



Sintesis, *Molecular Docking* dan Aktivitas Sitotoksik Senyawa Analog Kalkon Berbasis Alfa Tetralone terhadap Sel Kanker Payudara MCF-7

Synthesis, Molecular Docking, and Cytotoxic Activity of Alpha Tetralone Based Chalcone Analogue Compounds against MCF-7 Breast Cancer Cells

Agung Rahmadani^{1,*}, Indriana Tasya¹, Wahyu Yunita Lestari¹, Nurdianah Abdul Kadir¹, Mitha Saputri¹, Farah Erika¹, Usman¹, Sukemi¹, Hanggara Arifian², Supriatno Salam², Herman², Laode Rijai²

¹Program Studi Sarjana Pendidikan Kimia, Fakultas Keguruan dan Ilmu Pendidikan, Universitas Mulawarman, Samarinda, 75123, Indonesia

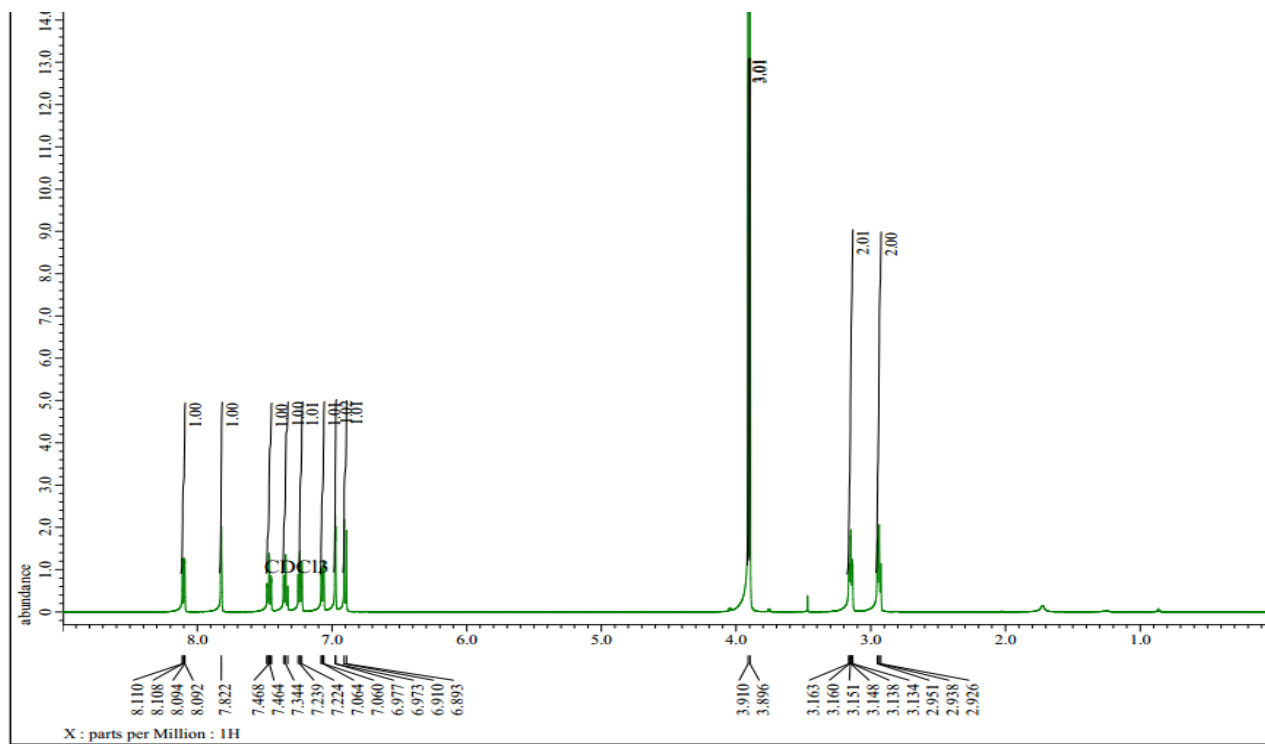
²Laboratorium Penelitian dan Pengembangan Kefarmasian "Farmaka Tropis", Fakultas Farmasi, Universitas Mulawarman, Samarinda, Kalimantan Timur, Indonesia

