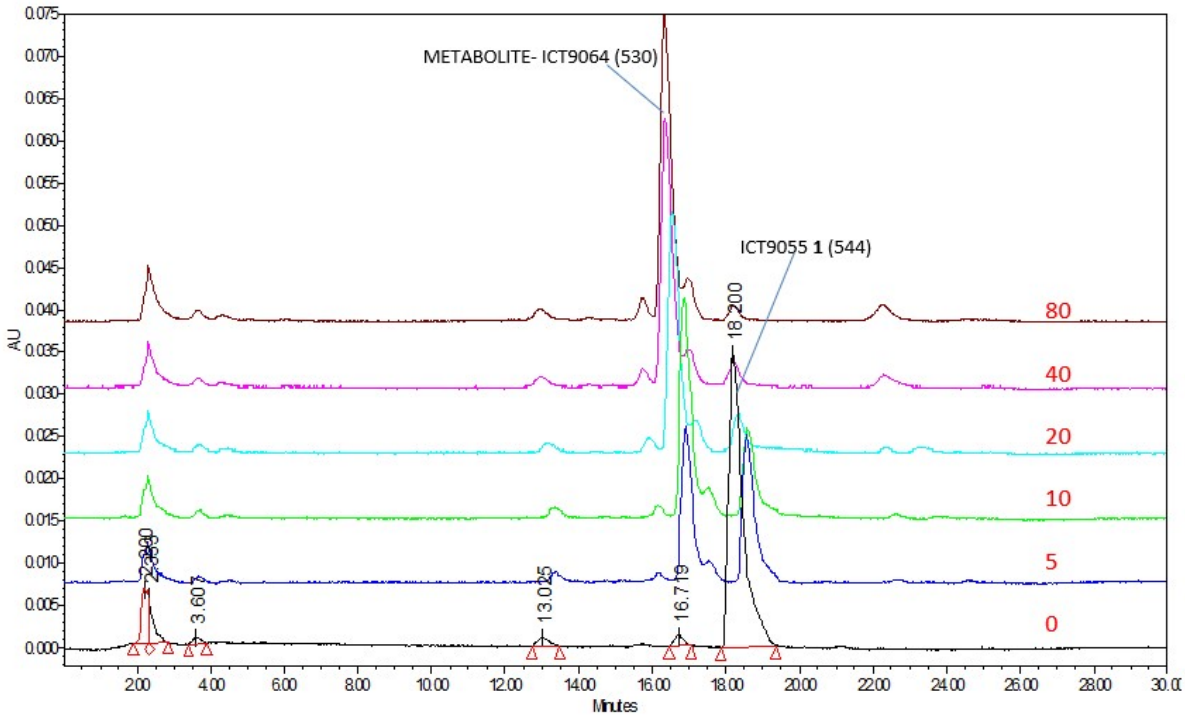
Table S1 Cytotoxicity of compounds on the cell lines used in the functional assays (measured by MTT assay). Cells (2000 cells/well for Sk-Mel-2; 1000 cells/well for U87MG) were incubated for 96 hours at 37 °C in a total volume of 200 µL/well (180 µL medium + 20 µL test compound solution). After 96 hours, the medium was replaced by fresh medium containing 0.5 mg/ml (end conc.) MTT per well, incubated for 4 h then the plate processed and read as described in Sutherland et al.[1]

Compound	IC_{50}/µM Sk-Mel-2	U87MG IC_{50}/µM
17 ICT9097	> 50	70.1 ± 18.8
18 ICT 9096	-	59.2 ± 16.9
19 ICT 9100	> 50	-
20ICT 9093	> 50	37.9 ± 9.1
21 ICT 9091	> 50	30.9 ± 8.1
22 ICT 9092	> 50	46.4 ± 3.5
23 ICT 9101	> 50	-
24ICT 9094	31.9 ± 2.0	46.7 ± 7.6
28 ICT 9082	> 100	32.5 ± 14.1
29 ICT 9084	> 50	36.2 ± 12.4
30 ICT 9081	> 10	160.8 ± 61.0
31 ICT 9083	> 100	-
32 ICT 9085	80.0 ± 19.6	40.9 ± 11.5
33 ICT 9087	40.0 ± 2.0	35.5 ± 2.0
34 ICT 9088	97.1 ± 3.2	51.3 ± 1.9
35 ICT 9089	15.2 ± 5.5	-
37ICT 9098	> 50	-
38 ICT 9102	> 50	-
39 ICT 9099	35.2 ± 6.5	-
40 ICT 9103	> 50	-
53 ICT 9072	33.5 ± 8.4	36.9 ± 8.0
54 ICT 9073	33.0 ± 10.5	18.9 ± 2.6
1 ICT9055	9.6 ± 5.7	36.9 ± 11.7
cRGDfV	42.5 ± 1.8	69.2 ± 25.5

