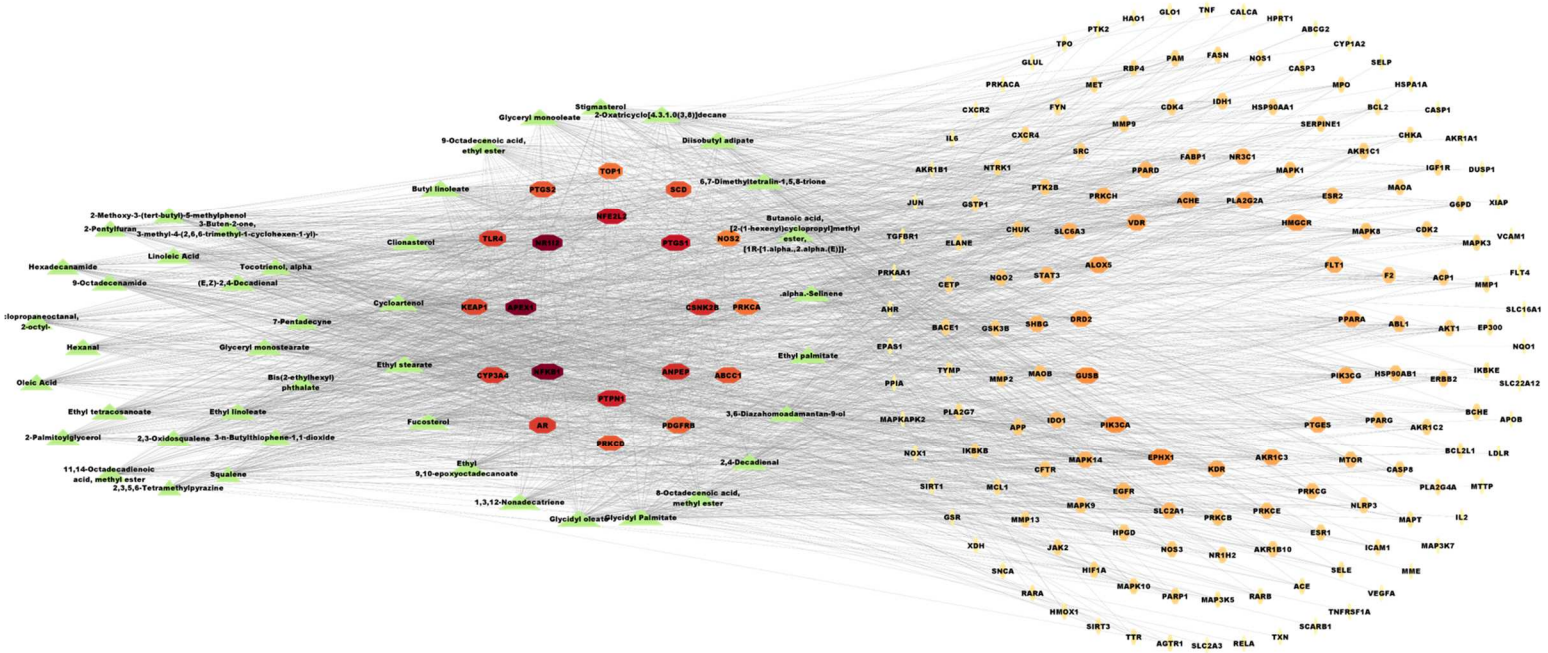
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Supplementary Materials

Supplementary Figure S1. Compounds-targets network: green triangle nodes are compounds and red shades octagonal nodes are targets.



Supplementary Table S1. Molecular docking results of the top 10 Hub genes and the 20 active compounds in LLPS.

Proteins	Compounds	Binding affinity (kcal/mol)	Interaction bonds	
			H-bonds/Covalent bonds/ Alkyl bonds/ Pi-sigma bonds/ Pi-Pi stacked/ Unfavorable acceptor-acceptor/ Unfavorable donor-donor	Van der Waals
NOS2 (4NOS)	Stigmasterol	-10.9	Trp194, Ala197, Arg199, Cys200, Met355, Phe369, Trp372, Tyr489	Pro198, Ile201, Gly202, Gln205, Ser242, Val352, Gly371, Met374, Glu377, Phe488
	Cycloartenol	-10.4	Trp194, Leu209, Ile244, Gln263, Phe369, Tyr489	Cys200, Ser242, Pro350, Ala351, Val352, Asn370, Gly371, Tyr373, Glu377, Aso382, Arg388
	Clionasterol	-10.1	Ala197, Arg199, Cys200, Met355, Phe369, Trp372, Tyr489	Trp194, Pro198, Ile201, Gly202, Gln205, Ser242, Val352, Gly371, Met374, Glu377, Phe488, Tyr490
	Fucosterol	-9.1	Ala197, Arg199, Val352, Met355, Arg381, Trp463, Pro467	Pro198, Cys200, Ile201, Phe369, Met374, Thr376, Glu377, Tyr486, Tyr491
	6,7-Dimethyltetralin-1,5,8-trione	-7.7	Trp194, Cys200, Phe369	Ala197, Leu209, Ser242, Met355, Asn370, Gly371, Tyr489
	alpha-Selinene	-7.3	Trp194, Cys200, Phe369	Gly202, Leu209, Ser242, Val352, Asn370, Gly371, Trp372, Tyr489
	Glyceryl monooleate	-7.0	Leu125, Trp194, Ala197, Pro198, Arg199, Cys200, Pro350, Val352, Met355, Phe369, Phe488, Tyr489, Tyr491	Gly202, Leu209, Ser242, Ala351, Asn370, Gly371, Trp372, Tyr490
	Butyl linoleate	-7.0	Leu125, Trp194, Ala197, Pro198, Arg199, Cys200, Leu209, Pro350, Val352, Met355, Phe369, Phe488, Tyr489, Tyr491	Ser242, Ala351, Asn370, Gly371, Trp372, Tyr490
	Butanoic acid, [2-(1-hexenyl)cyclopropyl]methyl ester, [1R-[1.alpha.,2.alpha.(E)]]-	-7.1	Leu125, Trp194, Ala197, Cys200, Met355, Phe369, Phe488, Tyr489, Tyr491	Pro198, Arg199, Leu209, Ser242, Asn370, Gly371, Tyr490
	Glycidyl oleate	-7.1	Leu125, Trp194, Ala197, Arg199, Cys200, Leu209, Met355, Phe369, Gly371 Phe488, Tyr489, Tyr491	Ser242, Pro350, Ala351, Val352, Asn370, Glu377, Tyr490

	1,3,12-Nonadecatriene	-6.5	Trp194, Leu209, Pro350, Phe369, Trp372, Tyr489	Ile201, Gly202, Gln205, Ser242, Ala351, Val352, Asn370, Gly371, Glu377
	Ethyl stearate	-6.2	Leu125, Trp194, Ala197, Arg199, Cys200, Phe369, Tyr489, Tyr491	Pro198, Leu209, Ser242, Val352, Met355, Asn370, Gly371, Phe488
	Glycidyl palmitate	-6.3	Trp194, Cys200, Leu209, Pro350, Val352, Phe369, Tyr373, Tyr489	Ser242, Ile244, Gln263, Arg266, Tyr347, Ala351, Asn370, Gly371, Trp372 Glu377, Asp382, Arg388
	Ethyl 9,10-epoxyoctadecanoate	-6.4	Leu125, Trp194, Ala197, Pro198, Arg199, Cys200, Leu209, Pro350, Phe369, Phe488, Tyr489, Tyr491	Ser242, Val352, Met355, Asn370, Gly371, Trp372, Glu377
	9-Octadecenoic acid, ethyl ester	-6.5	Leu125, Trp194, Ala197, Arg199, Cys200, Leu209, Phe369, Phe488, Tyr489, Tyr491	Pro198, Ser242, Val352, Met355, Asn370, Gly371, Glu377
	Diisobutyl adipate	-6.3	Leu125, Trp194, Pro198, Arg199, Phe369, Phe488, Tyr489, Tyr491	Ala197, Cys200, Leu209, Val352, Met355, Asn370, Gly371
	Ethyl palmitate	-6.1	Leu125, Trp194, Ala197, Pro198, Arg199, Cys200, Gly202, Met355, Phe369, Trp372, Phe488, Tyr491	Gln205, Gly371, Tyr489, Tyr490
