

Supplemental Data Table 1

BIOCHEMICAL	without imputation method				with imputation method				outlier deleted with imputation method			
	N of pairs used	CVw (95% CI)	CVb (95% CI)	ICC (95% CI)	N of pairs used	CVw (95% CI)	CVb (95% CI)	ICC (95% CI)	N of pairs used	CVw (95% CI)	CVb (95% CI)	ICC (95% CI)
1,2-propanediol	60	0.36 (0.28, 0.48)	0.16 (0.09, 0.30)	0.17 (0.03, 0.54)	60	0.36 (0.28, 0.48)	0.16 (0.09, 0.30)	0.17 (0.03, 0.54)	59	0.32 (0.25, 0.41)	0.16 (0.10, 0.27)	0.21 (0.06, 0.54)
1,3,7-trimethylurate	13	0.40 (0.20, 0.80)	0.57 (0.35, 0.93)	0.67 (0.34, 0.89)	60	0.33 (0.24, 0.44)	0.60 (0.52, 0.71)	0.78 (0.66, 0.86)	58	0.25 (0.19, 0.32)	0.37 (0.31, 0.44)	0.69 (0.55, 0.81)
1,3-dimethylurate	12	0.65 (0.22, 1.88)	0.96 (0.46, 1.97)	0.68 (0.35, 0.90)	60	0.98 (0.49, 1.96)	1.49 (0.95, 2.35)	0.70 (0.56, 0.81)	59	0.33 (0.25, 0.44)	0.40 (0.31, 0.50)	0.59 (0.42, 0.74)
1,5-anhydroglucitol (1,5-AG)	60	0.13 (0.11, 0.16)	0.34 (0.31, 0.37)	0.87 (0.79, 0.92)	60	0.13 (0.11, 0.16)	0.34 (0.31, 0.37)	0.87 (0.79, 0.92)	60	0.13 (0.11, 0.16)	0.34 (0.31, 0.37)	0.87 (0.79, 0.92)
1,6-anhydroglucose	34	0.87 (0.42, 1.78)	0.58 (0.19, 1.71)	0.31 (0.10, 0.65)	60	1.09 (0.56, 2.15)	0.80 (0.32, 2.01)	0.35 (0.17, 0.59)	59	0.79 (0.47, 1.32)	0.72 (0.41, 1.27)	0.46 (0.27, 0.65)
1,7-dimethylurate	27	0.44 (0.27, 0.71)	0.42 (0.25, 0.69)	0.47 (0.22, 0.74)	60	0.56 (0.37, 0.84)	0.71 (0.51, 0.98)	0.61 (0.45, 0.76)	59	0.50 (0.34, 0.72)	0.58 (0.42, 0.79)	0.57 (0.40, 0.73)
10-heptadecenoate (17:1n7)	60	0.30 (0.23, 0.39)	0.30 (0.23, 0.39)	0.50 (0.32, 0.68)	60	0.30 (0.23, 0.39)	0.30 (0.23, 0.39)	0.50 (0.32, 0.68)	59	0.27 (0.21, 0.35)	0.29 (0.23, 0.37)	0.53 (0.35, 0.70)
10-nonadecenoate (19:1n9)	60	0.32 (0.24, 0.41)	0.30 (0.23, 0.40)	0.48 (0.29, 0.67)	60	0.32 (0.24, 0.41)	0.30 (0.23, 0.40)	0.48 (0.29, 0.67)	59	0.28 (0.22, 0.37)	0.30 (0.24, 0.39)	0.53 (0.36, 0.71)
10-undecenoate (11:1n1)	60	0.22 (0.17, 0.27)	0.29 (0.24, 0.34)	0.64 (0.48, 0.77)	60	0.22 (0.17, 0.27)	0.29 (0.24, 0.34)	0.64 (0.48, 0.77)	60	0.22 (0.17, 0.27)	0.29 (0.24, 0.34)	0.64 (0.48, 0.77)
12-HETE	33	0.65 (0.33, 1.28)	1.16 (0.79, 1.69)	0.76 (0.59, 0.87)	60	0.90 (0.45, 1.81)	1.73 (1.21, 2.49)	0.79 (0.68, 0.87)	59	0.95 (0.44, 2.06)	2.01 (1.40, 2.90)	0.82 (0.72, 0.89)
13-HODE + 9-HODE	60	0.27 (0.21, 0.34)	0.19 (0.13, 0.26)	0.32 (0.15, 0.57)	60	0.27 (0.21, 0.34)	0.19 (0.13, 0.26)	0.32 (0.15, 0.57)	59	0.23 (0.18, 0.29)	0.16 (0.12, 0.23)	0.34 (0.16, 0.59)
1-arachidonoylglycerophosphocholine*	58	0.56 (0.39, 0.82)	0.19 (0.06, 0.57)	0.10 (0.01, 0.65)	60	0.58 (0.40, 0.84)	0.21 (0.07, 0.59)	0.11 (0.01, 0.60)	60	0.58 (0.40, 0.84)	0.21 (0.07, 0.59)	0.11 (0.01, 0.60)
1-arachidonoylglycerophosphoethanolamine*	60	0.21 (0.17, 0.26)	0.15 (0.11, 0.21)	0.34 (0.16, 0.58)	60	0.21 (0.17, 0.26)	0.15 (0.11, 0.21)	0.34 (0.16, 0.58)	59	0.18 (0.15, 0.22)	0.16 (0.13, 0.21)	0.45 (0.26, 0.65)
1-arachidonoylglycerophosphoinositol*	60	0.23 (0.19, 0.29)	0.11 (0.07, 0.18)	0.19 (0.05, 0.53)	60	0.23 (0.19, 0.29)	0.11 (0.07, 0.18)	0.19 (0.05, 0.53)	60	0.23 (0.19, 0.29)	0.11 (0.07, 0.18)	0.19 (0.05, 0.53)
1-docosahexaenoylglycerophosphocholine*	60	0.61 (0.41, 0.91)	0.27 (0.11, 0.67)	0.16 (0.03, 0.54)	60	0.61 (0.41, 0.91)	0.27 (0.11, 0.67)	0.16 (0.03, 0.54)	59	0.55 (0.38, 0.79)	0.21 (0.08, 0.54)	0.13 (0.02, 0.58)
1-docosapentaenoylglycerophosphocholine*	33	0.36 (0.25, 0.52)	0.14 (0.05, 0.37)	0.13 (0.01, 0.74)	60	0.47 (0.34, 0.66)	0.38 (0.25, 0.58)	0.40 (0.21, 0.62)	59	0.44 (0.32, 0.62)	0.42 (0.30, 0.60)	0.48 (0.29, 0.67)
1-eicosadienoylglycerophosphocholine*	55	0.41 (0.30, 0.55)	0.08 (0.01, 0.39)	0.03 (0.00, 0.99)	60	0.40 (0.30, 0.54)	0.17 (0.08, 0.34)	0.14 (0.02, 0.56)	59	0.35 (0.27, 0.46)	0.18 (0.10, 0.30)	0.20 (0.05, 0.54)
1-eicosatrienoylglycerophosphocholine*	60	0.37 (0.28, 0.50)	0.29 (0.20, 0.42)	0.38 (0.19, 0.60)	60	0.37 (0.28, 0.50)	0.29 (0.20, 0.42)	0.38 (0.19, 0.60)	58	0.32 (0.25, 0.42)	0.23 (0.16, 0.34)	0.35 (0.16, 0.59)
1-heptadecanoylglycerophosphocholine	51	0.48 (0.34, 0.69)	0.18 (0.07, 0.47)	0.12 (0.01, 0.64)	60	0.54 (0.38, 0.77)	0.23 (0.10, 0.54)	0.15 (0.03, 0.55)	59	0.48 (0.35, 0.67)	0.20 (0.09, 0.44)	0.15 (0.02, 0.56)
1-linoleoylglycerol (1-monolinolein)	20	0.38 (0.25, 0.59)	. (., .)	0.00 (., .)	60	0.43 (0.32, 0.58)	0.24 (0.13, 0.41)	0.23 (0.07, 0.54)	59	0.41 (0.30, 0.55)	0.26 (0.17, 0.42)	0.29 (0.12, 0.56)
1-linoleoylglycerophosphocholine	60	0.50 (0.37, 0.69)	. (., .)	0.00 (., .)	60	0.50 (0.37, 0.69)	. (., .)	0.00 (., .)	59	0.48 (0.35, 0.64)	. (., .)	0.00 (., .)
1-linoleoylglycerophosphoethanolamine*	60	0.27 (0.21, 0.34)	0.25 (0.20, 0.33)	0.47 (0.29, 0.66)	60	0.27 (0.21, 0.34)	0.25 (0.20, 0.33)	0.47 (0.29, 0.66)	60	0.27 (0.21, 0.34)	0.25 (0.20, 0.33)	0.47 (0.29, 0.66)
1-methylurate	31	0.43 (0.27, 0.70)	0.66 (0.48, 0.91)	0.70 (0.50, 0.85)	60	0.49 (0.33, 0.72)	0.86 (0.68, 1.07)	0.76 (0.63, 0.85)	59	0.40 (0.29, 0.55)	0.57 (0.46, 0.72)	0.67 (0.52, 0.80)
1-myristoylglycerophosphocholine	60	0.50 (0.35, 0.70)	0.27 (0.14, 0.50)	0.22 (0.07, 0.53)	60	0.50 (0.35, 0.70)	0.27 (0.14, 0.50)	0.22 (0.07, 0.53)	59	0.48 (0.34, 0.68)	0.32 (0.19, 0.53)	0.30 (0.13, 0.57)
1-oleoylglycerol (1-monolein)	51	0.66 (0.42, 1.05)	0.40 (0.19, 0.86)	0.27 (0.09, 0.57)	60	0.63 (0.42, 0.95)	0.38 (0.19, 0.75)	0.27 (0.10, 0.55)	58	0.40 (0.30, 0.55)	0.36 (0.25, 0.51)	0.44 (0.26, 0.65)
1-oleoylglycerophosphocholine	60	0.29 (0.23, 0.37)	0.14 (0.09, 0.23)	0.20 (0.05, 0.53)	60	0.29 (0.23, 0.37)	0.14 (0.09, 0.23)	0.20 (0.05, 0.53)	60	0.29 (0.23, 0.37)	0.14 (0.09, 0.23)	0.20 (0.05, 0.53)
1-oleoylglycerophosphoethanolamine	60	0.32 (0.25, 0.42)	0.32 (0.24, 0.42)	0.49 (0.31, 0.68)	60	0.32 (0.25, 0.42)	0.32 (0.24, 0.42)	0.49 (0.31, 0.68)	59	0.30 (0.23, 0.40)	0.28 (0.21, 0.37)	0.45 (0.26, 0.65)
1-palmitoleoylglycerophosphocholine*	60	0.54 (0.38, 0.77)	0.25 (0.11, 0.54)	0.17 (0.04, 0.54)	60	0.54 (0.38, 0.77)	0.25 (0.11, 0.54)	0.17 (0.04, 0.54)	59	0.54 (0.38, 0.77)	0.22 (0.09, 0.53)	0.15 (0.02, 0.56)
1-palmitoylglycerol (1-monopalmitin)	55	0.37 (0.27, 0.50)	0.32 (0.23, 0.45)	0.43 (0.24, 0.65)	60	0.37 (0.28, 0.50)	0.32 (0.23, 0.45)	0.43 (0.25, 0.64)	59	0.32 (0.25, 0.42)	0.32 (0.24, 0.42)	0.49 (0.31, 0.68)
1-palmitoylglycerophosphocholine	60	0.21 (0.17, 0.27)	0.09 (0.06, 0.15)	0.16 (0.03, 0.54)	60	0.21 (0.17, 0.27)	0.09 (0.06, 0.15)	0.16 (0.03, 0.54)	60	0.21 (0.17, 0.27)	0.09 (0.06, 0.15)	0.16 (0.03, 0.54)
1-palmitoylglycerophosphoethanolamine	60	0.49 (0.35, 0.68)	0.09 (0.02, 0.52)	0.04 (0.00, 0.98)	60	0.49 (0.35, 0.68)	0.09 (0.02, 0.52)	0.04 (0.00, 0.98)	60	0.49 (0.35, 0.68)	0.09 (0.02, 0.52)	0.04 (0.00, 0.98)
1-palmitoylglycerophosphoinositol*	26	0.27 (0.18, 0.39)	0.25 (0.17, 0.37)	0.47 (0.21, 0.74)	60	0.50 (0.35, 0.70)	0.42 (0.28, 0.63)	0.42 (0.23, 0.63)	60	0.50 (0.35, 0.70)	0.42 (0.28, 0.63)	0.42 (0.23, 0.63)
1-pentadecanoylglycerophosphocholine*	42	0.55 (0.36, 0.84)	0.17 (0.04, 0.69)	0.09 (0.00, 0.81)	60	0.62 (0.42, 0.92)	0.16 (0.03, 0.75)	0.06 (0.00, 0.85)	60	0.62 (0.42, 0.92)	0.16 (0.03, 0.75)	0.06 (0.00, 0.85)
1-stearoylglycerol (1-monostearin)	31	0.50 (0.31, 0.80)	0.26 (0.10, 0.64)	0.21 (0.03, 0.67)	60	0.86 (0.51, 1.44)	0.32 (0.08, 1.30)	0.12 (0.01, 0.59)	58	0.62 (0.41, 0.92)	0.32 (0.15, 0.70)	0.21 (0.06, 0.54)
1-stearoylglycerophosphocholine	60	0.28 (0.22, 0.35)	0.14 (0.09, 0.23)	0.20 (0.05, 0.53)	60	0.28 (0.22, 0.35)	0.14 (0.09, 0.23)	0.20 (0.05, 0.53)	59	0.25 (0.20, 0.32)	0.14 (0.09, 0.21)	0.23 (0.07, 0.54)
1-stearoylglycerophosphoinositol	58	0.55 (0.38, 0.79)	0.11 (0.02, 0.70)	0.04 (0.00, 0.98)	60	0.54 (0.38, 0.76)	0.10 (0.02, 0.64)	0.04 (0.00, 0.98)	59	0.52 (0.37, 0.75)	0.17 (0.06, 0.50)	0.10 (0.01, 0.65)
21-hydroxypregnenolone disulfate	37	0.22 (0.14, 0.36)	1.22 (1.12, 1.34)	0.97 (0.94, 0.98)	60	0.23 (0.16, 0.34)	1.27 (1.19, 1.36)	0.97 (0.95, 0.98)	59	0.18 (0.14, 0.23)	0.51 (0.47, 0.56)	0.89 (0.83, 0.94)
2-aminobutyrate	60	0.18 (0.15, 0.22)	0.21 (0.17, 0.25)	0.57 (0.40, 0.73)	60	0.18 (0.15, 0.22)	0.21 (0.17, 0.25)	0.57 (0.40, 0.73)	60	0.18 (0.15, 0.22)	0.21 (0.17, 0.25)	0.57 (0.40, 0.73)
2-arachidonoylglycerophosphocholine*	40	0.34 (0.24, 0.46)	0.21 (0.12, 0.35)	0.28 (0.09, 0.62)	60	0.39 (0.29, 0.52)	0.20 (0.12, 0.35)	0.21 (0.06, 0.53)	59	0.34 (0.26, 0.45)	0.22 (0.14, 0.34)	0.29 (0.12, 0.56)
2-arachidonoylglycerophosphoethanolamine*	28	0.25 (0.18, 0.35)	0.09 (0.04, 0.23)	0.13 (0.01, 0.80)	60	0.48 (0.35, 0.67)	0.13 (0.04, 0.43)	0.07 (0.00, 0.78)	60	0.48 (0.35, 0.67)	0.13 (0.04, 0.43)	0.07 (0.00, 0.78)
2-hydroxy-3-methylvalerate	16	0.38 (0.22, 0.65)	0.27 (0.13, 0.58)	0.34 (0.07, 0.78)	60	0.42 (0.30, 0.57)	0.48 (0.36, 0.63)	0.57 (0.40, 0.73)	59	0.32 (0.24, 0.42)	0.40 (0.32, 0.50)	0.61 (0.45, 0.76)
2-hydroxyacetaminophen sulfate*	8	0.41 (0.15, 1.13)	0.90 (0.56, 1.42)	0.83 (0.51, 0.96)	60	2.13 (0.52, 8.69)	2.79 (0.95, 8.16)	0.63 (0.47, 0.77)	59	0.71 (0.35, 1.42)	2.10 (1.66, 2.65)	0.90 (0.84, 0.94)
2-hydroxybutyrate (AHB)	60	0.25 (0.19, 0.31)	0.27 (0.22, 0.34)	0.56 (0.38, 0.72)	60	0.25 (0.19, 0.31)	0.27 (0.22, 0.34)	0.56 (0.38, 0.72)	59	0.22 (0.18, 0.28)	0.27 (0.23, 0.33)	0.60 (0.43, 0.75)
2-hydroxyglutarate	45	0.36 (0.26, 0.49)	0.11 (0.04, 0.30)	0.08 (0.00, 0.81)	60	0.42 (0.31, 0.57)	0.02 (0.00, 0.429)	0.00 (0.00, 1.00)	60	0.42 (0.31, 0.57)	0.02 (0.00, 0.429)	0.00 (0.00, 1.00)
2-hydroxyhippurate (salicylurate)	41	1.26 (0.37, 4.34)	2.81 (1.62, 4.90)	0.83 (0.72, 0.91)	60	1.49 (0.45, 4.92)	3.29 (1.91, 5.65)	0.83 (0.74, 0.89)	59	1.05 (0.40, 2.75)	2.87 (2.02, 4.08)	0.88 (0.81, 0.93)
2-hydroxyisobutyrate	57	0.31 (0.23, 0.41)	0.42 (0.34, 0.51)	0.65 (0.49, 0.78)	60	0.31 (0.23, 0.40)	0.41 (0.34, 0.50)	0.64 (0.49, 0.78)	59	0.23 (0.19, 0.29)	0.14 (0.09, 0.20)	0.25 (0.09, 0.54)
2-hydroxyoctanoate	25	0.18 (0.13, 0.25)	0.27 (0.22, 0.34)	0.71 (0.48, 0.86)	60	0.32 (0.24, 0.42)	0.32 (0.25, 0.42)	0.50 (0.32, 0.68)	59	0.25 (0.20, 0.32)	0.37 (0.31, 0.44)	0.69 (0.54, 0.80)
2-hydroxypalmitate	60	0.15 (0.12, 0.18)	0.14 (0.11, 0.17)	0.47 (0.29, 0.66)	60	0.15 (0.12, 0.18)	0.14 (0.11, 0.17)	0.47 (0.29, 0.66)	60	0.15 (0.12, 0.18)	0.14 (0.11, 0.17)	0.47 (0.29, 0.66)
2-hydroxystearate	60	0.22 (0.18, 0.28)	0.16 (0.12, 0.22)	0.35 (0.17, 0.59)	60	0.22 (0.18, 0.28)	0.16 (0.12, 0.22					

2-methoxyacetaminophen sulfate*	6	-5.15 (-52E3, 0.00)	(.,.)	0.00 (.,.)	60	6.25 (0.16, 251.6)	4.20 (0.02, 1023)	0.31 (0.13, 0.57)	58	0.94 (0.46, 1.93)	1.65 (1.10, 2.48)	0.75 (0.63, 0.85)
2-methylbutyroylcarnitine	55	0.17 (0.13, 0.21)	0.26 (0.23, 0.30)	0.71 (0.57, 0.82)	60	0.19 (0.16, 0.24)	0.27 (0.23, 0.32)	0.66 (0.51, 0.79)	60	0.19 (0.16, 0.24)	0.27 (0.23, 0.32)	0.66 (0.51, 0.79)
2-oleylglycerophosphocholine*	60	0.32 (0.24, 0.41)	0.18 (0.12, 0.28)	0.25 (0.09, 0.54)	60	0.32 (0.24, 0.41)	0.18 (0.12, 0.28)	0.25 (0.09, 0.54)	60	0.32 (0.24, 0.41)	0.18 (0.12, 0.28)	0.25 (0.09, 0.54)
2-oleylglycerophosphoethanolamine*	39	0.32 (0.23, 0.44)	0.03 (0.00, 1.35)	0.01 (0.00, 1.00)	60	0.45 (0.34, 0.60)	(.,.)	0.00 (.,.)	60	0.45 (0.34, 0.60)	(.,.)	0.00 (.,.)
