-1: activating signal cointegrator 1 TRRAP_770_792 0.6 STAF40: transformation/transcription domain-associated protein TRXR1_132_154 0.2 TR: thioredoxinreduactase TR1 | TIF1A_373_395_C394S | 0.2 | TIF1-a: transcription intermediary factor 1-alpha |
| TREF1_850_872 0.7 TREF1: transcriptional-regulating factor 1 TRIP4_149_171_C171S 0.4 ASC-1: activating signal cointegrator 1 TRRAP_770_792 0.6 STAF40: transformation/transcription domain-associated protein TRXR1_132_154 0.2 TR: thioredoxinreduactase TR1 | TIF1A_747_769 | 0.4 | |
| TRIP4_149_171_C171S 0.4 ASC-1: activating signal cointegrator 1 TRRAP_770_792 0.6 STAF40: transformation/transcription domain-associated protein TRXR1_132_154 0.2 TR: thioredoxinreduactase TR1 | TIP60_476_498 | 0.6 | Tip60: 60 kDa Tat interactive protein |
| TRRAP_770_792 0.6 STAF40: transformation/transcription domain-associated protein TRXR1_132_154 0.2 TR: thioredoxinreduactase TR1 | TREF1_850_872 | 0.7 | TREF1: transcriptional-regulating factor 1 |
| TRRAP_971_993 0.5 protein TRXR1_132_154 0.2 TR: thioredoxinreduactase TR1 | TRIP4_149_171_C171S | 0.4 | ASC-1: activating signal cointegrator 1 |
| TRXR1_132_154 0.2 TR: thioredoxinreduactase TR1 | TRRAP_770_792 | 0.6 | STAF40: transformation/transcription domain-associated |
| | TRRAP_971_993 | 0.5 | protein |
| ZNHI3_89_111 0.4 TRIP-3: thyroid receptor interacting protein 3 | TRXR1_132_154 | 0.2 | TR: thioredoxinreduactase TR1 |
| | | 0.4 | TRIP-3: thyroid receptor interacting protein 3 |

^aNegative interactions defined as: binding value>50, relative binding <1, p-value <0.05

For complete results, see Excel Table S2

^bRelative binding value shows each peptide binding relative to the control, 2% DMSO

Table S9. 31 peptides that negatively interact^a with the BPS/ERα complex derived from 23 coregulators

| Peptide | Relative binding value ^b | Coregulator |
|---------------------------|-------------------------------------|---|
| BL1S1_1_11 | 0.8 | BLOC-1: biogenesis of lysosome-related organelles complex-1 |
| | | subunit 1 |
| CBP_345_367_C367S | 0.6 | CBP: CREB-binding protein |
| CHD9_1023_1045 | 0.6 | CHD9: PPAR-alpha-interacting complex protein 320 kDa |
| CNOT1_1626_1648 | 0.4 | NOT1H: negative regulator of transcription subunit 1 homolog |
| CNOT1_1929_1951_C1932S | 0.3 | |
| DHX30_49_70 | 0.5 | DHX30: DEAH box protein 30 |
| GELS_376_398 | 0.5 | ADF: actin-depolymerizing factor |
| GNAQ_21_43 | 0.7 | Gαq : guanine nucleotide-binding protein alpha-q |
| HAIR_553_575_C567S | 0.4 | H: hairless |
| MAPE_249_271 | 0.7 | OIP4: OPA-interacting protein 4 |
| MAPE_300_322 | 0.7 | |
| MAPE_454_476_C472S | 0.4 | |
| MAPE_91_113 | 0.3 | |
| MGMT_86_108 | 0.7 | MGMT: methylated-DNA-protein-cysteine methyltransferase |
| NCOR1_2039_2061 | 0.6 | N-CoR1: nuclear receptor corespressor 1 |
| NCOR1_2251_2273 | 0.3 | |
| NCOR1_662_684_C662S | 0.6 | |
| NCOR2_2330_2352 | 0.3 | N-CoR2/SMRT: nuclear receptor corespressor 2 |
| NELFB_328_350 | 0.5 | NELF-B: negative elongation factor B |
| NRIP1_700_722 | 0.8 | RIP140: receptor-interacting protein 1 |
| PAK6_248_270 | 0.8 | PAK 6: serine/threonine –protein kinase PAK 6 |
| PCAF_178_200 | 0.2 | PCAF: P300/CBP-associated factor |
| PELP1_142_164 | 0.4 | PELP1: proline-, glutamic acid-, and leucine-rich protein 1 |
| PELP1_258_280 | 0.4 | |
| PPRC1_1159_1181 | 0.6 | PRC: PGC-related coactivator |
| PR285_1062_1084 | 0.4 | PDIP1: PPAR-gamma DBD-interacting protein 1 |
| PRDM2_948_970 | 0.6 | PRDP2/MTB-ZF: PR domain-containing protein 2 |
| RAD9A_348_370 | 0.4 | hRAD9: DNA repairexonuclease rad9 homolog A |
| TGFI1_325_347_C334S/C346S | 0.7 | TGFI1: transforming growth factor beta-1-induced transcript 1 |
| TGFI1_443_461_C452S/C455S | 0.6 | |
| TIF1A_373_395_C394S | 0.5 | TIF1-α: transcription intermediary factor 1-alpha |