	2,4-Decadienal	-5.9	Trp194, Ala197, Cys200, Leu209, Phe369, Tyr489	Arg199, Ser242, Asn370, Gly371
	3,6-Diazahomoadamantan-9-ol	-5.6	Gly253, Lys254, Asp256, Arg258, Gln310	Pro129, Gly313, Ala495, Thr498, His499, Val500
	2-Oxatricyclo[4.3.1.0(3,8)]decane	-5.2	Gln310, Gly313, His499	Pro129, Gly253, Lys254, Asp256, Arg258, Ala495, Thr498, Val500
KEAP1 (6TYP)	Stigmasterol	-9.9	Ala366, Arg415, Val465, Ala556, Val512	Tyr334, Ser363, Gly364, Leu365, Gly367, Arg380, Asn414, Gly462, Val463, Gly464, Ala466, Gly509, Ala510, Gly511, Cys513, Phe577, Ile559, Gly603, Val604, Gly605, Val606
	Cycloartenol	-10.1	ALa366, Gly367, Arg415, Tyr525, Ala556	Gly364, Leu365, Ile416, Val418, Gly462, Gly464, Val465, Ser508, Gly509, Ala510, Gly511, Val512, Ser555, Leu557, Gly558, Ile559, Gly603, Val604, Gly605, Val606
	Clionasterol	-9.2	Ala466, Cys513, Ala556	Gly364, Leu365. Ala366, Gly367, Arg415, Val418, Gly419, Gly462, Val463, Gly464, Val465, Val467, Gly509, Ala510, Gly511, Val512, Val514, Ile557, Gly558, Ile559, Thr560, Gky603, Val604, Val606, Ala607

Fucosterol	-8.3	Val465, Val467	Gly367, Cys368, Val418, Gly419, Val420, Ala466, Val512, Cys513, Val514, Ile559, Val561, Thr560, Ala607
6,7-Dimethyltetralin-1,5,8-trione	-7.7	Tyr334, Ser363, Arg380, Ser602	Gly364, Asn382, Arg415, Ala556, Tyr572, Phe577, Gly603
alpha-Selinene	-6.8	Ala366	Leu365, Gly376, Ile416, Gly417, Val418, Gly462, Val463, Gly464, Val465, Gly509, Ala510, Gly511, Leu557, Gly558, Ile559, Val604, Gly605, Val606
Glyceryl monooleate	-6.3	Tyr334, Ile416, Val463, Tyr525, Ala556, Tyr572, Phe577	Ser363, Gly364, Leu365, Ala366, Arg380, ARg415, Gly417, Gly462, Gly464, Gly509, Gln530, Ser555, Ser602, Gly603
Butyl linoleate	-6.0	Tyr334, Arg380, Arg415, Tyr525, Ala556, Tyr572	Ser363, Gly364, Asn414, Ser508, Gly509, Gln530, Ser555, Phe577, Ser602, Gly603
Butanoic acid, [2-(1-hexenyl)cyclopropyl]methyl ester, [1R-[1.alpha.,2.alpha.(E)]]-	-5.4	Arg415, Ser508, Ala556, Tyr572, Phe577	Tyr334, Gly462, Arg483, Gly509, Tyr525, Ser555, Ser602
Glycidyl oleate	-5.9	Tyr334, Arg415, Tyr525, Ala556, Tyr572, Phe577	Ser363, Gly364, Arg380, Gly462, Gly509, Gln530, Ser555, Ser602, Gly603
1,3,12-Nonadecatriene	-5.3	Tyr334, Arg415, Tyr525, Ala556, Tyr572, Phe577	Ser363, Gly364, Arg380, Gly509, Gln530, Ser555, Ser602, Gy603
Ethyl stearate	-5.7	Tyr334, Ser363, Arg380, Tyr525, Ala556, Tyr572	Gly364, Arg415, Gly509, Gln530, Ser555, Phe577, Ser602, Gly603
Glycidyl palmitate	-5.6	Tyr334, Asn414, Tyr525, Ala556, Tyr572, Phe577	Ser363, Gly364, Arg380, Arg415, Gln530, Ser555, Ser602
Ethyl 9,10-epoxyoctadecanoate	-5.8	Tyr525, Ser555, Ala556, Tyr572	Tyr334, Ser363, Gly364, Arg380, Asn414, Ile461, Gly462, Arg483, Ser508, Gly509, Phe577, Ser602, Gly603
9-Octadecenoic acid, ethyl ester	-5.6	Tyr334, Arg380, Arg415, Tyr525, Ala556, Tyr572, Phe577	Ser363, Gly364, Asn414, Gln530, Ser555, Ser602, Gly603
Diisobutyl adipate	-5.6	Gly367, Ala556, Gly605, Val606	Gly364, Leu365, Arg415, Ile416, Gly417, Val418, Gly462, Val463, Gly464, Val465, Gly509, Ala510, Val512, Leu556, Leu557 Ile559, Gly603, Val604

	Ethyl palmitate	-5.8	Tyr334, Arg380, Arg415, Tyr525, Tyr572, Phe577	Ser363, Gly364, Asn414, Arg483, Ser508, Gly509, Gln530, Ser555, Ala556, Ser602
	2,4-Decadienal	-5.0	Tyr334, Asn414, Arg415, Ala556, Tyr572, Phe577	Ser363, Gly364, Arg380, Ser555, Ser602
