# Supplementary materials：Establishment of HS-SPME-GC-QTOF analysis method and Molecular docking data

## 1. Fiber coating

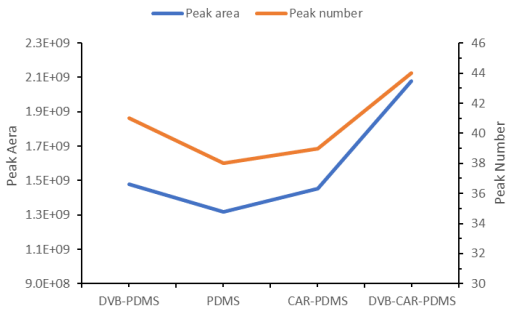
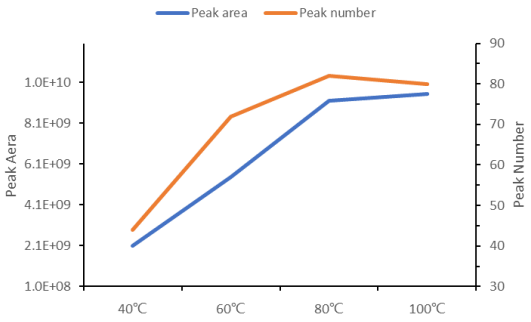
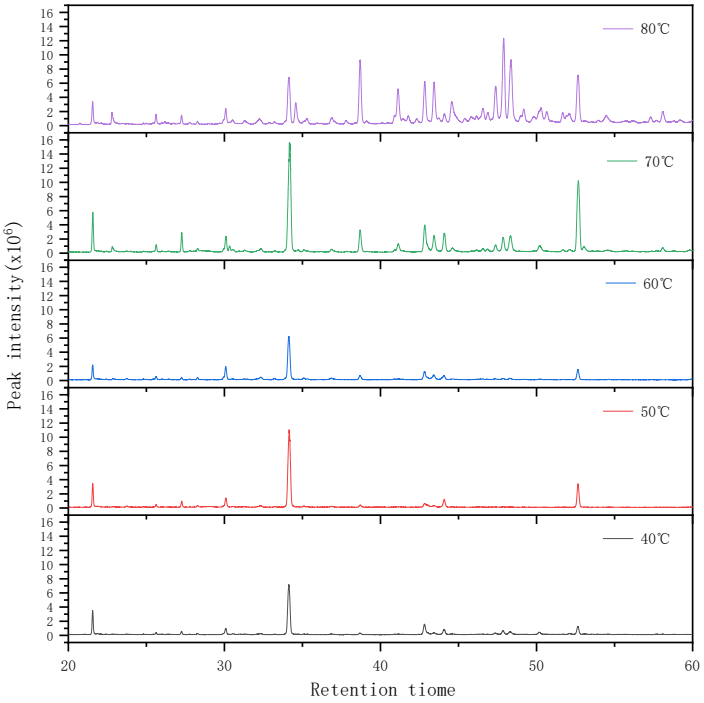



**Figure S1.** Effect of SPME fiber coating on the peak area and number of agarwood oil sample. (extraction temperature=40℃; extraction time=15min; desorption time=3min. The data were represented by the average of three replicate measurements.)

## 2. Extraction temperature



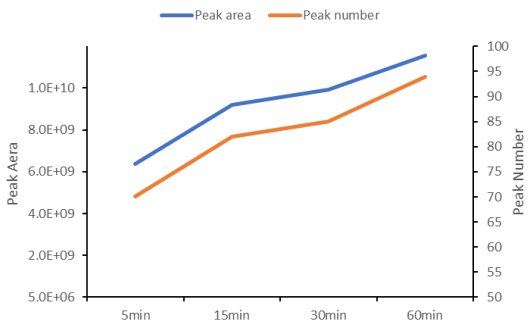

**(a)**



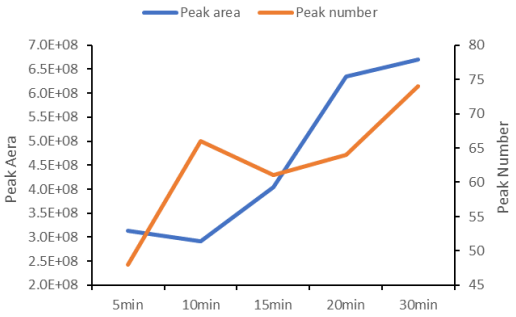

**(b)**

**Figure S2. (a)** Effect of extraction time on the peak area and number of agarwood oil sample by using DVB/CAR/PDMS fiber. (extraction time=15min; desorption time=3min. The data were represented by the average of three replicate measurements.) (**b**) The TIC chromatograph of different extraction temperature on serum sample by using DVB/PDMS fiber.