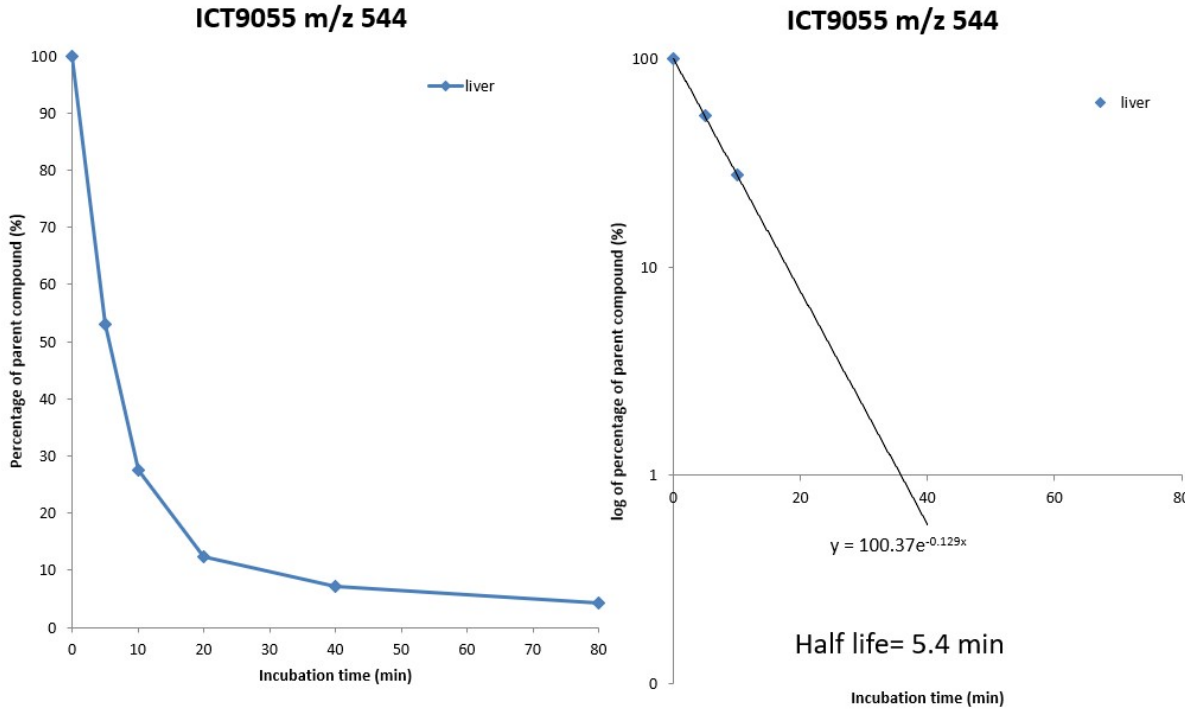
1. M. Sutherland, A. Gordon, F. O. Al-Shammari, A. Throup, A. Cilia La Corte, H. Philippou, S. D. Shnyder, L. H. Patterson and H. M. Sheldrake, *Cancers*, 2023, **15**, 4023.