	3,6-Diazahomoadamantan-9-ol	-6.2	Leu365, Gly367, Leu557, Ile559, Val606	Ala366, Cys368, Gly511, Val512, Gly558, Val604, Gly605, Ala607
	2-Oxatricyclo[4.3.1.0(3,8)]decane	-5.2	Tyr334, Arg415, Ala556	Ser363, Gly364, Arg380, Ser602, Gly603
PTGS2 (5IKQ)	Stigmasterol	-8.9	Leu294, Leu391, Tyr404, Ile408, Ala443, Val444	Ala202, Gln203, His207, Tyr385, His386, Trp387, His388, Leu390, Val447
	Cycloartenol	-8.7	Tyr385, Trp387, Tyr404, Ile408	Gln203, His207, Leu294, Val295, His386, His388, Leu390, Leu391, Gln405, Val444, Val447
	Clionasterol	-8.9	Leu294, Leu391, Ile408	Ala202, Gln203, Thr206, His207, Tyr385, His386, Trp387, His388, Leu390, Tyr404, Ala443, Val444, Val447
	Fucosterol	-8.7	His207, Lys211, Gln289, Val291, His388, Leu391	Ala202, Gln203, Thr206, Phe210, Thr212, His214, Tyr385, His386, Trp387, Leu390, Val447
	6,7-Dimethyltetralin-1,5,8-trione	-7.8	His207, His388	Ala199, Ala202, Gln203, Thr206, Phe210, Asn382, Tyr385, His386, Trp387, Leu390, Leu391
	alpha-Selinene	-8.0	Val349, Leu352, Val523, Ala527	Tyr348, Ser353, Tyr385, Trp387, Phe518, Met522, Gly526, Ser530
	Glyceryl monooleate	-6.8	Val349, Leu352, Ser353, Tyr385, Trp387, Phe518, Met522, Val523, Ala527, Leu531	His90, Val116, Arg120, Gln192, Tyr348, Gly354, Tyr355, Leu359, Phe381, Leu384, Arg513, Ala516, Ile517, Gly526, Ser530,
	Butyl linoleate	-6.7	His90, Val523, Val349, Tyr355, Tyr385, Trp387, Ala516, Ile517, Phe518, Met522, Val523, Ala527, Leu531	Val116, Arg120, Gln192, Tyr348, Leu352, Ser353, Leu359, Leu384, Arg513, Gly526, Ser530
	Butanoic acid, [2-(1-hexenyl)cyclopropyl]methyl ester, [1R-[1.alpha.,2.alpha.(E)]]-	-6.8	Val116, Arg120, Val349, Leu352, Tyr355, Leu359, Tyr385, Trp387, Phe518, Val523, Leu531	Met113, Tyr348, Ser353, Phe381, Leu384, MEt522, Gly526, Ala527, Ser530,
	Glycidyl oleate	-6.8	Arg120, Val349, Leu352, Tyr355, Leu384, Tyr385, Trp387, Phe518, Val523, Ala527	Val89, Leu93, Tyr115, Val116, Ser119, Tyr348, Ser353, Phe381, Met522, Gly526, Ser530, Leu531
	1,3,12-Nonadecatriene	-6.9	Val116, Ile345, Val349, Leu352, Tyr355, Leu359, Tyr385, Trp387, Phe518, Val523, Ala527, Leu531	Met113, Arg120, Trp348, Ser353, Phe381, Leu384, Met522, Gly526, Ser530

	Ethyl stearate	-5.9	Ala202, Val295, His388, Leu390, Leu391, Phe395, Tyr404, Phe407, Ile408, Val444, Val447	Ala199, Phe200, Gln203, Thr206, His207, Phe210, Leu294, Tyr385, His386, Trp387
	Glycidyl palmitate	-6.1	Val349, Leu352, Tyr355, Tyr385, Trp387, Ala527, Leu531	Val116, Arg120, Tyr348, Ser353, Leu359, Phe381, Leu384, Phe518, Met522, Val523 Gly526, Ser530
	Ethyl 9,10-epoxyoctadecanoate	-6.8	Val116, Ile345, Val349, Leu352, Tyr355, Leu359, Leu384, Tyr385, Trp387, Phe518, Met522, Val523, Ala527, Ser530, Leu531	Met113, Arg120, Tyr348, Ser353, Phe381, Glt526
	9-Octadecenoic acid, ethyl ester	-6.7	Arg120, Ile345, Val349, Leu352, Tyr355, Leu359, Leu384, Tyr385, Trp387, Phe518, Met522, Val523, Ala527, Leu531	Met113, Val116, Tyr348, Ser353, Phe381, Gly526, Ser530
	Diisobutyl adipate	-6.6	Val116, Tyr348, Val349, Leu352, Tyr355,, Leu359, Leu531	Met113, Arg120, Ser353, Tyr385, Trp387, Phe518, Met522, Val523, Gly526, Ala527, Ser530
	Ethyl palmitate	-6.7	Leu352, Tyr355, Tyr385, Trp387, Phe518, Val523, Ala527, Ser530	Val116, Arg120, Tyr348, Val349, Ser353, Leu359, Phe381, Leu384, Met522, Gly526
