Table 1: **The target hormone receptor used in AutoDock analysis.**

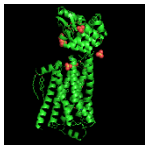
Target hormone	Target protein receptor (PDB)
Epinephrine (adrenaline)	β2 adrenoreceptor (PDB: 2rh1) • High resolution crystal structure of human B2-adrenergic G protein-coupled receptor • DOI: 10.2210/pdb2RH1/pdb • Classification: MEMBRANE PROTEIN/HYDROLASE • Organism(s): *Homo sapiens*, Escherichia virus T4 • Expression system: *Spodoptera frugiperda* Deposition author(s): Cherezov, V., Rosenbaum, D.M., Hanson, M.A., Rasmussen, S.G.F., Thian, F.S., Kobilka, T.S., Choi, H.J., Kuhn, P., Weis, W.I., Kobilka, B.K., Stevens, R.C., Accelerated Technologies Center for Gene to 3D Structure (ATCG3D), GPCR Network (GPCR)  3D structure of 2rh1

Table 2: **Results of the AutoDock analysis of Tri-B (vitamin B1, vitamin B6, vitamin B12 complex) ligand binding to the β2 adrenoreceptor (2rh1).**

Tri-B (ligand)	AutoDock analysis results	The chemical structure from PubChem CID
Vitamin B1 (thiamine)	mode | affinity | dist from best mode | (kcal/mol) | rmsd l.b.| rmsd u.b. -----+----------+----------+---------- 1 -7.4 0.000 0.000 2 -7.3 3.630 5.217 3 -7.0 1.639 2.188 4 -6.9 4.118 5.388 5 -6.8 2.035 2.637 6 -6.7 3.634 5.376 7 -6.7 4.671 5.778	Compound CID: 1130 MF: C12H17N4OS + MW: 265.36g/mol InChIKey: JZRWCGZRTZMZEH-UHFFFAOYSA-N IUPAC Name: 2-[3-[(4-amino-2-methylpyrimidin-5-yl)methyl]-4-methyl-1,3-thiazol-3-ium-5-yl]ethanol Create Date: 2004-09-16

	8 -6.7 2.878 5.030 9 -6.7 2.884 4.998	
Vitamin B6 (pyridoxine)	mode | affinity | dist from best mode | (kcal/mol) | rmsd l.b.| rmsd u.b. -----+------------+----------+---------- 1 -6.9 0.000 0.000 2 -6.6 2.794 4.391 3 -6.5 2.209 2.855 4 -6.4 2.180 2.672 5 -6.3 2.553 4.192 6 -6.2 2.535 3.622 7 -6.2 2.188 4.427 8 -6.1 2.084 2.827 9 -6.1 16.422 16.602	Compound CID: 104817 MF: C8H10NO5P-2 MW: 231.14g/mol InChIKey: RBCOYOYDYNXAFA-UHFFFAOYSA-L IUPAC Name: (5-hydroxy-4,6-dimethylpyridin-3-yl)methyl phosphate Create Date: 2005-08-08
Vitamin B12 (cobalamin)	mode | affinity | dist from best mode | (kcal/mol) | rmsd l.b.| rmsd u.b. -----+------------+----------+---------- 1 -15.5 0.000 0.000 2 -15.4 12.265 15.620 3 -15.1 0.968 1.731 4 -14.9 2.361 7.506 5 -14.2 2.123 7.384 6 -13.9 2.976 9.291 7 -13.9 2.846 8.072 8 -13.8 2.417 8.519 9 -13.7 2.504 6.569	Compound CID: 16686079 MF: C63H87CoN14O14P MW: 1354.4g/mol InChIKey: OWLMJFLNVIKMTJ-AKMVRCBCSA-M IUPAC Name: cobalt(2+);[(2R,5S)-5-(5,6-dimethylbenzimidazol-1-yl)-4-hydroxy-2-(hydroxymethyl)oxolan-3-yl] 1-[3-[(4Z,9Z,14Z)-2,13,18-tris(2-amino-2-oxoethyl)-7,12,17-tris(3-amino-3-oxopropyl)-3,5,8,8,13,15,18,19-octamethyl-2,7,12,17-tetrahydrocorrin-3-yl]propanoylamino]propan-2-yl phosphate;cyanide Create Date: 2007-08-23

Table 3: **Results of the GC–MS analysis of agarwood (AW) and the AutoDock analysis of AW ligand binding to β2 adrenoreceptor (2rh1).**

Compound separated by GC–MS analysis	The chemical (PubChem CID:)	RT (min) GC–MS analysis	Peak Area (%) GC–MS analysis	AutoDock analysis results
Doconexent	Compound CID: 445580 MF: C22H32O2 MW: 328.5g/mol InChIKey: MBMBGCFOFBJSGT-KUBAVDMBSA-N IUPAC Name: (4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoic acid Create Date: 2004-09-16	12.078	2.81	mode | affinity | dist from best mode | (kcal/mol) | rmsd l.b.| rmsd u.b. -----+------------+----------+---------- 1 -9.7 0.000 0.000 2 -9.4 2.885 5.696 3 -9.4 16.016 17.546 4 -9.4 3.197 6.007 5 -9.4 16.443 18.823 6 -9.3 2.611 6.017 7 -9.2 2.565 3.586 8 -9.1 2.683 4.555 9 -9.0 15.973 17.901