*Email Korespondensi: agungrahmadani@fkip.unmul.ac.id

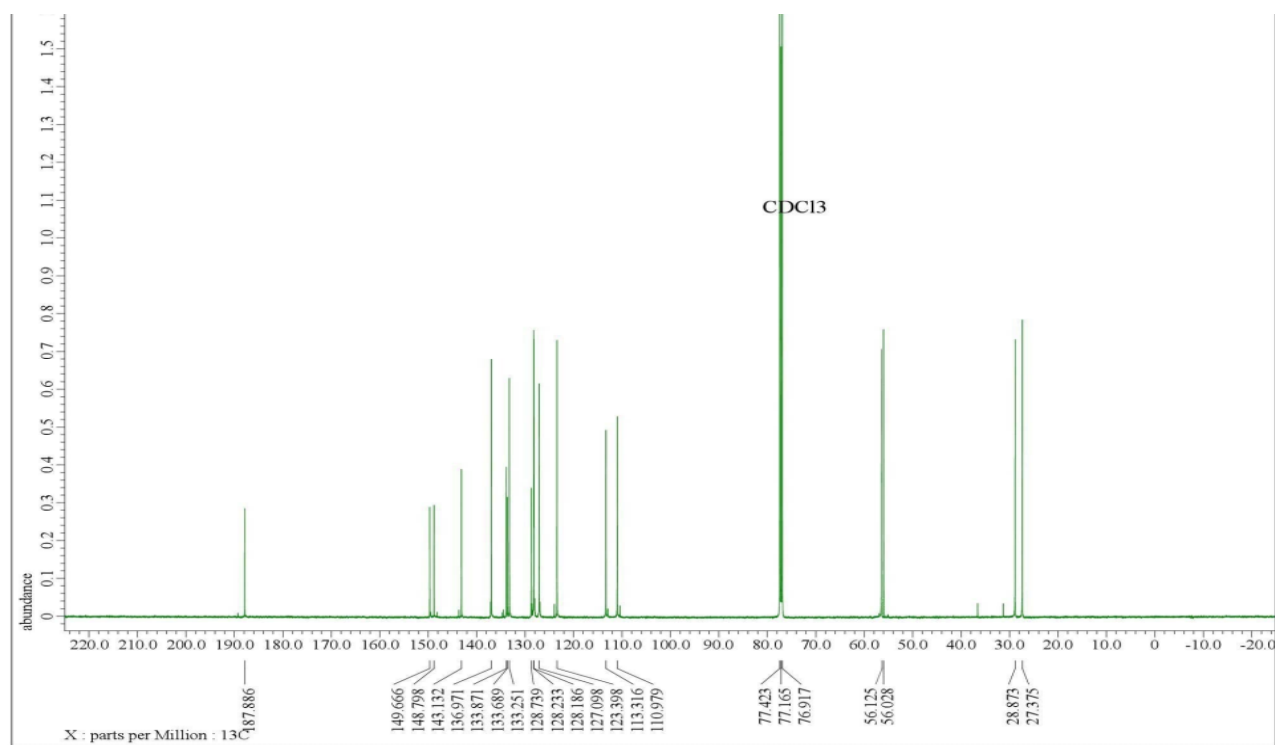
Data Pendukung

Daftar Gambar

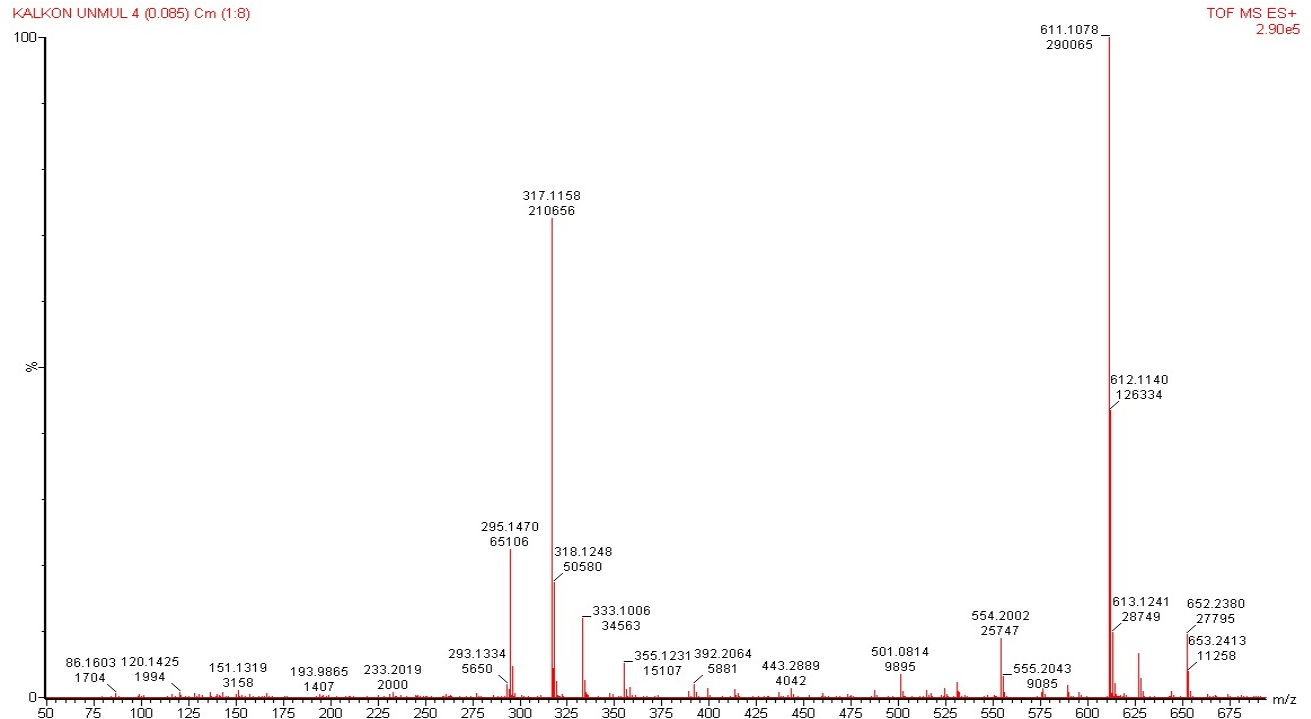
Gambar	Isi	Halaman
S1	Spektrum $^1\text{H-NMR}$ (500 MHz, CDCl_3) Senyawa Kalkon 1	3
S2	Spektrum $^{13}\text{C-NMR}$ (125 MHz, CDCl_3) Senyawa Kalkon 1	4
S3	Spektrum massa HR-TOF-MS (ES+) Senyawa Kalkon 1	5
S4	<i>Single Mass Analysis</i> Senyawa Kalkon 1	5
S5	Spektrum FTIR Senyawa Kalkon 1	6
S6	Morfologi Sel MCF-7 Hasil Uji Senyawa Kalkon 1	7
S7	Dokumentasi Well Plate Senyawa Kalkon 1 terhadap Sel MCF-7	7
S8	Spektrum $^1\text{H-NMR}$ (500 MHz, CDCl_3) Senyawa Kalkon 2	8
S9	Spektrum $^{13}\text{C-NMR}$ (125 MHz, CDCl_3) Senyawa Kalkon 2	9
S10	Spektrum massa HR-TOF-MS (ES+) Senyawa Kalkon 2	10
