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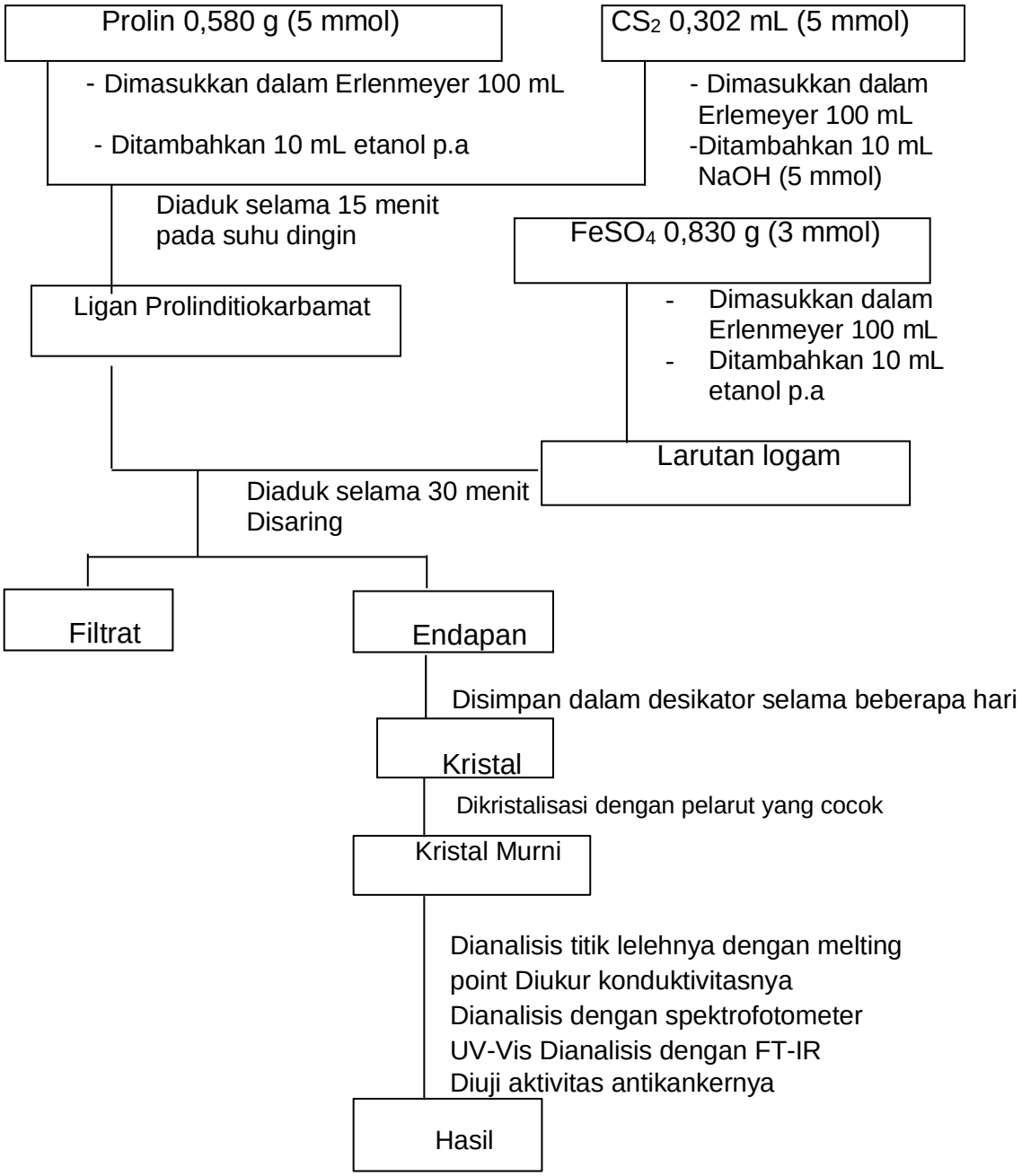
Lampiran 1. Bagan Kerja Sintesis, Analisis dan Uji Kanker Senyawa Kompleks Fe(II) dan Mn(II) dengan ProlinDitiokarbamat



Ket: Dengan cara yang sama dilakukan sintesis kompleks Mn(II) dengan ligan Prolinditiokarbamat.