Compound separated by GC–MS analysis	The chemical (PubChem CID:)	RT (min) GC–MS analysis	Peak Area (%) GC–MS analysis	AutoDock analysis results
Hexadecanoic acid, ethyl ester	Compound CID: 12366 MF: C18H36O2 MW: 284.5g/mol InChIKey: XIRNKXNNONJFQO-UHFFFAOYSA-N IUPAC Name: ethyl hexadecanoate Create Date: 2005-03-26	11.714	7.62	mode | affinity | dist from best mode | (kcal/mol) | rmsd l.b.| rmsd u.b. -----+------------+----------+---------- 1 -6.6 0.000 0.000 2 -6.3 16.642 19.151 3 -6.2 3.729 5.962 4 -6.1 17.390 19.379 5 -5.9 6.243 9.567 6 -5.9 17.099 19.982 7 -5.9 17.732 20.785 8 -5.9 6.879 10.221 9 -5.6 17.088 18.993

Compound separated by GC–MS analysis	The chemical (PubChem CID:)	RT (min) GC–MS analysis	Peak Area (%) GC–MS analysis	AutoDock analysis results
4-Isopropenyl-4,7-dimethyl-1-oxaspiro[2.5]octane	Compound CID: 543441 MF: C12H20O MW: 180.29g/mol InChIKey: HFKIFHWZVYAGCQ-UHFFFAOYSA-N IUPAC Name: 4,7-dimethyl-4-prop-1-en-2-yl-1-oxaspiro[2.5]octane Create Date: 2005-03-27	8.013	0.31	mode | affinity | dist from best mode | (kcal/mol) | rmsd l.b.| rmsd u.b. -----+------------+----------+---------- 1 -7.6 0.000 0.000 2 -7.6 13.164 14.367 3 -7.3 12.744 14.438 4 -7.3 12.956 14.627 5 -7.3 13.194 14.690 6 -7.2 16.942 18.104 7 -7.1 13.046 14.211 8 -7.1 13.276 14.196 9 -7.0 17.091 18.314

Compound separated by GC–MS analysis	The chemical (PubChem CID:)	RT (min) GC–MS analysis	Peak Area (%) GC–MS analysis	AutoDock analysis results
4,5-Di-epi-aristolochene	Compound CID: 6429376 MF: C15H24 MW: 204.35g/mol InChIKey: YONHOSLUBQJXPR-RMTCENKZSA-N IUPAC Name: (4S,4aR)-4,4a-dimethyl-6-prop-1-en-2-yl-2,3,4,5,6,7-hexahydro-1H-naphthalene Create Date: 2006-04-28	8.211	0.37	mode | affinity | dist from best mode | (kcal/mol) | rmsd l.b.| rmsd u.b. -----+------------+----------+---------- 1 -8.3 0.000 0.000 2 -8.3 18.729 20.364 3 -8.2 15.497 17.142 4 -8.1 1.156 2.842 5 -7.5 15.418 17.138 6 -7.5 0.755 3.504 7 -7.5 1.203 3.043 8 -7.4 0.790 3.549 9 -7.4 18.522 20.024

Compound separated by GC–MS analysis	The chemical (PubChem CID:)	RT (min) GC–MS analysis	Peak Area (%) GC–MS analysis	AutoDock analysis results
3-Buten-2-one, 4-(6,6-dimethyl-1-cyclohexen-1-yl)-	Compound CID: 5363747 MF: C12H18O MW: 178.27g/mol InChIKey: JXVNWAUWOPLPEA-BQYQJAHWSA-N IUPAC Name: (E)-4-(6,6-dimethylcyclohexen-1-yl)but-3-en-2-one Create Date: 2005-03-27	8.3635	0.69	mode | affinity | dist from best mode | (kcal/mol) | rmsd l.b.| rmsd u.b. -----+------------+----------+---------- 1 -7.7 0.000 0.000 2 -7.6 9.927 10.294 3 -7.5 16.441 17.657 4 -7.4 15.427 16.685 5 -7.3 9.039 9.413 6 -6.9 15.189 16.406 7 -6.9 1.659 3.564 8 -6.9 2.004 3.464 9 -6.9 15.840 16.881

Compound separated by GC–MS analysis	The chemical (PubChem CID:)	RT (min) GC–MS analysis	Peak Area (%) GC–MS analysis	AutoDock analysis results
Spiro[2,4,5,6,7,7a-hexahydro-2-oxo-4,4,7a-trimethylbenzofuran]-7,2'-(oxirane)	Compound CID: 536241 MF: C12H16O3 MW: 208.25g/mol InChIKey: XHEGXVAWDSUIIG-UHFFFAOYSA-N IUPAC Name: 4,4,7a-trimethylspiro[5,6-dihydro-1-benzofuran-7,2'-oxirane]-2-one Create Date: 2005-03-27	8.422	0.58	mode | affinity | dist from best mode | (kcal/mol) | rmsd l.b.| rmsd u.b. -----+------------+----------+--------- - 1 -8.5 0.000 0.000 2 -8.1 1.288 2.513 3 -8.1 1.060 2.358 4 -7.9 1.278 2.497 5 -7.7 1.604 2.462 6 -7.6 5.033 6.850 7 -7.6 15.883 17.306 8 -7.4 1.577 2.765 9 -7.4 15.976 17.569