2-palmitoylglycerophosphocholine*	60	0.45 (0.33, 0.61)	0.10 (0.02, 0.41)	0.04 (0.00, 0.95)	60	0.45 (0.33, 0.61)	0.10 (0.02, 0.41)	0.04 (0.00, 0.95)	60	0.45 (0.33, 0.61)	0.10 (0.02, 0.41)	0.04 (0.00, 0.95)
2-palmitoylglycerophosphoethanolamine*	51	0.36 (0.27, 0.48)	0.05 (0.01, 0.43)	0.02 (0.00, 1.00)	60	0.39 (0.29, 0.53)	0.18 (0.10, 0.34)	0.17 (0.04, 0.54)	60	0.39 (0.29, 0.53)	0.18 (0.10, 0.34)	0.17 (0.04, 0.54)
2-stearoylglycerophosphocholine*	58	0.32 (0.25, 0.42)	0.22 (0.15, 0.33)	0.33 (0.15, 0.58)	60	0.33 (0.25, 0.42)	0.22 (0.15, 0.32)	0.31 (0.13, 0.56)	59	0.25 (0.20, 0.32)	0.21 (0.16, 0.28)	0.40 (0.22, 0.62)
3-(4-hydroxyphenyl)lactate	60	0.14 (0.11, 0.17)	0.24 (0.21, 0.27)	0.75 (0.62, 0.84)	60	0.14 (0.11, 0.17)	0.24 (0.21, 0.27)	0.75 (0.62, 0.84)	60	0.14 (0.11, 0.17)	0.24 (0.21, 0.27)	0.75 (0.62, 0.84)
3-(cystein-S-yl)acetaminophen*	7	-2.71 (-244, -0.03)	(.,.)	0.00 (.,.)	60	-13.2 (-25E3, -0.01)	-4.51 (-18E9, 0.00)	0.10 (0.01, 0.63)	58	1.26 (0.51, 3.11)	1.94 (1.08, 3.49)	0.70 (0.56, 0.81)
3-carboxy-4-methyl-5-propyl-2-furanpropanoate	60	0.47 (0.32, 0.69)	0.80 (0.64, 1.00)	0.74 (0.62, 0.84)	60	0.47 (0.32, 0.69)	0.80 (0.64, 1.00)	0.74 (0.62, 0.84)	59	0.39 (0.27, 0.54)	0.76 (0.63, 0.90)	0.79 (0.68, 0.87)
3-dehydrocarnitine*	60	0.12 (0.09, 0.15)	0.45 (0.43, 0.48)	0.94 (0.90, 0.96)	60	0.12 (0.09, 0.15)	0.45 (0.43, 0.48)	0.94 (0.90, 0.96)	60	0.12 (0.09, 0.15)	0.45 (0.43, 0.48)	0.94 (0.90, 0.96)
3-hydroxy-2-ethylpropionate	53	0.23 (0.18, 0.29)	0.30 (0.25, 0.36)	0.63 (0.46, 0.78)	60	0.30 (0.23, 0.39)	0.29 (0.22, 0.38)	0.48 (0.30, 0.67)	59	0.27 (0.21, 0.35)	0.29 (0.23, 0.37)	0.55 (0.37, 0.71)
3-hydroxybutyrate (BHBA)	60	0.70 (0.44, 1.09)	0.50 (0.27, 0.94)	0.34 (0.16, 0.58)	60	0.70 (0.44, 1.09)	0.50 (0.27, 0.94)	0.34 (0.16, 0.58)	59	0.60 (0.40, 0.91)	0.50 (0.30, 0.82)	0.41 (0.22, 0.62)
3-hydroxydecanoate	60	0.34 (0.26, 0.44)	0.35 (0.27, 0.46)	0.53 (0.35, 0.70)	60	0.34 (0.26, 0.44)	0.35 (0.27, 0.46)	0.53 (0.35, 0.70)	59	0.26 (0.21, 0.34)	0.24 (0.18, 0.31)	0.45 (0.27, 0.65)
3-hydroxyisobutyrate	59	0.23 (0.18, 0.29)	0.26 (0.21, 0.32)	0.56 (0.39, 0.72)	60	0.23 (0.19, 0.29)	0.27 (0.22, 0.33)	0.57 (0.40, 0.73)	60	0.23 (0.19, 0.29)	0.27 (0.22, 0.33)	0.57 (0.40, 0.73)
3-indoxyl sulfate	60	0.28 (0.22, 0.36)	0.36 (0.30, 0.44)	0.63 (0.47, 0.76)	60	0.28 (0.22, 0.36)	0.36 (0.30, 0.44)	0.63 (0.47, 0.76)	59	0.23 (0.18, 0.30)	0.36 (0.31, 0.42)	0.71 (0.57, 0.82)
3-methoxytyrosine	57	0.30 (0.07, 1.34)	5.61 (5.17, 6.07)	1.00 (1.00, 1.00)	60	0.31 (0.07, 1.36)	5.73 (5.29, 6.21)	1.00 (1.00, 1.00)	59	0.27 (0.21, 0.35)	0.27 (0.21, 0.35)	0.49 (0.30, 0.67)
3-methyl-2-oxobutyrate	60	0.13 (0.11, 0.16)	0.15 (0.12, 0.17)	0.56 (0.39, 0.72)	60	0.13 (0.11, 0.16)	0.15 (0.12, 0.17)	0.56 (0.39, 0.72)	60	0.13 (0.11, 0.16)	0.15 (0.12, 0.17)	0.56 (0.39, 0.72)
3-methyl-2-oxovalerate	60	0.13 (0.11, 0.16)	0.18 (0.16, 0.21)	0.64 (0.49, 0.78)	60	0.13 (0.11, 0.16)	0.18 (0.16, 0.21)	0.64 (0.49, 0.78)	59	0.12 (0.10, 0.14)	0.18 (0.16, 0.21)	0.70 (0.56, 0.82)
3-methylhistidine	50	0.53 (0.36, 0.77)	0.14 (0.04, 0.58)	0.07 (0.00, 0.84)	60	0.60 (0.41, 0.88)	0.25 (0.10, 0.63)	0.15 (0.02, 0.55)	60	0.60 (0.41, 0.88)	0.25 (0.10, 0.63)	0.15 (0.02, 0.55)
3-methylxanthine	27	0.38 (0.25, 0.60)	0.42 (0.28, 0.64)	0.55 (0.29, 0.78)	60	0.47 (0.33, 0.67)	0.60 (0.46, 0.79)	0.63 (0.46, 0.76)	60	0.47 (0.33, 0.67)	0.60 (0.46, 0.79)	0.63 (0.46, 0.76)
3-phenylpropionate (hydrocinnamate)	42	0.54 (0.34, 0.85)	0.54 (0.34, 0.85)	0.50 (0.29, 0.71)	60	0.58 (0.38, 0.88)	0.71 (0.51, 1.00)	0.60 (0.44, 0.75)	59	0.51 (0.35, 0.76)	0.69 (0.52, 0.92)	0.64 (0.49, 0.78)
4-acetamidobutanoate	51	0.24 (0.19, 0.31)	0.27 (0.22, 0.34)	0.57 (0.38, 0.74)	60	0.28 (0.22, 0.36)	0.30 (0.24, 0.38)	0.53 (0.36, 0.70)	60	0.28 (0.22, 0.36)	0.30 (0.24, 0.38)	0.53 (0.36, 0.70)
4-acetamidophenol	7	4.04 (0.00, 3272)	(.,.)	0.00 (.,.)	60	81.00 (0.00, 11E21)	27.38 (0.00, 97E5)	10 (0.01, 0.63)	59	2.39 (0.55, 10.39)	2.03 (0.36, 11.47)	0.42 (0.23, 0.63)
4-acetaminophen sulfate	8	4.98 (0.00, 16809)	3.62 (0.00, 256E3)	0.35 (0.03, 0.89)	60	-14.6 (-98E3, 0.00)	-11.9 (-61E4, 0.00)	0.40 (0.21, 0.62)	58	1.46 (0.35, 6.11)	4.43 (2.76, 7.10)	0.90 (0.84, 0.94)
4-androsten-3beta,17beta-diol disulfate 1*	58	0.28 (0.18, 0.43)	1.37 (1.26, 1.49)	0.96 (0.94, 0.98)	60	0.28 (0.18, 0.43)	1.41 (1.29, 1.53)	0.96 (0.94, 0.98)	59	0.27 (0.17, 0.41)	1.39 (1.28, 1.51)	0.96 (0.94, 0.98)
4-androsten-3beta,17beta-diol disulfate 2*	58	0.17 (0.13, 0.23)	0.69 (0.64, 0.73)	0.94 (0.90, 0.96)	60	0.17 (0.13, 0.23)	0.71 (0.67, 0.76)	0.94 (0.91, 0.97)	59	0.16 (0.12, 0.20)	0.55 (0.51, 0.59)	0.92 (0.88, 0.95)
4-ethylphenylsulfate	11	0.48 (0.16, 1.42)	1.29 (0.86, 1.93)	0.88 (0.67, 0.96)	60	1.27 (0.57, 2.83)	1.20 (0.52, 2.81)	0.47 (0.29, 0.66)	59	0.86 (0.40, 1.84)	2.17 (1.61, 2.94)	0.86 (0.79, 0.92)
4-guanidinobutanoate	21	0.30 (0.20, 0.47)	0.29 (0.18, 0.46)	0.48 (0.20, 0.78)	60	0.33 (0.25, 0.43)	0.28 (0.20, 0.38)	0.42 (0.23, 0.63)	59	0.32 (0.25, 0.42)	0.25 (0.18, 0.35)	0.39 (0.20, 0.61)
4-hydroxyhippurate	43	0.34 (0.24, 0.47)	0.43 (0.33, 0.56)	0.62 (0.43, 0.78)	60	0.38 (0.28, 0.52)	0.53 (0.43, 0.67)	0.66 (0.51, 0.79)	59	0.33 (0.25, 0.44)	0.52 (0.44, 0.63)	0.72 (0.58, 0.82)
4-hydroxyphenylacetate	6	0.25 (0.11, 0.57)	0.49 (0.32, 0.75)	0.79 (0.38, 0.96)	60	0.80 (0.46, 1.39)	1.00 (0.64, 1.56)	0.61 (0.44, 0.75)	58	0.42 (0.29, 0.62)	0.89 (0.74, 1.07)	0.82 (0.71, 0.89)
4-methyl-2-oxpentanoate	60	0.13 (0.10, 0.15)	0.21 (0.19, 0.24)	0.74 (0.61, 0.84)	60	0.13 (0.10, 0.15)	0.21 (0.19, 0.24)	0.74 (0.61, 0.84)	60	0.13 (0.10, 0.15)	0.21 (0.19, 0.24)	0.74 (0.61, 0.84)
4-vinylphenol sulfate	55	1.56 (0.60, 4.05)	0.57 (0.04, 7.75)	0.12 (0.01, 0.62)	60	1.63 (0.63, 4.24)	0.70 (0.07, 6.52)	0.15 (0.03, 0.55)	59	0.84 (0.49, 1.45)	0.64 (0.31, 1.30)	0.36 (0.18, 0.60)
5-acetylamino-6-amino-3-methyluracil	10	0.88 (0.13, 5.99)	2.26 (1.07, 4.78)	0.87 (0.63, 0.96)	60	1.19 (0.41, 3.44)	3.17 (2.13, 4.72)	0.88 (0.81, 0.92)	59	0.61 (0.40, 0.91)	0.43 (0.24, 0.76)	0.33 (0.15, 0.58)
Salpha-androstan-3alpha,17beta-diol disulfate	5	0.38 (0.14, 1.04)	0.31 (0.09, 1.07)	0.40 (0.03, 0.94)	60	0.38 (0.27, 0.54)	0.78 (0.66, 0.93)	0.81 (0.70, 0.88)	57	0.14 (0.11, 0.18)	0.48 (0.45, 0.52)	0.92 (0.87, 0.95)
Salpha-androstan-3beta,17beta-diol disulfate	49	0.23 (0.17, 0.31)	0.63 (0.56, 0.70)	0.88 (0.81, 0.93)	60	0.24 (0.18, 0.33)	0.77 (0.70, 0.85)	0.91 (0.85, 0.94)	59	0.24 (0.18, 0.32)	0.80 (0.73, 0.87)	0.92 (0.87, 0.95)
Salpha-pregnan-3beta,20alpha-diol disulfate	33	0.44 (0.28, 0.70)	0.61 (0.43, 0.85)	0.65 (0.44, 0.82)	60	0.46 (0.32, 0.67)	0.76 (0.60, 0.95)	0.73 (0.60, 0.83)	58	0.29 (0.22, 0.40)	0.70 (0.61, 0.79)	0.85 (0.76, 0.91)
5-dodecanoate (12:1n7)	58	0.25 (0.20, 0.32)	0.25 (0.19, 0.31)	0.48 (0.30, 0.67)	60	0.25 (0.20, 0.32)	0.25 (0.20, 0.32)	0.50 (0.32, 0.68)	59	0.21 (0.17, 0.27)	0.25 (0.21, 0.31)	0.59 (0.42, 0.74)
5-methyluridine (ribothymidine)	22	0.14 (0.10, 0.19)	0.13 (0.09, 0.19)	0.49 (0.21, 0.77)	60	0.14 (0.11, 0.17)	0.12 (0.10, 0.15)	0.43 (0.24, 0.63)	60	0.14 (0.11, 0.17)	0.12 (0.10, 0.15)	0.43 (0.24, 0.63)
5-oxoproline	60	0.10 (0.08, 0.12)	0.17 (0.15, 0.19)	0.74 (0.60, 0.83)	60	0.10 (0.08, 0.12)	0.17 (0.15, 0.19)	0.74 (0.60, 0.83)	59	0.09 (0.07, 0.10)	0.16 (0.14, 0.18)	0.77 (0.65, 0.86)
7-alpha-hydroxy-3-oxo-4-cholestenoate (7-Hoca)	60	0.22 (0.18, 0.28)	0.16 (0.12, 0.22)	0.35 (0.17, 0.59)	60	0.22 (0.18, 0.28)	0.16 (0.12, 0.22)	0.35 (0.17, 0.59)	59	0.18 (0.15, 0.23)	0.17 (0.13, 0.21)	0.45 (0.27, 0.65)
7-methylguanine	57	0.36 (0.27, 0.47)	0.10 (0.04, 0.27)	0.08 (0.00, 0.76)	60	0.36 (0.27, 0.47)	0.18 (0.10, 0.31)	0.20 (0.05, 0.53)	59	0.29 (0.23, 0.37)	0.20 (0.14, 0.29)	0.32 (0.14, 0.58)
7-methylxanthine	31	0.44 (0.30, 0.64)	(.,.)	0.00 (.,.)	60	0.50 (0.36, 0.69)	0.16 (0.06, 0.45)	0.10 (0.01, 0.65)	59	0.44 (0.32, 0.60)	0.17 (0.07, 0.38)	0.13 (0.02, 0.58)
acetyl carnitine	60	0.19 (0.15, 0.23)	0.19 (0.15, 0.23)	0.51 (0.33, 0.69)	60	0.19 (0.15, 0.23)	0.19 (0.15, 0.23)	0.51 (0.33, 0.69)	60	0.19 (0.15, 0.23)	0.19 (0.15, 0.23)	0.51 (0.33, 0.69)
acetyl phosphate	60	0.15 (0.12, 0.18)	0.11 (0.09, 0.15)	0.36 (0.18, 0.60)	60	0.15 (0.12, 0.18)	0.11 (0.09, 0.15)	0.36 (0.18, 0.60)	60	0.15 (0.12, 0.18)	0.11 (0.09, 0.15)	0.36 (0.18, 0.60)
adenosine	21	0.73 (0.33, 1.59)	0.49 (0.15, 1.57)	0.31 (0.07, 0.73)	60	1.01 (0.54, 1.89)	0.78 (0.35, 1.76)	0.38 (0.19, 0.60)	58	0.90 (0.50, 1.60)	0.76 (0.38, 1.51)	0.42 (0.23, 0.63)
ADpSGEGDFXAEGGGV*	60	0.20 (0.16, 0.25)	0.32 (0.28, 0.37)	0.72 (0.59, 0.83)	60	0.20 (0.16, 0.25)	0.32 (0.28, 0.37)	0.72 (0.59, 0.83)	59	0.19 (0.15, 0.23)	0.33 (0.29, 0.37)	0.76 (0.63, 0.85)
adrenate (22:4n6)	60	0.21 (0.17, 0.26)	0.18 (0.14, 0.23)	0.43 (0.24, 0.63)	60	0.21 (0.17, 0.26)	0.18 (0.14, 0.23)	0.43 (0.24, 0.63)	60	0.21 (0.17, 0.26)	0.18 (0.14, 0.23)	0.43 (0.24, 0.63)
ADSGEGDFXAEGGGV*	60	0.32 (0.24, 0.43)	0.58 (0.49, 0.68)	0.76 (0.64, 0.85)	60	0.32 (0.24, 0.43)	0.58 (0.49, 0.68)	0.76 (0.64, 0.85)	59	0.28 (0.21, 0.37)	0.48 (0.41, 0.56)	0.74 (0.62, 0.84)
alanine	60	0.17 (0.14, 0.21)	0.19 (0.15, 0.23)	0.54 (0.36, 0.70)	60	0.17 (0.14, 0.21)	0.19 (0.15, 0.23)	0.54 (0.36, 0.70)	60	0.17 (0.14, 0.21)	0.19 (0.15, 0.23)	0.54 (0.36, 0.70)
alanyl leucine	27	0.32 (0.22, 0.47)	0.19 (0.10, 0.36)	0.25 (0.05, 0.69)	60	0.50 (0.36, 0.71)						

androsterone sulfate	58	0.28 (0.22, 0.37)	0.44 (0.37, 0.52)	0.70 (0.56, 0.82)	60	0.29 (0.22, 0.38)	0.47 (0.40, 0.55)	0.72 (0.59, 0.83)	58	0.24 (0.19, 0.32)	0.51 (0.45, 0.57)	0.81 (0.71, 0.88)
arabinose	47	0.23 (0.18, 0.29)	0.25 (0.19, 0.31)	0.54 (0.34, 0.73)	60	0.28 (0.22, 0.37)	0.31 (0.25, 0.39)	0.54 (0.37, 0.71)	60	0.28 (0.22, 0.37)	0.31 (0.25, 0.39)	0.54 (0.37, 0.71)
arabonate	49	0.30 (0.22, 0.39)	0.28 (0.21, 0.38)	0.47 (0.27, 0.68)	60	0.35 (0.26, 0.47)	0.35 (0.26, 0.46)	0.50 (0.32, 0.68)	60	0.35 (0.26, 0.47)	0.35 (0.26, 0.46)	0.50 (0.32, 0.68)
arachidonate (20:4n6)	60	0.14 (0.12, 0.17)	0.17 (0.15, 0.21)	0.60 (0.43, 0.75)	60	0.14 (0.12, 0.17)	0.17 (0.15, 0.21)	0.60 (0.43, 0.75)	59	0.13 (0.10, 0.16)	0.18 (0.15, 0.20)	0.65 (0.50, 0.78)
arginine	60	0.25 (0.20, 0.32)	0.12 (0.08, 0.20)	0.19 (0.05, 0.53)	60	0.25 (0.20, 0.32)	0.12 (0.08, 0.20)	0.19 (0.05, 0.53)	59	0.24 (0.19, 0.30)	0.15 (0.10, 0.22)	0.29 (0.11, 0.56)
asparagine	60	0.22 (0.18, 0.28)	0.14 (0.10, 0.20)	0.28 (0.11, 0.55)	60	0.22 (0.18, 0.28)	0.14 (0.10, 0.20)	0.28 (0.11, 0.55)	60	0.22 (0.18, 0.28)	0.14 (0.10, 0.20)	0.28 (0.11, 0.55)
aspartate	5	0.10 (0.06, 0.16)	(., .)	0.00 (., .)	60	0.33 (0.27, 0.42)	(., .)	0.00 (., .)	59	0.20 (0.17, 0.24)	(., .)	0.00 (., .)