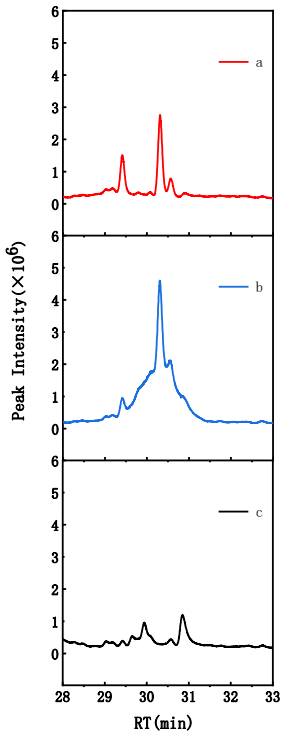
## 3. Extraction time




**(a)**




**(b)**




**(c)**

**Figure S3.** (**a**) Effect of extraction time on the peak area and number of agarwood oil sample by using DVB/CAR/PDMS fiber. (extraction temperature=80℃; desorption time=3min. The data were represented by the average of three replicate measurements.) (**b**) Effect of extraction time on the peak area and number of serum sample by using DVB/PDMS fiber. (extraction temperature=80℃; NaCl concentration=20mg. The data were represented by the average of two replicate measurements.) (**c**) Comparative TIC chromatograph analysis of different extraction time and salt concentration in RT29min-RT32min by using DVB/PDMS fiber.
(a: extraction time=20min, NaCl concentration=20mg; b: extraction time=20min, NaCl concentration=30mg; c: extraction time=30min, NaCl concentration=30mg;)

## 4. Salt concentration

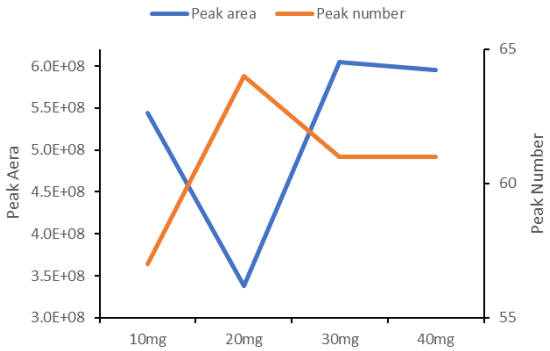



**Figure S4.** Effect of salt concentration on the peak area and number of serum sample by using DVB/PDMS fiber. (extraction temperature=80℃; extraction time=20min. The data were represented by the average of two replicate measurements.)