Compound separated by GC–MS analysis	The chemical (PubChem CID:)	RT (min) GC–MS analysis	Peak Area (%) GC–MS analysis	AutoDock analysis results
2,5-Octadecadiynoic acid, methyl ester	Compound CID: 42151 MF: C19H30O2 MW: 290.4g/mol InChIKey: XQDLQQYTXOVDQQ-UHFFFAOYSA-N IUPAC Name: methyl octadeca-2,5-diynoate Create Date: 2005-03-27	8.9195	0.15	mode | affinity | dist from best mode | (kcal/mol) | rmsd l.b.| rmsd u.b. -----+------------+----------+---------- 1 -6.3 0.000 0.000 2 -6.1 15.730 16.628 3 -6.1 2.374 2.558 4 -6.0 5.168 10.076 5 -5.9 15.785 18.570 6 -5.8 16.314 18.818 7 -5.8 1.057 2.040 8 -5.7 4.030 8.986 9 -5.5 2.072 4.362

Compound separated by GC–MS analysis	The chemical (PubChem CID:)	RT (min) GC–MS analysis	Peak Area (%) GC–MS analysis	AutoDock analysis results
Isoaromadendrene epoxide	Compound CID: 534398 MF: C15H24O MW: 220.35g/mol InChIKey: GLKQAHXBJLGAFT-UHFFFAOYSA-N IUPAC Name: 2,7,7,10-tetramethyl-3-oxatetracyclo[7.3.0.02,4.06,8]dodecane Create Date: 2005-03-27	9.0025	0.74	mode | affinity | dist from best mode | (kcal/mol) | rmsd l.b.| rmsd u.b. -----+------------+----------+---------- 1 -8.6 0.000 0.000 2 -8.3 1.278 2.606 3 -8.1 16.015 17.721 4 -8.1 1.965 3.007 5 -7.9 14.287 15.566 6 -7.9 15.947 17.576 7 -7.9 19.416 21.144 8 -7.9 16.121 18.121 9 -7.9 19.452 21.011

Compound separated by GC–MS analysis	The chemical (PubChem CID:)	RT (min) GC–MS analysis	Peak Area (%) GC–MS analysis	AutoDock analysis results
Aromadendrene oxide-(1)	Compound CID: 528759 MF: C15H24O MW: 220.35g/mol InChIKey: XPGWKKLDFXNBPJ-UHFFFAOYSA-N IUPAC Name: 1,1,7-trimethylspiro[2,3,4a,5,6,7,7a,7b-octahydro-1aH-cyclopropa[e]azulene-4,2'-oxirane] Create Date: 2005-03-27	10.3745	1.82	mode | affinity | dist from best mode | (kcal/mol) | rmsd l.b.| rmsd u.b. -----+------------+----------+---------- 1 -8.5 0.000 0.000 2 -8.3 1.138 3.183 3 -8.2 15.831 17.419 4 -8.2 15.936 17.628 5 -8.2 19.340 20.764 6 -8.2 15.630 17.556 7 -8.2 19.369 20.796 8 -8.0 16.145 18.153 9 -8.0 1.979 2.590

Compound separated by GC–MS analysis	The chemical (PubChem CID:)	RT (min) GC–MS analysis	Peak Area (%) GC–MS analysis	AutoDock analysis results
Octadecanoic acid, ethyl ester	Compound CID: 8122 MF: C20H40O2 MW: 312.5g/mol InChIKey: MVLVMROFTAUDAG-UHFFFAOYSA-N IUPAC Name: ethyl octadecanoate Create Date: 2005-03-26	12.958	10.06	mode | affinity | dist from best mode | (kcal/mol) | rmsd l.b.| rmsd u.b. -----+------------+----------+---------- 1 -6.7 0.000 0.000 2 -6.6 3.665 10.251 3 -6.3 3.304 3.935 4 -6.2 27.164 29.179 5 -6.0 4.619 10.354 6 -6.0 5.895 10.677 7 -5.9 5.190 10.543 8 -5.9 4.475 5.690 9 -5.8 27.478 27.882

Compound separated by GC–MS analysis	The chemical (PubChem CID:)	RT (min) GC–MS analysis	Peak Area (%) GC–MS analysis	AutoDock analysis results
Hexadecanamide	Compound CID: 69421 MF: C16H33NO MW: 255.44g/mol InChIKey: HSEMFIZWXHQJAE-UHFFFAOYSA-N IUPAC Name: hexadecanamide Create Date: 2005-03-26	13.009	30.6	mode | affinity | dist from best mode | (kcal/mol) | rmsd l.b.| rmsd u.b. -----+------------+----------+---------- 1 -6.7 0.000 0.000 2 -6.7 5.028 8.582 3 -6.6 28.386 29.626 4 -6.6 5.729 9.544 5 -6.5 2.460 2.639 6 -6.5 28.156 28.656 7 -6.4 1.818 3.279 8 -6.4 3.535 8.035 9 -6.3 2.631 4.428