aspartylphenylalanine	52	0.55 (0.37, 0.82)	0.38 (0.22, 0.68)	0.33 (0.14, 0.59)	60	0.56 (0.38, 0.82)	0.45 (0.28, 0.72)	0.39 (0.21, 0.61)	58	0.39 (0.29, 0.53)	0.42 (0.32, 0.56)	0.54 (0.36, 0.71)
azelate (nonanedioate)	60	0.69 (0.45, 1.06)	0.12 (0.01, 1.44)	0.03 (0.00, 1.00)	60	0.69 (0.45, 1.06)	0.12 (0.01, 1.44)	0.03 (0.00, 1.00)	59	0.23 (0.18, 0.29)	0.20 (0.16, 0.26)	0.44 (0.25, 0.64)
benzoate	60	0.17 (0.14, 0.21)	0.14 (0.11, 0.18)	0.42 (0.24, 0.63)	60	0.17 (0.14, 0.21)	0.14 (0.11, 0.18)	0.42 (0.24, 0.63)	59	0.15 (0.12, 0.19)	0.15 (0.12, 0.18)	0.49 (0.31, 0.68)
beta-hydroxyisovalerate	60	0.22 (0.18, 0.28)	0.26 (0.22, 0.32)	0.58 (0.41, 0.73)	60	0.22 (0.18, 0.28)	0.26 (0.22, 0.32)	0.58 (0.41, 0.73)	60	0.22 (0.18, 0.28)	0.26 (0.22, 0.32)	0.58 (0.41, 0.73)
betaine	60	0.14 (0.12, 0.18)	0.19 (0.17, 0.22)	0.64 (0.49, 0.78)	60	0.14 (0.12, 0.18)	0.19 (0.17, 0.22)	0.64 (0.49, 0.78)	60	0.14 (0.12, 0.18)	0.19 (0.17, 0.22)	0.64 (0.49, 0.78)
bilirubin (E,E)*	60	0.28 (0.22, 0.36)	0.24 (0.18, 0.32)	0.42 (0.23, 0.63)	60	0.28 (0.22, 0.36)	0.24 (0.18, 0.32)	0.42 (0.23, 0.63)	59	0.25 (0.20, 0.32)	0.23 (0.18, 0.30)	0.45 (0.26, 0.65)
bilirubin (E,Z or Z,E)*	42	0.44 (0.30, 0.64)	0.32 (0.19, 0.54)	0.35 (0.14, 0.63)	60	0.59 (0.40, 0.88)	0.44 (0.26, 0.75)	0.35 (0.17, 0.59)	60	0.59 (0.40, 0.88)	0.44 (0.26, 0.75)	0.35 (0.17, 0.59)
bilirubin (Z,Z)	58	0.31 (0.24, 0.40)	0.29 (0.22, 0.38)	0.47 (0.29, 0.67)	60	0.31 (0.24, 0.41)	0.29 (0.22, 0.38)	0.46 (0.28, 0.66)	59	0.21 (0.17, 0.27)	0.30 (0.26, 0.36)	0.67 (0.52, 0.79)
biliverdin	52	0.47 (0.33, 0.66)	0.34 (0.21, 0.55)	0.35 (0.16, 0.60)	60	0.51 (0.36, 0.72)	0.38 (0.24, 0.61)	0.36 (0.18, 0.59)	59	0.44 (0.32, 0.61)	0.37 (0.26, 0.55)	0.42 (0.23, 0.63)
bradykinin, des-arg(9)	44	0.92 (0.47, 1.81)	0.65 (0.25, 1.69)	0.33 (0.13, 0.62)	60	0.98 (0.52, 1.82)	0.89 (0.45, 1.76)	0.45 (0.27, 0.65)	58	0.78 (0.45, 1.34)	0.98 (0.64, 1.51)	0.61 (0.45, 0.76)
butyrylcarnitine	60	0.18 (0.14, 0.23)	0.39 (0.35, 0.43)	0.83 (0.73, 0.89)	60	0.18 (0.14, 0.23)	0.39 (0.35, 0.43)	0.83 (0.73, 0.89)	59	0.17 (0.14, 0.22)	0.38 (0.34, 0.42)	0.83 (0.74, 0.90)
caffeine	49	0.67 (0.40, 1.12)	0.74 (0.46, 1.18)	0.55 (0.35, 0.73)	60	0.76 (0.45, 1.28)	0.94 (0.62, 1.43)	0.61 (0.44, 0.75)	59	0.66 (0.41, 1.06)	0.86 (0.60, 1.23)	0.63 (0.47, 0.77)
caprate (10:0)	59	0.20 (0.16, 0.25)	0.18 (0.14, 0.23)	0.45 (0.27, 0.65)	60	0.20 (0.16, 0.25)	0.19 (0.15, 0.24)	0.46 (0.28, 0.66)	60	0.20 (0.16, 0.25)	0.19 (0.15, 0.24)	0.46 (0.28, 0.66)
caproate (6:0)	60	0.18 (0.14, 0.22)	0.14 (0.11, 0.18)	0.39 (0.21, 0.61)	60	0.18 (0.14, 0.22)	0.14 (0.11, 0.18)	0.39 (0.21, 0.61)	60	0.18 (0.14, 0.22)	0.14 (0.11, 0.18)	0.39 (0.21, 0.61)
caprylate (8:0)	60	0.19 (0.16, 0.24)	0.17 (0.14, 0.22)	0.44 (0.26, 0.64)	60	0.19 (0.16, 0.24)	0.17 (0.14, 0.22)	0.44 (0.26, 0.64)	60	0.19 (0.16, 0.24)	0.17 (0.14, 0.22)	0.44 (0.26, 0.64)
carnitine	60	0.08 (0.07, 0.10)	0.17 (0.16, 0.19)	0.82 (0.72, 0.89)	60	0.08 (0.07, 0.10)	0.17 (0.16, 0.19)	0.82 (0.72, 0.89)	60	0.08 (0.07, 0.10)	0.17 (0.16, 0.19)	0.82 (0.72, 0.89)
catechol sulfate	60	0.38 (0.28, 0.51)	0.44 (0.34, 0.57)	0.57 (0.40, 0.73)	60	0.38 (0.28, 0.51)	0.44 (0.34, 0.57)	0.57 (0.40, 0.73)	59	0.30 (0.23, 0.39)	0.43 (0.35, 0.52)	0.67 (0.52, 0.79)
C-glycosyltryptophan*	60	0.09 (0.07, 0.11)	0.21 (0.19, 0.23)	0.85 (0.77, 0.91)	60	0.09 (0.07, 0.11)	0.21 (0.19, 0.23)	0.85 (0.77, 0.91)	60	0.09 (0.07, 0.11)	0.21 (0.19, 0.23)	0.85 (0.77, 0.91)
chiro-inositol	14	1.59 (0.21, 12.12)	1.41 (0.14, 13.85)	0.44 (0.13, 0.81)	60	1.66 (0.60, 4.57)	1.33 (0.37, 4.71)	0.39 (0.21, 0.61)	58	1.36 (0.56, 3.34)	1.53 (0.69, 3.41)	0.56 (0.38, 0.72)
cholate	25	2.15 (0.29, 15.88)	1.53 (0.09, 25.39)	0.34 (0.10, 0.71)	60	2.69 (0.52, 13.95)	2.41 (0.38, 15.12)	0.45 (0.26, 0.65)	57	1.94 (0.51, 7.45)	2.74 (1.06, 7.11)	0.67 (0.51, 0.79)
cholesterol	60	0.12 (0.10, 0.15)	0.17 (0.15, 0.20)	0.66 (0.51, 0.79)	60	0.12 (0.10, 0.15)	0.17 (0.15, 0.20)	0.66 (0.51, 0.79)	58	0.10 (0.08, 0.12)	0.18 (0.16, 0.20)	0.75 (0.63, 0.85)
choline	60	0.11 (0.09, 0.13)	0.13 (0.11, 0.15)	0.60 (0.43, 0.75)	60	0.11 (0.09, 0.13)	0.13 (0.11, 0.15)	0.60 (0.43, 0.75)	60	0.11 (0.09, 0.13)	0.13 (0.11, 0.15)	0.60 (0.43, 0.75)
cis-aconitate	60	0.19 (0.15, 0.24)	0.25 (0.22, 0.30)	0.64 (0.48, 0.77)	60	0.19 (0.15, 0.24)	0.25 (0.22, 0.30)	0.64 (0.48, 0.77)	59	0.17 (0.14, 0.21)	0.26 (0.22, 0.30)	0.69 (0.54, 0.80)
citrate	60	0.18 (0.15, 0.23)	0.14 (0.11, 0.19)	0.37 (0.19, 0.60)	60	0.18 (0.15, 0.23)	0.14 (0.11, 0.19)	0.37 (0.19, 0.60)	60	0.18 (0.15, 0.23)	0.14 (0.11, 0.19)	0.37 (0.19, 0.60)
citrulline	58	0.11 (0.09, 0.13)	0.26 (0.24, 0.29)	0.86 (0.78, 0.91)	60	0.11 (0.09, 0.14)	0.28 (0.26, 0.30)	0.86 (0.78, 0.91)	59	0.10 (0.08, 0.12)	0.26 (0.24, 0.28)	0.87 (0.80, 0.92)
cortisol	60	0.27 (0.21, 0.35)	0.24 (0.18, 0.32)	0.44 (0.25, 0.64)	60	0.27 (0.21, 0.35)	0.24 (0.18, 0.32)	0.44 (0.25, 0.64)	60	0.27 (0.21, 0.35)	0.24 (0.18, 0.32)	0.44 (0.25, 0.64)
cortisone	54	0.18 (0.14, 0.22)	0.13 (0.10, 0.18)	0.36 (0.17, 0.61)	60	0.19 (0.15, 0.24)	0.15 (0.12, 0.20)	0.39 (0.20, 0.61)	60	0.19 (0.15, 0.24)	0.15 (0.12, 0.20)	0.39 (0.20, 0.61)
cotinine	6	0.14 (0.07, 0.27)	0.35 (0.27, 0.46)	0.87 (0.55, 0.97)	60	0.15 (0.12, 0.20)	0.75 (0.71, 0.79)	0.96 (0.94, 0.98)	57	0.07 (0.05, 0.09)	0.65 (0.63, 0.66)	0.99 (0.98, 0.99)
creatine	60	0.27 (0.21, 0.35)	0.47 (0.41, 0.55)	0.75 (0.63, 0.85)	60	0.27 (0.21, 0.35)	0.47 (0.41, 0.55)	0.75 (0.63, 0.85)	59	0.24 (0.18, 0.30)	0.46 (0.41, 0.53)	0.79 (0.69, 0.87)
creatinine	59	0.10 (0.08, 0.12)	0.21 (0.20, 0.23)	0.83 (0.74, 0.90)	60	0.12 (0.10, 0.14)	0.20 (0.18, 0.23)	0.75 (0.62, 0.84)	59	0.10 (0.08, 0.12)	0.21 (0.20, 0.23)	0.83 (0.74, 0.90)
cyclo(leu-pro)	20	0.42 (0.26, 0.66)	(., .)	0.00 (., .)	60	0.51 (0.36, 0.72)	0.18 (0.07, 0.47)	0.11 (0.01, 0.61)	58	0.37 (0.28, 0.50)	0.22 (0.14, 0.36)	0.26 (0.09, 0.55)
cysteine	60	0.22 (0.18, 0.28)	0.20 (0.15, 0.25)	0.44 (0.26, 0.64)	60	0.22 (0.18, 0.28)	0.20 (0.15, 0.25)	0.44 (0.26, 0.64)	60	0.22 (0.18, 0.28)	0.20 (0.15, 0.25)	0.44 (0.26, 0.64)
cysteine-glutathione disulfide	58	0.21 (0.16, 0.26)	0.43 (0.38, 0.48)	0.81 (0.71, 0.89)	60	0.22 (0.17, 0.28)	0.43 (0.38, 0.48)	0.79 (0.68, 0.87)	59	0.21 (0.16, 0.26)	0.44 (0.39, 0.49)	0.82 (0.72, 0.89)
decanoylearnitine	60	0.29 (0.22, 0.40)	0.66 (0.58, 0.75)	0.83 (0.74, 0.90)	60	0.29 (0.22, 0.40)	0.66 (0.58, 0.75)	0.83 (0.74, 0.90)	59	0.25 (0.19, 0.34)	0.65 (0.58, 0.73)	0.87 (0.79, 0.92)
dehydroisoandrosterone sulfate (DHEA-S)	60	0.20 (0.15, 0.28)	0.93 (0.87, 1.00)	0.96 (0.93, 0.97)	60	0.20 (0.15, 0.28)	0.93 (0.87, 1.00)	0.96 (0.93, 0.97)	58	0.15 (0.12, 0.20)	0.72 (0.68, 0.76)	0.96 (0.93, 0.97)
deoxycarnitine	59	0.09 (0.08, 0.11)	0.17 (0.15, 0.19)	0.77 (0.65, 0.86)	60	0.09 (0.08, 0.11)	0.17 (0.16, 0.19)	0.77 (0.65, 0.86)	60	0.09 (0.08, 0.11)	0.17 (0.16, 0.19)	0.77 (0.65, 0.86)
deoxycholate	17	1.27 (0.29, 5.54)	1.00 (0.15, 6.51)	0.38 (0.10, 0.78)	60	1.31 (0.59, 2.93)	1.02 (0.36, 2.87)	0.38 (0.19, 0.60)	59	0.76 (0.46, 1.24)	0.59 (0.31, 1.10)	0.38 (0.19, 0.60)
desmethylnaproxen sulfate*	4	0.54 (0.12, 2.40)	0.63 (0.18, 2.26)	0.58 (0.09, 0.95)	60	1.80 (0.52, 6.21)	2.66 (1.15, 6.15)	0.68 (0.54, 0.80)	57	1.03 (0.36, 2.92)	3.21 (2.30, 4.49)	0.91 (0.85, 0.94)
dihomo-linoleate (20:2n6)	60	0.30 (0.23, 0.38)	0.31 (0.24, 0.40)	0.52 (0.34, 0.69)	60	0.30 (0.23, 0.38)	0.31 (0.24, 0.40)	0.52 (0.34, 0.69)	60	0.30 (0.23, 0.38)	0.31 (0.24, 0.40)	0.52 (0.34, 0.69)
dihomo-linolenate (20:3n3 or n6)	60	0.16 (0.13, 0.20)	0.23 (0.20, 0.26)	0.67 (0.51, 0.79)	60	0.16 (0.13, 0.20)	0.23 (0.20, 0.26)	0.67 (0.51, 0.79)	60	0.16 (0.13, 0.20)	0.23 (0.20, 0.26)	0.67 (0.51, 0.79)
dimethylarginine (SDMA + ADMA)	60	0.18 (0.15, 0.22)	0.13 (0.10, 0.17)	0.34 (0.16, 0.58)	60	0.18 (0.15, 0.22)	0.13 (0.10, 0.17)	0.34 (0.16, 0.58)	59	0.16 (0.13, 0.20)	0.12 (0.09, 0.16)	0.35 (0.17, 0.59)
dimethylglycine	52	0.24 (0.19, 0.32)	0.31 (0.26, 0.38)	0.62 (0.45, 0.77)	60	0.29 (0.22, 0.37)	0.32 (0.25, 0.40)	0.55 (0.38, 0.72)	59	0.27 (0.21, 0.35)	0.34 (0.28, 0.42)	0.62 (0.45, 0.76)
docosahexaenoate (DHA; 22:6n3)	60	0.20 (0.16, 0.25)	0.41 (0.37, 0.46)	0.81 (0.71, 0.88)	60	0.20 (0.16, 0.25)	0.41 (0.37, 0.46)	0.81 (0.71, 0.88)	60	0.20 (0.16, 0.25)	0.41 (0.37, 0.46)	0.81 (0.71, 0.88)
docosapentaenoate (n3 DPA; 22:5n3)	60	0.30 (0.23, 0.39)	0.41 (0.34, 0.50)	0.66 (0.50, 0.78)	60	0.30 (0.23, 0.39)	0.41 (0.34, 0.50)	0.66 (0.50, 0.78)	59	0.27 (0.21, 0.35)	0.39 (0.33, 0.47)	0.67 (0.52, 0.80)
docosapentaenoate (n6 DPA; 22												

epiandrosterone sulfate	56	0.36 (0.27, 0.49)	0.47 (0.37, 0.59)	0.63 (0.46, 0.77)	60	0.37 (0.27, 0.50)	0.51 (0.41, 0.64)	0.66 (0.50, 0.78)	59	0.24 (0.18, 0.31)	0.56 (0.50, 0.63)	0.84 (0.76, 0.90)
erythritol	60	0.15 (0.13, 0.19)	0.30 (0.27, 0.33)	0.79 (0.68, 0.87)	60	0.15 (0.13, 0.19)	0.30 (0.27, 0.33)	0.79 (0.68, 0.87)	59	0.14 (0.11, 0.18)	0.30 (0.27, 0.33)	0.81 (0.71, 0.89)
erythronate*	60	0.14 (0.12, 0.17)	0.28 (0.26, 0.31)	0.80 (0.69, 0.88)	60	0.14 (0.12, 0.17)	0.28 (0.26, 0.31)	0.80 (0.69, 0.88)	60	0.14 (0.12, 0.17)	0.28 (0.26, 0.31)	0.80 (0.69, 0.88)
erythrose	56	0.36 (0.27, 0.48)	0.06 (0.01, 0.32)	0.03 (0.00, 1.00)	60	0.41 (0.30, 0.54)	0.10 (0.03, 0.33)	0.06 (0.00, 0.84)	60	0.41 (0.30, 0.54)	0.10 (0.03, 0.33)	0.06 (0.00, 0.84)
fructose	60	0.55 (0.38, 0.79)	0.22 (0.09, 0.54)	0.14 (0.02, 0.56)	60	0.55 (0.38, 0.79)	0.22 (0.09, 0.54)	0.14 (0.02, 0.56)	58	0.41 (0.30, 0.55)	0.30 (0.20, 0.46)	0.36 (0.18, 0.60)
gamma-CEHC	48	0.33 (0.24, 0.44)	0.29 (0.21, 0.41)	0.44 (0.23, 0.66)	60	0.35 (0.26, 0.46)	0.41 (0.32, 0.52)	0.58 (0.41, 0.73)	60	0.35 (0.26, 0.46)	0.41 (0.32, 0.52)	0.58 (0.41, 0.73)
gamma-glutamylalanine	60	0.29 (0.23, 0.38)	0.31 (0.24, 0.39)	0.53 (0.35, 0.70)	60	0.29 (0.23, 0.38)	0.31 (0.24, 0.39)	0.53 (0.35, 0.70)	60	0.29 (0.23, 0.38)	0.31 (0.24, 0.39)	0.53 (0.35, 0.70)
gamma-glutamylglutamate	14	0.26 (0.16, 0.42)	0.04 (0.00, 0.78)	0.03 (0.00, 1.00)	60	0.39 (0.31, 0.51)	(..)	0.00 (..)	60	0.39 (0.31, 0.51)	(..)	0.00 (..)