^aNegative interactions defined as: binding value>50, relative binding <1, p-value <0.05

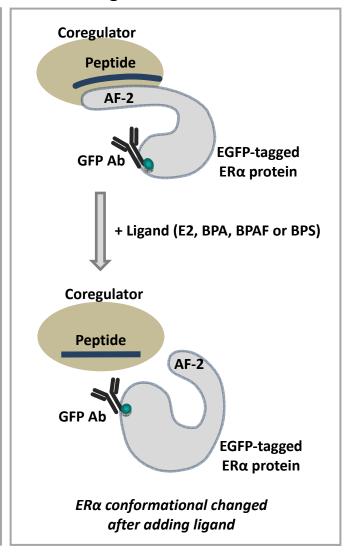
For complete results, see Excel Table S2

^bRelative binding value shows each peptide binding relative to the control, 2% DMSO

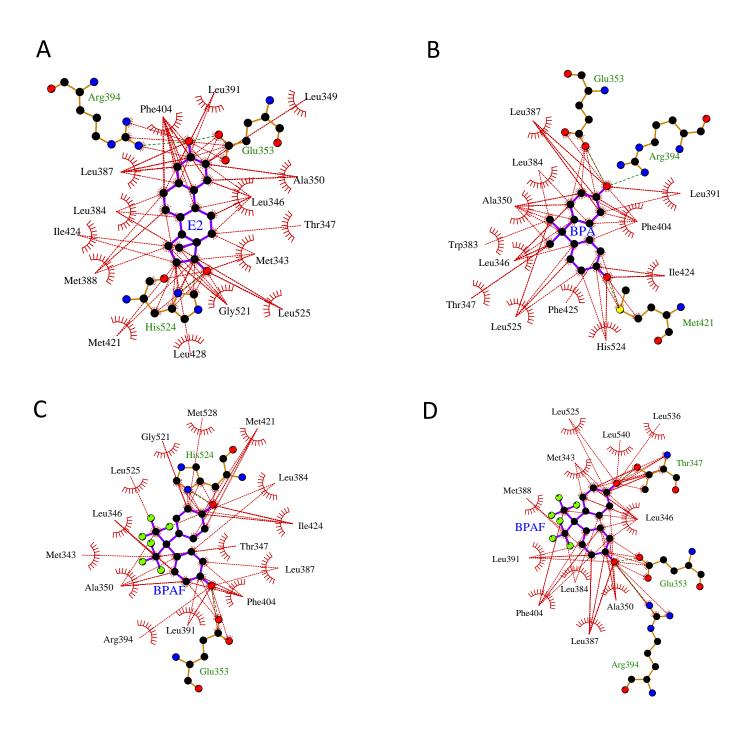
Positive interaction

Coregulator **Peptide** AF-2 **GFP Ab** EGFP-tagged **ERα** protein + Ligand (E2, BPA, BPAF or BPS) Coregulator **Peptide** AF-2 GFP Ab **EGFP-tagged ERα** protein ERα conformational changed after adding ligand