**Table S1.** Chemical composition of the 79 compounds putatively identified in agarwood oil sample.

| Number | RT | Formula | Compound | Peak area/% | CAS | Similarity |
|---|---|---|---|---|---|---|
| 1 | 7.169 | C8H10O | Benzene, (methoxymethyl)- | 0.16 | 538-86-3 | 76.53 |
| 2 | 7.938 | C7H6O | Benzaldehyde | 0.29 | 100-52-7 | 87.2 |
| 3 | 11.59 | C10H16O | Carveol | 1.43 | 99-48-9 | 75.54 |
| 4 | 12.075 | C9H10O | Benzene, 1-ethenyl-4-methoxy- | 0.07 | 637-69-4 | 84.1 |
| 5 | 16.047 | C12H18 | 6,7-Dimethyl-1,2,3,5,8,8a-hexahydronaphthalene | 0.1 | 107914-92-1 | 81.54 |
| 6 | 16.433 | C10H12O | Benzenepropanal, .beta.-methyl- | 2.43 | 16251-77-7 | 85.35 |
| 7 | 16.948 | C10H12O | 2-Butanone, 4-phenyl- | 0.11 | 2550-26-7 | 84.73 |
| 8 | 18.921 | C11H10 | Naphthalene, 2-methyl- | 0.24 | 91-57-6 | 71.57 |
| 9 | 19.845 | C11H10 | Naphthalene, 1-methyl- | 0.11 | 90-12-0 | 80.92 |
| 10 | 21.425 | C11H16O | 4-(2-Methyl-cyclohex-1-enyl)-but-3-en-2-one | 0.29 | 41437-92-7 | 79.26 |
| 11 | 22.114 | C12H18O | 2,7-Methanonaphthalene-3-methanol, 1,2,3,4,4a,7,8,8a-octahydro- | 0.09 | 56045-33-1 | 80.62 |
| 12 | 24.529 | C15H24 | Bicyclo[5.2.0]nonane, 4-methylene-2,8,8-trimethyl-2-vinyl- | 0.19 | 1000159-38-2 | 81.55 |
| 13(Z1) | 24.835 | C15H24 | Bicyclo[5.2.0]nonane,2-methylene-4,8,8-trimethyl-4-vinyl- | 0.68 | 242794-76-9 | 81.02 |
| 14(Z2) | 25.656 | C14H24O | Spiro[2.5]octane,5,5-dimethyl-4-(3-oxobutyl)- | 1.72 | 77143-32-9 | 79.02 |
| 15 | 26.694 | C15H22O | (1aR,4aS,8aS)-4a,8,8-Trimethyl-1,1a,4,4a,5,6,7,8-octahydrocyclopropa[d]naphthalene-2-carbaldehyde | 0.08 | 470-41-7 | 79.55 |
| 16 | 27.13 | C15H22O | Ylangenal | 0.07 | 41610-68-8 | 80.72 |
| 17 | 27.785 | C15H24 | .alpha.-Guaiene | 0.61 | 3691-12-1 | 87.15 |
| 18 | 28.058 | C15H24 | 4,7-Methanoazulene, 1,2,3,4,5,6,7,8-octahydro-1,4,9,9-tetramethyl-, [1S-(1.alpha.,4.alpha.,7.alpha.)]- | 0.34 | 514-51-2 | 84.92 |
| 19(Z3) | 28.327 | C15H24O | (1R,3aR,5aR,9aS)-1,4,4,7-Tetramethyl-1,2,3,3a,4,5a18,9-octahydrocyclopenta[c]benzofuran | 1.54 | 104188-25-2 | 76.87 |
| 20 | 28.7 | C15H24 | (4S,4aR,6R)-4,4a-Dimethyl-6-(prop-1-en-2-yl)-1,2,3,4,4a,5,6,7-octahydronaphthalene | 0.22 | 54868-40-5 | 85.01 |
| 21 | 28.972 | C15H24O | (1R,4S,5S)-1,8-Dimethyl-4-(prop-1-en-2-yl)spiro[4.5]dec-7-ene | 0.08 | 43219-80-3 | 83.99 |
| 22 | 29.268 | C15H24O | Caryophyllene oxide | 0.14 | 1139-30-6 | 82.24 |
| 23(Z4) | 30.27 | C15H24O | 1H-Cycloprop[e]azulen-7-ol,decahydro-1,1,7-trimethyl-4-methylene-,[1aR-(1aα,4aα,7β,7aβ,7bα)]- | 4.87 | 6750-60-3 | 89.51 |
| 24 | 30.363 | C15H24O | Tricyclo[5.2.2.0(1,6)]undecan-3-ol, 2-methylene-6,8,8-trimethyl- | 3.47 | 1000159-37-6 | 86.33 |
| 25(Z5) | 30.592 | C15H24 | 4a,8-Dimethyl-2-(prop-1-en-2-yl)-1,2,3,4,4a,5,6,7-octahydronaphthalene | 1.24 | 103827-22-1 | 78.54 |
| 26 | 31.184 | C15H24 | .beta.-Guaiene | 0.17 | 88-84-6 | 87.53 |