Compound separated by GC–MS analysis	The chemical (PubChem CID:)	RT (min) GC–MS analysis	Peak Area (%) GC–MS analysis	AutoDock analysis results
Glycerol 1-palmitate	Compound CID: 14900 MF: C19H38O4 MW: 330.5g/mol InChIKey: QHZLMUACJMDIAE-UHFFFAOYSA-N IUPAC Name: 2,3-dihydroxypropyl hexadecanoate Create Date: 2005-03-26	14.8645	0.9	mode | affinity | dist from best mode | (kcal/mol) | rmsd l.b.| rmsd u.b. -----+------------+----------+---------- 1 -7.4 0.000 0.000 2 -6.8 6.051 10.046 3 -6.7 17.955 19.910 4 -6.7 18.641 20.636 5 -6.6 9.229 13.553 6 -6.4 4.569 8.233 7 -6.4 7.274 11.540 8 -6.4 17.225 19.002 9 -6.4 6.924 10.589

Compound separated by GC–MS analysis	The chemical (PubChem CID:)	RT (min) GC–MS analysis	Peak Area (%) GC–MS analysis	AutoDock analysis results
Oleic acid	Compound CID: 445639 MF: C18H34O2 MW: 282.5g/mol InChIKey: ZQPPMHVWECSIRJ-KTKRTIGZSA-N IUPAC Name: (Z)-octadec-9-enoic acid Create Date: 2004-09-16	15.605	0.2	mode | affinity | dist from best mode | (kcal/mol) | rmsd l.b.| rmsd u.b. -----+------------+----------+---------- 1 -6.5 0.000 0.000 2 -6.4 17.750 20.380 3 -6.4 4.719 9.039 4 -6.4 28.078 28.832 5 -6.4 17.225 19.403 6 -6.0 28.249 29.880 7 -5.8 16.900 18.674 8 -5.8 21.043 21.620 9 -5.8 16.406 17.908

Compound separated by GC–MS analysis	The chemical (PubChem CID:)	RT (min) GC–MS analysis	Peak Area (%) GC–MS analysis	AutoDock analysis results
9-Octadecenoic acid (Z)-, phenylmethyl ester	Compound CID: 5368218 MF: C25H40O2 MW: 372.6g/mol InChIKey: CGFITOCWTCRCSL-KTKRTIGZSA-N IUPAC Name: benzyl (Z)-octadec-9-enoate Create Date: 2005-03-27	17.817	0.34	mode | affinity | dist from best mode | (kcal/mol) | rmsd l.b.| rmsd u.b. -----+------------+----------+---------- 1 -8.9 0.000 0.000 2 -8.8 16.998 21.207 3 -8.6 17.087 18.534 4 -8.5 4.048 6.439 5 -8.3 18.886 22.569 6 -8.3 17.946 19.810 7 -8.2 3.322 11.693 8 -8.1 3.646 9.035 9 -8.1 20.559 22.915

Compound separated by GC–MS analysis	The chemical (PubChem CID:)	RT (min) GC–MS analysis	Peak Area (%) GC–MS analysis	AutoDock analysis results
Quinazolin-4(3H)-one, 2-(4-methoxybenzylthio)-3-methyl-	Compound CID: 578769 MF: C17H16N2O2S MW: 312.4g/mol InChIKey: SJZAPCLSPJEYPR-UHFFFAOYSA-N IUPAC Name: 2-[(4-methoxyphenyl)methylsulfanyl]-3-methylquinazolin-4-one Create Date: 2005-03-27	18.355	3.72	mode | affinity | dist from best mode | (kcal/mol) | rmsd l.b.| rmsd u.b. -----+------------+----------+---------- 1 -9.4 0.000 0.000 2 -8.7 0.986 1.171 3 -8.4 3.794 5.979 4 -8.4 1.633 2.532 5 -8.3 3.082 5.014 6 -8.2 2.022 6.016 7 -8.1 2.587 2.864 8 -7.9 2.683 4.384 9 -7.3 13.996 15.868