S11	<i>Single Mass Analysis</i> Senyawa Kalkon 2	10
S12	Spektrum FTIR Senyawa Kalkon 2	11
S13	Morfologi Sel MCF-7 Hasil Uji Senyawa Kalkon 2	12
S14	Dokumentasi Well Plate Senyawa Kalkon 2 terhadap Sel MCF-7	12



Gambar S1. Spektrum ¹H-NMR (500 MHz, CDCl₃) Senyawa Kalkon 1



Gambar S2. Spektrum ¹³C-NMR (125 MHz, CDCl₃) Senyawa Kalkon 1



Gambar S3. Spektrum massa HR-TOF-MS (ES+) Senyawa Kalkon 1

Single Mass Analysis

Tolerance = 100.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

107 formula(e) evaluated with 50 results within limits (up to 50 closest results for each mass)

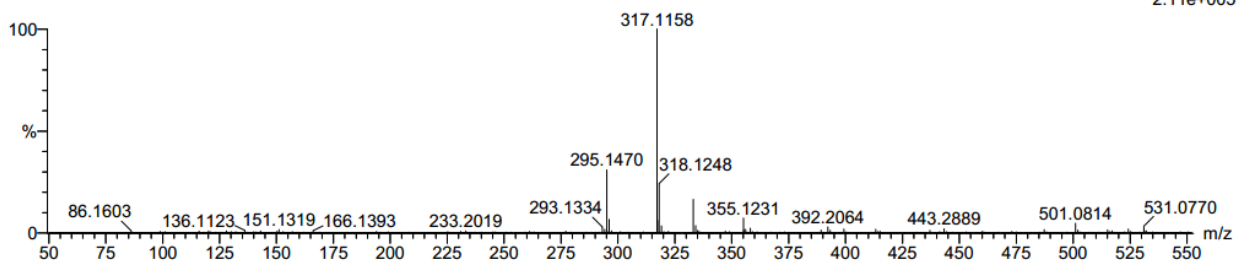
Elements Used:

C: 0-500 H: 0-1000 O: 0-200 Na: 0-1

KALKON UNMUL 4 (0.085) Cm (1:8)

