**Medium to use**

**Unconstrained elements**

|  |  |  |  |
| --- | --- | --- | --- |
| **Elements** | **Recon ID** | **lb** | **ub** |
| **H2O** | h2o[e] |  |  |
| **O2** | o2[e] |  |  |
| **H** | h[e] |  |  |
| **O2S** | o2s[e] |  |  |
| **CO2** | Co2[e] |  |  |
| **Pi** | pi[e] |  |  |
| **H2O2** | h2o2[e] |  |  |
| **HCO3** | hco3[e] |  |  |
| **H2CO3** | h2co3[e] |  |  |
| **CO** | co[e] |  |  |

**Plasmax medium**

- Article: Vande Voorde et al. *Improving the metabolic fidelity of cancer models with a physiological cell culture medium*. Science Advances. 2019;5: eaau7314 (<10.1126/sciadv.aau7314>)

- Detailed information gathered from supplementary table S1 (<https://advances.sciencemag.org/content/advances/suppl/2018/12/21/5.1.eaau7314.DC1/aau7314_SM.pdf>)

- Medium: <https://ximbio.com/reagent/156371/plasmaxsuptmsup-cell-culture-medium-coming-soon#datasheet>

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | **Elements** | **Recon ID** | **Concentration in Medium (μM)** | **lb** | **ub** |
| **Proteinogenic Amino Acids** | L-Alanine | ala\_L[e] | 510 |  |  |
| L-Arginine | arg\_L[e] | 64 |  |  |
| L-Asparagine | asn\_L[e] | 41 |  |  |
| L-Aspartic acid | asp\_L[e] | 6 |  |  |
| L-Cysteine | cys\_L[e] | 33 |  |  |
| L-Glutamate | glu\_L[e] | 98 |  |  |
| L-Glutamine | gln\_L[e] | 650 |  |  |
| Glycine | gly[e] | 330 |  |  |
| L-Histidine | his\_L[e] | 120 |  |  |
| L-Isoleucine | ile\_L[e] | 140 |  |  |
| L-Leucine | leu\_L[e] | 170 |  |  |
| L-Lysine | lys\_L[e] | 220 |  |  |
| L-Methionine | met\_L[e] | 30 |  |  |
| L-Phenylalanine | phe\_L[e] | 68 |  |  |
| L-Proline | pro\_L[e] | 360 |  |  |
| L-Serine | ser\_L[e] | 140 |  |  |
| L-Threonine | thr\_L[e] | 240 |  |  |
| L-Tryptophan | trp\_L[e] | 78 |  |  |
| L-Tyrosine | tyr\_L[e] | 74 |  |  |
| L-Valine | val\_L[e] | 230 |  |  |
| **Non-proteinogenic Amino Acids** | α-Aminobutyrate | C02356[e] | 41 |  |  |
| L-Citrulline | citr\_L[e] | 55 |  |  |
| L-Cystine | Lcystin[e] | 65 |  |  |
| L-Homocysteine | hcys\_L[e] | 9 |  |  |
| 4-Hydroxy-L-proline | 4hpro\_LT[e] | 13 |  |  |
| L-Ornithine | orn[e] | 80 |  |  |
| L-Pyroglutamate | 5oxpro[e] | 20 |  |  |
| **Amino Acids Derivatives** | L-Acetyl glycine | acgly[e] | 70 |  |  |
| L-Carnosine | carn[e] | 6 |  |  |
| Glutathione (reduced) | gthrd[e] | 37 |  |  |
| Taurine | taur[e] | 130 |  |  |
| N-Trimethylglycine (betaine) | glyb[e] | 72 |  |  |
| **Other Components** | Acetate | ac[e] | 42 |  |  |
| Acetone | acetone[e] | 55 |  |  |
| Acetyl carnitine | acrn[e] | 5 |  |  |
| Citrate | cit[e] | 114 |  |  |
| Carnitine | crn[e] | 46 |  |  |
| Creatine | creat[e] | 37 |  |  |
| Creatinine | crtn[e] | 74 |  |  |
| Formate | for[e] | 33 |  |  |
| D-Glucose | glc\_D[e] | 5560 |  |  |
| Glycerol | glyc[e] | 82 |  |  |
| 2-Hydroxybutyrate | 2hb[e] | 31 |  |  |
| 3-Hydroxybutyrate | bhb[e] | 77 |  |  |
| 3-Hydroxyisobutyrate | 3hmp[e] | 20 |  |  |
| Hypoxanthine | hxan[e] | 5 |  |  |
| Lactate | lac\_L[e]; lac\_D[e] | 500 |  |  |
| Methyl acetoacetate | - | 41 |  |  |
| Phenol Red | - | 25 |  |  |
| Pyruvate | pyr[e] | 100 |  |  |
| Succinate | succ[e] | 23 |  |  |
| Uracil | ura[e] | 2 |  |  |
| Urate | urate[e] | 270 |  |  |
| Urea | urea[e] | 3000 |  |  |
| Uridine | uri[e] | 3 |  |  |
| **Inorganic Salts** | Ammonium Chloride | nh4[e] and cl[e] | 50 |  |  |
| Calcium Chloride | ca2[e] and cl[e] | 1800 |  |  |
| Magnesium Sulfate | - and so4[e] | 813 |  |  |
| Potassium Chloride | K[e] and cl[e] | 5330 |  |  |
| Sodium Bicarbonate | na1[e] and hco3[e] | 26191 |  |  |
| Sodium Chloride | na1[e] and cl[e] | 118706 |  |  |
| Sodium Phosphate monobasic | na1[e] and pi[e] | 1010 |  |  |
| **Trace Elements** | Ammonium Metavanadate | - | 0.0026 |  |  |
| Cupric Sulfate | - | 0.0052 |  |  |
| Ferric Nitrate | - | 0.1238 |  |  |
| Ferric Sulfate | - | 1.048 |  |  |
| Manganous Chloride | - | 0.0002 |  |  |
| Sodium Selenite | - | 0.0289 |  |  |
| Zinc Sulfate | - | 1.5 |  |  |
| Ascorbate | ascb\_L | 62 |  |  |
| D-Biotin | btn | 4.1 |  |  |
| Choline | chol | 7.1 |  |  |
| Folate | fol | 2.3 |  |  |
| Myo-Inositol | inost | 11.1 |  |  |
| Niacinamide | ncam | 8.2 |  |  |
| D-Pantothenic acid hemicalcium | - | 4.2 |  |  |
| Pyridoxine | pydxn | 4.9 |  |  |
| Riboflavin | ribflv | 0.3 |  |  |
| Thiamine | thm | 3 |  |  |
| Vitamin B12 | cbl1 | 0.005 |  |  |