	2,4-Decadienal	-5.3	Val349, Leu352, Tyr355, Phe518, Met522, Val523, Ala527	Arg120, Tyr348, Ser353, Phe381, Tyr385, Trp387, Gly526, Ser530
	3,6-Diazahomoadamantan-9-ol	-5.5	Pro84, Ser119, Arg120, Glu524	Lys83, Pro86, Val89, Tyr115, His122
	2-Oxatricyclo[4.3.1.0(3,8)]decane	-5.6	Val349, Leu352, Phe518, Val523, Ala527	Ser353
PTGS1 (6Y3C)	Stigmasterol	-8.4	Pro128, Arg374, Arg376, Pro538	Ser126, Pro127, Phe142, Val145, Gly225, His226, Asp229, Arg333, Leu334, Ile337, Asn375, Asn537
	Cycloartenol	-8.2	Leu93, Leu112,	Arg83, Pro84, Pro86, Thr89, Leu92, Trp100, Leu115, Val116, Val119, Arg120, Leu357, Gly471, Glu524
	Clionasterol	-7.8	Phe356	Gln192, Glu347, Gln350, Gln351, Gly354, Tyr355, Leu564, Val578, Ser579, Phe580, Arg581
	Fucosterol	-7.6	Arg79, Arg83	His43, Gln44, Thr62, Gly63, Tyr64, Thr76, Asn80, Val119, Asn122, Leu123, Gly471
	6,7-Dimethyltetralin-1,5,8-trione	-8.1	Ala202, Gln203, His207, His388	Ala199, Thr206, Phe210, Tyr385, Trp387, Leu390, Met391
	alpha-Selinene	-6.6	His207, His386	Ala202, Gln203, Thr206, Phe210, Asn382, Tyr385, His388, Val447

Glyceryl monooleate	-6.0	Cys36, Tyr39, Cys47, Arg49, Pro153, Pro156	Asn34, Cys41, Gln42, His43, Gln44, Gly45, Val48, Asp135, Tyr136, Leu152, Ser154, Gln461, Glu465, Lys468, Arg469
Butyl linoleate	-5.7	Cys36, Tyr39, Gln44, Gly45, Ile46, Cys47, Pro153	Pro40, Cys41, Gln42, His43, Val48, Arg49, Tyr130, Asp135, Tyr136, Ile137, Leu152, Gln461, Arg469
Butanoic acid, [2-(1-hexenyl)cyclopropyl]methyl ester, [1R-[1.alpha.,2.alpha.(E)]]-	-6.0	Phe205, Phe209, Val344, Tyr348, Val349, Leu352, Tyr385, Trp387, Leu534	Ser353, Phe381, Leu384, Phe518, Met522, Ile523, Gly526, Ala527, Ser530, Gly533,
Glycidyl oleate	-6.2	Cys36, Tyr39, Ile46, Cys47, Tyr130, Pro153, Pro156, Glu465, Lys468	Pro40, Cys41, Gln42, His43, Gln44, Gly45, Asp135, Leu152, Ser154, Gln461, Arg469
1,3,12-Nonadecatriene	-6.5	Ala199, Ala202, Phe210, Leu295, Tyr385, His386, Trp387, His388, Leu390, Met391, Phe395, Tyr404, Phe407, Leu408, Ile444	Gln203, Thr206, Asn382
Ethyl stearate	-7.2	Arg120, Phe205, Phe209, Val228, Val344, Tyr348, Val349, Leu352, Ser353, Tyr355, Leu359, Ile377, Phe381, Trp387, Phe518, Ile523, Ala527, Leu531, Leu534	Val116, Gly227, Asn375, Tyr385, Met522, Gly526, Ser530, Gly533
Glycidyl palmitate	-5.9	Phe205, Gly227, Tyr348, Val349, Leu352, Ile377, Phe381, Tyr385, Trp387, Phe518, Ile523, Ala527, Leu534	Arg120, Phe209, Val228, Val344, Ser353, Asn375, Arg376, Ala378, Leu384, Gly526, Phe529, Ser530, Gly533
Ethyl 9,10-epoxyoctadecanoate	-6.4	Phe205, Val344, Tyr348, Val349, Leu352, Tyr355, Leu359, Ile377, Phe381, Tyr385, Ile523, Ala527, Phe529, Ser530, Leu534	Arg120, Phe209, Gly227, Val228, Ser353, Asn375, Trp387, Phe518, Met522, Gly526, Gly533
9-Octadecenoic acid, ethyl ester	-6.2	Val116, Phe205, Phe209, Val344, Tyr348, Val349, Leu352, Tyr355, Leu359, Ile377, Tyr385, Trp387, Ile523, Ala527, Ser530, Leu531, Gly533, Leu534,	Arg120, Gly227, Val228, Ser353, Asn375, Phe381, Leu384, Phe518, Met522, Gly526, Phe529
Diisobutyl adipate	-6.1	Cys36, Cys41, Pro153, Pro156, Gln461, Lys468	Tyr39, Gln42, His43, Gln44, Gly45, Cys47, Asp135, Leu152, Ser154, Val155, Glu465, Arg469
Ethyl palmitate	-5.7	Cys36, Tyr39, Gln44, Gly45, Ile46, Cys47, Tyr130, Pro153, Pro156, Lys468, Arg469	Cys41, Gln42, His43, Asp135, Leu152, Ser154, Gln461, Glu465