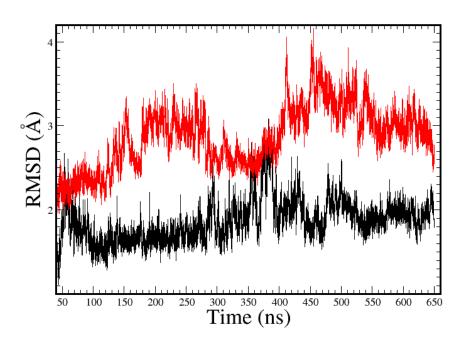
Negative interaction



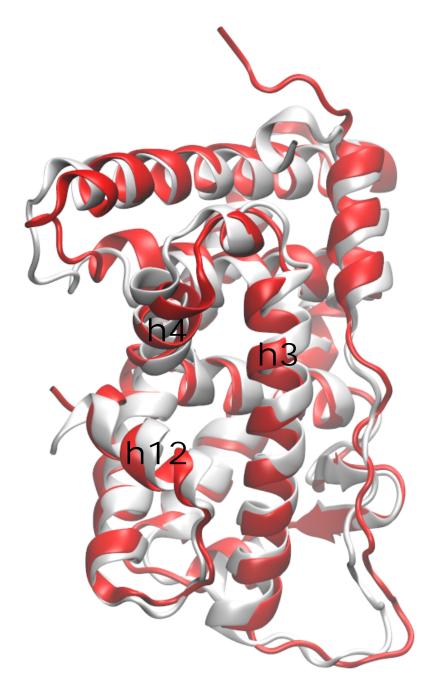
Supplemental Figure S1. Working model of the MARCONI assay. Cell lysates ware isolated from the EGFP-tagged full-length human ER α -transfected U2OS cells. For MARCONI, 25 μL assay mixtures that contain cell lysates, 25 nM of Alexa488-conjugated GFP-antibody (Invitrogen), and 0.2 mM ligand (E2, BPA, BPAF or BPS, pre-diluted in DMSO, final concentration 2%) were prepared on ice. The ligand-modulated coregulator interactions with the EGFP-tagged ER α was assessed using a PamChip® plate which contained the 154 coregulator-derived binding peptides. The positive interaction means that ligand increases peptide binding and negative interaction means that the ligand decreases peptide binding to ER α .



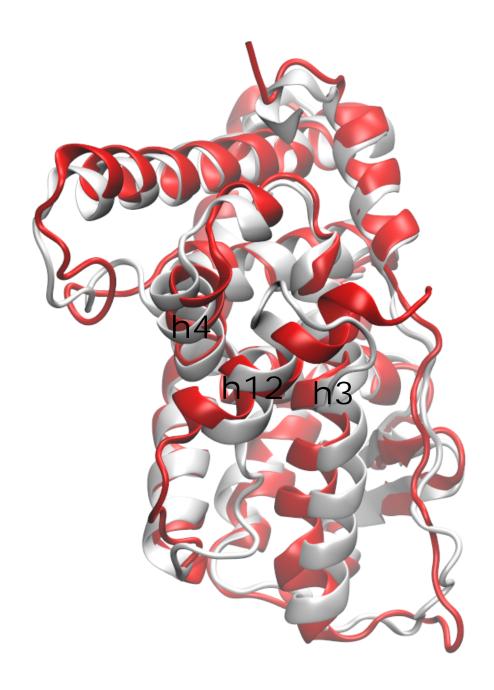
Supplemental Figure S2. Ligand interactions from the reported X-ray crystal structures. The ligand interactions with ER that were found in the X-ray crystal structures (A) E2, (B) BPA, and (C and D) BPAF in two conformations.



Supplemental Figure S3. Root mean square deviations (RMSD) of ligand-free ER structures started at agonist (black) and antagonist (red) forms. The X-ray crystal structures were used as the reference structures for RMSD calculations and all backbone heavy atoms of each residue were used to calculate the average RMSD at each time point.

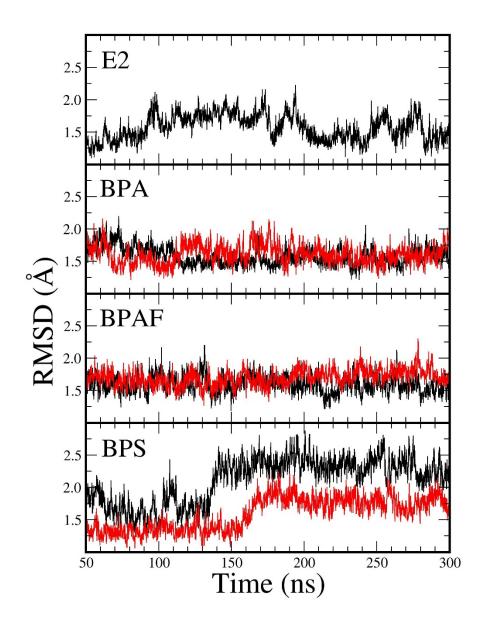


Supplemental Figure S4. Ligand free conformations of ER α (starting with aqueous agonist form). Starting conformation is in white and the final conformation is in red. The three helices that are involved in creating the coregulator surface are marked.