gamma-glutamylglutamine	60	0.14 (0.12, 0.17)	0.17 (0.14, 0.20)	0.59 (0.42, 0.74)	60	0.14 (0.12, 0.17)	0.17 (0.14, 0.20)	0.59 (0.42, 0.74)	59	0.13 (0.11, 0.16)	0.18 (0.15, 0.21)	0.64 (0.49, 0.78)
gamma-glutamylisoleucine*	55	0.22 (0.17, 0.28)	0.23 (0.18, 0.29)	0.52 (0.34, 0.70)	60	0.22 (0.17, 0.27)	0.26 (0.22, 0.32)	0.59 (0.42, 0.74)	60	0.22 (0.17, 0.27)	0.26 (0.22, 0.32)	0.59 (0.42, 0.74)
gamma-glutamylleucine	60	0.14 (0.12, 0.18)	0.23 (0.20, 0.26)	0.72 (0.59, 0.83)	60	0.14 (0.12, 0.18)	0.23 (0.20, 0.26)	0.72 (0.59, 0.83)	59	0.13 (0.10, 0.16)	0.21 (0.18, 0.23)	0.72 (0.58, 0.83)
gamma-glutamylmethionine	51	0.27 (0.21, 0.35)	0.11 (0.05, 0.21)	0.13 (0.01, 0.62)	60	0.32 (0.25, 0.41)	0.18 (0.11, 0.28)	0.24 (0.08, 0.54)	59	0.30 (0.24, 0.39)	0.18 (0.12, 0.28)	0.27 (0.10, 0.55)
gamma-glutamylphenylalanine	60	0.25 (0.20, 0.32)	0.07 (0.03, 0.16)	0.07 (0.00, 0.81)	60	0.25 (0.20, 0.32)	0.07 (0.03, 0.16)	0.07 (0.00, 0.81)	60	0.25 (0.20, 0.32)	0.07 (0.03, 0.16)	0.07 (0.00, 0.81)
gamma-glutamylthreonine*	51	0.30 (0.23, 0.39)	0.23 (0.17, 0.33)	0.39 (0.19, 0.63)	60	0.31 (0.24, 0.40)	0.27 (0.20, 0.36)	0.42 (0.24, 0.63)	60	0.31 (0.24, 0.40)	0.27 (0.20, 0.36)	0.42 (0.24, 0.63)
gamma-glutamyltyrosine	59	0.17 (0.14, 0.21)	0.18 (0.15, 0.22)	0.52 (0.34, 0.70)	60	0.18 (0.14, 0.22)	0.19 (0.16, 0.23)	0.54 (0.36, 0.71)	60	0.18 (0.14, 0.22)	0.19 (0.16, 0.23)	0.54 (0.36, 0.71)
gamma-glutamylvaline	60	0.19 (0.15, 0.23)	0.18 (0.15, 0.23)	0.48 (0.30, 0.67)	60	0.19 (0.15, 0.23)	0.18 (0.15, 0.23)	0.48 (0.30, 0.67)	60	0.19 (0.15, 0.23)	0.18 (0.15, 0.23)	0.48 (0.30, 0.67)
gamma-tocopherol	39	0.35 (0.24, 0.49)	0.34 (0.24, 0.48)	0.49 (0.27, 0.71)	60	0.48 (0.34, 0.69)	0.48 (0.34, 0.69)	0.50 (0.32, 0.68)	59	0.47 (0.33, 0.67)	0.54 (0.40, 0.73)	0.57 (0.39, 0.73)
gluconate	59	0.27 (0.21, 0.35)	0.15 (0.09, 0.23)	0.23 (0.07, 0.54)	60	0.27 (0.22, 0.35)	0.16 (0.11, 0.24)	0.26 (0.09, 0.54)	60	0.27 (0.22, 0.35)	0.16 (0.11, 0.24)	0.26 (0.09, 0.54)
glucose	60	0.10 (0.08, 0.12)	0.12 (0.11, 0.15)	0.61 (0.45, 0.75)	60	0.10 (0.08, 0.12)	0.12 (0.11, 0.15)	0.61 (0.45, 0.75)	60	0.10 (0.08, 0.12)	0.12 (0.11, 0.15)	0.61 (0.45, 0.75)
glutamate	60	0.27 (0.21, 0.35)	0.23 (0.18, 0.31)	0.42 (0.24, 0.63)	60	0.27 (0.21, 0.35)	0.23 (0.18, 0.31)	0.42 (0.24, 0.63)	58	0.21 (0.17, 0.26)	0.18 (0.14, 0.23)	0.44 (0.25, 0.64)
glutamine	60	0.09 (0.07, 0.11)	0.10 (0.08, 0.12)	0.54 (0.36, 0.71)	60	0.09 (0.07, 0.11)	0.10 (0.08, 0.12)	0.54 (0.36, 0.71)	60	0.09 (0.07, 0.11)	0.10 (0.08, 0.12)	0.54 (0.36, 0.71)
glutaroyl carnitine	60	0.16 (0.13, 0.20)	0.22 (0.19, 0.26)	0.66 (0.51, 0.79)	60	0.16 (0.13, 0.20)	0.22 (0.19, 0.26)	0.66 (0.51, 0.79)	59	0.15 (0.12, 0.18)	0.24 (0.21, 0.27)	0.72 (0.58, 0.82)
glycerate	60	0.29 (0.23, 0.38)	0.20 (0.14, 0.29)	0.32 (0.14, 0.57)	60	0.29 (0.23, 0.38)	0.20 (0.14, 0.29)	0.32 (0.14, 0.57)	59	0.19 (0.16, 0.24)	0.18 (0.14, 0.23)	0.46 (0.28, 0.66)
glycerol	60	0.28 (0.22, 0.37)	0.37 (0.30, 0.45)	0.63 (0.47, 0.77)	60	0.28 (0.22, 0.37)	0.37 (0.30, 0.45)	0.63 (0.47, 0.77)	59	0.22 (0.17, 0.28)	0.36 (0.31, 0.41)	0.72 (0.59, 0.83)
glycerol 3-phosphate (G3P)	59	-8.21 (-892, -0.08)	(..)	0.00 (..)	60	-8.10 (-794, -0.08)	(..)	0.00 (..)	59	1.13 (0.57, 0.24)	0.57 (0.15, 0.21)	0.20 (0.05, 0.54)
glycerophosphorylcholine (GPC)	60	0.28 (0.22, 0.36)	0.25 (0.18, 0.33)	0.43 (0.24, 0.64)	60	0.28 (0.22, 0.36)	0.25 (0.18, 0.33)	0.43 (0.24, 0.64)	58	0.22 (0.17, 0.27)	0.25 (0.20, 0.30)	0.57 (0.39, 0.73)
glycine	60	0.16 (0.13, 0.19)	0.22 (0.19, 0.26)	0.66 (0.51, 0.79)	60	0.16 (0.13, 0.19)	0.22 (0.19, 0.26)	0.66 (0.51, 0.79)	59	0.14 (0.11, 0.17)	0.22 (0.19, 0.25)	0.72 (0.58, 0.82)
glycochenodeoxycholate	59	0.94 (0.50, 1.78)	1.09 (0.63, 1.89)	0.57 (0.40, 0.73)	60	0.97 (0.51, 1.85)	1.12 (0.64, 1.96)	0.57 (0.40, 0.73)	58	0.83 (0.45, 1.52)	1.26 (0.85, 1.87)	0.70 (0.55, 0.81)
glycocholate	47	1.11 (0.48, 2.54)	1.34 (0.67, 2.66)	0.59 (0.40, 0.76)	60	1.22 (0.54, 2.73)	1.50 (0.78, 2.89)	0.60 (0.44, 0.75)	58	0.79 (0.43, 1.45)	1.36 (0.95, 1.93)	0.75 (0.62, 0.84)
glycochenolate sulfate*	59	0.25 (0.20, 0.32)	0.41 (0.35, 0.48)	0.72 (0.59, 0.83)	60	0.26 (0.20, 0.33)	0.40 (0.34, 0.47)	0.71 (0.57, 0.82)	60	0.26 (0.20, 0.33)	0.40 (0.34, 0.47)	0.71 (0.57, 0.82)
glycodeoxycholate	27	0.72 (0.27, 1.91)	1.88 (1.29, 2.73)	0.87 (0.75, 0.94)	60	0.87 (0.41, 1.85)	2.13 (1.56, 2.90)	0.86 (0.77, 0.91)	58	0.69 (0.33, 1.45)	2.32 (1.86, 2.90)	0.92 (0.87, 0.95)
glycolate (hydroxyacetate)	53	0.28 (0.22, 0.36)	0.15 (0.10, 0.25)	0.23 (0.07, 0.56)	60	0.31 (0.24, 0.40)	0.17 (0.11, 0.27)	0.24 (0.08, 0.54)	60	0.31 (0.24, 0.40)	0.17 (0.11, 0.27)	0.24 (0.08, 0.54)
glycolithocholate sulfate*	58	0.57 (0.37, 0.88)	0.79 (0.58, 1.08)	0.66 (0.50, 0.79)	60	0.57 (0.38, 0.87)	0.78 (0.58, 1.06)	0.65 (0.50, 0.78)	60	0.57 (0.38, 0.87)	0.78 (0.58, 1.06)	0.65 (0.50, 0.78)
glycylphenylalanine	19	0.22 (0.15, 0.32)	0.12 (0.06, 0.24)	0.23 (0.03, 0.77)	60	0.22 (0.18, 0.28)	0.29 (0.24, 0.34)	0.63 (0.47, 0.77)	58	0.19 (0.15, 0.24)	0.28 (0.25, 0.33)	0.70 (0.55, 0.81)
guanosine	58	0.18 (0.15, 0.23)	0.31 (0.28, 0.36)	0.75 (0.62, 0.84)	60	0.19 (0.15, 0.23)	0.33 (0.29, 0.37)	0.76 (0.63, 0.85)	59	0.18 (0.14, 0.22)	0.34 (0.30, 0.38)	0.79 (0.68, 0.87)
heme*	60	0.71 (0.45, 1.10)	0.22 (0.05, 0.91)	0.09 (0.00, 0.70)	60	0.71 (0.45, 1.10)	0.22 (0.05, 0.91)	0.09 (0.00, 0.70)	58	0.43 (0.31, 0.58)	0.24 (0.14, 0.42)	0.24 (0.08, 0.54)
heptanoate (7:0)	60	0.19 (0.16, 0.24)	0.17 (0.13, 0.21)	0.43 (0.24, 0.63)	60	0.19 (0.16, 0.24)	0.17 (0.13, 0.21)	0.43 (0.24, 0.63)	60	0.19 (0.16, 0.24)	0.17 (0.13, 0.21)	0.43 (0.24, 0.63)
hexadecanedioate	57	0.29 (0.22, 0.37)	0.33 (0.26, 0.42)	0.57 (0.40, 0.73)	60	0.30 (0.23, 0.38)	0.35 (0.28, 0.44)	0.58 (0.41, 0.74)	59	0.29 (0.22, 0.37)	0.35 (0.28, 0.43)	0.60 (0.43, 0.75)
hexanoylcarnitine	60	0.26 (0.20, 0.35)	0.68 (0.61, 0.76)	0.87 (0.80, 0.92)	60	0.26 (0.20, 0.35)	0.68 (0.61, 0.76)	0.87 (0.80, 0.92)	59	0.23 (0.17, 0.31)	0.71 (0.65, 0.78)	0.90 (0.84, 0.94)
hippurate	60	0.98 (0.54, 1.78)	0.57 (0.20, 1.60)	0.25 (0.09, 0.54)	60	0.98 (0.54, 1.78)	0.57 (0.20, 1.60)	0.25 (0.09, 0.54)	58	0.72 (0.45, 1.17)	0.59 (0.33, 1.06)	0.40 (0.22, 0.62)
histidine	60	0.11 (0.09, 0.13)	0.10 (0.09, 0.13)	0.48 (0.30, 0.67)	60	0.11 (0.09, 0.13)	0.10 (0.09, 0.13)	0.48 (0.30, 0.67)	60	0.11 (0.09, 0.13)	0.10 (0.09, 0.13)	0.48 (0.30, 0.67)
homocitrulline	56	0.35 (0.26, 0.47)	0.35 (0.26, 0.47)	0.50 (0.31, 0.69)	60	0.36 (0.27, 0.48)	0.38 (0.29, 0.50)	0.53 (0.36, 0.70)	59	0.32 (0.25, 0.42)	0.36 (0.28, 0.46)	0.55 (0.37, 0.71)
homostachydrine*	58	0.31 (0.23, 0.40)	0.45 (0.37, 0.54)	0.68 (0.53, 0.80)	60	0.32 (0.24, 0.43)	0.46 (0.38, 0.56)	0.68 (0.53, 0.80)	59	0.31 (0.23, 0.41)	0.49 (0.41, 0.58)	0.71 (0.57, 0.82)
HWEASXX*	40	0.72 (0.40, 1.28)	0.60 (0.30, 1.20)	0.41 (0.20, 0.67)	60	0.81 (0.48, 1.37)	0.76 (0.43, 1.33)	0.47 (0.28, 0.66)	58	0.65 (0.41, 1.04)	0.84 (0.58, 1.20)	0.63 (0.46, 0.77)
hyodeoxycholate	22	1.03 (0.37, 2.88)	0.54 (0.08, 3.84)	0.22 (0.03, 0.74)	60	1.64 (0.61, 4.41)	1.18 (0.30, 4.67)	0.34 (0.16, 0.58)	59	0.91 (0.50, 1.66)	0.96 (0.54, 1.70)	0.53 (0.35, 0.70)
hypoxanthine	42	0.30 (0.22, 0.40)	0.23 (0.15, 0.34)	0.36 (0.16, 0.64)	60	0.34 (0.26, 0.44)	0.24 (0.16, 0.35)	0.33 (0.15, 0.58)	59	0.31 (0.24, 0.41)	0.26 (0.19, 0.36)	0.42 (0.23, 0.63)
ibuprofen	15	-3.18 (-137, -0.07)	-2.02 (-753, -0.01)	0.29 (0.04, 0.80)	60	-6.92 (-421, -0.11)	-4.86 (-1691, -0.01)	0.33 (0.15, 0.58)	59	14.74 (0.00, 87E4	27.68 (0.08, 9619)	0.78 (0.66, 0.86)
indoleacetate	60	0.20 (0.16, 0.26)	0.61 (0.56, 0.66)	0.90 (0.84, 0.94)	60	0.20 (0.16, 0.26)	0.61 (0.56, 0.66)	0.90 (0.84, 0.94)	59	0.17 (0.13, 0.22)	0.55 (0.51, 0.59)	0.91 (0.86, 0.95)
indolelactate	53	0.26 (0.20, 0.34)	0.28 (0.22, 0.36)	0.53 (0.34, 0.71)	60	0.28 (0.22, 0.36)	0.34 (0.27, 0.42)	0.59 (0.43, 0.74)	60	0.28 (0.22, 0.36)	0.34 (0.27, 0.42)	0.59 (0.43, 0.74)
indolepropionate	54	0.42 (0.30, 0.60)	0.58 (0.45, 0.75)	0.65 (0.48, 0.78)	60	0.43 (0.31, 0.61)	0.64 (0.50, 0.81)	0.68 (0.54, 0.80)	58	0.31 (0.24, 0.42)	0.50 (0.42, 0.60)	0.72 (0.58, 0.83)
inosine	59	0.24 (0.19, 0.32)	0.51 (0.45, 0.58)	0.81 (0.71, 0.88)	60	0.24 (0.19, 0.32)	0.52 (0.46, 0.58)	0.82 (0.72, 0.89)	60	0.24 (0.19, 0.32)	0.52 (0.46, 0.58)	0.82 (0.72, 0.89)
inositol 1-phosphate (I1P)	48	0.35 (0.26, 0.47)	0.23 (0.15, 0.37)	0								

kynurenine	60	0.15 (0.13, 0.19)	0.16 (0.14, 0.20)	0.53 (0.36, 0.70)	60	0.15 (0.13, 0.19)	0.16 (0.14, 0.20)	0.53 (0.36, 0.70)	59	0.10 (0.08, 0.12)	0.18 (0.16, 0.20)	0.78 (0.67, 0.86)
lactate	60	0.14 (0.12, 0.18)	0.15 (0.13, 0.19)	0.53 (0.36, 0.70)	60	0.14 (0.12, 0.18)	0.15 (0.13, 0.19)	0.53 (0.36, 0.70)	59	0.13 (0.11, 0.16)	0.16 (0.13, 0.19)	0.60 (0.43, 0.75)
lathosterol	6	0.21 (0.10, 0.43)	0.24 (0.13, 0.45)	0.57 (0.12, 0.92)	60	0.57 (0.38, 0.85)	0.57 (0.38, 0.85)	0.50 (0.32, 0.68)	59	0.57 (0.38, 0.85)	0.64 (0.44, 0.92)	0.56 (0.38, 0.72)
laurate (12:0)	60	0.14 (0.12, 0.17)	0.09 (0.06, 0.12)	0.27 (0.10, 0.55)	60	0.14 (0.12, 0.17)	0.09 (0.06, 0.12)	0.27 (0.10, 0.55)	60	0.14 (0.12, 0.17)	0.09 (0.06, 0.12)	0.27 (0.10, 0.55)
laurylcarnitine	60	0.34 (0.26, 0.45)	0.37 (0.29, 0.48)	0.54 (0.37, 0.71)	60	0.34 (0.26, 0.45)	0.37 (0.29, 0.48)	0.54 (0.37, 0.71)	59	0.26 (0.21, 0.34)	0.37 (0.31, 0.45)	0.67 (0.51, 0.79)
leucine	60	0.09 (0.07, 0.10)	0.13 (0.11, 0.14)	0.68 (0.53, 0.80)	60	0.09 (0.07, 0.10)	0.13 (0.11, 0.14)	0.68 (0.53, 0.80)	59	0.08 (0.06, 0.09)	0.12 (0.11, 0.14)	0.73 (0.59, 0.83)
leucylleucine	15	0.30 (0.18, 0.51)	0.42 (0.29, 0.62)	0.66 (0.36, 0.88)	60	0.65 (0.43, 0.99)	0.42 (0.22, 0.81)	0.29 (0.12, 0.56)	60	0.65 (0.43, 0.99)	0.42 (0.22, 0.81)	0.29 (0.12, 0.56)
linoleate (18:2n6)	60	0.22 (0.17, 0.27)	0.18 (0.14, 0.24)	0.42 (0.23, 0.63)	60	0.22 (0.17, 0.27)	0.18 (0.14, 0.24)	0.42 (0.23, 0.63)	59	0.20 (0.16, 0.25)	0.18 (0.15, 0.23)	0.47 (0.28, 0.66)
linolenate [alpha or gamma; (18:3n3 or 6)]	60	0.39 (0.29, 0.53)	0.34 (0.24, 0.47)	0.42 (0.24, 0.63)	60	0.39 (0.29, 0.53)	0.34 (0.24, 0.47)	0.42 (0.24, 0.63)	59	0.30 (0.23, 0.39)	0.30 (0.23, 0.38)	0.49 (0.31, 0.68)
lysine	60	0.22 (0.18, 0.27)	0.12 (0.08, 0.18)	0.23 (0.07, 0.54)	60	0.22 (0.18, 0.27)	0.12 (0.08, 0.18)	0.23 (0.07, 0.54)	60	0.22 (0.18, 0.27)	0.12 (0.08, 0.18)	0.23 (0.07, 0.54)
malate	53	0.31 (0.23, 0.40)	0.19 (0.12, 0.29)	0.27 (0.09, 0.57)	60	0.32 (0.25, 0.42)	0.22 (0.15, 0.32)	0.31 (0.13, 0.57)	59	0.24 (0.19, 0.31)	0.18 (0.13, 0.25)	0.36 (0.18, 0.60)
mannitol	47	13.84 (0.00, 181E)	11.85 (0.00, 765E)	0.42 (0.22, 0.66)	60	13.66 (0.00, 5697E)	12.34 (0.00, 125E)	0.45 (0.27, 0.65)	57	1.92 (0.53, 6.90)	2.33 (0.81, 6.68)	0.60 (0.42, 0.75)
mannose	60	0.16 (0.13, 0.20)	0.21 (0.18, 0.24)	0.63 (0.47, 0.76)	60	0.16 (0.13, 0.20)	0.21 (0.18, 0.24)	0.63 (0.47, 0.76)	59	0.15 (0.12, 0.18)	0.21 (0.18, 0.24)	0.68 (0.53, 0.80)
margarate (17:0)	60	0.28 (0.22, 0.37)	0.30 (0.24, 0.39)	0.53 (0.36, 0.70)	60	0.28 (0.22, 0.37)	0.30 (0.24, 0.39)	0.53 (0.36, 0.70)	60	0.28 (0.22, 0.37)	0.30 (0.24, 0.39)	0.53 (0.36, 0.70)
methionine	60	0.10 (0.09, 0.13)	0.12 (0.10, 0.14)	0.57 (0.39, 0.72)	60	0.10 (0.09, 0.13)	0.12 (0.10, 0.14)	0.57 (0.39, 0.72)	60	0.10 (0.09, 0.13)	0.12 (0.10, 0.14)	0.57 (0.39, 0.72)
methyl palmitate	36	2.48 (0.39, 15.83)	0.91 (0.01, 141.2)	0.12 (0.01, 0.74)	60	2.14 (0.62, 7.40)	0.92 (0.05, 16.43)	0.16 (0.03, 0.55)	59	0.43 (0.31, 0.58)	0.33 (0.22, 0.50)	0.38 (0.20, 0.61)
methylglutaryl carnitine	37	0.25 (0.17, 0.37)	0.71 (0.63, 0.81)	0.89 (0.80, 0.94)	60	0.27 (0.20, 0.37)	0.84 (0.76, 0.93)	0.91 (0.85, 0.94)	58	0.21 (0.16, 0.29)	0.81 (0.75, 0.88)	0.94 (0.90, 0.96)
metoprolol	4	0.73 (0.07, 8.06)	1.69 (0.60, 4.76)	0.84 (0.39, 0.98)	60	0.57 (0.36, 0.90)	1.06 (0.83, 1.36)	0.78 (0.66, 0.86)	58	0.23 (0.17, 0.32)	0.79 (0.72, 0.87)	0.92 (0.87, 0.95)
metoprolol acid metabolite*	17	1.48 (0.29, 7.64)	0.72 (0.03, 20.74)	0.19 (0.01, 0.82)	60	2.96 (0.52, 16.80)	1.62 (0.07, 38.62)	0.23 (0.07, 0.54)	59	-5.65 (-158, -0.20)	-3.23 (-1092, -0.01)	0.25 (0.08, 0.54)
myo-inositol	60	0.18 (0.15, 0.23)	0.19 (0.15, 0.23)	0.52 (0.34, 0.69)	60	0.18 (0.15, 0.23)	0.19 (0.15, 0.23)	0.52 (0.34, 0.69)	59	0.17 (0.14, 0.21)	0.20 (0.17, 0.24)	0.59 (0.42, 0.74)
myristate (14:0)	60	0.19 (0.15, 0.24)	0.15 (0.12, 0.20)	0.39 (0.21, 0.61)	60	0.19 (0.15, 0.24)	0.15 (0.12, 0.20)	0.39 (0.21, 0.61)	60	0.19 (0.15, 0.24)	0.15 (0.12, 0.20)	0.39 (0.21, 0.61)
myristoleate (14:1n5)	60	0.33 (0.25, 0.44)	0.33 (0.25, 0.43)	0.50 (0.31, 0.68)	60	0.33 (0.25, 0.44)	0.33 (0.25, 0.43)	0.50 (0.31, 0.68)	58	0.27 (0.21, 0.34)	0.32 (0.26, 0.39)	0.59 (0.42, 0.74)
N-(2-furoyl)glycine	1	(., .)	(., .)	(., .)	60	0.03 (0.02, 0.03)	0.00 (0.00, .)	0.00 (0.00, .)	59	(., .)	(., .)	(., .)