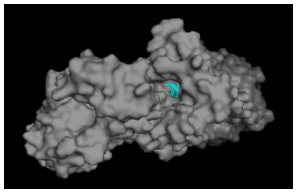
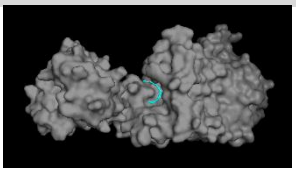
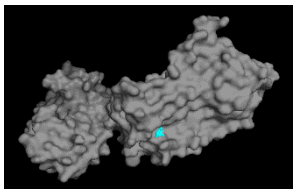
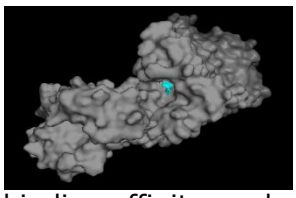
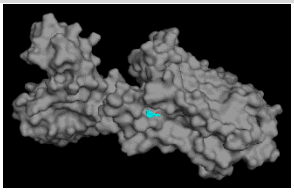
Compound separated by GC–MS analysis	The chemical (PubChem CID:)	RT (min) GC–MS analysis	Peak Area (%) GC–MS analysis	AutoDock analysis results
Cholesterol	Compound CID: 5997 MF: C27H46O MW: 386.7g/mol InChIKey: HVYWMOMLDIMFJA-DPAQBDIFSA-N IUPAC Name: (3S,8S,9S,10R,13R,14S,17R)-10,13-dimethyl-17-[(2R)-6-methylheptan-2-yl]-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3-ol Create Date: 2004-09-16	20.5395	1.02	mode | affinity | dist from best mode | (kcal/mol) | rmsd l.b.| rmsd u.b. -----+------------+----------+---------- 1 -10.6 0.000 0.000 2 -9.7 2.585 6.516 3 -9.4 2.737 6.587 4 -9.3 18.475 21.148 5 -9.3 15.348 17.516 6 -9.2 15.182 16.656 7 -9.2 18.147 20.428 8 -9.2 25.496 26.443 9 -9.1 2.264 4.561

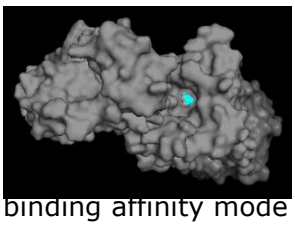
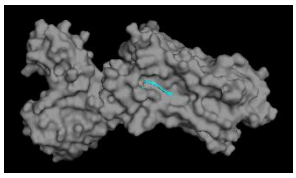
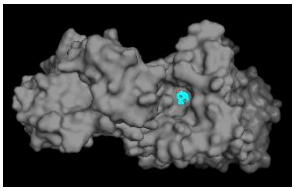
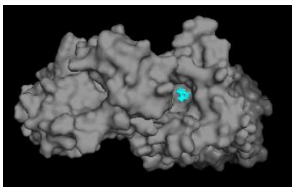
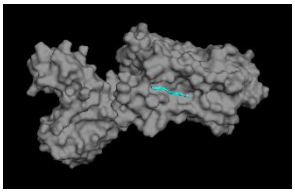
Compound separated by GC–MS analysis	The chemical (PubChem CID:)	RT (min) GC–MS analysis	Peak Area (%) GC–MS analysis	AutoDock analysis results
Stigmasterol	Compound CID: 5280794 MF: C29H48O MW: 412.7g/mol InChIKey: HCXVJBMSMIARIN-PHZDYDNGSA-N IUPAC Name: (3S,8S,9S,10R,13R,14S,17R)-17-[(E,2R,5S)-5-ethyl-6-methylhept-3-en-2-yl]-10,13-dimethyl-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3-ol Create Date: 2005-06-08	22.6465	2.36	mode | affinity | dist from best mode | (kcal/mol) | rmsd l.b.| rmsd u.b. -----+------------+----------+---------- 1 -11.2 0.000 0.000 2 -11.1 1.410 2.112 3 -11.1 1.790 3.162 4 -10.9 12.998 14.353 5 -10.9 13.050 14.463 6 -10.8 7.743 10.195 7 -10.7 19.180 21.337 8 -10.7 18.654 21.417 9 -10.7 16.772 19.236

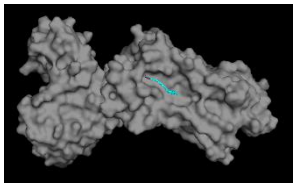
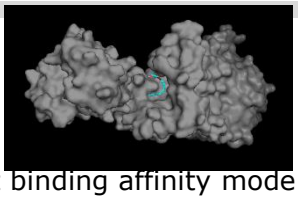
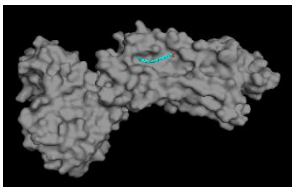
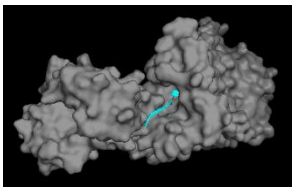
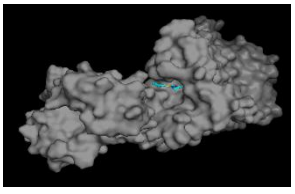
Compound separated by GC–MS analysis	The chemical (PubChem CID:)	RT (min) GC–MS analysis	Peak Area (%) GC–MS analysis	AutoDock analysis results
Aromadendrene, dehydro-	Compound CID: 589433 MF: C15H22 MW: 202.33g/mol InChIKey: WILLVGWOOMVDNT-UHFFFAOYSA-N IUPAC Name: 1,1,7-trimethyl-4-methylidene-2,3,6,7,7a,7b-hexahydro-1aH-cyclopropa[e]azulene Create Date: 2005-03-27	7.0905	0.33	mode | affinity | dist from best mode | (kcal/mol) | rmsd l.b.| rmsd u.b. -----+------------+----------+---------- 1 -8.5 0.000 0.000 2 -8.2 0.527 3.201 3 -8.2 0.533 3.381 4 -8.1 15.642 17.375 5 -8.1 15.777 17.624 6 -8.1 19.192 20.858 7 -8.1 14.410 15.713 8 -8.1 19.008 20.951 9 -8.1 15.746 17.698