TOF MS ES+

2.11e+005

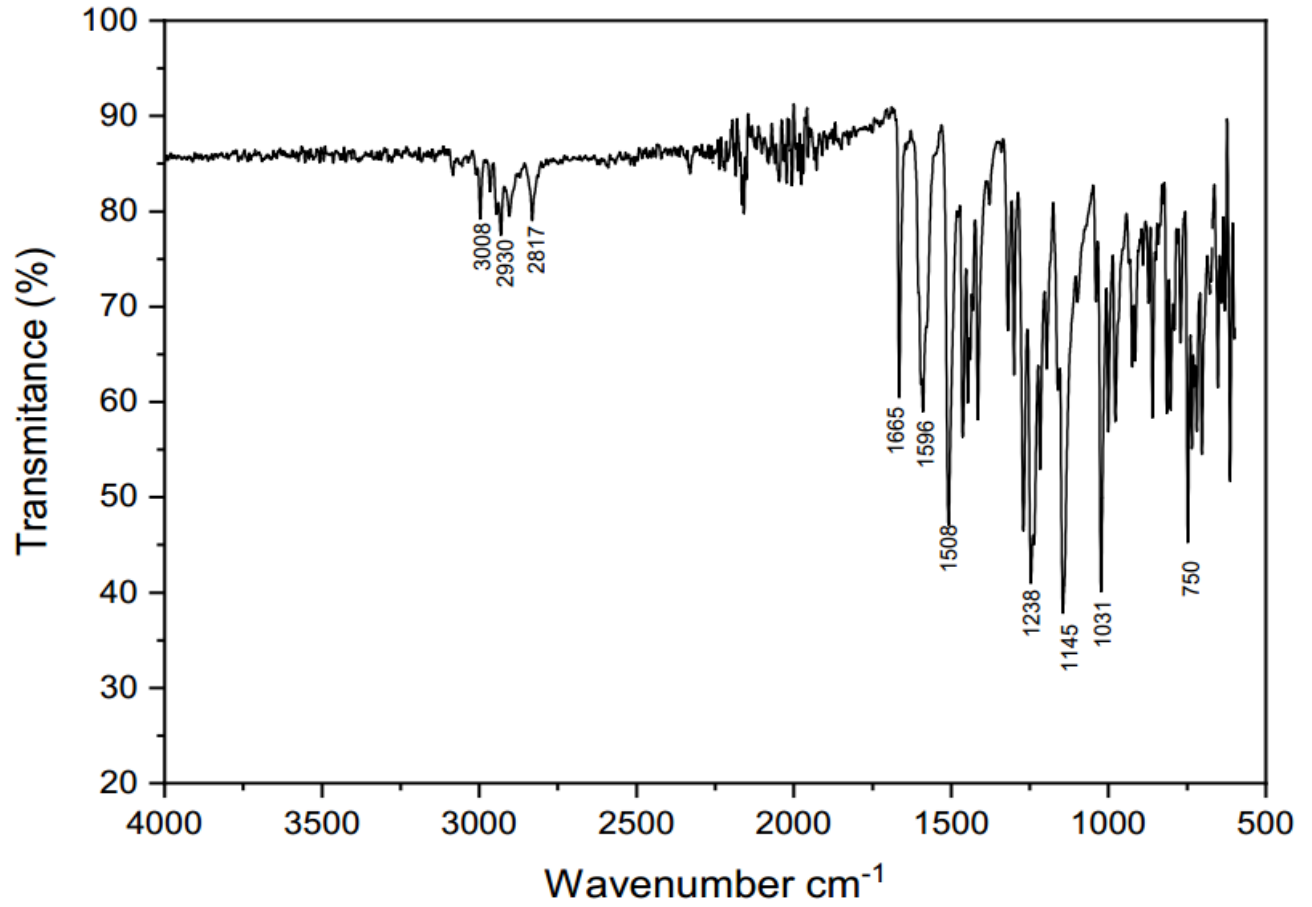


Minimum:

Maximum: 100.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
317.1158	317.1154	0.4	1.3	10.5	308.2	8.4	C19 H18 O3 Na