N1-methyadenosine	60	0.21 (0.17, 0.27)	0.16 (0.12, 0.22)	0.37 (0.18, 0.60)	60	0.21 (0.17, 0.27)	0.16 (0.12, 0.22)	0.37 (0.18, 0.60)	59	0.20 (0.16, 0.25)	0.18 (0.14, 0.23)	0.44 (0.25, 0.64)
N2,N2-dimethylguanosine	16	0.18 (0.12, 0.27)	0.09 (0.04, 0.20)	0.19 (0.01, 0.83)	60	0.22 (0.18, 0.28)	0.13 (0.09, 0.19)	0.25 (0.09, 0.54)	60	0.22 (0.18, 0.28)	0.13 (0.09, 0.19)	0.25 (0.09, 0.54)
N6-acetyllysine	60	0.19 (0.15, 0.23)	0.22 (0.18, 0.26)	0.57 (0.40, 0.73)	60	0.19 (0.15, 0.23)	0.22 (0.18, 0.26)	0.57 (0.40, 0.73)	60	0.19 (0.15, 0.23)	0.22 (0.18, 0.26)	0.57 (0.40, 0.73)
N6-carbamoylthreonyladenosine	23	0.14 (0.10, 0.19)	0.07 (0.04, 0.14)	0.22 (0.03, 0.73)	60	0.18 (0.14, 0.22)	0.12 (0.08, 0.16)	0.30 (0.13, 0.56)	58	0.14 (0.11, 0.17)	0.12 (0.09, 0.15)	0.41 (0.22, 0.63)
N-acetylalanine	60	0.10 (0.09, 0.13)	0.18 (0.16, 0.20)	0.75 (0.63, 0.85)	60	0.10 (0.09, 0.13)	0.18 (0.16, 0.20)	0.75 (0.63, 0.85)	60	0.10 (0.09, 0.13)	0.18 (0.16, 0.20)	0.75 (0.63, 0.85)
N-acetyl-beta-alanine	60	0.35 (0.27, 0.47)	0.26 (0.18, 0.38)	0.35 (0.16, 0.59)	60	0.35 (0.27, 0.47)	0.26 (0.18, 0.38)	0.35 (0.16, 0.59)	59	0.33 (0.25, 0.43)	0.27 (0.20, 0.38)	0.41 (0.22, 0.62)
N-acetyl glycine	44	0.58 (0.36, 0.92)	0.58 (0.37, 0.93)	0.50 (0.30, 0.71)	60	0.58 (0.39, 0.86)	0.61 (0.42, 0.89)	0.53 (0.35, 0.70)	59	0.47 (0.33, 0.67)	0.59 (0.45, 0.78)	0.62 (0.45, 0.76)
N-acetylornithine	60	0.31 (0.24, 0.42)	0.50 (0.42, 0.60)	0.72 (0.58, 0.82)	60	0.31 (0.24, 0.42)	0.50 (0.42, 0.60)	0.72 (0.58, 0.82)	59	0.28 (0.22, 0.37)	0.45 (0.38, 0.54)	0.72 (0.58, 0.83)
N-acetylserine	49	0.22 (0.17, 0.28)	0.20 (0.15, 0.26)	0.46 (0.26, 0.68)	60	0.28 (0.22, 0.35)	0.24 (0.18, 0.32)	0.42 (0.24, 0.63)	59	0.26 (0.20, 0.33)	0.26 (0.21, 0.33)	0.51 (0.33, 0.69)
N-acetylthreonine	49	0.18 (0.14, 0.22)	0.17 (0.13, 0.21)	0.47 (0.27, 0.68)	60	0.20 (0.16, 0.25)	0.24 (0.19, 0.29)	0.57 (0.40, 0.73)	60	0.20 (0.16, 0.25)	0.24 (0.19, 0.29)	0.57 (0.40, 0.73)
naproxen	4	0.61 (0.11, 3.36)	0.84 (0.24, 2.89)	0.66 (0.14, 0.96)	60	1.69 (0.51, 5.68)	2.83 (1.37, 5.83)	0.74 (0.61, 0.84)	57	0.96 (0.38, 2.45)	2.79 (2.03, 3.85)	0.89 (0.83, 0.94)
N-methyl proline	47	0.63 (0.36, 1.12)	1.22 (0.91, 1.64)	0.79 (0.66, 0.88)	60	0.65 (0.39, 1.09)	1.26 (0.96, 1.64)	0.79 (0.68, 0.87)	59	0.65 (0.38, 1.12)	1.40 (1.09, 1.80)	0.82 (0.73, 0.89)
nonadecanoate (19:0)	60	0.26 (0.20, 0.33)	0.23 (0.18, 0.30)	0.44 (0.26, 0.65)	60	0.26 (0.20, 0.33)	0.23 (0.18, 0.30)	0.44 (0.26, 0.65)	60	0.26 (0.20, 0.33)	0.23 (0.18, 0.30)	0.44 (0.26, 0.65)
octadecanedioate	51	0.32 (0.24, 0.43)	0.28 (0.20, 0.39)	0.44 (0.24, 0.66)	60	0.39 (0.29, 0.53)	0.30 (0.20, 0.44)	0.37 (0.19, 0.60)	60	0.39 (0.29, 0.53)	0.30 (0.20, 0.44)	0.37 (0.19, 0.60)
octanoylcarnitine	60	0.38 (0.26, 0.53)	0.85 (0.73, 1.00)	0.84 (0.75, 0.90)	60	0.38 (0.26, 0.53)	0.85 (0.73, 1.00)	0.84 (0.75, 0.90)	59	0.25 (0.18, 0.35)	0.90 (0.82, 0.99)	0.93 (0.88, 0.96)
oleate (18:1n9)	60	0.31 (0.24, 0.40)	0.23 (0.16, 0.32)	0.35 (0.17, 0.59)	60	0.31 (0.24, 0.40)	0.23 (0.16, 0.32)	0.35 (0.17, 0.59)	60	0.31 (0.24, 0.40)	0.23 (0.16, 0.32)	0.35 (0.17, 0.59)
oleoylcarnitine	60	0.27 (0.21, 0.35)	0.29 (0.23, 0.37)	0.54 (0.36, 0.70)	60	0.27 (0.21, 0.35)	0.29 (0.23, 0.37)	0.54 (0.36, 0.70)	60	0.27 (0.21, 0.35)	0.29 (0.23, 0.37)	0.54 (0.36, 0.70)
ornithine	57	0.30 (0.23, 0.39)	0.25 (0.19, 0.35)	0.42 (0.23, 0.63)	60	0.33 (0.25, 0.43)	0.27 (0.19, 0.37)	0.40 (0.22, 0.62)	59	0.29 (0.23, 0.38)	0.27 (0.21, 0.36)	0.46 (0.28, 0.66)
p-acetamidophenylglucuronide	7	8.83 (0.00, 21E6)	1.66 (0.00, 13E33)	0.03 (0.00, 1.00)	60	909.2 (0.00, 5E235)	592.2 (0.00, .)	0.30 (0.12, 0.56)	59	1.79 (0.45, 7.05)	3.52 (1.75, 7.07)	0.79 (0.69, 0.87)
palmitate (16:0)	60	0.18 (0.14, 0.22)	0.15 (0.12, 0.19)	0.41 (0.23, 0.62)	60	0.18 (0.14, 0.22)	0.15 (0.12, 0.19)	0.41 (0.23, 0.62)	60	0.18 (0.14, 0.22)	0.15 (0.12, 0.19)	0.41 (0.23, 0.62)
palmitoleate (16:1n7)	60	0.31 (0.24, 0.41)	0.34 (0.27, 0.43)	0.54 (0.37, 0.71)	60	0.31 (0.24, 0.41)	0.34 (0.27, 0.43)	0.54 (0.37, 0.71)	59	0.27 (0.21, 0.35)	0.33 (0.27, 0.41)	0.60 (0.44, 0.75)
palmitoyl sphingomyelin	60	0.12 (0.10, 0.15)	0.25 (0.23, 0.28)	0.82 (0.72, 0.89)	60	0.12 (0.10, 0.15)	0.25 (0.23, 0.28)	0.82 (0.72, 0.89)	59	0.11 (0.09, 0.13)	0.23 (0.21, 0.26)	0.83 (0.73, 0.89)
palmitoylcarnitine	60	0.27 (0.21, 0.34)	0.10 (0.05, 0.19)	0.11 (0.01, 0.61)	60	0.27 (0.21, 0.34)	0.10 (0.05, 0.19)	0.11 (0.01, 0.61)	59	0.26 (0.20, 0.33)	0.11 (0.06, 0.19)	0.15 (0.03, 0.55)
pantothenate	50	0.24 (0.18, 0.31)	0.48 (0.42, 0.55)	0.80 (0.69, 0.88)	60	0.26 (0.20, 0.34)	0.59 (0.53, 0.67)	0.84 (0.75, 0.90)	59	0.23 (0.18, 0.30)	0.54 (0.49, 0.61)	0.85 (0.76, 0.91)
paraxanthine	45	0.54 (0.35, 0.84)	0.54 (0.35, 0.84)	0.50 (0.29, 0.70)	60	0.63 (0.41, 0.98)	0.76 (0.53, 1.10)	0.59 (0.42, 0.74)	58	0.55 (0.37, 0.83)	0.69 (0.50, 0.95)	0.61 (0.44, 0.76)
p-cresol sulfate	60	0.34 (0.26, 0.45)	0.36 (0.28, 0.47)	0.53 (0.35, 0.70)	60	0.34 (0.26, 0.45)	0.36 (0.28, 0.47)	0.53 (0.35, 0.70)	57	0.20 (0.16, 0.26)	0.42 (0.38, 0.47)	0.81 (0.71, 0.89)
pelargonate (9:0)	60	0.21 (0.17, 0.26)	0.18 (0.14, 0.23)	0.42 (0.23, 0.63)	60	0.21 (0.17, 0.26)	0.18 (0.14, 0.23)	0.42 (0.23, 0.63)	59	0.20 (0.16, 0.25)	0.17 (0.13, 0.22)	0.42 (0.24, 0.63)
phenol sulfate	60	0.54 (0.34, 0.86)	1.14 (0.92, 1.42)	0.81 (0.71, 0.89)	60	0.54 (0.34, 0.86)	1.14 (0.92, 1.42)	0.81 (0.71, 0.89)	59	0.41 (0.28, 0.62)	1.07 (0.92, 1.25)	0.87 (0.80, 0.92)
phenylacetate	25											

pipecolate	60	0.77 (0.47, 1.28)	0.65 (0.36, 1.18)	0.42 (0.23, 0.63)	60	0.77 (0.47, 1.28)	0.65 (0.36, 1.18)	0.42 (0.23, 0.63)	57	0.45 (0.31, 0.65)	0.70 (0.56, 0.89)	0.71 (0.57, 0.82)
piperine	56	1.36 (0.56, 3.28)	1.26 (0.48, 3.26)	0.46 (0.27, 0.66)	60	1.39 (0.58, 3.35)	1.34 (0.54, 3.33)	0.48 (0.30, 0.67)	58	0.74 (0.45, 1.23)	0.79 (0.49, 1.27)	0.53 (0.35, 0.70)
pregn steroid monosulfate*	60	0.29 (0.19, 0.44)	1.30 (1.19, 1.43)	0.95 (0.92, 0.97)	60	0.29 (0.19, 0.44)	1.30 (1.19, 1.43)	0.95 (0.92, 0.97)	59	0.27 (0.19, 0.37)	0.85 (0.77, 0.94)	0.91 (0.85, 0.94)
pregnen-diol disulfate*	59	0.18 (0.11, 0.28)	1.56 (1.49, 1.65)	0.99 (0.98, 0.99)	60	0.18 (0.11, 0.28)	1.58 (1.50, 1.66)	0.99 (0.98, 0.99)	59	0.17 (0.12, 0.25)	1.21 (1.15, 1.28)	0.98 (0.97, 0.99)
pro-hydroxy-pro	60	0.26 (0.20, 0.34)	0.52 (0.46, 0.60)	0.80 (0.70, 0.88)	60	0.26 (0.20, 0.34)	0.52 (0.46, 0.60)	0.80 (0.70, 0.88)	58	0.20 (0.16, 0.26)	0.51 (0.46, 0.56)	0.87 (0.79, 0.92)
proline	60	0.11 (0.09, 0.14)	0.23 (0.21, 0.25)	0.80 (0.70, 0.88)	60	0.11 (0.09, 0.14)	0.23 (0.21, 0.25)	0.80 (0.70, 0.88)	60	0.11 (0.09, 0.14)	0.23 (0.21, 0.25)	0.80 (0.70, 0.88)
propionylcarnitine	60	0.16 (0.13, 0.20)	0.29 (0.26, 0.33)	0.76 (0.64, 0.85)	60	0.16 (0.13, 0.20)	0.29 (0.26, 0.33)	0.76 (0.64, 0.85)	60	0.16 (0.13, 0.20)	0.29 (0.26, 0.33)	0.76 (0.64, 0.85)
pseudouridine	60	0.14 (0.11, 0.17)	0.16 (0.13, 0.19)	0.58 (0.41, 0.73)	60	0.14 (0.11, 0.17)	0.16 (0.13, 0.19)	0.58 (0.41, 0.73)	59	0.12 (0.10, 0.15)	0.16 (0.14, 0.19)	0.62 (0.45, 0.76)
pyridoxate	60	31.90 (0.00, 287E12)	12.23 (0.00, 7E21)	0.13 (0.02, 0.58)	60	31.90 (0.00, 287E7)	12.23 (0.00, 7E21)	0.13 (0.02, 0.58)	59	0.47 (0.29, 0.76)	1.39 (1.18, 1.64)	0.90 (0.84, 0.94)
pyroglutamine*	60	0.26 (0.20, 0.35)	0.59 (0.52, 0.67)	0.83 (0.74, 0.90)	60	0.26 (0.20, 0.35)	0.59 (0.52, 0.67)	0.83 (0.74, 0.90)	58	0.20 (0.16, 0.26)	0.56 (0.51, 0.62)	0.89 (0.82, 0.93)
pyroglutamylglycine	13	0.17 (0.10, 0.27)	0.33 (0.26, 0.42)	0.80 (0.54, 0.93)	60	0.56 (0.38, 0.82)	0.40 (0.23, 0.68)	0.34 (0.16, 0.58)	59	0.27 (0.21, 0.35)	0.40 (0.33, 0.47)	0.68 (0.53, 0.80)
pyruvate	58	0.34 (0.26, 0.45)	0.26 (0.19, 0.38)	0.38 (0.19, 0.61)	60	0.35 (0.26, 0.45)	0.26 (0.19, 0.38)	0.37 (0.19, 0.60)	60	0.35 (0.26, 0.45)	0.26 (0.19, 0.38)	0.37 (0.19, 0.60)
quinate	35	0.42 (0.25, 0.70)	1.02 (0.83, 1.26)	0.86 (0.74, 0.92)	60	0.55 (0.32, 0.94)	1.56 (1.29, 1.88)	0.89 (0.82, 0.93)	59	0.59 (0.33, 1.04)	1.71 (1.40, 2.08)	0.89 (0.83, 0.94)
saccharin	11	0.88 (0.25, 3.13)	0.41 (0.03, 6.40)	0.17 (0.00, 0.92)	60	2.83 (0.56, 14.38)	0.92 (0.01, 135.2)	0.10 (0.01, 0.66)	57	1.23 (0.58, 2.60)	0.58 (0.12, 2.84)	0.18 (0.04, 0.55)
salicylate	55	3.06 (0.30, 31.42)	5.51 (1.51, 20.08)	0.76 (0.64, 0.86)	60	2.53 (0.41, 15.62)	4.39 (1.53, 12.54)	0.75 (0.62, 0.84)	59	0.95 (0.35, 2.53)	3.15 (2.35, 4.24)	0.92 (0.87, 0.95)
salicyluric glucuronide*	25	0.83 (0.34, 2.00)	1.06 (0.53, 2.11)	0.62 (0.37, 0.82)	60	1.03 (0.50, 2.10)	1.50 (0.92, 2.45)	0.68 (0.53, 0.80)	59	0.97 (0.44, 2.15)	2.09 (1.44, 3.02)	0.82 (0.72, 0.89)
scyrollo-inositol	54	0.24 (0.19, 0.32)	0.44 (0.38, 0.51)	0.76 (0.63, 0.86)	60	0.27 (0.21, 0.35)	0.46 (0.39, 0.53)	0.74 (0.61, 0.84)	60	0.27 (0.21, 0.35)	0.46 (0.39, 0.53)	0.74 (0.61, 0.84)
sebacate (decanedioate)	60	0.57 (0.39, 0.83)	0.16 (0.04, 0.60)	0.07 (0.00, 0.76)	60	0.57 (0.39, 0.83)	0.16 (0.04, 0.60)	0.07 (0.00, 0.76)	58	0.21 (0.17, 0.26)	0.19 (0.15, 0.25)	0.47 (0.28, 0.66)
serine	60	0.20 (0.16, 0.25)	0.16 (0.12, 0.21)	0.38 (0.20, 0.61)	60	0.20 (0.16, 0.25)	0.16 (0.12, 0.21)	0.38 (0.20, 0.61)	60	0.20 (0.16, 0.25)	0.16 (0.12, 0.21)	0.38 (0.20, 0.61)
serotonin (5HT)	60	0.16 (0.13, 0.20)	0.37 (0.33, 0.40)	0.84 (0.76, 0.90)	60	0.16 (0.13, 0.20)	0.37 (0.33, 0.40)	0.84 (0.76, 0.90)	60	0.16 (0.13, 0.20)	0.37 (0.33, 0.40)	0.84 (0.76, 0.90)
stachydrine	60	0.50 (0.34, 0.74)	0.84 (0.66, 1.06)	0.74 (0.61, 0.84)	60	0.50 (0.34, 0.74)	0.84 (0.66, 1.06)	0.74 (0.61, 0.84)	59	0.49 (0.33, 0.74)	0.92 (0.74, 1.14)	0.78 (0.66, 0.86)
stearate (18:0)	60	0.19 (0.15, 0.23)	0.17 (0.13, 0.21)	0.44 (0.26, 0.64)	60	0.19 (0.15, 0.23)	0.17 (0.13, 0.21)	0.44 (0.26, 0.64)	60	0.19 (0.15, 0.23)	0.17 (0.13, 0.21)	0.44 (0.26, 0.64)
stearidonate (18:4n3)	59	0.51 (0.35, 0.74)	0.54 (0.38, 0.77)	0.53 (0.35, 0.70)	60	0.52 (0.36, 0.76)	0.56 (0.39, 0.79)	0.53 (0.36, 0.70)	58	0.36 (0.27, 0.48)	0.44 (0.34, 0.56)	0.60 (0.43, 0.75)
stearoyl sphingomyelin	60	0.23 (0.18, 0.29)	0.31 (0.26, 0.37)	0.64 (0.48, 0.77)	60	0.23 (0.18, 0.29)	0.31 (0.26, 0.37)	0.64 (0.48, 0.77)	60	0.23 (0.18, 0.29)	0.31 (0.26, 0.37)	0.64 (0.48, 0.77)
stearoylcarnitine	55	0.28 (0.22, 0.36)	0.23 (0.17, 0.32)	0.41 (0.22, 0.63)	60	0.29 (0.23, 0.38)	0.25 (0.18, 0.33)	0.41 (0.23, 0.63)	60	0.29 (0.23, 0.38)	0.25 (0.18, 0.33)	0.41 (0.23, 0.63)
suberate (octanedioate)	20	0.20 (0.14, 0.29)	0.22 (0.16, 0.31)	0.55 (0.26, 0.81)	60	0.79 (0.49, 1.29)	0.15 (0.01, 1.88)	0.04 (0.00, 0.98)	58	0.43 (0.31, 0.59)	0.37 (0.26, 0.53)	0.43 (0.24, 0.64)
succinate	60	0.13 (0.10, 0.15)	0.14 (0.12, 0.17)	0.56 (0.38, 0.72)	60	0.13 (0.10, 0.15)	0.14 (0.12, 0.17)	0.56 (0.38, 0.72)	58	0.10 (0.08, 0.12)	0.15 (0.13, 0.17)	0.71 (0.56, 0.82)
succinylcarnitine	59	0.17 (0.14, 0.21)	0.24 (0.20, 0.28)	0.67 (0.51, 0.79)	60	0.17 (0.14, 0.22)	0.23 (0.20, 0.28)	0.64 (0.49, 0.78)	60	0.17 (0.14, 0.22)	0.23 (0.20, 0.28)	0.64 (0.49, 0.78)
taurochenodeoxycholate	37	0.79 (0.42, 1.50)	0.48 (0.17, 1.37)	0.27 (0.07, 0.63)	60	1.14 (0.56, 2.30)	0.84 (0.32, 2.18)	0.35 (0.17, 0.59)	59	0.64 (0.41, 1.00)	0.69 (0.45, 1.04)	0.53 (0.36, 0.70)
taurocholate	10	-15.1 (-22E9, 0.00)	-4.56 (-1E31, 0.00)	0.08 (0.00, 1.00)	60	6.97 (0.12, 390.8)	3.20 (0.00, 2058)	0.17 (0.04, 0.54)	59	0.59 (0.38, 0.93)	0.90 (0.67, 1.21)	0.70 (0.55, 0.81)