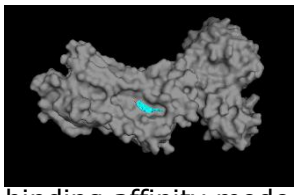
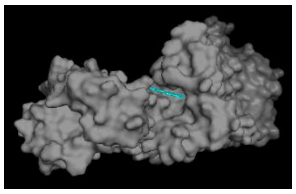
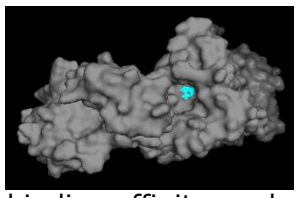
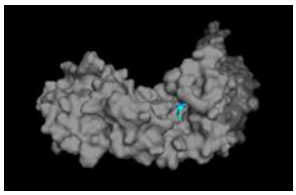
Notes: RT = Retention time (minutes); PA = peak area (%). GC–MS analysis was carried out for the ethanoic extracts using Agilent Technologies (G3440B). The components of the plant extract were characterized by computer simulations of spectra in the commercial libraries WILEY and NIST (National Institute of Standards and Technology).

Table 4: **Prediction of the best interaction of ligands with β2 adrenoreceptor (2rh1) in the AutoDock analysis.**

Compound separated by GC–MS analysis	The chemical (PubChem CID)	Global binding energy of the highest binding affinity (kcal/mole)
Doconexent	Compound CID: 445580	−9.7  3D structure of 2rh1 in the best binding affinity mode with doconexent
Hexadecanoic acid, ethyl ester	Compound CID: 12366	−6.6  3D structure of 2rh1 in the best binding affinity mode with hexadecanoic acid, ethyl ester
4-Isopropenyl-4,7-dimethyl-1-oxaspiro[2.5]octane	Compound CID: 543441	−7.6  3D structure of 2rh1 in the best binding affinity mode with 4-isopropenyl-4,7-dimethyl-1-oxaspiro[2.5]octane
4,5-Di-epi-aristolochene	Compound CID: 6429376	−8.3  3D structure of 2rh1 in the best binding affinity mode with 4,5-di-epi-aristolochene
3-Buten-2-one, 4-(6,6-dimethyl-1-cyclohexen-1-yl)	Compound CID: 5363747	−7.7  3D structure of 2rh1 in the best binding affinity mode with 3-buten-2-one, 4-(6,6-dimethyl-1-cyclohexen-1-yl)

Compound separated by GC–MS analysis	The chemical (PubChem CID)	Global binding energy of the highest binding affinity (kcal/mole)
Spiro[2,4,5,6,7,7a-hexahydro-2-oxo-4,4,7a-trimethylbenzofuran]-7,2'-(oxirane)	Compound CID: 536241	−8.5  3D structure of 2rh1 in the best binding affinity mode with spiro[2,4,5,6,7,7a-hexahydro-2-oxo-4,4,7a-trimethylbenzofuran]-7,2'-(oxirane)
2,5-Octadecadiynoic acid, methyl ester	Compound CID: 42151	−6.3  3D structure of 2rh1 in the best binding affinity mode with 2,5-octadecadiynoic acid, methyl ester
Isoaromadendrene epoxide	Compound CID: 534398	−8.6  3D structure of 2rh1 in the best binding affinity mode with isoaromadendrene epoxide
Aromadendrene oxide-(1)	Compound CID: 528759	−8.5  3D structure of 2rh1 in the best binding affinity mode with aromadendrene oxide-(1)
Octadecanoic acid, ethyl ester	Compound CID: 8122	−6.7  3D structure of 2rh1 in the best binding affinity mode with A Octadecanoic acid, ethyl ester

Compound separated by GC–MS analysis	The chemical (PubChem CID)	Global binding energy of the highest binding affinity (kcal/mole)
Hexadecanamide	Compound CID: 69421	−6.7  3D structure of 2rh1 in the best binding affinity mode with hexadecanamide
Glycerol 1-palmitate	Compound CID: 14900	−7.4  3D structure of 2rh1 in the best binding affinity mode with glycerol 1-palmitate
Oleic acid	Compound CID: 445639	−6.5  3D structure of 2rh1 in the best binding affinity mode with oleic acid
9-Octadecenoic acid (Z)-, phenylmethyl ester	Compound CID: 5368218	−8.9  3D structure of 2rh1 in the best binding affinity mode with 9-octadecenoic acid (Z)-, phenylmethyl ester
Quinazolin-4(3H)-one, 2-(4-methoxybenzylthio)-3-methyl-	Compound CID: 578769	−9.4  3D structure of 2rh1 in the best binding affinity mode with quinazolin-4(3H)-one, 2-(4-methoxybenzylthio)-3-methyl

