Table 1. Assignment of resonances in the 700 MHz ^{1}H HRMAS-NMR spectrum of *C. elegans* based on the literature (1)

Metabolite	Moieties (key)	Chemical shift (multiplicity)
Cholesterol	C18 (1) and (2)	0.59 (m), 0.67 (m)
Fatty acids	$C\underline{H}_3(CH_2)_n$(3), $C\underline{H}_3CH_2CH_2C$=C(4), $C\underline{H}_3CH_2$(5), $CH_3CH_2C\underline{H}_2$(16), $C\underline{H}_2CH_2CH_2CO$(17), $C\underline{H}_2CH_2CH_2CO$(19), $C\underline{H}_2CH_2CO$(20), $C\underline{H}_2CH_2C$=C(24)	0.89(m), 0.91(m) 0.93(m), 1.17(m) 1.29(m), 1.34(m) 1.41(m), 1.60(m)
Isoleucine	δCH_3(6), βCH_3(12), βCH(31), αCH(83)	0.94(t), 1.01(d), 1.99(m),3.71(d)
Leucine	δCH_3(7), δ'CH_3(8), βCH_2-γCH(28), αCH(84)	0.95(d), 0.96(d), 1.73(m), 3.74(m)
α-hydroxy-*N*-valerate	CH_3(9)	0.97(m)
Valine	CH_3(10), CH_3(14), βCH(39), αCH(79)	0.99(d), 1.05(d), 2.26(m), 3.62(d)
Lactate	CH_3(18)	1.33(m)
Penicillamine	CH_3(21)	1.46(s)
Alanine	CH_3(22), αCH(87)	1.48(d), 3.79(q)
Saccharopine	Hδ and Hβii(23), $C\underline{H}_2$COOH(37)	1.53(m), 2.19(m)
α-keto-β-methyl-*N*-valerate	CH_2(25), CH_2(27)	1.64(m), 1.70(m)
Arginine	γCH_2(26), βCH_2(30), αCH(86)	1.68(m), 1.92(m), 3.78(m)
Lysine	βCH2(29), εCH_2(57), αCH(85)	1.84(m), 3.03(t), 3.77(m)
Proline	βCH_2(32), δCH_2(72), αCH(96)	2.03(m), 3.38(m), 4.13(m)
N-acetyl-glutamate	CH_3(33)	2.05(s)
Isovalerate	CH_2(34)	2.06(d)

Glutamate/Glutamine	βCH_2(35)	2.08(m)
Methionine	S-CH_3(36), S-CH_2(47), αCH(89)	2.14(m), 2.64(m), 3.85(m)
Homocysteine	βCH_2(38)	2.22(m)
Glutamate	γCH_2(40)	2.35(m)
Pyroglutamate	CH_2 (41), CH_2(45)	2.41(m), 2.49(m)
Glutamine	γCH_2(42)	2.46(d)
Succinate	CH_2(43)	2.46(s)
β-alanine	C$\underline{H_2}$COOH(46), NCH_2(66)	2.55(m), 3.18(m)
Aspartate	βCH_2(48) and (53)	2.68(d), 2.82(dd)
N-acetyl-L-aspartate	CH_2(49)	2.70(d)
α-ketobutyrate	CH_2(50)	2.73(m)
Dimethylamine	CH_3(51)	2.74(s)
Sarcosine	CH_3(52)	2.76(s)
Asparagine	βCH_2(54) and (56)	2.87(d), 2.97(d)
Melatonin	CH_2CH_2NH(55)	2.94(m)
Tyrosine	βCH_2(58), βCH_2 (67) aromatic(111)	3.05(d), 3.20(d), 6.9 (m) and 7.19(m)
Ornithine	δCH_2(59)	3.08(m)
Indole-3-lactate	CH_2(60)	3.10(m)
Cysteine	CH_2(61)	3.11(m)
Phenylalanine	βCH_2(62), βCH2(70), aromatic(115)	3.13(m), 3.29(m), 7.42(m)
Histidine	βCH_2(63), αCH(93)	3.14(m), 3.97(dd)
Homocarnosine	αCH_2(55)	3.16(m)

β-glucose	H_2(68), H_4(73), H_3(75), CH_2-C6(91), H_1(105)	3.25(m), 3.41(t), 3.48(t), 3.92(dd), 4.64(d)
Trimethylamine-*N*-oxyde (TMAO)	CH_3(69)	3.27(s)
5-methoxytriptamine	CH_2NH_2(70)	3.33(m)
α-glucose	H_4(74), H_2(76), CH_2-C6(82), H_1(107)	3.42(t), 3.52(dd), 3.70(dd), 5.23(d)
Glycerol	CH_2(77), CH_2(80), C2-H(90)	3.56(dd), 3.65(dd), 3.87(m)
Threonine	αCH(78), βCH(98)	3.60(d), 4.26(m)
Choline in lipids	NCH_2(81)	3.67(m)
Glycerate	CH_2(88)	3.84(d)
Serine	βCH_2(92), βCH_2(94),	3.96(dd), 4.00(dd)
Glyceryl of lipids	CH_2OCOR(95), CHOCOR(106)	4.09(m), 5.20(m)
Inosine	H_5'(97), H_4'(102), H_2'(110), H_8(119), H_2(120)	4.23(m), 4.44(m), 6.10(d), 8.23(s), 8.35(s)
Unknown	(99)	4.34(m)
Unknown	(100)	4.39(m)
Dihydroxyacetone	CH_2(101)	4.42(s)
Folate	CH_2(103)	4.53(s)
β-galactose	H_1(104)	4.57(d)
Unsaturated lipids	=C<u>H</u>CH_2CH_2(108)	5.33(m)
Uracil	H_5(109)	5.80(d)
Indole	H_6(112), H_7(116)	7.22(t), 7.53(d)
Phenylacetate	H_2, H_4 and H_6(113)	7.33(t)

β-phenylpyruvate	H_4(114)	7.38(t)
Anserine	H_2(117)	7.97(s)
Adenine	H_8(118)	8.19(s)
Formate	CH(121)	8.46(s)
Picolinate	H_6(122)	8.52(s)

1. Nicholson JK, Foxall PJD, Spraul M, Farrant RD, Lindon JC (1995) *Anal Chem* 67:793-811.