2,4-Decadienal	-5.3	Arg120, Val349, Leu352, Tyr355, Trp387, Phe518, Ala527	Tyr348m Ser353, Met522, Ile523, Gly526, Ser530,

	3,6-Diazahomoadamantan-9-ol	-5.5	Ile523	Val349, Leu352, Ser353, Leu384, Trp387, Phe518, Met522, Gly526, Ala527, Ser530
	2-Oxatricyclo[4.3.1.0(3,8)]decane	-6.3	Val349, Leu352, Phe518, Ile523, Ala527	Ser353, Trp387, Ser530, Gly526
NR1I2 (6P2B)	Stigmasterol	-7.8	Lys170, Leu174, Leu213, Leu215, Trp223	Phe172, Pro175, Val177, Gly217, Glu218, Asn224, Tyr225, Arg303
	Cycloartenol	-8.1	Phe172, Leu174, Leu215, Trp223	Pro175, Gly176, Val177, Asn224, Tyr225, Lys226
	Clionasterol	-7.1	Trp223, Tyr225	Leu174, Pro175, Gly176, Val177, Leu215, Asn224, Lys226, Pro228
	Fucosterol	-6.8	Lys277, Pro354, Ala405	Ser274, Gly278, Arg353, Asn404, Thr408, Gln409, Leu412, Phe429, Gly430
	6,7-Dimethyltetralin-1,5,8-trione	-7.3	Val211, Trp299	Leu209, Met243, Gln285, Phe288, Tyr306, Met323, Leu324, His327
	alpha-Selinene	-7.9	Phe288, Trp299, Tyr306	Leu209, Val211, Met243, Met246, Gln285, Met323, His327, His407
	Glyceryl monooleate	-6.2	Leu209, Lys210, Val211, Met243, Phe288, Trp299, Tyr306	Leu206, Leu239, Leu240, Met246, Ser247, Gln285, Met323, His327, His407
	Butyl linoleate	-6.7	Val211, Leu240, Met243, Ser247, Phe288, Trp299, Tyr306, His327	Leu206, Leu209, Ala244, Gln285, Leu308, Met323, Leu324, His407, Leu411, Ile414, Phe420, Met425,
	Butanoic acid, [2-(1-hexenyl)cyclopropyl]methyl ester, [1R-[1.alpha.,2.alpha.(E)]]-	-6.2	Met243, Cys284, Phe288, Trp299, Tyr306, His407, Leu411, Met425, Phe429	Met246, Ser247, Phe251, Phe281, Gln285, Met323, His327
	Glycidyl oleate	-6.2	Leu209, Val211, Met243, Met246, Phe281, Phe288, Trp299, Tyr306, Met323, His327, His407	Leu206, Leu240, Ser247, Cys284, Gln285, Leu324, Ile414, Phe420
	1,3,12-Nonadecatriene	-5.9	Leu209, Val211, Met243, Phe288, Trp299, Tyr306, Met323, His327, His407	Leu240, Ser247, Gln285, Leu308, Leu324
	Ethyl stearate	-5.6	Leu209, Val211, Leu240, Met243, Ser247, Phe288, Trp299, Tyr306, His407, Phe420	Gln285, Met323, His327, Leu411, Met425
	Glycidyl palmitate	-6.2	Leu209, Val211, Met243, Gln285, Phe288, Trp299, Tyr306, Met323, His407	Ser247, Phe281, Cys284, Leu308, Leu324, His327, Leu411, Phe420, Met425
	Ethyl 9,10-epoxyoctadecanoate	-6.3	Leu209, Val211, Met243, Gln285, Phe288, Trp299, Tyr306, Met323, His407	Leu206, Leu240, Leu324, Arg410, Leu411, Ile414, Phe420
	9-Octadecenoic acid, ethyl ester	-5.6	Leu209, Val211, Met243, Phe288, Trp299, Tyr306, Met323, His327, His407	Leu206, Leu240, Met246, Ser247, Gln285, Leu324

	Diisobutyl adipate	-6.3	Leu206, Leu240, Ser247, Gln285, Phe288, Trp299, His407, Leu411, Ile414	Met243, Ala244, Cys284, His327, Phe420, Met425
	Ethyl palmitate	-5.9	Leu209, Val211, Met243, Ser247, Phe288, Trp299, Tyr306, Leu308, Leu324, His407	Aka244, Phe281, Gln285, Met323, His327, Leu411, Phe420, Met425
	2,4-Decadienal	-5.4	Ser247, Phe288, Trp299, Tyr306, His407	Met243, Met246, Phe281, Gln285
	3,6-Diazahomoadamantan-9-ol	-5.5	His327	Val211, Met243, Gln285, Phe288, Trp299, Tyr306, Met323
	2-Oxatricyclo[4.3.1.0(3,8)]decane	-6.4	Met243, Phe288, Trp299, Tyr306	Val211, Met246, Gln285
PRKCA (6AR4)	Stigmasterol	-7.7	Ile35, Ile37, Phe53, Ala87, Ile90	Leu32, Ile33, Gly34, Thr56, Gln91
	Cycloartenol	-7.3	Leu32, Phe53, Ala87, Ile90	Lys27, Asn31, Ile33, Gly34, Ile35, Ser36, Ile37, Gln91
	Clionasterol	-7.9	Phe53, Ala87	Leu32, Ile33, Gly34, Ile35, Ser36, Ile37, Asp54, Thr56, Val86, Ile90, Gln91