Compound separated by GC–MS analysis	The chemical (PubChem CID)	Global binding energy of the highest binding affinity (kcal/mole)
Cholesterol	Compound CID: 5997	−10.6  3D structure of 2rh1 in the best binding affinity mode with cholesterol
Stigmasterol	Compound CID: 5280794	−11.2  3D structure of 2rh1 in the best binding affinity mode with stigmasterol
Aromadendrene, dehydro-	Compound CID: 589433	−8.5  3D structure of 2rh1 in the best binding affinity mode with aromadendrene, dehydro-
Vitamin B1	Compound CID: 1130	−7.4  3D structure of 2rh1 in the best binding affinity mode with vitamin B1

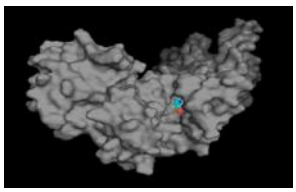
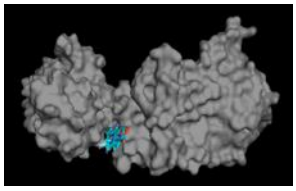
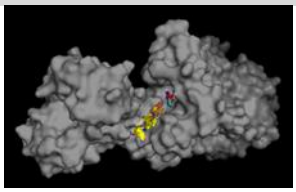
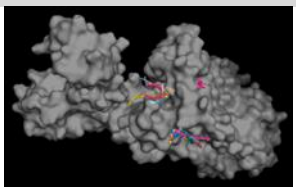
Compound separated by GC–MS analysis	The chemical (PubChem CID)	Global binding energy of the highest binding affinity (kcal/mole)
Vitamin B6	Compound CID: 104817	−6.9  3D structure of 2rh1 in the best binding affinity mode with Vitamin B6
Vitamin B12	Compound CID: 16686079	−15.5  3D structure of 2rh1 in the best binding affinity mode with vitamin B12
Tri- B (synergetic effect)		 3D structure of 2rh1 in the best binding affinity mode with Tri-B (synergetic effect) Mean the best binding energy of affinity mode=-9.93
Agarwood (synergetic effect)		 3D structure of 2rh1 in the best binding affinity mode with compounds extracted from agarwood (synergetic effect) Mean the best binding energy of affinity mode=-8.21

Table 5. **Biochemical comparison of the different groups in the animal study.**

	Control (n = 10)	**Epinephrine$^{\$}$ (n = 10)**	**Epinephrine + Tri-B$^{\#}$ (n = 10)**	**Tri-B$^{\$}$ (n = 10)**	**AW$^{\$}$ (n = 10)**	**Epinephrine + AW$^{\#}$ (n = 10)**	***F* (*p*-level)**
Serum							
Total cholesterol (mg/dl)	$76.5^{e} \pm 0.2$	$220.8^{a} \pm 0.6$	$103.1^{c} \pm 1.7$	$78.2^{d} \pm 0.6$	$76.5^{e} \pm 0.6$	$123.1^{b} \pm 1.7$	26879.40^{*} ($<0.001^{*}$)
% change		↑188.6	↓53.3	↑2.2	0.0	↓44.2	
TG (mg/dl)	$82.4^{d} \pm 0.2$	$165.4^{a} \pm 1$	$93.3^{b} \pm 2.1$	$83.7^{cd} \pm 1.9$	$85.6^{c} \pm 2.1$	$94.4^{b} \pm 2.4$	3125.457^{*} ($<0.001^{*}$)
% change		↑100.7	↓43.6	↑1.6	↑3.9	↓42.9	
HDL-C (mg/dl)	$34.8^{a} \pm 0.5$	$26.3^{c} \pm 2.1$	$31.5^{b} \pm 1.2$	$34.5^{a} \pm 1.6$	$35.1^{a} \pm 1.6$	$31.4^{b} \pm 1.2$	54.237^{*} ($<0.001^{*}$)
% change		↓24.4	↑19.8	↓0.9	↑0.9	↑19.4	
LDL-C (mg/dl)	$36.9^{c} \pm 0.4$	$173.9^{a} \pm 0.9$	$124.8^{b} \pm 2.1$	$37.7^{c} \pm 0.5$	$36.4^{c} \pm 0.9$	$123.3^{b} \pm 2.8$	14790.47^{*} ($<0.001^{*}$)
% change		↑371.3	↓28.2	↑2.2	↓1.4	↓29.1	
Serum cortisol (ng /ml)	$75.6^{c} \pm 0.7$	$123.4^{a} \pm 1.3$	$94.9^{b} \pm 1.5$	$74.9^{c} \pm 0.9$	$74.3^{c} \pm 1.7$	$94.9^{b} \pm 1.5$	2130.179^{*} ($<0.001^{*}$)
% change		↑63.2	↓23.1	↓0.9	↓1.7	↓23.1	
IL-1β (pg/ml)	$92^{d} \pm 0.9$	$294.8^{a} \pm 3$	$158.1^{b} \pm 1$	$92^{d} \pm 1.1$	$92.1^{d} \pm 0.9$	$153.2^{c} \pm 1.1$	27207.17^{*} ($<0.001^{*}$)
% change		↑220.4	↓46.4	0.0	↑0.1	↓48.0	
AST (U/L)	$13.3^{e} \pm 0.1$	$25.2^{a} \pm 0.1$	$15.3^{c} \pm 0.1$	$13.5^{d} \pm 0.1$	$13.5^{d} \pm 0.1$	$17.3^{b} \pm 0.2$	13452.50^{*} ($<0.001^{*}$)
% change		↑89.5	↓39.3	↑1.5	↑1.5	↓31.3	
ALT (U/L)	$0.72^{d} \pm 0.02$	$6.54^{a} \pm 0.02$	$1.24^{c} \pm 0.03$	$0.72^{d} \pm 0.03$	$0.74^{d} \pm 0.03$	$1.85^{b} \pm 0.03$	69865.62^{*} ($<0.001^{*}$)
% change		↑808.3	↓81.0	0.0	↑2.8	↓71.7	
Liver Tissue							
NO (μm)	$26.3^{c} \pm 0.2$	$72.3^{a} \pm 0.5$	$43^{b} \pm 1.9$	$27.3^{c} \pm 1.5$	$25.8^{c} \pm 2$	$42.5^{b} \pm 1.5$	1569.964^{*} ($<0.001^{*}$)