Gambar S4. Single Mass Analysis Senyawa Kalkon 1



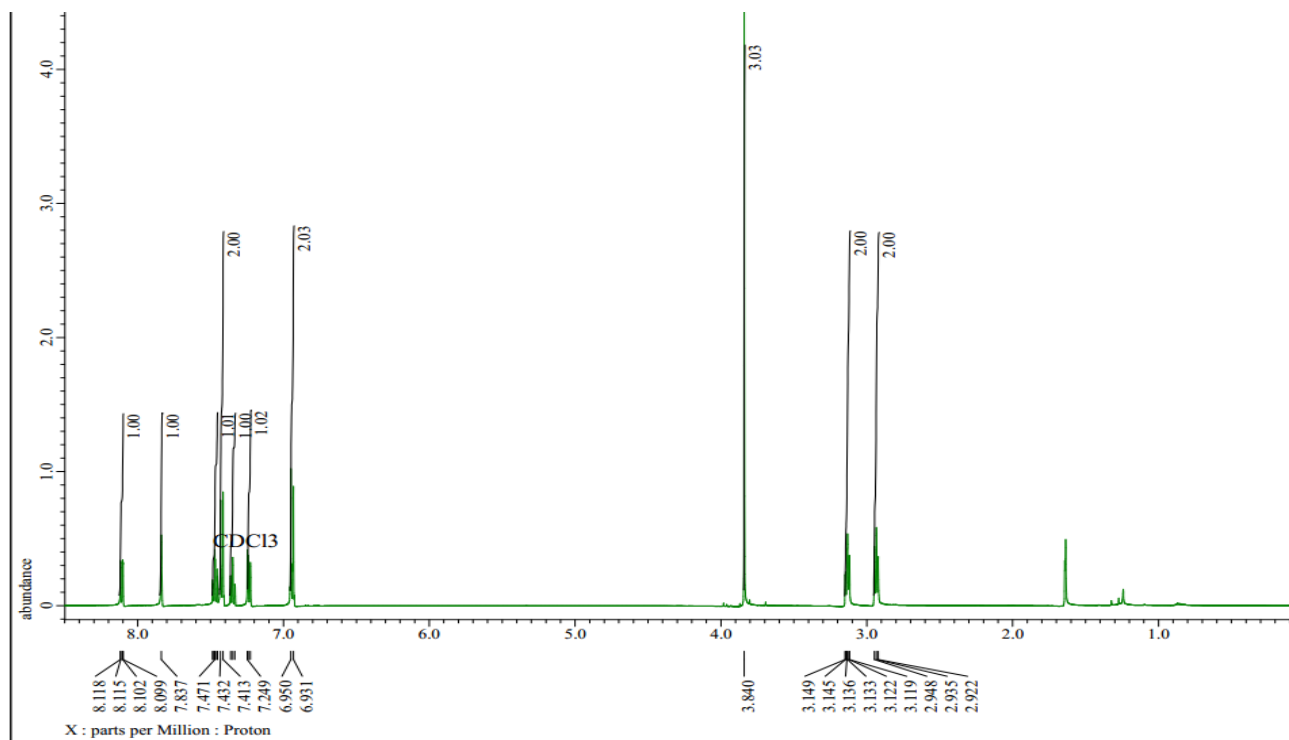
Gambar S5. Spektrum FTIR Senyawa Kalkon 1



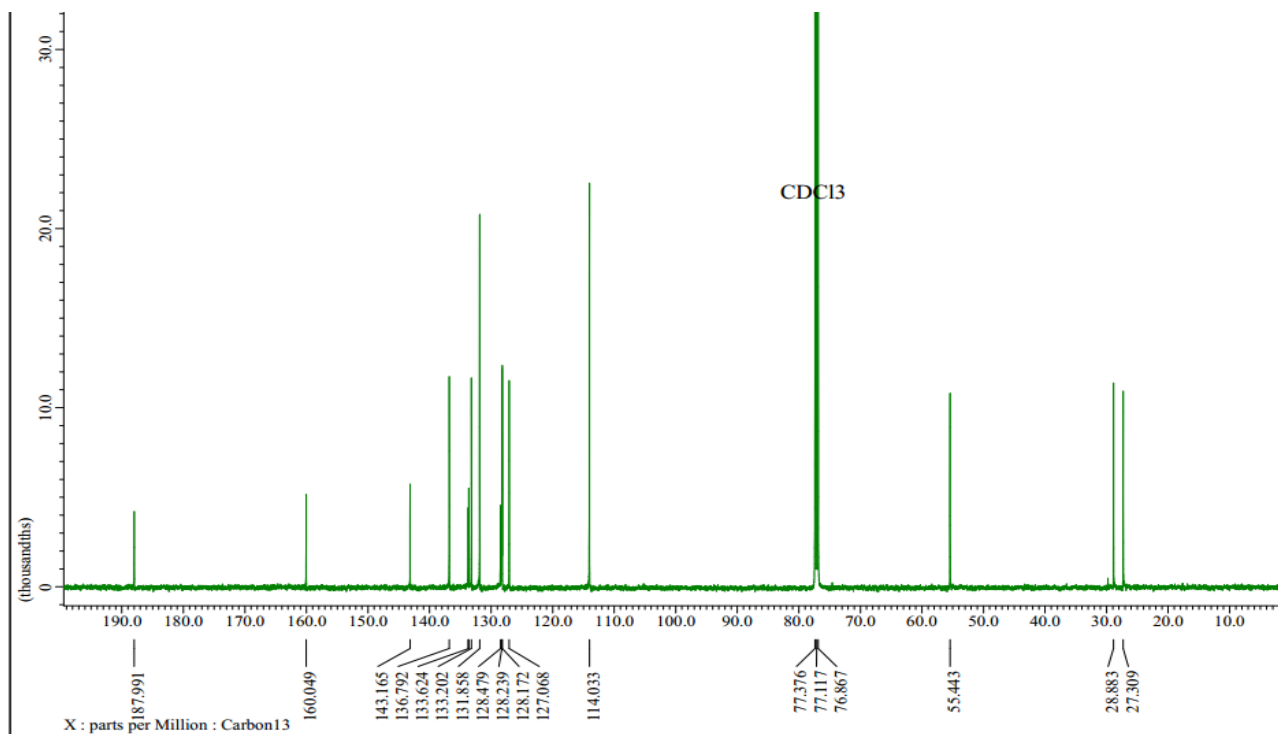
Gambar S6. Morfologi Sel MCF-7 Hasil Uji Senyawa Kalkon 1