	Fucosterol	-5.8	Leu32, Ile35, Ile37	Gly34, Ser36, Phe53, Lys83, Val84, Ala87, Gln91
	6,7-Dimethyltetralin-1,5,8-trione	-6.1	Leu32, Ile33, Gly34	Ile35, Phe53, Ala87, Ile90, Gln91
	alpha-Selinene	-6.9	Leu32, Ile35, Ile37, Ala87, Ile90	Ile33, Gly34, Ser36, Gln91
	Glyceryl monooleate	-5.4	Asp28, Gln30, Leu32, Ile35, Ile37, Phe53, Thr56 Ala87, Ile90	Ile33, Gly34, Ser36, Asn55, Pro57, Gln91
	Butyl linoleate	-5.7	Leu32, Ile33, Gly34, Ile35, Ile37, Phe53, Lys83, Val84, Ala87, Lys88, Ile90	Lys27, Ser36, Gln91
	Butanoic acid, [2-(1-hexenyl)cyclopropyl]methyl ester, [1R-[1.alpha.,2.alpha.(E)]]-	-5.3	Leu32, Phe53	Ile33, Gly34, Ile35, Ser36, Ile37, Ala87, Ile90, Gln91
	Glycidyl oleate	-5.5	Leu32, Ile35, Ile37, Phe53, Asp54, Ala87, Ile90	Lys27, Asp28, Asn31, Ile33, Gly34, Ser36, Asn55, Thr56, Gln91
	1,3,12-Nonadecatriene	-4.9	Leu32, Ile33, Ile35, Ile37, Phe53, Ala87, Ile90	Gly34, Ser36, Gln91
	Ethyl stearate	-5.6	Leu32, Ile33, Ile35, Ile37 Phe53, Lys83, Val84, Ala87, Ile90	Asp28, Gln30, Gly34, Ser36, Thr56, Gln91
	Glycidyl palmitate	-5.0	Leu32, Ser36, Ile35, Ile37, Phe53, Ala87, Ile90	Ile33, Gly34, Val50, Lys83, Gln91
	Ethyl 9,10-epoxyoctadecanoate	-5.9	Leu32, Ile33, Gly34, Ile35, Ile37, Phe53, Ala87, Ile90	Ser36, Thr56, Gln91
	9-Octadecenoic acid, ethyl ester	-5.3	Gln30, Leu32, Ile33, Ile35, Ile37, Phe53, Ala87, Ile90	Asp28, Gly34, Ser36, Asp54, Asn55, Thr56, Gln91

	Diisobutyl adipate	-5.5	Leu32, Ile33, Gly34, Ile35, Ile37, Phe53, Lys83, Ala87	Ser36, Ile90, Gln91
	Ethyl palmitate	-5.3	Leu32, Ile35, Ile37, Phe53, Ala87, Ile90	Ile33, Gly34, Ser36, Gln91
	2,4-Decadienal	-5.2	Leu32, Ile33, Ile35, Ile37, Ala87, Ile90	Gly34, Ser36, Gln91
	3,6-Diazahomoadamantan-9-ol	-4.0	Asn102	Tyr48, Gly67, Asp68, Glu69, Lys103, Leu104
	2-Oxatricyclo[4.3.1.0(3,8)]decane	-5.2	Leu32, Ile33, Ala87, Ile90	Gly34, Ile35, Ile37, Gln91
PRKCD (1YRK)	Stigmasterol	-7.6	Phe27, Tyr52, Ala77	Gln25, Glu54, Trp55, Met74, Glu78
	Cycloartenol	-7.6	Phe27, Tyr52, Ala77	Gln25, Glu54, Trp55
	Clionasterol	-7.0	Gln25, Phe27, Tyr52, Glu54, Trp55	Glu54, Trp55, Ala77
	Fucosterol	-6.6	Phe27	Gln25, Tyr52, Pro53, Glu54, Trp55, Ala76
	6,7-Dimethyltetralin-1,5,8-trione	-5.9	Phe27	Gln25, Tyr52, Glu54, Trp55
	alpha-Selinene	-5.7	Phe27	Tyr52, Pro53, Glu54, Trp55
	Glyceryl monooleate	-4.8	Phe27, Tyr52, Trp55, Ala77, Glu78	Gln25, Ala29, Lys31, Thr50, Pro53, Glu54, Met74
	Butyl linoleate	-4.2	Phe27, Tyr52, Ala77	Gln25, Pro53, Glu54, Ala76
	Butanoic acid, [2-(1-hexenyl)cyclopropyl]methyl ester, [1R-[1.alpha.,2.alpha.(E)]]-	-4.7	Phe27, Tyr52, Trp55, Ala77	Gln25, Pro53, Glu54
	Glycidyl oleate	-4.4	Phe27, Tyr52, Trp55	Ala23, Gln25, Glu54, Pro53
	1,3,12-Nonadecatriene	-4.3	Phe27 Tyr52, Trp55	Gln25, Pro26, Pro53, Glu54, Ala77
	Ethyl stearate	-4.2	Phe27, Tyr52, Trp55, Ala77	Gln25, Pro26, Cys28, Pro53, Glu54
	Glycidyl palmitate	-4.0	Gln25, Phe27, Tyr52, Glu54, Trp55	Cys28, Pro53
	Ethyl 9,10-epoxyoctadecanoate	-3.9	Phe27, Tyr52, Ala77	Ala23, Asn24, Gln25, Pro53, Glu54, Trp55, Arg75, Ala76
	9-Octadecenoic acid, ethyl ester	-4.0	Phe27, Ala76, Ala77	Als23, Asn24, Gln25, Tyr52, Pro53, Glu54, Trp55, Arg75
	Diisobutyl adipate	-4.1	Phe27, Trp55	Gln25, Pro26, Cys28, Tyr52, Pro53, Glu54, Ala76
	Ethyl palmitate	-3.9	Ala23, Phe27, Tyr52	Gln25, Pro53, Glu54, Trp55