Metabolic stability of ICT9055 (1) and its free acid metabolite ICT9064

A



B



C

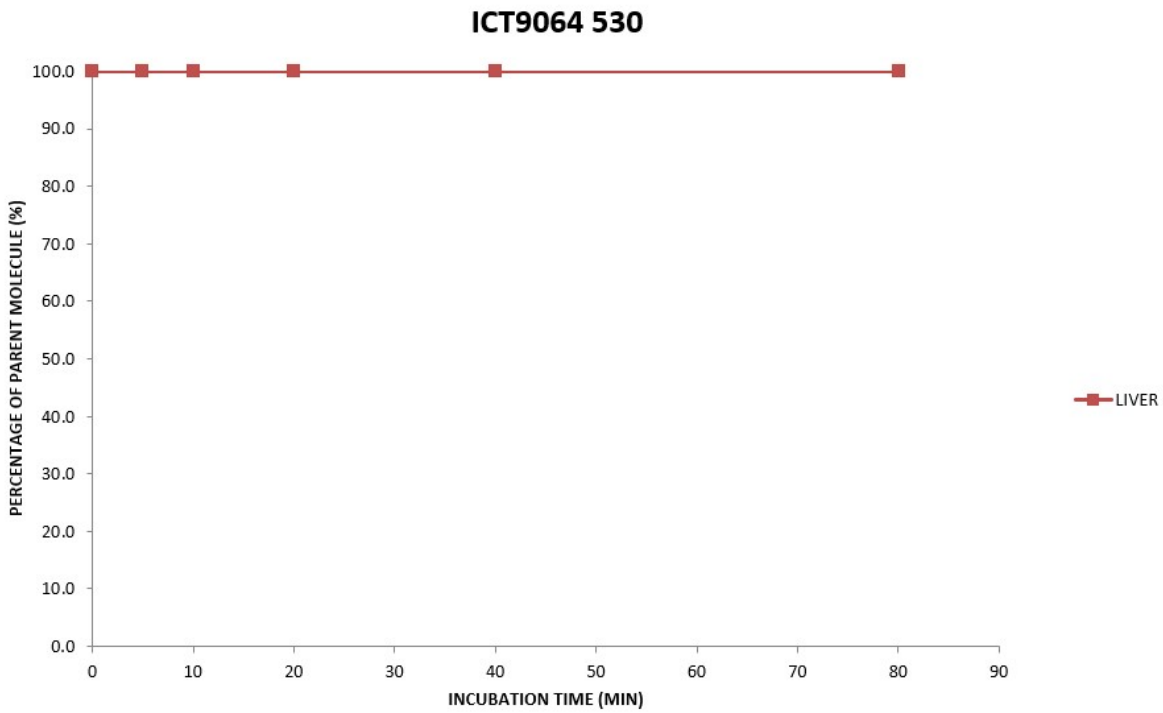
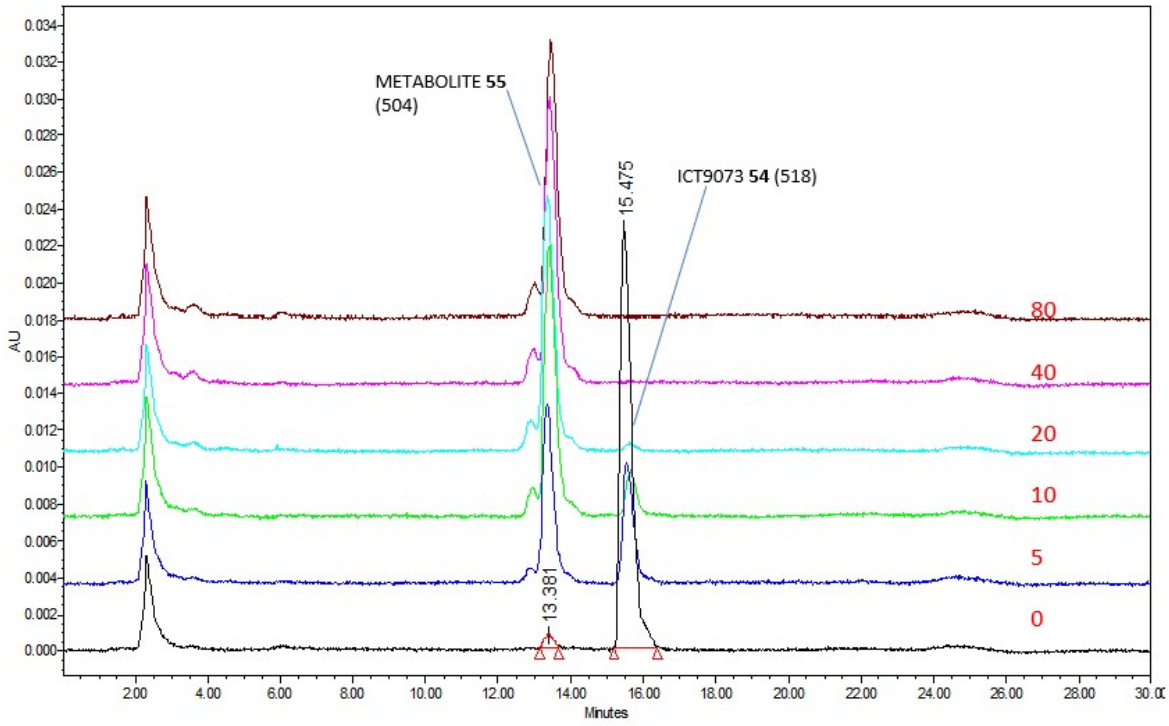