Media	Media +Sel	Cisplatin	Pelarut	Konsentrasi Sampel (µg/mL)							
				7,81	15,63	31,25	62,50	125,00	250,00	500,00	1000,00

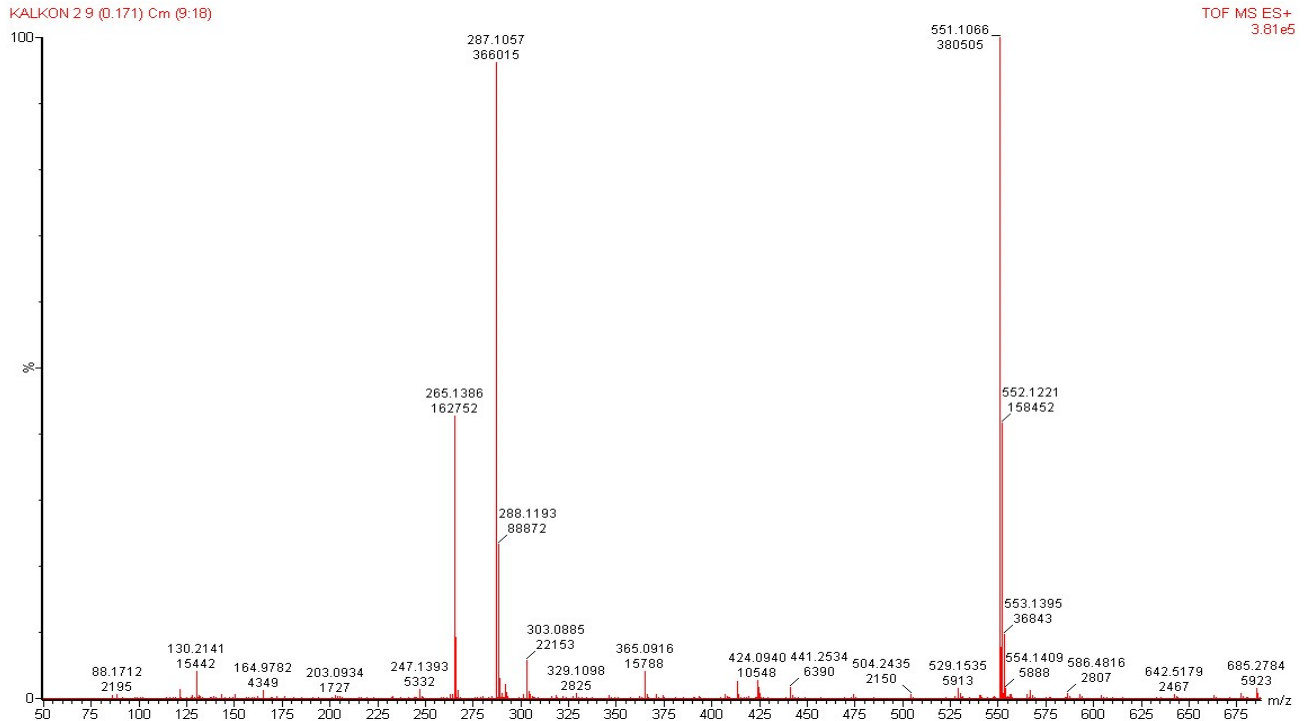
Gambar S7. Dokumentasi Well Plate Senyawa Kalkon 1 terhadap Sel MCF-7