| 27(Z6) | 31.39 | C15H24 | (1R,3aS,8aS)-7-Isopropyl-1,4-dimethyl-1,2,3,3a,6,8a-hexahydroazulene | 2.2 | 36577-33-0 | 88.25 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 28(Z7) | 32.468 | C15H26O | 2H-3,9a-Methano-1-benzoxepin,octahydro-2,2,5a,9-tetramethyl-,[3R(3α,5aα,9α,9aα)]- | 4.92 | 5956-09-2 | 88.55 |
| 29(Z8) | 33.29 | C15H24O | (R)-2-((4aS,8aR)-4a-Methylene-1,4,4a,5,6,7,8,8a-octahydronaphthalen-2-yl)propan-1-ol | 1.36 | 28102-68-3 | 74.9 |
| 30 | 34.051 | C15H24O | 2-(4a,8-Dimethyl-1,2,3,4,4a,5,6,7-octahydro-naphthalen-2-yl)-prop-2-en-1-ol | 2.51 | 1000190-51-8 | 83.57 |
| 31(Z9) | 35.235 | C15H26O | 1,4-Dimethyl-7-(prop-1-en-2-yl)decahydroazulen-4-ol | 1.73 | 21698-41-9 | 76.36 |
| 32(Z10) | 35.445 | C15H26O2 | Cedran-diol,(8S,14)- | 1.38 | 62600-05-9 | 85.16 |
| 33 | 36.23 | C24H40O2 | 10,12-Tricosadiynoic acid, methyl ester | 0.38 | 1000333-59-4 | 81.06 |
| 34(Z11) | 36.982 | C15H24O | 2-((2R,4aR,8aR)-4a,8-Dimethyl-1,2,3,4,4a,5,6,8a-octahydronaphthalen-2-yl)prop-2-en-1-ol | 3.56 | 65018-15-7 | 89.11 |
| 35 | 38.066 | C15H24 | Bicyclo[5.3.0]decane, 2-methylene-5-(1-methylvinyl)-8-methyl- | 0.93 | 1000159-39-3 | 90.35 |
| 36(Z12) | 39.021 | C15H26O | 2-((4aS,8R,8aR)-4a,8-Dimethyl)-3,4,4a,5,6,7,8,8a-octahydronaphthalen-2-yl)propan-2-ol | 6.31 | 194607-96-0 | 71.71 |
| 37(Z13) | 40.547 | C15H24O | 2-((2R,4aR,8aS)-4a-Methyl-8-methylenedecahydronaphthalen-2-yl)prop-2-en-1-ol | 0.15 | 515-20-8 | 81.27 |
| 38(Z14) | 41.286 | C15H24O | (E)-2-((8R,8aS)-8,8a-Dimethyl-3,4,6,7,8,8a-hexahydronaphthalen-2(1H)-ylidene)propan-1-ol | 4.71 | 22387-74-2 | 75.9 |
| 39(Z15) | 41.758 | C15H24O | Aristol-1(10)-en-9-ol | 3.39 | 1372763-27-3 | 79.1 |
| 40 | 42.397 | C15H24O | Alloaromadendrene oxide-(1) | 0.31 | | |
| 41 | 42.656 | C15H24O | 7-Oxabicyclo[4.1.0]heptane, 2,2,6-trimethyl-1-(3-methyl-1,3-butadienyl)-5-methylene- | 0.22 | 70038-20-9 | 79.73 |
| 42 | 43.072 | C15H24O | .beta.-Oplopenone | 0.28 | 28305-60-4 | 85.07 |
| 43 | 43.255 | C23H34O2 | 4,7,10,13,16,19-Docosahexaenoic acid, methyl ester, (all-Z)- | 0.11 | 2566-90-7 | 82.21 |
| 44(Z16) | 43.614 | C15H24O | Aromadendrene oxide-(2) | 0.9 | 1000156-12-7 | 82.29 |
| 45 | 44.266 | C15H24 | .gamma.-HIMACHALENE | 0.2 | 1000140-08-0 | 87.3 |
| 46(Z17) | 44.858 | C15H24 | 1H-Cyclopropa[a]naphthalene,decahydro-1,1,3a-trimethyl-7-methylene-,[1aS-(1aα,3aα,7aβ,7bα)]- | 3.61 | 20071-49-2 | 89 |
| 47 | 45.041 | C15H26O | 1H-Benzocyclohepten-7-ol, 2,3,4,4a,5,6,7,8-octahydro-1,1,4a,7-tetramethyl-, cis- | 1.4 | 6892-80-4 | 85.68 |
| 48 | 45.61 | C15H24O | Cedren-13-ol, 8- | 0.28 | 18319-35-2 | 83.49 |
| 49(Z18) | 45.999 | C15H24 | 1H-Cyclopropa[a]naphthalene,1a,2,3,3a,4,5,6,7b-octahydro-1,1,3a,7-tetramethyl-,[1aR-(1aα,3aα,7bα)]- | 0.19 | 489-29-2 | 92 |
| 50(Z19) | 46.378 | C15H24 | Guaia-1(10),11-diene | 0.66 | 3691-11-0 | 93.79 |
| 51(Z20) | 46.874 | C15H24 | β-Guaiene | 1.76 | 88-84-6 | 85.53 |