	2,4-Decadienal	-4.2	Phe27, Tyr52, Ala77	Met74, Glu78
	3,6-Diazahomoadamantan-9-ol	-4.0	Ala19, Glu22, Asn24	Gln18, Glu20, Asp21
	2-Oxatricyclo[4.3.1.0(3,8)]decane	-3.9	Phe27	Tyr52, Pro53, Glu54
NFKB1	Stigmasterol	-7.2	Tyr60, Val61, Ala62, Val145	Glu63, Leu143, His144, Thr146, Lys149, Thr153, Arg157

(1SCV)	Cycloartenol	-7.1	Phe56, Arg57, Lys79	Lys52, Gly55, Arg59, His67, Gly68, Gly69, Pro71, Ser74, Ser75, Lys80, Ser81, Ser243
	Clionasterol	-6.7	Pro71, Ser74, Lys79, Lys80	Lys52, Gly55, Phe56, Arg57, Arg59, His67, Gly68, Gly69, Ser75, Ser81
	Fucosterol	-6.9	Val61, Leu143, Val145, Lys149	Pro65, Ser113, Val115, His144, Thr146, Thr153, Arg157
	6,7-Dimethyltetralin-1,5,8-trione	-6.2	Ser113, Val145, Thr153, Arg157	Val61, Leu143, His144, Thr146, Lys149, Ala156
	alpha-Selinene	-5.6	Val61, Val115, Leu143, Val145	Ala111, His112, Ser113, Asp121, His144, Lys149, Thr153, Arg157
	Glyceryl monooleate	-5.5	Arg59, Pro65, Ser113, Gly122, Val115, Leu143, Arg157	Val61, Gly64, His67, Gly68, Gly69, Leu114, Gly116, Glu120, Asp121, Asn139, Gly141, Ile142, Thr153
	Butyl linoleate	-4.9	Arg59, Val61, Pro65, Val115, Leu143	Gly64, Gly68, Gly69, Gky116, Lys117, Asn139, Leu140, Gly141, Ile142
	Butanoic acid, [2-(1-hexenyl)cyclopropyl]methyl ester, [1R-[1.alpha.,2.alpha.(E)]]-	-4.9	Val61, Ala62, Leu143, Val145, Thr153	Tyr60, Ala111, His112, Ser113, His144, Thr146, Lys149, Arg157
	Glycidyl oleate	-4.8	Tyr60, Val61, Ala62, Ser113, Gly122, Leu143, Val145, Arg157	Val115, Asp121, His144, Thr146, Lys149, Thr153
	1,3,12-Nonadecatriene	-5	Tyr60, Val61, Ala62, Leu143, Val145, Lys147, Lys149	Ala111, His112, Ser113, His144, Thr146, Thr153, Arg157
	Ethyl stearate	-4.3	Val61, Ser113, Leu143, Val145, Lys149, Arg157	Tyr60, Ala62, Val115, Asp121, Gly122, His144, Thr146, Thr153
	Glycidyl palmitate	-4.7	Arg59, Val61, Pro65, Val115, Asp121, Gly122, Leu143	Tyr60, Gly64, Ser113, Gly116, Cys119, Glu120, Arg157
	Ethyl 9,10-epoxyoctadecanoate	-5.2	Arg59, Val61, Val115, Leu143, Val145, Lys149, Thr153, Arg157	Gly64, Pro65, His67, Gly68, Ala111, His112, Ser113, Asp121, Gly141, Ile142
	9-Octadecenoic acid, ethyl ester	-5.1	Phe56, Arg59, Val61, Val115, Leu143, Lys149, Thr153	Gly64, Pro65, His67, Gly68, Ser113, Gly141, Ile142, His144, Val145, Thr146, Arg157
	Diisobutyl adipate	-4.9	Val61, Ala62, Thr146, Arg157	Tyr60, Ala111, His112, Ser113, Leu143, His144, Val145, Lys149, Thr153
	Ethyl palmitate	-4.7	Arg59, Val61, Pro65, Val115, Leu143	Tyr60, Gly64, His67, Gly68, Gly69, Gly116, Asn139, Leu140 Gly141, Ile142

	2,4-Decadienal	-4.7	Arg59, Val61, Pro65, His67, Gly68, Val115, Leu143	Gly64, Gly141
	3,6-Diazahomoadamantan-9-ol	-4.4	Ser249	Ser243, Lys244, Asn250, Asp274, Lys275, Phe310
	2-Oxatricyclo[4.3.1.0(3,8)]decane	-4.1	Val61, Pro65, Val115, Leu143	Gly64
NFE2L2 (7X5E)	Stigmasterol	-6.7	Phe481, Arg499, Arg502, Arg503, Lys506	Asn482, Met485, Asn507, Ala510
	Cycloartenol	-7.4	Lys506	Val478, Arg499, Arg502, Arg503
	Clionasterol	-6.3	Val478, Arg499, Arg502, Arg503	Pro477, Phe481, Lys506
	Fucosterol	-6.2	Val478, Arg499, Arg502, Arg503	Phe 481, Asn482, Arg502, Lys506
	6,7-Dimethyltetralin-1,5,8-trione	-6.2	Arg502, Arg503, Lys506	Val478, Phe481, Arg499
	alpha-Selinene	-6.2	Phe481, Arg499, Arg502, Arg503	Lys506
	Glyceryl monooleate	-4.5	Phe481, Arg499, Arg502, Arg503, Lys506	Ala496, Asp500
	Butyl linoleate	-4.3	Val478, Phe281, Arg499, Arg502, Arg503	Ans482, Lys506