% change		↑174.9	↓40.5	↑3.8	↓1.9	↓41.2	
MDA (nmol/g tissue)	$2.9^{c} \pm 0.01$	$19.5^{a} \pm 0.2$	$13.4^{b} \pm 1.4$	$2.6^{c} \pm 0.1$	$2.6^{c} \pm 0.3$	$13.2^{b} \pm 1.3$	841.899^{*} ($<0.001^{*}$)
% change		↑572.4	↓31.3	↓10.3	↓10.3	↓32.3	
COX-2 activities (nmol/min/ml)	$3.4^{c} \pm 0.2$	$9.3^{a} \pm 0.3$	$5.6^{b} \pm 0.3$	$2.5^{d} \pm 0.1$	$2.5^{d} \pm 0.2$	$5.5^{b} \pm 0.4$	1056.026^{*} ($<0.001^{*}$)
% change		↑173.5	↓39.8	↓26.5	↓26.5	↓40.9	
LOX activities (µmol/mg protein)	$0.08^{c} \pm 0.01$	$0.3^{a} \pm 0.01$	$0.11^{b} \pm 0.01$	$0.09^{c} \pm 0.01$	$0.09^{c} \pm 0.01$	$0.12^{b} \pm 0.01$	556.280^{*} ($<0.001^{*}$)
% change		↑275.0	↓63.3	↑12.5	↑12.5	↓60.0	
TNF-α (pg/ml)	$26.6^{c} \pm 0.4$	$99.1^{a} \pm 0.7$	$43.9^{b} \pm 1.8$	$26.4^{c} \pm 1.2$	$26.2^{c} \pm 2.2$	$43.9^{b} \pm 2.4$	3047.457^{*} ($<0.001^{*}$)
% change		↑272.6	↓55.7	↓0.8	↓1.5	↓55.7	

Table 6: **Biochemical comparison of the two groups in the human study.**

	Normal range	**Group 1 (n = 119)**	**Group 2 (n = 119)**	**% change**	***t***	***p***
NO (µmol/l)	24–25	84.7 ± 10.6	39 ± 3.8	↓54	44.143^{*}	$<0.001^{*}$
MDA (nmol/ml)	4–5	54.1 ± 3.3	23.4 ± 2.8	↓56.7	78.082^{*}	$<0.001^{*}$
COX-2 activity (ng/mL)	Not detectable	5.6 ± 0.2	2.6 ± 0.2	↓53.6	100.995^{*}	$<0.001^{*}$
LOX activity (ng/mL)	Not detectable	1.7 ± 0.2	0.8 ± 0.2	↓52.9	43.338^{*}	$<0.001^{*}$
Serum cortisol (ng/ml)	185 – 624	555.1 ± 36.2	377.4 ± 20.5	↓32	46.590^{*}	$<0.001^{*}$
IL-1β (pg/ml^{-1})	0.0 –1.65	132.1 ± 13.7	64 ± 6.8	↓51.6	48.433^{*}	$<0.001^{*}$
TNF-α (pg/ml)	Not detectable–8.1	75.9 ± 4.5	52.6 ± 5.6	↓30.7	35.373^{*}	$<0.001^{*}$
Total cholesterol (mg/dl)	Up to 200	216.1 ± 9.1	199.2 ± 7.5	↓7.8	15.683^{*}	$<0.001^{*}$
TG (mg/dl)	Up to 200	254.3 ± 8.3	196.7 ± 4.6	↓22.7	66.376^{*}	$<0.001^{*}$
HDL-C (mg/dl)	>35	32.8 ± 1.5	36.6 ± 1.1	↑11.6	22.706^{*}	$<0.001^{*}$

LDL-C (mg/dl)	Up to 105	101 ± 0.9	92.6 ± 2.3	↓8.3	36.917*	<0.001*
AST (U/L)	F: up to 31 M: up to 35	40.6 ± 3.7	37 ± 1.3	↓8.9	9.858*	<0.001*
ALT (U/L)	F: up to 31 M: up to 41	40.3 ± 1.4	35.6 ± 1.1	↓11.7	28.473*	<0.001*