Figure S2: A. Timecourse of conversion of methyl ester **1** (ICT9055) to carboxylic acid (ICT9064) in mouse liver homogenate. B. Determination of half-life of **1** (ICT9055) **i**n mouse liver homogenate. C. The metabolite, carboxylic acid (ICT9064) is highly stable in liver, with a half life of >80 minutes.

A



B

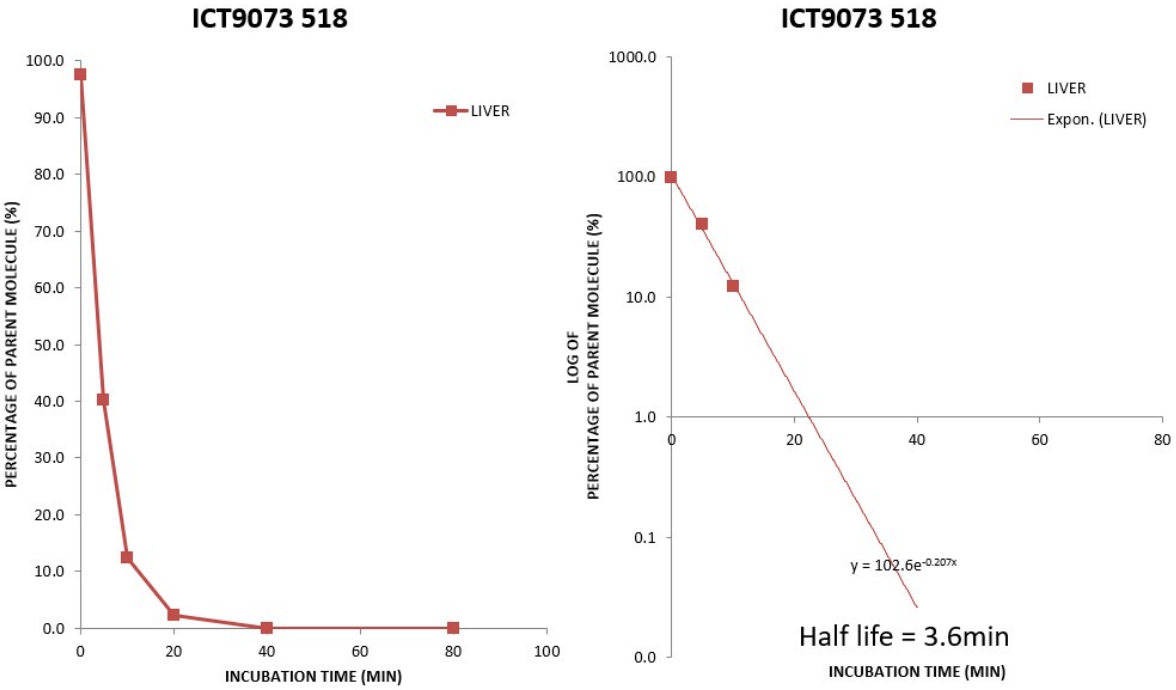


Figure S3. A. Timecourse of conversion of methyl ester **54** (ICT9073) to carboxylic acid **55** in mouse liver homogenate. The metabolite appears to be stable in liver. B. Determination of half-life of **54** in mouse liver homogenate.