

Supporting Information

Discovery of Novel Peroxisome Proliferator-Activated Receptor A (PPAR α) Agonists by Virtual Screening and Biological Evaluation

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Notes

The authors declare no competing financial interest.

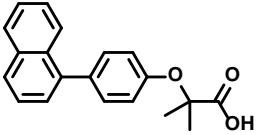
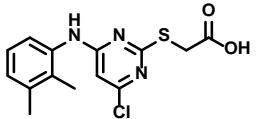
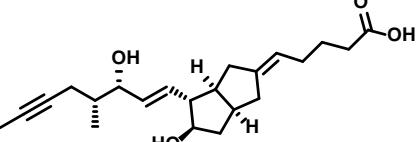
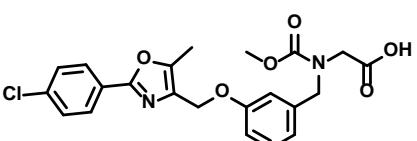
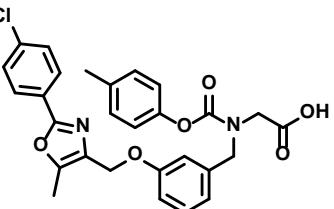
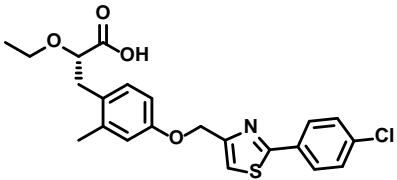
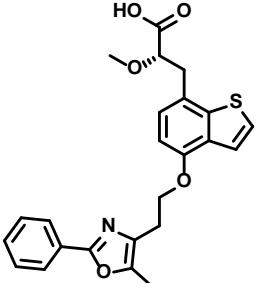
Table of Contents

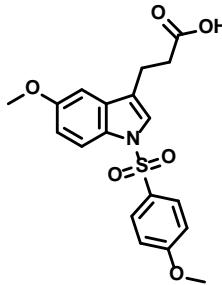
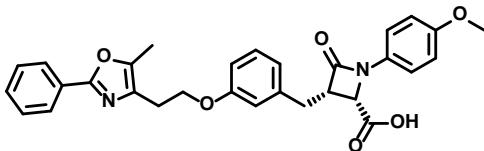
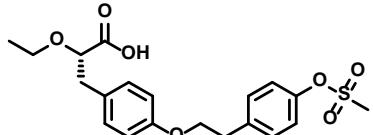
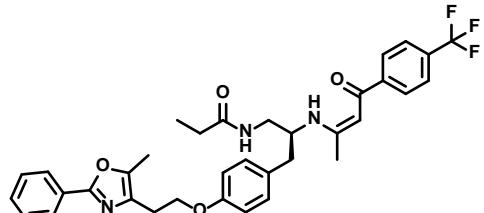
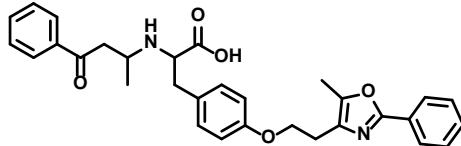
| | |
|--|---|
| 1. Table S1. Primer pairs used in real-time PCR assay..... | 2 |
| 2. Table S2. The crystal structures of PPAR α LBD in complex with different ligands have been reported till now..... | 3 |
| 3. Table S3. The structures of 14 compounds purchased..... | 5 |

Table S1. Primer pairs used in real-time PCR assay

| Gene name | Forward primer 5'-3' | Reverse primer 5'-3' |
|---------------|-------------------------|-------------------------|
| <i>IL15</i> | TTGGGAACCATAAGATTGTGCAG | GGGTGAACATCACTTCCGTAT |
| <i>IL6</i> | ACTCACCTCTCAGAACGAATTG | CCATCTTCCAAGGTTCAAGTTG |
| <i>ACADVL</i> | ACAGATCAGGTGTTCCCATACC | CTTGGCGGGATCGTCACCTT |
| <i>ACADM</i> | ACAGGGGTTCAGACTGCTATT | TCCTCCGTTGGTTATCCACAT |
| <i>CPT1A</i> | ATCAATCGGACTCTGGAAACGG | TCAGGGAGTAGCGCATGGT |
| <i>CD36</i> | CTTGCGCTTAATGAGACTGGGAC | GCAACAAACATCACCACACCA |
| <i>ACTB</i> | CATGTACGTTGCTATCCAGGC | CTCCTTAATGTCACGCACGAT |
| <i>Il6</i> | TAGTCCTCCTACCCCAATTCC | TTGGTCCTTAGCCACTCCTTC |
| <i>Il18</i> | GACTCTGCGTCAACTTCAAGG | CAGGCTGTCTTGTCACGA |
| <i>Gapdh</i> | TGACCTCAACTACATGGTCTACA | CTTCCCATTCTCGGCCCTG |

Table S2. The crystal structures of PPAR α LBD in complex with different ligands have been reported till now.

| PDB ID | Resolution (Å) | Year | Ligand |
|-------------------|----------------|------------|--|
| 5HYK ¹ | 1.83 | 11/23/2016 |  |
| 4BCR ² | 2.5 | 5/29/2013 |  |
| 3SP6 ³ | 2.21 | 7/20/2011 |  |
| 3KDT ⁴ | 2.7 | 4/28/2010 |  |
| 3KDU ⁴ | 2.07 | 4/28/2010 |  |
| 3FEI ⁵ | 2.4 | 10/20/2009 |  |
| 3G8I ⁶ | 2.2 | 6/2/2009 |  |

| | | | |
|-----------------------------------|------|------------|--|
| 3ET1 ⁷ | 2.5 | 2/17/2009 |  |
| 2REW ^a | 2.35 | 11/27/2007 |  |
| 1I7G ⁸ | 2.2 | 3/9/2002 |  |
| 1KKQ ⁹ (antagonist) | 3.0 | 2/20/2002 |  |
| 1K7L ¹⁰ | 2.5 | 12/5/2001 |  |

^a There is no reference for this crystal structure.

Table S3. The structures of 14 compounds were purchased from ChemDiv.

| Compd. | Structure | IDNUMBER | MW | LogP ^a | Glide Gscore |
|--------|-----------|-----------|--------|-------------------|-----------------|
| A-1 | | 3019-0307 | 386.38 | 1.55 | -7.96 |
| A-2 | | G818-0013 | 337.76 | 1.98 | -8.25 |
| A-3 | | 3570-0508 | 351.19 | 4.78 | -8.23 |
| A-4 | | 3793-4708 | 452.55 | 4.45 | -8.89 |

| | | | | | |
|------------|--|-----------|--------|------|--------|
| A-5 | | 4327-3056 | 358.42 | 3.42 | -7.99 |
| A-6 | | 7202-2780 | 413.43 | 3.97 | -9.24 |
| A-7 | | 8008-4201 | 315.33 | 2.22 | -7.22 |
| A-8 | | 8018-7032 | 378.39 | 2.21 | -10.88 |
| A-9 | | D135-0107 | 362.43 | 4.03 | -9.09 |

| | | | | | |
|-------------|--|-----------|--------|------|--------|
| A-10 | | D135-0118 | 422.49 | 3.99 | -8.94 |
| A-11 | | D135-0119 | 414.48 | 3.23 | -9.05 |
| A-12 | | D317-5172 | 388.47 | 3.89 | -7.99 |
| A-13 | | F136-0100 | 452.90 | 2.08 | -11.45 |
| A-14 | | F296-0408 | 431.55 | 4.36 | -9.87 |

^a The LogP values are obtained from the ChemDiv database.

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