	Butanoic acid, [2-(1-hexenyl)cyclopropyl]methyl ester, [1R-[1.alpha.,2.alpha.(E)]]-	-4.4	Arg499, Arg502, Arg503	Val478, Phe481, Ala496, Lys506
	Glycidyl oleate	-4.7	Phe481, Arg499, Arg502, Arg503	Val478, Ala496, Lys506
	1,3,12-Nonadecatriene	-4.4	Val478, Phe481, Arg499, Arg502, Arg503, Lys506	Asn482
	Ethyl stearate	-4.2	Phe481, Ala496, Arg499, Arg502, Arg503	Lys506
	Glycidyl palmitate	-4	Phe481, Arg499, Arg502, Arg503, Lys506	Val478, Asn482
	Ethyl 9,10-epoxyoctadecanoate	-4.6	Phe481, Arg499, Lys506, Ala510	Val478, Asn507
	9-Octadecenoic acid, ethyl ester	-3.9	Phe481, ALa496, Arg499, Arg502, Arg503	Val478, Asn482
	Diisobutyl adipate	-4.9	Phe481, Ala496, Arg502, Arg503	Val478, Arg499, Asp500, Lys506
	Ethyl palmitate	-4.2	Phe481, Ala496, Arg499, Arg502, Arg503	Val478, Asp500, Lys506
	2,4-Decadienal	-4.2	Phe481, Arg499, Arg502, Arg503	
	3,6-Diazahomoadamantan-9-ol	-4.6	Arg503	Phe481, Arg499, Arg502, Lys506
	2-Oxatricyclo[4.3.1.0(3,8)]decane	-4.6	Arg499, Arg502, Arg503	Phe481, Lys506
TLR4 (3FXI)	Stigmasterol	-6.8	Ala291, Val316, Val338, Ser381, Arg382	Arg234, Arg289, Tyr292, Ser317, Glu336, Thr357, Thr359, Ser360, Asp379
	Cycloartenol	-7.0	Ala291, Val316, His179, Leu180	Asp181, Ser107, Asp109, Lys230, Thr232, Arg234, Val259, Phe263, Arg289, Tyr292, Ser317
	Clionasterol	-6.7	Ala291, Val316, Val338, Asp379, Ser381, Arg382	Arg234, Arg289, Tyr292, Ser317, Glu336, Thr357, Thr359, Ser360

Fucosterol	-5.7	Ala291, Val316	Arg234, Phe263, Arg264, Tyr292, Ser317, Asn339
6,7-Dimethyltetralin-1,5,8-trione	-5.7	Arg264, Tyr292, Thr319	Leu293, Asp294, Tyr296, Ser317, Val318, Lys362
alpha-Selinene	-5.6	Leu212	Pro214, Met215, Asn235, Asn236, Phe237, Asp238, Glu266, Gly267
Glyceryl monooleate	-4.0	His179, Asp181, Ser183, Asp209, Lys230	
Butyl linoleate	-4.3	Tyr296, Thr319, Lys362	Arg264, Tyr292, Leu293, Asp294, Tyr295, Ser317, Val318, Arg322, Lys341
Butanoic acid, [2-(1-hexenyl)cyclopropyl]methyl ester, [1R-[1.alpha.,2.alpha.(E)]]-	-4.0	Arg234, Phe263, Arg264, Ala291, Val316, Val338	Glu262, Arg289, Ser317
Glycidyl oleate	-3.9	His179, Lys230, Thr232	Glu154, Asn156, Leu180, Asp181, Ser207, Leu208, Asp209, Arg257
1,3,12-Nonadecatriene	-3.2	Leu212, Pro214	Asn235, Asn236, Phe237, Asp238, Glu266, Gly267
Ethyl stearate	-4.4	Lys230, Thr232, Arg234, Phe263, Arg264, Ala291, Tyr292, Val316	Asp209, Ser211, Val259, Arg289, Ser317
Glycidyl palmitate	-4	Val134, Ala158, His159, Ser211, Leu212, Arg234, Phe263	Asn156, Asp181, Ser183, Ser184, Asp209, Lys230, Thr232, Val259
Ethyl 9,10-epoxyoctadecanoate	-4.1	Lys230, Thr232, Arg234, Phe263, Arg264, Tyr292, Val316	Asp209, Ser211, Val259, Arg289, Ala291, Ser317
9-Octadecenoic acid, ethyl ester	-4.2	Tyr295, Tyr296, Thr319, Lys362	Tyr292, Leu293, Asp294, Asp298, Ser317, Val318, Arg322, Lys341
Diisobutyl adipate	-4.6	Arg234, Phe263, Arg264, Arg289, Ser317	Lys230, Thr232, Val259, Asn265, Ala291, Tyr292, Val316
Ethyl palmitate	-4.1	Val259, Phe263, Arg264, Arg289, Ala291, Tyr292, Val316	Lys230, Thr232, Arg234, Asn265, Ser317
2,4-Decadienal	-3.8	Phe263, Arg264, Ala291, Tyr292, Val316	Arg234, Arg289, Ser317
3,6-Diazahomoadamantan-9-ol	-4.6	Asn235, Phe237, Asp238	Leu212, Asn213, Pro214, Met215, Asn236, Gly267
2-Oxatricyclo[4.3.1.0(3,8)]decane	-4.5	Tyr292, Thr319	Leu293, Asp294, Tyr296, Ser317, Val318, Lys341, Lys362