taurocholenate sulfate*	44	0.41 (0.29, 0.59)	0.35 (0.23, 0.54)	0.42 (0.22, 0.67)	60	0.53 (0.36, 0.77)	0.52 (0.36, 0.76)	0.49 (0.31, 0.68)	57	0.34 (0.25, 0.46)	0.50 (0.41, 0.61)	0.68 (0.53, 0.80)
taurodeoxycholate	29	1.24 (0.40, 3.82)	1.15 (0.34, 3.88)	0.46 (0.21, 0.73)	60	1.35 (0.57, 3.20)	1.38 (0.59, 3.21)	0.51 (0.33, 0.69)	59	0.76 (0.44, 1.32)	1.16 (0.80, 1.66)	0.70 (0.56, 0.81)
taurolithocholate 3-sulfate	39	0.67 (0.38, 1.17)	0.68 (0.39, 1.18)	0.51 (0.29, 0.72)	60	0.65 (0.42, 1.02)	0.68 (0.44, 1.04)	0.52 (0.34, 0.69)	59	0.49 (0.34, 0.72)	0.64 (0.48, 0.86)	0.63 (0.47, 0.77)
tetradecanedioate	54	0.40 (0.29, 0.55)	0.27 (0.17, 0.43)	0.32 (0.13, 0.58)	60	0.41 (0.30, 0.56)	0.33 (0.23, 0.48)	0.39 (0.21, 0.61)	59	0.39 (0.29, 0.53)	0.34 (0.24, 0.48)	0.43 (0.24, 0.64)
theobromine	59	0.79 (0.48, 1.31)	0.40 (0.15, 1.07)	0.20 (0.05, 0.54)	60	0.79 (0.48, 1.30)	0.41 (0.16, 1.07)	0.22 (0.06, 0.53)	60	0.79 (0.48, 1.30)	0.41 (0.16, 1.07)	0.22 (0.06, 0.53)
theophylline	41	0.55 (0.20, 1.48)	2.94 (2.44, 3.54)	0.97 (0.94, 0.98)	60	0.65 (0.25, 1.75)	3.52 (2.93, 4.23)	0.97 (0.95, 0.98)	59	0.46 (0.32, 0.68)	0.78 (0.63, 0.98)	0.74 (0.61, 0.84)
threitol	58	0.36 (0.27, 0.47)	0.23 (0.15, 0.36)	0.30 (0.12, 0.57)	60	0.36 (0.27, 0.48)	0.24 (0.16, 0.36)	0.30 (0.13, 0.56)	60	0.36 (0.27, 0.48)	0.24 (0.16, 0.36)	0.30 (0.13, 0.56)
threonate	60	0.24 (0.19, 0.30)	0.30 (0.25, 0.36)	0.61 (0.44, 0.75)	60	0.24 (0.19, 0.30)	0.30 (0.25, 0.36)	0.61 (0.44, 0.75)	60	0.24 (0.19, 0.30)	0.30 (0.25, 0.36)	0.61 (0.44, 0.75)
threonine	47	0.15 (0.12, 0.20)	0.28 (0.25, 0.32)	0.77 (0.64, 0.87)	60	0.39 (0.29, 0.52)	0.36 (0.27, 0.50)	0.47 (0.29, 0.66)	59	0.33 (0.25, 0.43)	0.37 (0.29, 0.47)	0.57 (0.39, 0.73)
threonylphenylalanine	16	0.27 (0.19, 0.40)	(..,..)	0.00 (..,..)	60	0.33 (0.26, 0.43)	0.17 (0.10, 0.28)	0.20 (0.05, 0.53)	58	0.30 (0.23, 0.39)	0.20 (0.13, 0.29)	0.30 (0.12, 0.57)
thymol sulfate	25	0.48 (0.28, 0.81)	0.43 (0.24, 0.78)	0.45 (0.18, 0.74)	60	0.92 (0.51, 1.67)	0.90 (0.49, 1.66)	0.49 (0.31, 0.68)	58	0.72 (0.42, 1.22)	1.05 (0.73, 1.51)	0.68 (0.53, 0.80)
tiglylcarnitine	59	0.19 (0.15, 0.23)	0.24 (0.20, 0.28)	0.61 (0.45, 0.76)	60	0.19 (0.15, 0.24)	0.24 (0.20, 0.29)	0.61 (0.45, 0.76)	60	0.19 (0.15, 0.24)	0.24 (0.20, 0.29)	0.61 (0.45, 0.76)
trans-4-hydroxyproline	55	0.53 (0.36, 0.77)	0.29 (0.15, 0.57)	0.23 (0.07, 0.55)	60	0.55 (0.38, 0.80)	0.33 (0.18, 0.62)	0.27 (0.10, 0.55)	59	0.46 (0.33, 0.64)	0.29 (0.17, 0.49)	0.28 (0.10, 0.55)
tryptophan	60	0.08 (0.06, 0.09)	0.14 (0.12, 0.15)	0.77 (0.65, 0.86)	60	0.08 (0.06, 0.09)	0.14 (0.12, 0.15)	0.77 (0.65, 0.86)	60	0.08 (0.06, 0.09)	0.14 (0.12, 0.15)	0.77 (0.65, 0.86)
tryptophan betaine	57	0.39 (0.26, 0.56)	0.94 (0.81, 1.10)	0.86 (0.77, 0.91)	60	0.39 (0.27, 0.57)	0.98 (0.84, 1.14)	0.86 (0.78, 0.91)	59	0.42 (0.29, 0.60)	0.75 (0.62, 0.92)	0.76 (0.64, 0.85)
tyrosine	60	0.08 (0.07, 0.10)	0.14 (0.13, 0.16)	0.74 (0.62, 0.84)	60	0.08 (0.07, 0.10)	0.14 (0.13, 0.16)	0.74 (0.62, 0.84)	60	0.08 (0.07, 0.10)	0.14 (0.13, 0.16)	0.74 (0.62, 0.84)
undecanedioate	60	0.69 (0.45, 1.06)	0.04 (0.00, 143.7)	0.00 (0.00, 1.00)	60	0.69 (0.45, 1.06)	0.04 (0.00, 143.7)	0.00 (0.00, 1.00)	59	0.17 (0.14, 0.21)	0.17 (0.14, 0.21)	0.49 (0.31, 0.68)
undecanoate (11:0)	58	0.13 (0.11, 0.16)	0.13 (0.10, 0.16)	0.47 (0.29, 0.67)	60	0.14 (0.11, 0.17)	0.13 (0.10, 0.16)	0.46 (0.28, 0.66)	60	0.14 (0.11, 0.17)	0.13 (0.10, 0.16)	0.46 (0.28, 0.66)
urate	60	0.10 (0.08, 0.12)	0.17 (0.15, 0.19)	0.74 (0.61, 0.84)	60	0.10 (0.08, 0.12)	0.17 (0.15, 0.19)	0.74 (0.61, 0.84)	60	0.10 (0.08, 0.12)	0.17 (0.15, 0.19)	0.74 (0.61, 0.84)
urea	60	0.18 (0.14, 0.22)	0.17 (0.14, 0.21)	0.49 (0.31, 0.68)	60	0.18 (0.14, 0.22)	0.17 (0.14, 0.21)	0.49 (0.31, 0.68)	59	0.15 (0.13, 0.19)	0.17 (0.14, 0.20)	0.54 (0.36, 0.71)
uridine	60	0.10 (0.08, 0.12)	0.13 (0.12, 0.15)	0.64 (0.48, 0.77)	60	0.10 (0.08, 0.12)	0.13 (0.12, 0.15)	0.64 (0.48, 0.77)	60	0.10 (0.08, 0.12)	0.13 (0.12, 0.15)	0.64

X-02249_201	60	0.26 (0.20, 0.34)	0.39 (0.33, 0.46)	0.69 (0.54, 0.80)	60	0.26 (0.20, 0.34)	0.39 (0.33, 0.46)	0.69 (0.54, 0.80)	59	0.25 (0.19, 0.32)	0.41 (0.35, 0.48)	0.73 (0.59, 0.83)
X-02269_201	58	0.49 (0.32, 0.75)	1.03 (0.84, 1.26)	0.81 (0.71, 0.89)	60	0.50 (0.33, 0.77)	1.05 (0.86, 1.29)	0.82 (0.72, 0.89)	59	0.25 (0.18, 0.36)	1.05 (0.96, 1.14)	0.95 (0.91, 0.97)
X-02973	60	0.15 (0.12, 0.18)	0.05 (0.03, 0.09)	0.12 (0.01, 0.59)	60	0.15 (0.12, 0.18)	0.05 (0.03, 0.09)	0.12 (0.01, 0.59)	60	0.15 (0.12, 0.18)	0.05 (0.03, 0.09)	0.12 (0.01, 0.59)
X-03003	59	0.25 (0.20, 0.32)	0.12 (0.07, 0.19)	0.18 (0.04, 0.54)	60	0.26 (0.21, 0.33)	0.12 (0.08, 0.20)	0.18 (0.04, 0.53)	60	0.26 (0.21, 0.33)	0.12 (0.08, 0.20)	0.18 (0.04, 0.53)
X-03056_200	60	0.24 (0.19, 0.30)	0.28 (0.23, 0.34)	0.59 (0.42, 0.74)	60	0.24 (0.19, 0.30)	0.28 (0.23, 0.34)	0.59 (0.42, 0.74)	59	0.21 (0.17, 0.27)	0.27 (0.22, 0.32)	0.61 (0.44, 0.75)
X-03088	52	0.26 (0.20, 0.34)	0.06 (0.02, 0.18)	0.05 (0.00, 0.94)	60	0.31 (0.24, 0.39)	0.13 (0.07, 0.23)	0.14 (0.02, 0.56)	60	0.31 (0.24, 0.39)	0.13 (0.07, 0.23)	0.14 (0.02, 0.56)
X-03094	60	0.23 (0.18, 0.29)	0.18 (0.14, 0.24)	0.38 (0.20, 0.61)	60	0.23 (0.18, 0.29)	0.18 (0.14, 0.24)	0.38 (0.20, 0.61)	60	0.23 (0.18, 0.29)	0.18 (0.14, 0.24)	0.38 (0.20, 0.61)
X-04272	58	0.22 (0.18, 0.28)	0.06 (0.03, 0.14)	0.08 (0.00, 0.75)	60	0.25 (0.20, 0.30)	(..)	0.00 (..)	59	0.24 (0.19, 0.30)	0.06 (0.02, 0.15)	0.05 (0.00, 0.91)
X-04357	60	0.44 (0.32, 0.61)	0.30 (0.18, 0.48)	0.31 (0.13, 0.57)	60	0.44 (0.32, 0.61)	0.30 (0.18, 0.48)	0.31 (0.13, 0.57)	58	0.31 (0.24, 0.41)	0.28 (0.21, 0.38)	0.45 (0.27, 0.65)
X-04494	44	0.26 (0.20, 0.35)	0.19 (0.13, 0.28)	0.34 (0.14, 0.62)	60	0.37 (0.28, 0.49)	0.16 (0.09, 0.31)	0.16 (0.03, 0.54)	60	0.37 (0.28, 0.49)	0.16 (0.09, 0.31)	0.16 (0.03, 0.54)
X-04495	58	0.35 (0.26, 0.47)	0.33 (0.24, 0.44)	0.47 (0.28, 0.66)	60	0.35 (0.26, 0.46)	0.33 (0.25, 0.45)	0.48 (0.29, 0.67)	58	0.25 (0.20, 0.33)	0.32 (0.27, 0.39)	0.62 (0.45, 0.76)
X-04498	57	0.34 (0.25, 0.44)	0.32 (0.24, 0.43)	0.48 (0.29, 0.67)	60	0.34 (0.26, 0.45)	0.33 (0.25, 0.44)	0.49 (0.31, 0.68)	58	0.27 (0.21, 0.34)	0.30 (0.24, 0.38)	0.56 (0.38, 0.72)
X-04499	52	0.22 (0.17, 0.28)	0.27 (0.22, 0.33)	0.61 (0.43, 0.76)	60	0.25 (0.20, 0.32)	0.29 (0.24, 0.36)	0.57 (0.40, 0.73)	60	0.25 (0.20, 0.32)	0.29 (0.24, 0.36)	0.57 (0.40, 0.73)
X-04500	23	0.57 (0.23, 1.43)	1.71 (1.26, 2.33)	0.90 (0.79, 0.96)	60	0.96 (0.41, 2.22)	2.46 (1.78, 3.42)	0.87 (0.79, 0.92)	59	1.01 (0.39, 2.61)	2.86 (2.04, 4.00)	0.89 (0.82, 0.93)
X-04598	41	0.46 (0.31, 0.68)	0.17 (0.06, 0.48)	0.12 (0.01, 0.70)	60	0.60 (0.41, 0.89)	0.32 (0.16, 0.67)	0.22 (0.07, 0.53)	59	0.50 (0.35, 0.70)	0.26 (0.13, 0.50)	0.21 (0.06, 0.54)
X-04807	60	0.36 (0.27, 0.47)	0.16 (0.08, 0.29)	0.16 (0.03, 0.54)	60	0.36 (0.27, 0.47)	0.16 (0.08, 0.29)	0.16 (0.03, 0.54)	60	0.36 (0.27, 0.47)	0.16 (0.08, 0.29)	0.16 (0.03, 0.54)
X-04874	60	0.23 (0.18, 0.28)	0.15 (0.11, 0.21)	0.30 (0.12, 0.56)	60	0.23 (0.18, 0.28)	0.15 (0.11, 0.21)	0.30 (0.12, 0.56)	60	0.23 (0.18, 0.28)	0.15 (0.11, 0.21)	0.30 (0.12, 0.56)
X-05415	16	0.38 (0.22, 0.67)	0.23 (0.09, 0.58)	0.26 (0.03, 0.79)	60	0.71 (0.45, 1.12)	0.51 (0.27, 0.96)	0.34 (0.16, 0.58)	59	0.61 (0.40, 0.92)	0.51 (0.31, 0.83)	0.41 (0.22, 0.62)
X-05907	60	0.21 (0.17, 0.26)	0.17 (0.13, 0.22)	0.41 (0.22, 0.62)	60	0.21 (0.17, 0.26)	0.17 (0.13, 0.22)	0.41 (0.22, 0.62)	60	0.21 (0.17, 0.26)	0.17 (0.13, 0.22)	0.41 (0.22, 0.62)
X-06126_201	60	0.53 (0.37, 0.75)	0.36 (0.21, 0.61)	0.32 (0.14, 0.57)	60	0.53 (0.37, 0.75)	0.36 (0.21, 0.61)	0.32 (0.14, 0.57)	58	0.42 (0.31, 0.58)	0.38 (0.27, 0.54)	0.45 (0.26, 0.65)
X-06226	59	0.22 (0.18, 0.28)	0.15 (0.11, 0.21)	0.31 (0.13, 0.57)	60	0.23 (0.18, 0.29)	0.16 (0.11, 0.22)	0.31 (0.14, 0.57)	60	0.23 (0.18, 0.29)	0.16 (0.11, 0.22)	0.31 (0.14, 0.57)
X-06267	59	0.28 (0.22, 0.36)	0.14 (0.09, 0.23)	0.21 (0.06, 0.54)	60	0.28 (0.22, 0.36)	0.15 (0.09, 0.23)	0.21 (0.06, 0.53)	60	0.28 (0.22, 0.36)	0.15 (0.09, 0.23)	0.21 (0.06, 0.53)
X-06307	53	0.30 (0.23, 0.40)	0.23 (0.16, 0.33)	0.35 (0.16, 0.61)	60	0.34 (0.26, 0.44)	0.20 (0.13, 0.31)	0.26 (0.09, 0.54)	60	0.34 (0.26, 0.44)	0.20 (0.13, 0.31)	0.26 (0.09, 0.54)
X-06346	60	0.18 (0.15, 0.23)	0.07 (0.04, 0.12)	0.13 (0.02, 0.57)	60	0.18 (0.15, 0.23)	0.07 (0.04, 0.12)	0.13 (0.02, 0.57)	60	0.18 (0.15, 0.23)	0.07 (0.04, 0.12)	0.13 (0.02, 0.57)
X-06351	14	0.35 (0.20, 0.61)	0.19 (0.06, 0.53)	0.22 (0.01, 0.84)	60	0.65 (0.43, 0.98)	0.26 (0.09, 0.73)	0.14 (0.02, 0.56)	59	0.64 (0.42, 0.97)	0.34 (0.15, 0.75)	0.22 (0.06, 0.54)
X-07765_201	52	0.89 (0.47, 1.66)	0.98 (0.55, 1.73)	0.55 (0.36, 0.72)	60	0.99 (0.52, 1.88)	1.10 (0.62, 1.97)	0.56 (0.38, 0.72)	59	0.85 (0.49, 1.45)	0.60 (0.28, 1.28)	0.33 (0.15, 0.58)
X-08402	59	0.24 (0.19, 0.31)	0.28 (0.22, 0.34)	0.56 (0.38, 0.72)	60	0.25 (0.19, 0.31)	0.28 (0.23, 0.35)	0.57 (0.39, 0.72)	59	0.18 (0.14, 0.22)	0.30 (0.27, 0.34)	0.75 (0.62, 0.84)
X-08766	27	0.32 (0.22, 0.48)	0.10 (0.03, 0.35)	0.08 (0.00, 0.94)	60	0.37 (0.28, 0.49)	0.25 (0.17, 0.38)	0.32 (0.14, 0.57)	60	0.37 (0.28, 0.49)	0.25 (0.17, 0.38)	0.32 (0.14, 0.57)
X-09026	60	0.18 (0.15, 0.22)	0.14 (0.10, 0.18)	0.36 (0.18, 0.59)	60	0.18 (0.15, 0.22)	0.14 (0.10, 0.18)	0.36 (0.18, 0.59)	60	0.18 (0.15, 0.22)	0.14 (0.10, 0.18)	0.36 (0.18, 0.59)
X-09706	60	0.28 (0.22, 0.35)	0.12 (0.07, 0.21)	0.15 (0.02, 0.55)	60	0.28 (0.22, 0.35)	0.12 (0.07, 0.21)	0.15 (0.02, 0.55)	60	0.28 (0.22, 0.35)	0.12 (0.07, 0.21)	0.15 (0.02, 0.55)
X-09789_201	60	0.30 (0.22, 0.39)	0.57 (0.49, 0.66)	0.78 (0.67, 0.87)	60	0.30 (0.22, 0.39)	0.57 (0.49, 0.66)	0.78 (0.67, 0.87)	59	0.27 (0.20, 0.35)	0.56 (0.49, 0.64)	0.82 (0.72, 0.89)
X-10346_201	12	0.40 (0.20, 0.79)	0.36 (0.17, 0.77)	0.45 (0.11, 0.83)	60	0.52 (0.35, 0.78)	0.86 (0.68, 1.11)	0.73 (0.60, 0.83)	59	0.55 (0.37, 0.84)	0.78 (0.58, 1.04)	0.66 (0.51, 0.79)
X-10395	60	0.18 (0.15, 0.23)	0.18 (0.14, 0.22)	0.48 (0.30, 0.67)	60	0.18 (0.15, 0.23)	0.18 (0.14, 0.22)	0.48 (0.30, 0.67)	59	0.17 (0.14, 0.21)	0.19 (0.16, 0.23)	0.55 (0.37, 0.71)
X-10429	28	0.30 (0.21, 0.44)	0.12 (0.05, 0.30)	0.13 (0.01, 0.78)	60	0.53 (0.37, 0.75)	0.27 (0.14, 0.54)	0.21 (0.06, 0.53)	60	0.53 (0.37, 0.75)	0.27 (0.14, 0.54)	0.21 (0.06, 0.53)
X-10500	60	0.15 (0.12, 0.18)	0.20 (0.18, 0.24)	0.66 (0.50, 0.78)	60	0.15 (0.12, 0.18)	0.20 (0.18, 0.24)	0.66 (0.50, 0.78)	58	0.12 (0.10, 0.15)	0.22 (0.20, 0.25)	0.76 (0.64, 0.85)
X-10510	60	0.24 (0.19, 0.30)	0.29 (0.24, 0.35)	0.60 (0.44, 0.75)	60	0.24 (0.19, 0.30)	0.29 (0.24, 0.35)	0.60 (0.44, 0.75)	58	0.19 (0.15, 0.24)	0.31 (0.27, 0.35)	0.73 (0.59, 0.83)
X-11204	60	0.16 (0.13, 0.20)	0.17 (0.14, 0.21)	0.54 (0.37, 0.71)	60	0.16 (0.13, 0.20)	0.17 (0.14, 0.21)	0.54 (0.37, 0.71)	60	0.16 (0.13, 0.20)	0.17 (0.14, 0.21)	0.54 (0.37, 0.71)
X-11247	46	1.38 (0.54, 3.53)	0.66 (0.09, 4.70)	0.19 (0.03, 0.59)	60	1.18 (0.58, 2.37)	0.46 (0.08, 2.75)	0.13 (0.02, 0.57)	59	1.13 (0.58, 2.20)	0.23 (0.01, 6.29)	0.04 (0.00, 9.7)
X-11261	60	0.33 (0.25, 0.43)	0.45 (0.37, 0.55)	0.65 (0.50, 0.78)	60	0.33 (0.25, 0.43)	0.45 (0.37, 0.55)	0.65 (0.50, 0.78)	60	0.33 (0.25, 0.43)	0.45 (0.37, 0.55)	0.65 (0.50, 0.78)