| 52(Z21) | 47.25 | C15H24 | (-)-Aristolene | 1.8 | 6831-16-9 | 85.71 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 53(Z22) | 47.712 | C15H26O | 1H-Cycloprop[e]azulen-4-ol,decahydro-1,1,4,7-tetramethyl-,[1aR-(1aα,4β,7α,7aβ,7bα)]- | 1.48 | 552-02-3 | 86.63 |
| 54(Z23) | 48.361 | C15H24 | Naphthalene,1,2,3,5,6,7,8,8a-octahydro-1,8a-dimethyl-7-(1-methylethenyl)-,[1S-(1α,7α,8aα)]- | 4.06 | 10219-75-7 | 90.93 |
| 55 | 48.873 | C15H24 | Azulene, 1,2,3,3a,4,5,6,7-octahydro-1,4-dimethyl-7-(1-methylethenyl)-, [1R-(1.alpha.,3a.beta.,4.alpha.,7.beta.)]- | 2.95 | 22567-17-5 | 92.06 |
| 56 | 48.906 | C15H24 | Longifolene | 1.38 | 475-20-7 | 93.68 |
| 57 | 50.286 | C15H22 | 3,5,11-Eudesmatriene | 1.6 | 193615-07-5 | 86.42 |
| 58 | 50.516 | C15H22O2 | 7-(1,3-Dimethylbuta-1,3-dienyl)-1,6,6-trimethyl-3,8-dioxatricyclo[5.1.0.0(2,4)]octane | 1.58 | 1000190-22-7 | 84.99 |
| 59(Z24) | 50.822 | C15H24O | Tricyclo[4.4.0.0(2,7)]dec-8-ene-3-methanol,α,α,6,8-tetramethyl-,stereoisomer | 2.33 | 41370-56-3 | 76.55 |
| 60 | 51.131 | C15H24O | 4a,5-Dimethyl-3-(prop-1-en-2-yl)-1,2,3,4,4a,5,6,7-octahydronaphthalen-1-ol | 0.67 | 61847-19-6 | 89.41 |
| 61 | 52.239 | C15H22O3 | Hydroxyvalerenic acid | 7.11 | 1619-16-5 | 83.34 |
| 62 | 52.718 | C15H22O2 | Curcumenol | 0.11 | 19431-84-6 | 80.88 |
| 63 | 52.971 | C15H22O | 1(2H)-Naphthalenone, 3,4,4a,5,6,7-hexahydro-4a,5-dimethyl-3-(1-methylethenyl)-, [3S-(3.alpha.,4a.alpha.,5.alpha.)]- | 0.7 | 562-23-2 | 84.88 |
| 64 | 53.506 | C15H24O2 | Bicyclo[4.4.0]dec-2-ene-4-ol, 2-methyl-9-(prop-1-en-3-ol-2-yl)- | 0.64 | 1000196-79-7 | 84.67 |
| 65 | 54.604 | C15H24O | (-)-Spathulenol | 0.27 | 77171-55-2 | 82.96 |
| 66 | 55.891 | C15H24O | (1R,7S,E)-7-Isopropyl-4,10-dimethylenecyclodec-5-enol | 0.78 | 81968-62-9 | 84.5 |
| 67 | 56.403 | C15H22O | (1aR,4aS,8aS)-4a,8,8-Trimethyl-1,1a,4,4a,5,6,7,8-octahydrocyclopropa[d]naphthalene-2-carbaldehyde | 0.13 | 470-41-7 | 85.43 |
| 68 | 56.975 | C15H22O | 4,6,6-Trimethyl-2-(3-methylbuta-1,3-dienyl)-3-oxatricyclo[5.1.0.0(2,4)]octane | 0.15 | 1000190-22-2 | 84.02 |
| 69 | 57.245 | C15H22O | (E)-3-((4S,7R,7aR)-3,7-Dimethyl-2,4,5,6,7,7a-hexahydro-1H-inden-4-yl)-2-methylacrylaldehyde | 0.29 | 4176-16-3 | 85.79 |
| 70 | 57.993 | C15H22O | 3-epi-Cedrenal | 0.71 | 1000465-27-6 | 84.54 |
| 71 | 58.399 | C15H22O | 2H-Cyclopropa[a]naphthalen-2-one, 1,1a,4,5,6,7,7a,7b-octahydro-1,1,7,7a-tetramethyl-, (1a.alpha.,7.alpha.,7a.alpha.,7b.alpha.)- | 2.87 | 6831-17-0 | 85.68 |
| 72 | 58.855 | C15H22O | Squamulosone | 0.32 | 34413-94-0 | 85.76 |
| 73 | 59.929 | C15H22O | 2-((2R,4aR,8aR)-4a,8-Dimethyl-1,2,3,4,4a,5,6,8a-octahydronaphthalen-2-yl)acrylaldehyde | 0.8 | 4586-01-0 | 87.9 |
| 74 | 60.435 | C15H24O | 2-(4a,8-Dimethyl-1,2,3,4,4a,5,6,7-octahydro-naphthalen-2-yl)-prop-2-en-1-ol | 0.13 | 1000190-51-8 | 81.67 |
| 75 | 60.85 | C15H24O | 2-((2R,4aR)-4a,8-Dimethyl-1,2,3,4,4a,5,6,7-octahy | 0.1 | 65018-14-6 | 80.89 |