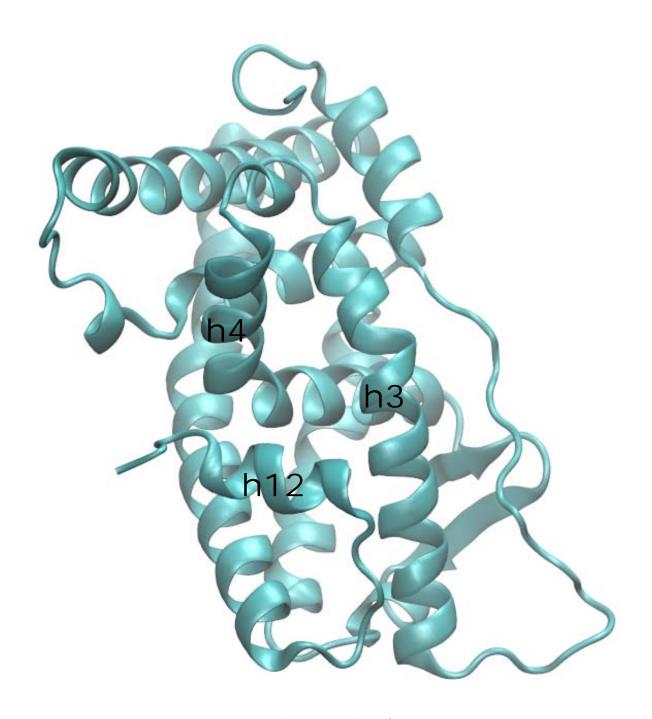
Supplemental Figure S5. Ligand free conformations of $\text{ER}\alpha$ (starting with antagonist form).

Starting conformation is in white and the final conformation is in red.

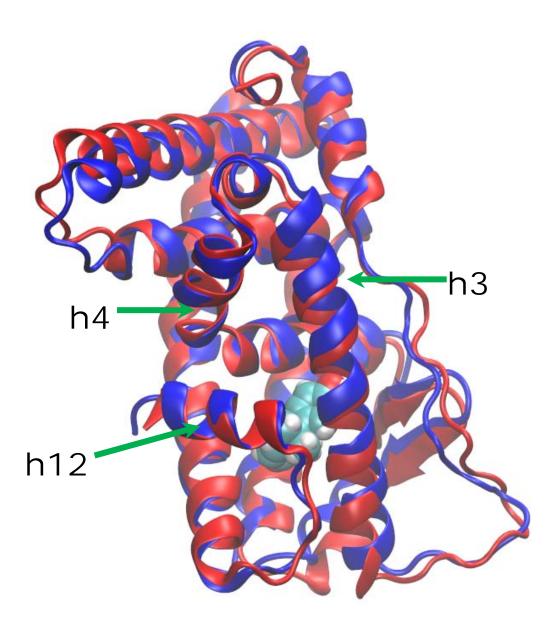


Supplemental Figure S6. Root mean square deviations (RMSD) of various ligand bound-ER structures.

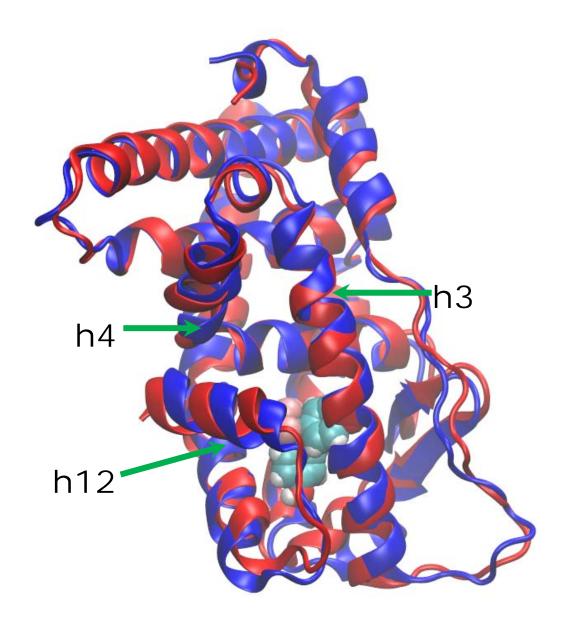
The X-ray crystal structures were used as the reference structures for these calculations and all backbone heavy atoms of each residue were used to calculate the average RMSD at each time point. For BPA, BPAF, and BPS, the black curve corresponds to the starting ligand in conformation "1" and the red curve to the ligand in conformation "2".