X-11299	56	0.75 (0.42, 1.33)	1.28 (0.91, 1.79)	0.75 (0.62, 0.84)	60	0.77 (0.43, 1.38)	1.36 (0.98, 1.89)	0.76 (0.63, 0.85)	59	0.65 (0.39, 1.11)	1.29 (0.99, 1.69)	0.80 (0.69, 0.87)
X-11308	60	0.18 (0.14, 0.23)	0.50 (0.46, 0.55)	0.89 (0.82, 0.93)	60	0.18 (0.14, 0.23)	0.50 (0.46, 0.55)	0.89 (0.82, 0.93)	58	0.13 (0.10, 0.17)	0.51 (0.48, 0.54)	0.94 (0.90, 0.96)
X-11315	60	0.16 (0.13, 0.20)	0.48 (0.45, 0.52)	0.90 (0.84, 0.94)	60	0.16 (0.13, 0.20)	0.48 (0.45, 0.52)	0.90 (0.84, 0.94)	58	0.13 (0.10, 0.16)	0.39 (0.36, 0.42)	0.90 (0.84, 0.94)
X-11317	60	0.21 (0.17, 0.27)	0.23 (0.19, 0.29)	0.54 (0.36, 0.71)	60	0.21 (0.17, 0.27)	0.23 (0.19, 0.29)	0.54 (0.36, 0.71)	60	0.21 (0.17, 0.27)	0.23 (0.19, 0.29)	0.54 (0.36, 0.71)
X-11319	60	0.16 (0.13, 0.19)	0.13 (0.11, 0.17)	0.42 (0.23, 0.63)	60	0.16 (0.13, 0.19)	0.13 (0.11, 0.17)	0.42 (0.23, 0.63)	60	0.16 (0.13, 0.19)	0.13 (0.11, 0.17)	0.42 (0.23, 0.63)
X-11327	60	0.21 (0.17, 0.27)	0.16 (0.12, 0.22)	0.36 (0.18, 0.59)	60	0.21 (0.17, 0.27)	0.16 (0.12, 0.22)	0.36 (0.18, 0.59)	60	0.21 (0.17, 0.27)	0.16 (0.12, 0.22)	0.36 (0.18, 0.59)
X-11333	24	0.26 (0.18, 0.38)	0.20 (0.12, 0.33)	0.37 (0.12, 0.72)	60	0.25 (0.20, 0.32)	0.32 (0.26, 0.39)	0.61 (0.44, 0.75)	58	0.22 (0.17, 0.27)	0.33 (0.29, 0.39)	0.71 (0.56, 0.82)
X-11334	40	0.30 (0.21, 0.43)	0.60 (0.51, 0.72)	0.80 (0.67, 0.89)	60	0.33 (0.24, 0.45)	0.65 (0.55, 0.76)	0.80 (0.69, 0.87)	59	0.33 (0.25, 0.44)	0.35 (0.27, 0.45)	0.53 (0.35, 0.70)
X-11372	60	0.13 (0.10, 0.16)	0.40 (0.37, 0.42)	0.90 (0.85, 0.94)	60	0.13 (0.10, 0.16)	0.40 (0.37, 0.42)	0.90 (0.85, 0.94)	59	0.10 (0.08, 0.13)	0.39 (0.37, 0.42)	0.93 (0.89, 0.96)
X-11378	56	0.34 (0.26, 0.46)	0.30 (0.22, 0.42)	0.44 (0.25, 0.65)	60	0.55 (0.38, 0.79)	0.30 (0.15, 0.59)	0.23 (0.07, 0.54)	59	0.38 (0.28, 0.51)	0.35 (0.25, 0.48)	0.46 (0.27, 0.66)
X-11381_201	60	0.17 (0.14, 0.21)	0.29 (0.25, 0.33)	0.74 (0.60, 0.83)	60	0.17 (0.14, 0.21)	0.29 (0.25, 0.33)	0.74 (0.60, 0.83)	60	0.17 (0.14, 0.21)	0.29 (0.25, 0.33)	0.74 (0.60, 0.83)
X-11412	51	0.24 (0.19, 0.31)	0.14 (0.09, 0.22)	0.25 (0.08, 0.57)	60	0.28 (0.22, 0.36)	0.16 (0.10, 0.24)	0.24 (0.08, 0				

X-11440	56	0.62 (0.37, 1.06)	1.30 (1.01, 1.68)	0.81 (0.71, 0.89)	60	0.64 (0.38, 1.08)	1.35 (1.06, 1.73)	0.82 (0.72, 0.89)	59	0.25 (0.19, 0.34)	0.75 (0.68, 0.83)	0.90 (0.84, 0.94)
X-11441	8	0.42 (0.18, 1.00)	0.40 (0.16, 0.99)	0.47 (0.09, 0.89)	60	0.42 (0.30, 0.57)	0.39 (0.28, 0.54)	0.47 (0.29, 0.66)	59	0.36 (0.27, 0.49)	0.45 (0.35, 0.57)	0.60 (0.44, 0.75)
X-11442	17	0.33 (0.20, 0.55)	0.32 (0.19, 0.54)	0.48 (0.18, 0.80)	60	0.47 (0.33, 0.66)	0.48 (0.35, 0.67)	0.52 (0.34, 0.69)	58	0.37 (0.27, 0.51)	0.51 (0.41, 0.64)	0.66 (0.50, 0.79)
X-11444	58	0.18 (0.15, 0.23)	0.36 (0.32, 0.40)	0.79 (0.68, 0.87)	60	0.19 (0.15, 0.24)	0.38 (0.34, 0.43)	0.80 (0.69, 0.87)	59	0.18 (0.14, 0.22)	0.40 (0.36, 0.44)	0.83 (0.74, 0.90)
X-11452	45	0.70 (0.38, 1.30)	1.21 (0.85, 1.73)	0.75 (0.60, 0.86)	60	0.72 (0.41, 1.26)	1.34 (0.99, 1.81)	0.78 (0.66, 0.86)	59	0.69 (0.42, 1.12)	0.91 (0.63, 1.32)	0.64 (0.48, 0.77)
X-11469	57	0.39 (0.27, 0.56)	0.83 (0.70, 0.98)	0.82 (0.72, 0.89)	60	0.40 (0.28, 0.57)	0.85 (0.72, 1.00)	0.82 (0.72, 0.89)	59	0.31 (0.23, 0.43)	0.72 (0.63, 0.83)	0.84 (0.75, 0.90)
X-11470	47	0.23 (0.17, 0.30)	0.42 (0.36, 0.49)	0.77 (0.64, 0.87)	60	0.25 (0.19, 0.33)	0.51 (0.45, 0.58)	0.81 (0.70, 0.88)	59	0.23 (0.18, 0.31)	0.54 (0.48, 0.61)	0.84 (0.75, 0.90)
X-11476	51	0.28 (0.21, 0.36)	0.17 (0.11, 0.27)	0.28 (0.10, 0.58)	60	0.33 (0.25, 0.43)	0.19 (0.12, 0.30)	0.25 (0.09, 0.54)	59	0.29 (0.23, 0.38)	0.19 (0.13, 0.28)	0.30 (0.12, 0.56)
X-11478	59	0.52 (0.36, 0.75)	0.47 (0.31, 0.71)	0.45 (0.26, 0.65)	60	0.53 (0.36, 0.76)	0.48 (0.32, 0.72)	0.46 (0.28, 0.65)	59	0.42 (0.31, 0.58)	0.45 (0.33, 0.61)	0.53 (0.35, 0.70)
X-11483	43	0.55 (0.34, 0.89)	0.77 (0.54, 1.08)	0.66 (0.48, 0.80)	60	0.60 (0.38, 0.94)	0.96 (0.72, 1.27)	0.72 (0.58, 0.82)	57	0.42 (0.29, 0.61)	0.88 (0.73, 1.05)	0.81 (0.71, 0.89)
X-11485	14	0.24 (0.15, 0.40)	0.28 (0.18, 0.43)	0.57 (0.23, 0.85)	60	0.31 (0.24, 0.40)	0.34 (0.26, 0.43)	0.54 (0.36, 0.71)	58	0.24 (0.19, 0.31)	0.26 (0.20, 0.32)	0.52 (0.34, 0.70)
X-11491	31	0.48 (0.27, 0.86)	1.05 (0.81, 1.37)	0.83 (0.69, 0.91)	60	0.54 (0.33, 0.87)	1.30 (1.06, 1.59)	0.85 (0.77, 0.91)	58	0.44 (0.31, 0.62)	0.62 (0.48, 0.79)	0.67 (0.51, 0.79)
X-11497	60	0.19 (0.16, 0.24)	0.23 (0.19, 0.28)	0.59 (0.42, 0.74)	60	0.19 (0.16, 0.24)	0.23 (0.19, 0.28)	0.59 (0.42, 0.74)	60	0.19 (0.16, 0.24)	0.23 (0.19, 0.28)	0.59 (0.42, 0.74)
X-11521	55	0.27 (0.21, 0.35)	0.24 (0.18, 0.32)	0.43 (0.24, 0.64)	60	0.28 (0.22, 0.37)	0.27 (0.21, 0.35)	0.47 (0.29, 0.66)	60	0.28 (0.22, 0.37)	0.27 (0.21, 0.35)	0.47 (0.29, 0.66)
X-11529	46	0.29 (0.20, 0.42)	0.88 (0.78, 0.99)	0.90 (0.84, 0.95)	60	0.31 (0.22, 0.44)	1.01 (0.90, 1.12)	0.91 (0.86, 0.95)	58	0.26 (0.20, 0.34)	0.55 (0.48, 0.63)	0.82 (0.72, 0.89)
X-11530	56	0.59 (0.38, 0.91)	0.76 (0.54, 1.07)	0.62 (0.46, 0.77)	60	0.59 (0.39, 0.91)	0.74 (0.53, 1.04)	0.61 (0.45, 0.75)	59	0.53 (0.36, 0.78)	0.56 (0.39, 0.80)	0.52 (0.34, 0.70)
X-11537	60	0.43 (0.31, 0.60)	0.40 (0.28, 0.56)	0.45 (0.27, 0.65)	60	0.43 (0.31, 0.60)	0.40 (0.28, 0.56)	0.45 (0.27, 0.65)	60	0.43 (0.31, 0.60)	0.40 (0.28, 0.56)	0.45 (0.27, 0.65)
X-11538	60	0.25 (0.19, 0.31)	0.32 (0.27, 0.39)	0.63 (0.47, 0.77)	60	0.25 (0.19, 0.31)	0.32 (0.27, 0.39)	0.63 (0.47, 0.77)	60	0.25 (0.19, 0.31)	0.32 (0.27, 0.39)	0.63 (0.47, 0.77)
X-11540	60	0.42 (0.31, 0.58)	0.32 (0.21, 0.48)	0.36 (0.18, 0.59)	60	0.42 (0.31, 0.58)	0.32 (0.21, 0.48)	0.36 (0.18, 0.59)	60	0.42 (0.31, 0.58)	0.32 (0.21, 0.48)	0.36 (0.18, 0.59)
X-11546	40	1.32 (0.47, 3.66)	1.32 (0.48, 3.66)	0.50 (0.28, 0.72)	60	1.51 (0.57, 3.97)	1.63 (0.67, 3.99)	0.54 (0.36, 0.71)	58	1.19 (0.53, 2.67)	1.47 (0.77, 2.83)	0.60 (0.43, 0.75)
X-11550	60	0.11 (0.09, 0.14)	0.17 (0.15, 0.19)	0.68 (0.54, 0.80)	60	0.11 (0.09, 0.14)	0.17 (0.15, 0.19)	0.68 (0.54, 0.80)	60	0.11 (0.09, 0.14)	0.17 (0.15, 0.19)	0.68 (0.54, 0.80)
X-11556	57	0.32 (0.24, 0.41)	0.23 (0.16, 0.33)	0.34 (0.16, 0.59)	60	0.32 (0.25, 0.42)	0.22 (0.15, 0.32)	0.31 (0.13, 0.57)	59	0.28 (0.22, 0.36)	0.26 (0.20, 0.34)	0.46 (0.28, 0.66)
X-11561	14	0.10 (0.07, 0.15)	0.08 (0.04, 0.13)	0.36 (0.07, 0.80)	60	0.11 (0.09, 0.13)	0.14 (0.12, 0.16)	0.62 (0.46, 0.76)	59	0.10 (0.08, 0.12)	0.15 (0.13, 0.17)	0.68 (0.53, 0.80)
X-11564	60	0.16 (0.13, 0.20)	0.24 (0.20, 0.27)	0.68 (0.53, 0.80)	60	0.16 (0.13, 0.20)	0.24 (0.20, 0.27)	0.68 (0.53, 0.80)	60	0.16 (0.13, 0.20)	0.24 (0.20, 0.27)	0.68 (0.53, 0.80)
X-11593	60	0.21 (0.17, 0.26)	0.30 (0.26, 0.35)	0.67 (0.52, 0.79)	60	0.21 (0.17, 0.26)	0.30 (0.26, 0.35)	0.67 (0.52, 0.79)	60	0.21 (0.17, 0.26)	0.30 (0.26, 0.35)	0.67 (0.52, 0.79)
X-11687_200	30	0.15 (0.11, 0.20)	0.17 (0.13, 0.22)	0.54 (0.30, 0.77)	60	0.16 (0.13, 0.20)	0.21 (0.18, 0.25)	0.64 (0.48, 0.77)	59	0.14 (0.12, 0.18)	0.21 (0.18, 0.24)	0.68 (0.54, 0.80)
X-11786	60	0.59 (0.41, 0.85)	(.,.)	0.00 (.,.)	60	0.59 (0.41, 0.85)	(.,.)	0.00 (.,.)	59	0.46 (0.33, 0.63)	0.10 (0.02, 0.44)	0.04 (0.00, 0.95)
X-11787	60	0.09 (0.07, 0.10)	0.19 (0.18, 0.21)	0.83 (0.74, 0.90)	60	0.09 (0.07, 0.10)	0.19 (0.18, 0.21)	0.83 (0.74, 0.90)	60	0.09 (0.07, 0.10)	0.19 (0.18, 0.21)	0.83 (0.74, 0.90)
X-11793	58	0.28 (0.22, 0.36)	0.20 (0.14, 0.29)	0.34 (0.16, 0.59)	60	0.28 (0.22, 0.36)	0.22 (0.16, 0.30)	0.39 (0.20, 0.61)	60	0.28 (0.22, 0.36)	0.22 (0.16, 0.30)	0.39 (0.20, 0.61)
X-11795	60	0.18 (0.14, 0.22)	0.44 (0.40, 0.48)	0.86 (0.78, 0.91)	60	0.18 (0.14, 0.22)	0.44 (0.40, 0.48)	0.86 (0.78, 0.91)	59	0.15 (0.12, 0.19)	0.46 (0.43, 0.50)	0.91 (0.85, 0.94)
X-11799	10	1.36 (0.19, 0.57)	0.37 (0.00, 0.472)	0.07 (0.00, 1.00)	60	1.44 (0.61, 3.43)	0.86 (0.20, 3.67)	0.26 (0.10, 0.55)	58	0.89 (0.50, 1.59)	0.73 (0.36, 1.47)	0.40 (0.21, 0.62)
X-11805	55	0.46 (0.33, 0.64)	0.31 (0.19, 0.52)	0.32 (0.14, 0.58)	60	0.47 (0.34, 0.65)	0.35 (0.22, 0.54)	0.36 (0.17, 0.59)	59	0.46 (0.33, 0.65)	0.38 (0.25, 0.57)	0.40 (0.22, 0.62)
X-11818	59	0.39 (0.29, 0.52)	0.33 (0.23, 0.46)	0.41 (0.23, 0.63)	60	0.39 (0.29, 0.53)	0.33 (0.24, 0.47)	0.42 (0.24, 0.63)	59	0.30 (0.23, 0.40)	0.40 (0.33, 0.49)	0.64 (0.48, 0.77)
X-11820	60	0.21 (0.16, 0.26)	0.29 (0.25, 0.34)	0.66 (0.51, 0.79)	60	0.21 (0.16, 0.26)	0.29 (0.25, 0.34)	0.66 (0.51, 0.79)	60	0.21 (0.16, 0.26)	0.29 (0.25, 0.34)	0.66 (0.51, 0.79)
X-11837_200	31	0.54 (0.32, 0.90)	0.38 (0.19, 0.79)	0.33 (0.11, 0.67)	60	0.66 (0.43, 1.02)	0.55 (0.32, 0.93)	0.41 (0.22, 0.62)	58	0.51 (0.35, 0.75)	0.59 (0.42, 0.82)	0.57 (0.39, 0.73)
X-11838	8	0.76 (0.22, 0.57)	(.,.)	0.00 (.,.)	60	1.01 (0.55, 1.87)	0.49 (0.13, 1.75)	0.19 (0.04, 0.53)	58	0.56 (0.38, 0.81)	0.32 (0.17, 0.62)	0.25 (0.08, 0.55)
X-11843	30	0.29 (0.20, 0.43)	0.51 (0.41, 0.64)	0.76 (0.58, 0.88)	60	0.34 (0.24, 0.48)	0.83 (0.72, 0.95)	0.86 (0.78, 0.91)	59	0.30 (0.21, 0.41)	0.81 (0.72, 0.91)	0.88 (0.81, 0.93)
X-11849	8	0.32 (0.13, 0.76)	0.75 (0.52, 1.09)	0.85 (0.55, 0.96)	60	0.94 (0.51, 1.72)	0.88 (0.46, 1.68)	0.47 (0.28, 0.66)	59	0.82 (0.46, 1.50)	1.24 (0.83, 1.84)	0.69 (0.55, 0.81)
X-11850	32	0.28 (0.19, 0.43)	0.71 (0.60, 0.83)	0.86 (0.74, 0.93)	60	0.35 (0.24, 0.51)	1.04 (0.92, 1.18)	0.90 (0.84, 0.94)	58	0.29 (0.21, 0.41)	0.87 (0.78, 0.97)	0.90 (0.84, 0.94)
X-11853	57	0.18 (0.14, 0.22)	0.17 (0.13, 0.21)	0.46 (0.27, 0.66)	60	0.19 (0.16, 0.24)	0.16 (0.13, 0.21)	0.42 (0.24, 0.63)	60	0.19 (0.16, 0.24)	0.16 (0.13, 0.21)	0.42 (0.24, 0.63)
X-11860	60	0.21 (0.17, 0.26)	0.09 (0.06, 0.15)	0.16 (0.03, 0.54)	60	0.21 (0.17, 0.26)	0.09 (0.06, 0.15)	0.16 (0.03, 0.54)	59	0.20 (0.16, 0.24)	0.11 (0.07, 0.16)	0.24 (0.08, 0.54)
X-11880	58	0.16 (0.13, 0.20)	0.41 (0.38, 0.45)	0.87 (0.79, 0.92)	60	0.18 (0.14, 0.22)	0.40 (0.36, 0.45)	0.84 (0.74, 0.90)	60	0.18 (0.14, 0.22)	0.40 (0.36, 0.45)	0.84 (0.74, 0.90)
X-11904	4	1.11 (0.07, 18.50)	1.26 (0.11, 15.02)	0.56 (0.08, 0.95)	60	0.35 (0.26, 0.47)	0.43 (0.34, 0.54)	0.60 (0.43, 0.74)	59	0.19 (0.16, 0.24)	0.12 (0.09, 0.17)	0.29 (0.12, 0.56)
X-11905	19	0.40 (0.23, 0.70)	0.39 (0.22, 0.68)	0.48 (0.18, 0.79)	60	0.47 (0.34, 0.66)	0.40 (0.27, 0.59)	0.42 (0.23, 0.63)	58	0.47 (0.33, 0.65)	0.36 (0.23, 0.55)	0.37 (0.19, 0.60)
X-12038	60	0.22 (0.18, 0.28)	0.31 (0.26, 0.37)	0.66 (0.51, 0.79)	60	0.22 (0.18, 0.28)	0.31 (0.26, 0.37)	0.66 (0.51, 0.79)	60	0.22 (0.18, 0.28)	0.31 (0.26, 0.37)	0.66 (0.51, 0.79)
X-12039	21	0.46 (0.23, 0.91)	1.00 (0.73, 1.38)	0.83 (0.65, 0.92)	60	0.52 (0.33, 0.82)	1.21 (1.00, 1.47)	0.85 (0.76, 0.91)	58	0.36 (0.24, 0.53)	1.06 (0.93, 1.21)	0.90 (0.84, 0.94)
X-12051	60	0.47 (0.34, 0.65)	0.23 (0.11, 0.45)	0.19 (0.04, 0.53)	60	0.47 (0.34, 0.65)	0.23 (0.11, 0.45)	0.19 (0.04, 0.53)	60	0.47 (0.34, 0.65)	0.23 (0.11, 0.45)	0.19 (0.04, 0.53)
X-12056	33	1.81 (0.44, 7.41)	0.37 (0.00, 386.0)	0.04 (0.00, 1.00)	60	1.37 (0.62, 3.04)	0.31 (0.01, 10.78)	0.05 (0.00, 0.93)	58	0.93 (0.53, 1.65)	0.20 (0.01, 2.86)	0.04 (0.00, 0.96)
X-12063	37	0.17 (0.12, 0.24)	0.59 (0.53, 0.64)	0.92 (0.86, 0.96)	60	0.19 (0.14, 0.25)	0.70 (0.65, 0.75)	0.93 (0.89, 0.96)	60	0.19 (0.14, 0.25)	0.70 (0.65, 0.75)	0.93 (0.89, 0.96)