| | | | | | | |
|---|---|---|---|---|---|---|
| | | | dronaphthalen-2-yl)prop-2-en-1-ol | | | |
| 76 | 62.367 | C16H24O2 | Methyl 2-((2R,4aR)-4a,8-dimethyl-1,2,3,4,4a,5,6,7-octahydronaphthalen-2-yl)acrylate | 0.11 | 132342-55-3 | 90.54 |
| 77(Z25) | 63.415 | C15H22O | 2(3H)-Naphthalenone,4,4a,5,6,7,8-hexahydro-4a,5-dimethyl-3-(1-methylethylidene)-,(4ar-cis)- | 2.39 | 19598-45-9 | 90.66 |
| 78 | 63.987 | C15H22O2 | Valerenic acid | 0.28 | 3569-10-6 | 86.26 |
| 79 | 69.109 | C15H22O2 | (3R,3aR,4aS,5R,9aS)-3,5,8-Trimethyl-3a,4,4a,5,6,7,9,9a-octahydroazuleno[6,5-b]furan-2(3H)-one | 0.08 | 66873-38-9 | 87.15 |

**Table S2.** Docking results of twenty five components with four targets

| **Ligand** | **Receptor** | **affinity (kcal/mol)** |
|---|---|---|
| Z1 | GABRA1 | -11 |
| Z10 | GABRA1 | -11.6 |
| Z11 | GABRA1 | -10.7 |
| Z12 | GABRA1 | -10.9 |
| Z13 | GABRA1 | -9.2 |
| Z14 | GABRA1 | -10.2 |
| Z15 | GABRA1 | -9.4 |
| Z16 | GABRA1 | -11.1 |
| Z17 | GABRA1 | -11.6 |
| Z18 | GABRA1 | -11.5 |
| Z19 | GABRA1 | -10.6 |
| Z2 | GABRA1 | -9.5 |
| Z20 | GABRA1 | -10.5 |
| Z21 | GABRA1 | -11.8 |
| Z22 | GABRA1 | -10.8 |
| Z23 | GABRA1 | -10.7 |
| Z24 | GABRA1 | -9.3 |
| Z25 | GABRA1 | -9.4 |
| Z3 | GABRA1 | -12 |
| Z4 | GABRA1 | -11.6 |
| Z5 | GABRA1 | -9.8 |
| Z6 | GABRA1 | -10.5 |
| Z7 | GABRA1 | -11.6 |
| Z8 | GABRA1 | -10.7 |
| Z9 | GABRA1 | -8.7 |
| Z1 | GRIA1 | -10 |
| Z10 | GRIA1 | -10.3 |
| Z11 | GRIA1 | -9.7 |
| Z12 | GRIA1 | -9.7 |
| Z13 | GRIA1 | -9.7 |