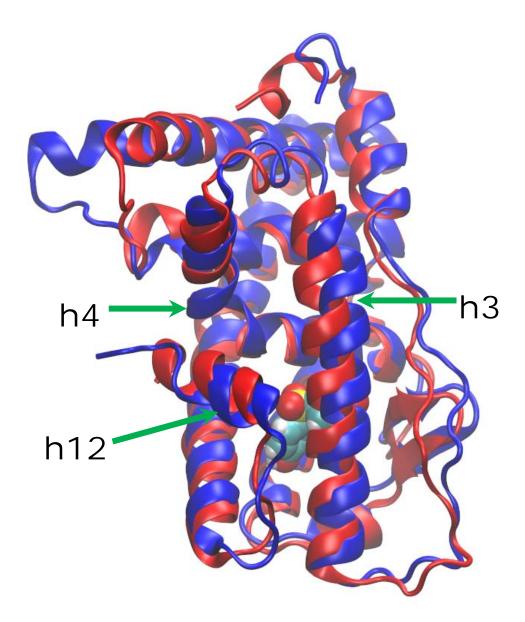
Supplemental Figure S7. E2-bound conformation of ER α (in which h12 is in agonist conformation). The final conformation of ER α with E2 from the MD simulation.



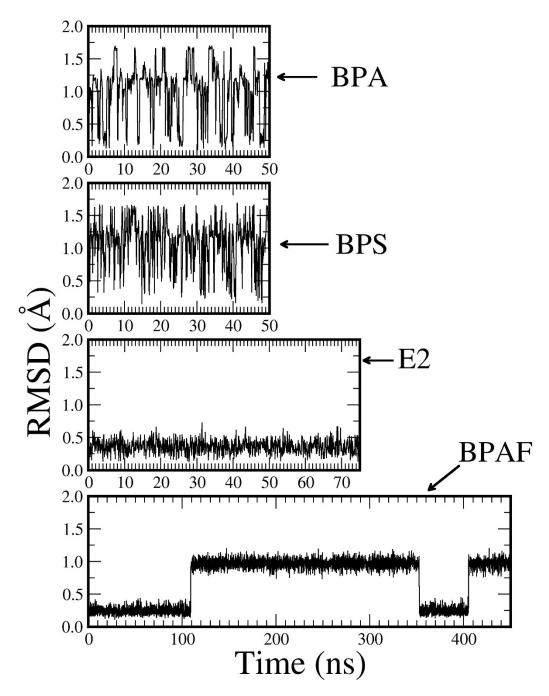
Supplemental Figure S8. BPA-bound conformations of ER α . The final conformation of ER α with BPA started in conformation 1 is shown in the blue ribbon; The final conformation of ER α with BPA started in conformation 2 is shown in the red ribbon. BPA is shown in space filling in the ligand binding site of ER α .



Supplemental Figure S9. BPAF-bound conformations of ER α . The final conformation of ER α with BPAF started in conformation 1 is show in the blue ribbon; The final conformation of ER α with BPAF started in conformation 2 is shown in the red ribbon. BPAF is shown in space filling in the ligand binding site of ER α .



Supplemental Figure S10. BPS-bound conformations of ER α . The final conformation of ER α with BPS started in conformation 1 is shown in the blue ribbon; The final conformation of ER α with BPS started in conformation 2 is shown in the red ribbon. BPS is shown in space filling in the ligand binding site of ER α .



Supplemental Figure S11. Root mean square deviations (RMSD) of the ligands in their aqueous environments. Starting structures were used as the reference structures for these calculations and all heavy atoms of the ligand were used to calculate the average RMSD at each time point.