X-12092	59	0.30 (0.22, 0.40)	0.67 (0.59, 0.77)	0.84 (0.74, 0.90)	60	0.30 (0.22, 0.40)	0.67 (0.59, 0.77)	0.84 (0.74, 0.90)	58	0.21 (0.16, 0.28)	0.74 (0.68, 0.80)	0.92 (0.88, 0.95)
X-12093	30	0.40 (0.26, 0.60)	0.28 (0.16, 0.51)	0.34 (0.11, 0.68)	60	0.40 (0.30, 0.54)	0.29 (0.19, 0.44)	0.34 (0.16, 0.58)	60	0.40 (0.30, 0.54)	0.29 (0.19, 0.44)	0.34 (0.16,

X-12205	60	0.20 (0.16, 0.25)	0.17 (0.13, 0.22)	0.43 (0.24, 0.64)	60	0.20 (0.16, 0.25)	0.17 (0.13, 0.22)	0.43 (0.24, 0.64)	60	0.20 (0.16, 0.25)	0.17 (0.13, 0.22)	0.43 (0.24, 0.64)
X-12212	3	0.18 (0.07, 0.45)	0.08 (0.01, 0.64)	0.16 (0.00, 1.00)	60	2.02 (0.64, 6.36)	(.,.)	0.00 (.,.)	59	0.67 (0.44, 1.02)	0.08 (0.00, 2.75)	0.01 (0.00, 1.00)
X-12216	16	0.16 (0.11, 0.23)	0.16 (0.11, 0.24)	0.52 (0.21, 0.82)	60	0.21 (0.16, 0.26)	0.31 (0.26, 0.36)	0.69 (0.55, 0.81)	59	0.18 (0.15, 0.23)	0.31 (0.28, 0.36)	0.75 (0.62, 0.84)
X-12217	31	0.64 (0.36, 1.14)	0.47 (0.21, 1.03)	0.35 (0.12, 0.68)	60	0.69 (0.44, 1.10)	0.68 (0.42, 1.09)	0.49 (0.31, 0.68)	59	0.43 (0.31, 0.61)	0.61 (0.48, 0.78)	0.66 (0.51, 0.79)
X-12230	30	0.42 (0.27, 0.65)	0.41 (0.27, 0.65)	0.50 (0.25, 0.74)	60	0.70 (0.45, 1.11)	0.45 (0.22, 0.91)	0.29 (0.11, 0.56)	58	0.46 (0.32, 0.65)	0.56 (0.42, 0.75)	0.60 (0.44, 0.75)
X-12231	35	0.70 (0.39, 1.26)	0.41 (0.15, 1.11)	0.26 (0.06, 0.64)	60	0.65 (0.42, 1.01)	0.57 (0.35, 0.94)	0.44 (0.25, 0.64)	58	0.45 (0.32, 0.64)	0.46 (0.33, 0.64)	0.50 (0.32, 0.69)
X-12244	60	0.20 (0.16, 0.25)	0.20 (0.16, 0.25)	0.51 (0.33, 0.69)	60	0.20 (0.16, 0.25)	0.20 (0.16, 0.25)	0.51 (0.33, 0.69)	60	0.20 (0.16, 0.25)	0.20 (0.16, 0.25)	0.51 (0.33, 0.69)
X-12437	32	0.33 (0.23, 0.47)	0.01 (0.00, 946.4)	0.00 (0.00, 1.00)	60	0.44 (0.32, 0.59)	0.12 (0.04, 0.37)	0.07 (0.00, 0.80)	60	0.44 (0.32, 0.59)	0.12 (0.04, 0.37)	0.07 (0.00, 0.80)
X-12442	60	0.33 (0.25, 0.43)	0.35 (0.27, 0.45)	0.53 (0.35, 0.70)	60	0.33 (0.25, 0.43)	0.35 (0.27, 0.45)	0.53 (0.35, 0.70)	59	0.26 (0.21, 0.34)	0.35 (0.29, 0.43)	0.64 (0.48, 0.77)
X-12456	10	0.21 (0.12, 0.36)	0.21 (0.12, 0.36)	0.50 (0.13, 0.87)	60	0.25 (0.20, 0.32)	0.27 (0.21, 0.34)	0.53 (0.35, 0.70)	59	0.22 (0.17, 0.28)	0.29 (0.25, 0.35)	0.64 (0.48, 0.77)
X-12465	47	0.54 (0.36, 0.81)	0.27 (0.12, 0.61)	0.21 (0.05, 0.58)	60	0.56 (0.38, 0.81)	0.37 (0.21, 0.65)	0.31 (0.13, 0.56)	59	0.46 (0.33, 0.64)	0.25 (0.14, 0.46)	0.23 (0.07, 0.54)
X-12510	55	0.29 (0.22, 0.39)	0.42 (0.35, 0.51)	0.67 (0.51, 0.80)	60	0.30 (0.23, 0.40)	0.48 (0.40, 0.57)	0.71 (0.58, 0.82)	59	0.29 (0.22, 0.38)	0.51 (0.44, 0.60)	0.76 (0.64, 0.85)
X-12511_201	53	0.28 (0.21, 0.37)	0.39 (0.32, 0.48)	0.66 (0.50, 0.79)	60	0.30 (0.23, 0.40)	0.45 (0.38, 0.54)	0.69 (0.54, 0.80)	59	0.27 (0.21, 0.35)	0.45 (0.38, 0.53)	0.73 (0.60, 0.84)
X-12644	60	0.25 (0.20, 0.32)	0.31 (0.26, 0.38)	0.61 (0.45, 0.76)	60	0.25 (0.20, 0.32)	0.31 (0.26, 0.38)	0.61 (0.45, 0.76)	60	0.25 (0.20, 0.32)	0.31 (0.26, 0.38)	0.61 (0.45, 0.76)
X-12645	19	0.35 (0.22, 0.58)	0.26 (0.14, 0.51)	0.36 (0.09, 0.75)	60	0.81 (0.49, 1.33)	0.46 (0.19, 1.11)	0.25 (0.08, 0.54)	60	0.81 (0.49, 1.33)	0.46 (0.19, 1.11)	0.25 (0.08, 0.54)
X-12696	58	0.16 (0.13, 0.19)	0.23 (0.20, 0.26)	0.68 (0.53, 0.80)	60	0.16 (0.13, 0.20)	0.24 (0.21, 0.28)	0.68 (0.53, 0.80)	60	0.16 (0.13, 0.20)	0.24 (0.21, 0.28)	0.68 (0.53, 0.80)
X-12715	3	0.27 (0.09, 0.77)	0.13 (0.01, 1.18)	0.18 (0.00, 1.00)	60	0.30 (0.23, 0.39)	0.36 (0.29, 0.45)	0.59 (0.43, 0.74)	59	0.25 (0.20, 0.32)	0.34 (0.28, 0.41)	0.65 (0.49, 0.78)
X-12717	26	0.91 (0.37, 2.26)	0.97 (0.41, 2.28)	0.53 (0.27, 0.77)	60	1.12 (0.53, 2.38)	1.39 (0.76, 2.55)	0.60 (0.44, 0.75)	59	0.68 (0.40, 1.15)	1.22 (0.91, 1.64)	0.76 (0.64, 0.85)
X-12728	17	1.30 (0.32, 5.31)	(.,.)	0.00 (.,.)	60	1.67 (0.62, 4.47)	0.88 (0.14, 5.71)	0.22 (0.06, 0.53)	58	1.58 (0.60, 4.18)	1.18 (0.32, 4.34)	0.36 (0.18, 0.60)
X-12729	0	(.,.)	(.,.)	(.,.)	60	(.,.)	(.,.)	(.,.)	60	(.,.)	(.,.)	(.,.)
X-12734	20	0.00 (.,.)	4.45 (0.06, 350.6)	0.00 (.,.)	60	1.87 (0.63, 5.55)	0.65 (0.03, 14.83)	0.11 (0.01, 0.62)	59	0.70 (0.44, 1.10)	0.51 (0.27, 0.94)	0.35 (0.16, 0.59)
X-12741	1	(.,.)	(.,.)	(.,.)	60	0.01 (0.01, 0.01)	0.00 (0.00, .)	0.00 (0.00, .)	59	(.,.)	(.,.)	(.,.)
X-12759	10	0.17 (0.10, 0.30)	0.42 (0.33, 0.53)	0.86 (0.61, 0.96)	60	0.41 (0.21, 0.79)	2.30 (2.05, 2.58)	0.97 (0.95, 0.98)	59	0.41 (0.20, 0.85)	2.60 (2.32, 2.91)	0.98 (0.96, 0.99)
X-12761	3	4.89 (0.00, 984E4)	6.67 (0.00, 278E3)	0.65 (0.10, 0.97)	60	1.37 (0.51, 3.66)	2.28 (1.26, 4.11)	0.74 (0.60, 0.83)	59	0.16 (0.12, 0.21)	0.84 (0.79, 0.89)	0.97 (0.94, 0.98)
X-12776	52	0.37 (0.27, 0.50)	0.23 (0.14, 0.37)	0.27 (0.10, 0.57)	60	0.44 (0.32, 0.60)	0.17 (0.08, 0.38)	0.13 (0.02, 0.58)	60	0.44 (0.32, 0.60)	0.17 (0.08, 0.38)	0.13 (0.02, 0.58)
X-12798	59	0.16 (0.13, 0.20)	0.46 (0.43, 0.50)	0.90 (0.83, 0.94)	60	0.16 (0.13, 0.20)	0.48 (0.44, 0.52)	0.90 (0.84, 0.94)	60	0.16 (0.13, 0.20)	0.48 (0.44, 0.52)	0.90 (0.84, 0.94)
X-12816	29	0.56 (0.27, 1.17)	1.44 (1.08, 1.92)	0.87 (0.75, 0.94)	60	0.72 (0.36, 1.44)	2.08 (1.64, 2.64)	0.89 (0.83, 0.93)	59	0.63 (0.38, 1.04)	1.15 (0.87, 1.51)	0.77 (0.65, 0.86)
X-12829	31	0.48 (0.29, 0.79)	0.55 (0.36, 0.85)	0.56 (0.33, 0.77)	60	0.52 (0.35, 0.77)	0.74 (0.56, 0.97)	0.67 (0.51, 0.79)	58	0.41 (0.29, 0.58)	0.65 (0.52, 0.81)	0.71 (0.57, 0.82)
X-12830	19	0.45 (0.25, 0.83)	0.51 (0.30, 0.88)	0.56 (0.27, 0.82)	60	0.47 (0.34, 0.67)	0.47 (0.33, 0.67)	0.50 (0.32, 0.68)	58	0.43 (0.31, 0.61)	0.59 (0.46, 0.76)	0.66 (0.50, 0.78)
X-12844	59	0.16 (0.13, 0.20)	0.28 (0.25, 0.32)	0.75 (0.63, 0.85)	60	0.16 (0.13, 0.20)	0.30 (0.27, 0.34)	0.77 (0.65, 0.86)	60	0.16 (0.13, 0.20)	0.30 (0.27, 0.34)	0.77 (0.65, 0.86)
X-12846	41	0.16 (0.12, 0.22)	0.44 (0.40, 0.49)	0.88 (0.79, 0.93)	60	0.20 (0.15, 0.25)	0.51 (0.46, 0.56)	0.87 (0.80, 0.92)	60	0.20 (0.15, 0.25)	0.51 (0.46, 0.56)	0.87 (0.80, 0.92)
X-12851	33	0.67 (0.32, 1.37)	1.31 (0.91, 1.89)	0.79 (0.64, 0.89)	60	0.80 (0.41, 1.55)	1.78 (1.32, 2.40)	0.83 (0.74, 0.90)	57	0.50 (0.28, 0.89)	1.80 (1.53, 2.11)	0.93 (0.88, 0.96)
X-12855	35	0.44 (0.29, 0.67)	0.39 (0.24, 0.63)	0.44 (0.21, 0.70)	60	0.47 (0.33, 0.67)	0.54 (0.39, 0.73)	0.56 (0.39, 0.72)	60	0.47 (0.33, 0.67)	0.54 (0.39, 0.73)	0.56 (0.39, 0.72)
X-13429	41	0.41 (0.28, 0.60)	0.46 (0.33, 0.65)	0.56 (0.35, 0.75)	60	0.49 (0.34, 0.71)	0.62 (0.47, 0.83)	0.62 (0.45, 0.76)	59	0.42 (0.30, 0.59)	0.61 (0.48, 0.77)	0.67 (0.52, 0.80)
X-13435	60	0.18 (0.14, 0.23)	0.35 (0.32, 0.40)	0.79 (0.68, 0.87)	60	0.18 (0.14, 0.23)	0.35 (0.32, 0.40)	0.79 (0.68, 0.87)	59	0.17 (0.14, 0.21)	0.36 (0.32, 0.40)	0.82 (0.72, 0.89)
X-13478	60	0.11 (0.09, 0.15)	0.65 (0.62, 0.68)	0.97 (0.95, 0.98)	60	0.11 (0.09, 0.15)	0.65 (0.62, 0.68)	0.97 (0.95, 0.98)	60	0.11 (0.09, 0.15)	0.65 (0.62, 0.68)	0.97 (0.95, 0.98)
X-13483	55	0.45 (0.33, 0.62)	0.10 (0.02, 0.43)	0.05 (0.00, 0.93)	60	0.50 (0.36, 0.71)	0.11 (0.02, 0.52)	0.04 (0.00, 0.95)	60	0.50 (0.36, 0.71)	0.11 (0.02, 0.52)	0.04 (0.00, 0.95)
X-13496	58	0.17 (0.14, 0.21)	0.17 (0.13, 0.21)	0.49 (0.30, 0.68)	60	0.19 (0.16, 0.24)	0.17 (0.13, 0.21)	0.43 (0.24, 0.63)	60	0.19 (0.16, 0.24)	0.17 (0.13, 0.21)	0.43 (0.24, 0.63)
X-13619	60	0.23 (0.19, 0.29)	0.03 (0.01, 0.16)	0.02 (0.00, 1.00)	60	0.23 (0.19, 0.29)	0.03 (0.01, 0.16)	0.02 (0.00, 1.00)	60	0.23 (0.19, 0.29)	0.03 (0.01, 0.16)	0.02 (0.00, 1.00)
X-13658	44	0.17 (0.11, 0.24)	0.95 (0.89, 1.01)	0.97 (0.95, 0.98)	60	0.18 (0.13, 0.25)	1.07 (1.01, 1.14)	0.97 (0.96, 0.98)	59	0.15 (0.11, 0.20)	0.93 (0.88, 0.97)	0.98 (0.96, 0.98)
X-13741	31	0.44 (0.27, 0.70)	0.57 (0.40, 0.82)	0.63 (0.40, 0.81)	60	0.58 (0.39, 0.89)	0.71 (0.51, 1.00)	0.60 (0.43, 0.75)	59	0.58 (0.38, 0.89)	0.80 (0.58, 1.09)	0.65 (0.50, 0.78)
X-13835	7	0.21 (0.11, 0.41)	0.18 (0.08, 0.39)	0.42 (0.05, 0.90)	60	0.16 (0.13, 0.20)	0.17 (0.14, 0.21)	0.53 (0.35, 0.70)	59	0.12 (0.10, 0.15)	0.08 (0.06, 0.11)	0.31 (0.13, 0.57)
X-14056	60	0.23 (0.18, 0.29)	0.23 (0.18, 0.29)	0.49 (0.31, 0.68)	60	0.23 (0.18, 0.29)	0.23 (0.18, 0.29)	0.49 (0.31, 0.68)	60	0.23 (0.18, 0.29)	0.23 (0.18, 0.29)	0.49 (0.31, 0.68)
X-14086	40	0.32 (0.23, 0.45)	0.33 (0.24, 0.46)	0.52 (0.30, 0.73)	60	0.34 (0.25, 0.45)	0.46 (0.38, 0.57)	0.65 (0.50, 0.78)	59	0.29 (0.22, 0.38)	0.46 (0.39, 0.55)	0.71 (0.57, 0.82)
X-14189	46	0.45 (0.31, 0.65)	0.35 (0.22, 0.56)	0.39 (0.18, 0.64)	60	0.48 (0.34, 0.67)	0.43 (0.29, 0.63)	0.45 (0.26, 0.65)	59	0.35 (0.26, 0.46)	0.39 (0.30, 0.50)	0.56 (0.38, 0.72)
X-14205	38	0.27 (0.20, 0.37)	0.36 (0.28, 0.45)	0.64 (0.43, 0.80)	60	0.31 (0.24, 0.41)	0.46 (0.38, 0.56)	0.69 (0.54, 0.80)	59	0.30 (0.23, 0.40)	0.48 (0.40, 0.57)	0.72 (0.58, 0.82)
X-14208	51	0.22 (0.17, 0.29)	0.41 (0.36, 0.48)	0.77 (0.64, 0.86)	60	0.24 (0.19, 0.32)	0.54 (0.48, 0.60)	0.83 (0.74, 0.89)	60	0.24 (0.19, 0.32)	0.54 (0.48, 0.60)	0.83 (0.74, 0.89)
X-14216	23	0.28 (0.19, 0.41)	0.22 (0.13, 0.36)	0.38 (0.12, 0.73)	60	0.27 (0.21, 0.35)	0.33 (0.27, 0.41)	0.59 (0.43, 0.74)	58	0.23 (0.18, 0.29)	0.31 (0.27, 0.37)	0.66 (0.50, 0.79)
X-14400	59	0.27 (0.21, 0.35)	0.22 (0.17, 0.30)	0.40 (0.22, 0.62)	60	0.27 (0.21, 0.35)	0.24 (0.18, 0.31)	0.43 (0.25, 0.64)	60	0.27 (0.21, 0.35)	0.24 (0.18, 0.31)	0.43 (0.25, 0.64)
X-14473	44	0.32 (0.24, 0.44)	0.23 (0.15, 0.36)	0.35 (0.14, 0.63)	60	0.36 (0.27, 0.48)	0.39 (0.30, 0.51)	0.54 (0.36, 0.71)	59	0.33 (0.25, 0.44)	0.42 (0.33, 0.52)	0.61 (0.45, 0.76)
X-14478	60	0.36 (0.27, 0.49)	0.44 (0.35, 0.56)	0.59 (0.43, 0.74)	60	0.36 (0.27, 0.49)	0.44 (0.35, 0.56)	0.59 (0.43, 0.74)	59	0.27 (0.21, 0.35)	0.43 (0.37, 0.51)	0.72 (0.58, 0.82)
X-14532	13	0.27 (0.15, 0.46)	0.39 (0.27, 0.57)	0.69 (0.37, 0.89)	60	0.33 (0.25, 0.44)	0.49 (0.40, 0.59)	0.69 (0.54, 0.80)	59	0.26 (0.20, 0.35)	0.54 (0.47, 0.61)	

X-14662	22	0.20 (0.13, 0.32)	0.74 (0.65, 0.84)	0.93 (0.85, 0.97)	60	0.46 (0.31, 0.68)	0.93 (0.77, 1.13)	0.81 (0.70, 0.88)	58	0.30 (0.21, 0.43)	0.98 (0.88, 1.09)	0.91 (0.86, 0.95)
X-14939	57	0.48 (0.33, 0.70)	0.60 (0.45, 0.81)	0.61 (0.44, 0.76)	60	0.49 (0.34, 0.70)	0.63 (0.48, 0.84)	0.63 (0.47, 0.76)	59	0.38 (0.28, 0.52)	0.54 (0.44, 0.67)	0.68 (0.52, 0.80)
X-15222	60	0.14 (0.12, 0.17)	0.19 (0.17, 0.22)	0.65 (0.49, 0.78)	60	0.14 (0.12, 0.17)	0.19 (0.17, 0.22)	0.65 (0.49, 0.78)	60	0.14 (0.12, 0.17)	0.19 (0.17, 0.22)	0.65 (0.49, 0.78)
X-15479	55	0.26 (0.20, 0.34)	0.39 (0.33, 0.47)	0.69 (0.54, 0.81)	60	0.27 (0.21, 0.35)	0.44 (0.38, 0.52)	0.73 (0.60, 0.83)	59	0.25 (0.19, 0.32)	0.47 (0.41, 0.54)	0.79 (0.67, 0.87)
X-15483	32	0.20 (0.16, 0.25)	. (., .)	0.00 (., .)	60	0.28 (0.23, 0.34)	. (., .)	0.00 (., .)	59	0.22 (0.18, 0.27)	0.06 (0.03, 0.14)	0.08 (0.00, 0.73)
X-15486	41	0.50 (0.32, 0.76)	0.50 (0.32, 0.77)	0.50 (0.29, 0.72)	60	0.49 (0.34, 0.71)	0.57 (0.42, 0.78)	0.57 (0.40, 0.73)	59	0.41 (0.30, 0.56)	0.50 (0.38, 0.65)	0.60 (0.43, 0.75)
X-15492	56	0.23 (0.18, 0.30)	0.30 (0.25, 0.37)	0.63 (0.46, 0.77)	60	0.23 (0.18, 0.30)	0.33 (0.28, 0.39)	0.67 (0.52, 0.79)	60	0.23 (0.18, 0.30)	0.33 (0.28, 0.39)	0.67 (0.52, 0.79)
xanthine	48	0.48 (0.33, 0.69)	0.07 (0.00, 0.92)	0.02 (0.00, 1.00)	60	0.52 (0.37, 0.73)	0.24 (0.11, 0.51)	0.18 (0.04, 0.54)	60	0.52 (0.37, 0.73)	0.24 (0.11, 0.51)	0.18 (0.04, 0.54)
xylitol	3	0.15 (0.08, 0.29)	. (., .)	0.00 (., .)	60	0.40 (0.30, 0.53)	0.16 (0.08, 0.33)	0.15 (0.02, 0.55)	58	0.32 (0.24, 0.41)	0.15 (0.09, 0.26)	0.19 (0.05, 0.54)