Gambar S8. Spektrum ¹H-NMR (500 MHz, CDCl₃) Senyawa Kalkon 2



Gambar S9. Spektrum ^{13}C -NMR (125 MHz, CDCl_3) Senyawa Kalkon 2



Gambar S10. Spektrum massa HR-TOF-MS (ES+) Senyawa Kalkon 2

Elemental Composition Report

Single Mass Analysis

Tolerance = 50.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

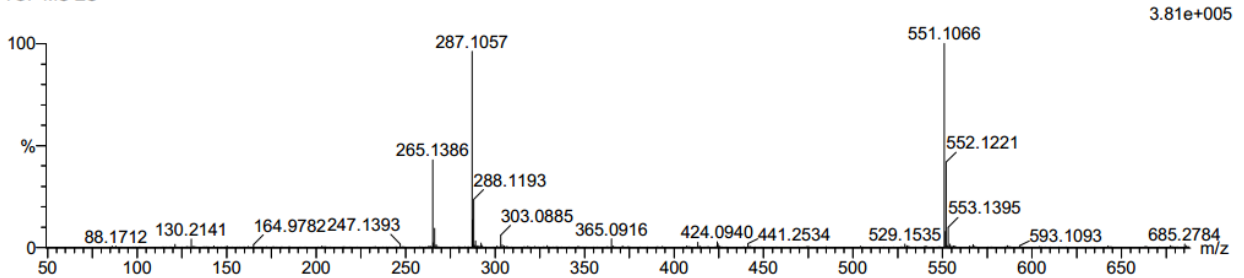
96 formula(e) evaluated with 22 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-500 H: 0-1000 O: 0-200 Na: 0-1

KALKON 2 9 (0.171) Cm (9:18)

TOF MS ES+



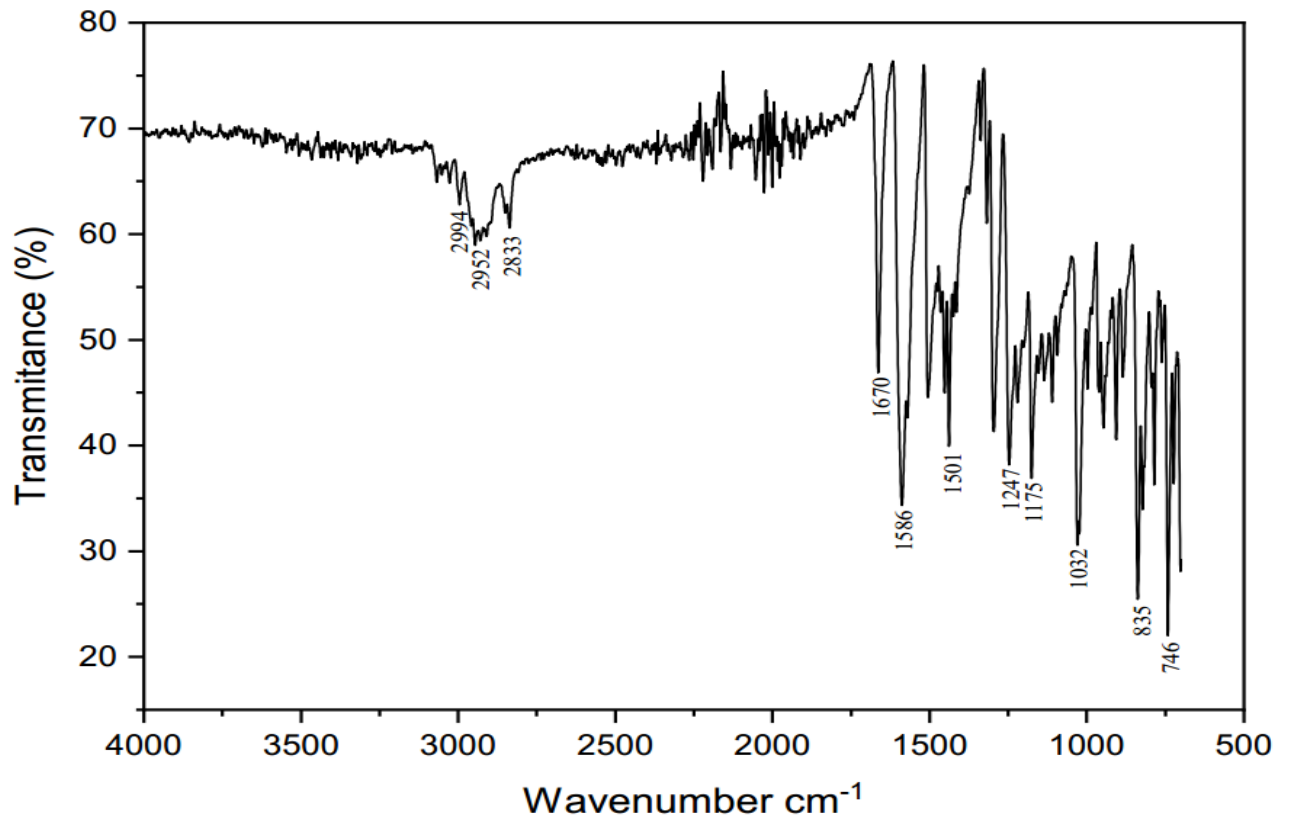
Minimum:

Maximum: 50.0 10.0 -1.5

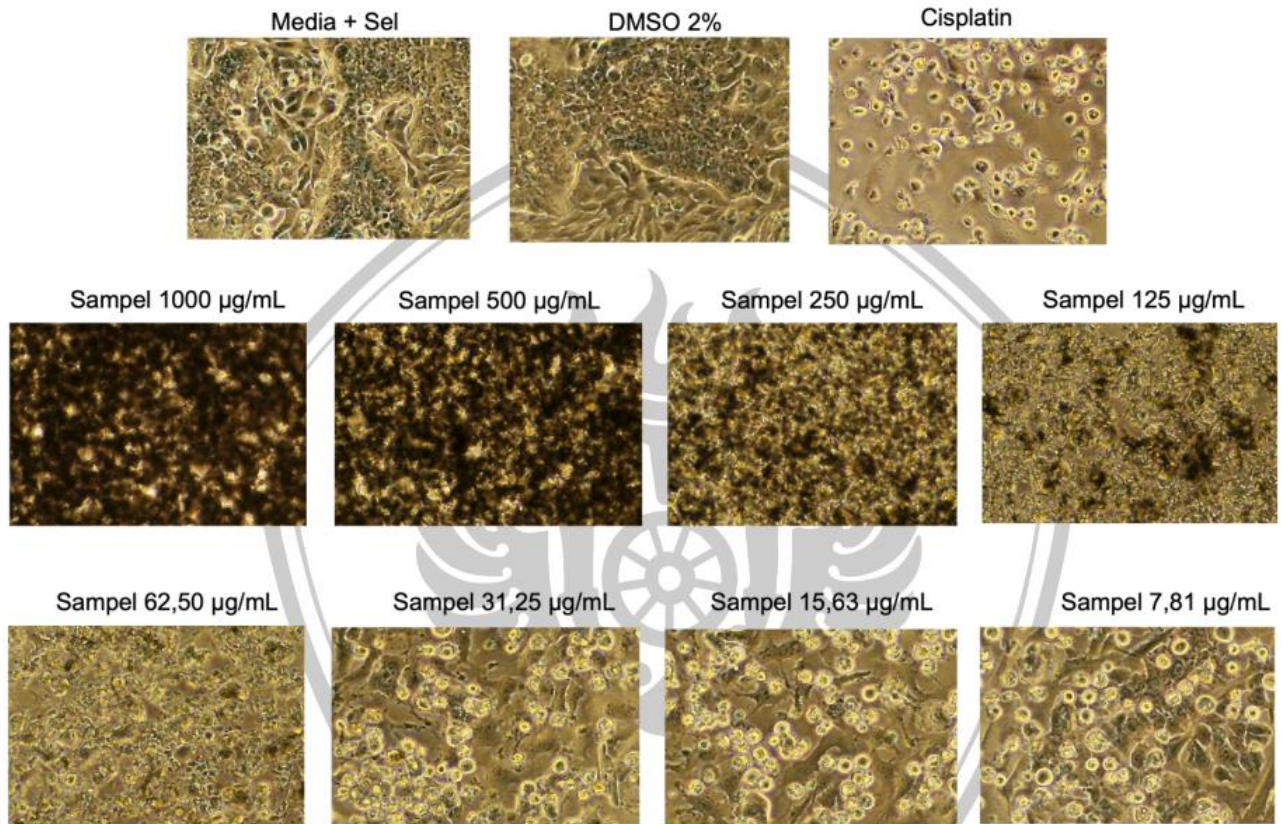
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
------	------------	-----	-----	-----	-------	--------------	---------

287.1057	287.1048	0.9	3.1	10.5	313.0	6.3	C18 H16 O2 Na
----------	----------	-----	-----	------	-------	-----	---------------

Gambar S11. Single Mass Analysis Senyawa Kalkon 2



Gambar S12. Spektrum FTIR Senyawa Kalkon 2



Gambar S13. Morfologi Sel MCF-7 Hasil Uji Senyawa Kalkon 2

Media	Media +Sel	Cisplatin	Pelarut	Konsentrasi Sampel (µg/mL)							
				7,81	15,63	31,25	62,50	125,00	250,00	500,00	1000,00

Gambar S14. Dokumentasi Well Plate Senyawa Kalkon 2 terhadap Sel MCF-7