| | | |
|---|---|---|
| Z14 | GRIA1 | -9.3 |
| Z15 | GRIA1 | -8.9 |
| Z16 | GRIA1 | -10.7 |
| Z17 | GRIA1 | -10.6 |
| Z18 | GRIA1 | -10.6 |
| Z19 | GRIA1 | -9.6 |
| Z2 | GRIA1 | -8.8 |
| Z20 | GRIA1 | -9.6 |
| Z21 | GRIA1 | -10.7 |
| Z22 | GRIA1 | -9.9 |
| Z23 | GRIA1 | -9.9 |
| Z24 | GRIA1 | -10 |
| Z25 | GRIA1 | -10 |
| Z3 | GRIA1 | -10.5 |
| Z4 | GRIA1 | -10.2 |
| Z5 | GRIA1 | -10.2 |
| Z6 | GRIA1 | -9.6 |
| Z7 | GRIA1 | -10.7 |
| Z8 | GRIA1 | -9.7 |
| Z9 | GRIA1 | -9.2 |
| Z1 | HTR1A | -10.3 |
| Z10 | HTR1A | -10.7 |
| Z11 | HTR1A | -8.4 |
| Z12 | HTR1A | -10.6 |
| Z13 | HTR1A | -8.2 |
| Z14 | HTR1A | -9.8 |
| Z15 | HTR1A | -8.7 |
| Z16 | HTR1A | -10.9 |
| Z17 | HTR1A | -11 |
| Z18 | HTR1A | -11 |
| Z19 | HTR1A | -10.5 |
| Z2 | HTR1A | -8.8 |
| Z20 | HTR1A | -8.5 |
| Z21 | HTR1A | -11.2 |
| Z22 | HTR1A | -10.3 |
| Z23 | HTR1A | -10.1 |
| Z24 | HTR1A | -10.1 |
| Z25 | HTR1A | -10.4 |
| Z3 | HTR1A | -10.8 |
| Z4 | HTR1A | -10.9 |
| Z5 | HTR1A | -10.3 |
| Z6 | HTR1A | -10.5 |
| Z7 | HTR1A | -11.1 |

| | | |
|---|---|---|
| Z8 | HTR1A | -7.7 |
| Z9 | HTR1A | -8 |
| Z1 | HTR2A | -9.5 |
| Z10 | HTR2A | -9.9 |
| Z11 | HTR2A | -9.3 |
| Z12 | HTR2A | -9.8 |
| Z13 | HTR2A | -9.3 |
| Z14 | HTR2A | -8.8 |
| Z15 | HTR2A | -8.4 |
| Z16 | HTR2A | -10.6 |
| Z17 | HTR2A | -10.3 |
| Z18 | HTR2A | -10.3 |
| Z19 | HTR2A | -9.2 |
| Z2 | HTR2A | -8.3 |
| Z20 | HTR2A | -9.2 |
| Z21 | HTR2A | -10.3 |
| Z22 | HTR2A | -9.6 |
| Z23 | HTR2A | -9.7 |
| Z24 | HTR2A | -9.1 |
| Z25 | HTR2A | -9.6 |
| Z3 | HTR2A | -10.7 |
| Z4 | HTR2A | -10.2 |
| Z5 | HTR2A | -9.8 |
| Z6 | HTR2A | -9.2 |
| Z7 | HTR2A | -10.7 |
| Z8 | HTR2A | -9.3 |
| Z9 | HTR2A | -9 |