Lampiran 2. Perhitungan Hasil Rendamen Senyawa Kompleks

1. Kompleks Fe(II)Prolinditiokarbamat

Dik: Berat praktek = 0,2103 g

$FeSO_4.4H_2O$ + Prolin + CS_2	⟶	Fe(II)Prolinditioarbamat	
3 mmol	5 mmol		
3 mmol	3 mmol	⟶	3 mmol
0 mmol	2 mmol		3 mmol

Berat teori = mmol Fe(II)ProDtc x Mr Fe(II)ProDtc
= 3 mmol x 247,117 g/mol
= 0,003 mol x 247,117 g/mol
= 0,7413 gr

$$\text{Persen Rendamen} = \frac{\text{g praktek}}{\text{g teori}} \text{x100\%}$$

$$\text{Persen Berat Rendamen} = \frac{0{,}2103}{0{,}7413} \text{ x100\% = 28.37 \%}$$

2. Kompleks Mn(II)Proinditiokarbamat

Dik: Berat praktek = 0,1750 g

$MnSO_4.5H_2O$ + prolin + CS_2	⟶	Mn(II)prolinditiokarbamat	
3 mmol	5 mmol		
3 mmol	3 mmol	⟶	3 mmol
0 mmol	2 mmol		3 mmol

Berat teori = mmol Mn(II)ProDtc x Mr Mn(II)ProDtc
= 3 mmol x 246,2107 g/mol
= 0,003 mol x 246,2107 g/mo/
= 0,7386 g

$$\text{Persen Rendamen} = \frac{\text{g praktek}}{\text{g teori}} \text{x100\%}$$

$$\text{Persen Rendamen} = \frac{0{,}1750}{0{,}7386} \text{x100\% = 23,70\%}$$

Lampiran 3. Hasil Uji Sitotoksisitas Senyawa Kompleks dan Logam terhadap sel kanker *MCF-7*

Tabel 8 . Absorbansi Hasil Uji Fe(II)Prolinditiokarbamat terhadap sel *MCF-7*

Panjang Gelombang /nm	Media	Media +Sel	Cisplatin	DMSO 2%	Konsentrasi Sampel (µg/mL)							
					300,00	150,00	75,00	37,50	18,75	9,38	4,69	2,34
570	0,4883	0,7990	0,6416	0,7762	0,8500	0,8136	0,8192	0,8020	0,7978	0,7755	0,8227	0,8018
	0,4891	0,7937	0,6403	0,7863	0,8245	0,8192	0,8188	0,8055	0,8119	0,8199	0,8089	0,7922
600	0,6259	0,2279	0,4004	0,2384	0,2924	0,2506	0,2390	0,2417	0,2365	0,2122	0,2322	0,2378
	0,6264	0,2341	0,4545	0,2653	0,2636	0,2460	0,2499	0,2395	0,2424	0,2569	0,2431	0,2459
Corrected Absorbance	-0,1375	0,7085	0,3788	0,6753	0,6951	0,7005	0,7176	0,6977	0,6987	0,7008	0,7279	0,7015
		0,6970	0,3233	0,6585	0,6983	0,7108	0,7065	0,7034	0,7070	0,7005	0,7031	0,6837

Tabel 9. Absorbansi Hasil Uji Mn(II)Prolinditiokarbamat terhadap sel *MCF-7*

Panjang Gelombang /nm	Media	Media +Sel	Cisplatin	DMSO 2%	Konsentrasi Sampel (µg/mL)							
					300,00	150,00	75,00	37,50	18,75	9,38	4,69	2,34
570	0,4811	0,8023	0,6349	0,8284	0,7117	0,7336	0,7486	0,7570	0,7783	0,8035	0,7947	0,7998
	0,4859	0,7878	0,6149	0,7871	0,7210	0,7290	0,7618	0,7866	0,7784	0,8103	0,7988	0,7955
600	0,6179	0,2915	0,4804	0,2820	0,3814	0,3381	0,3097	0,2756	0,2638	0,2536	0,2388	0,2466
	0,6227	0,2667	0,4911	0,2531	0,3898	0,3521	0,2969	0,2633	0,2374	0,2450	0,2370	0,2427
Corrected Absorbance	-0,1368	0,6477	0,2913	0,6833	0,4672	0,5324	0,5759	0,6183	0,6514	0,6867	0,6927	0,6902
		0,6579	0,2607	0,6708	0,4681	0,5137	0,6017	0,6601	0,6779	0,7021	0,6987	0,6896

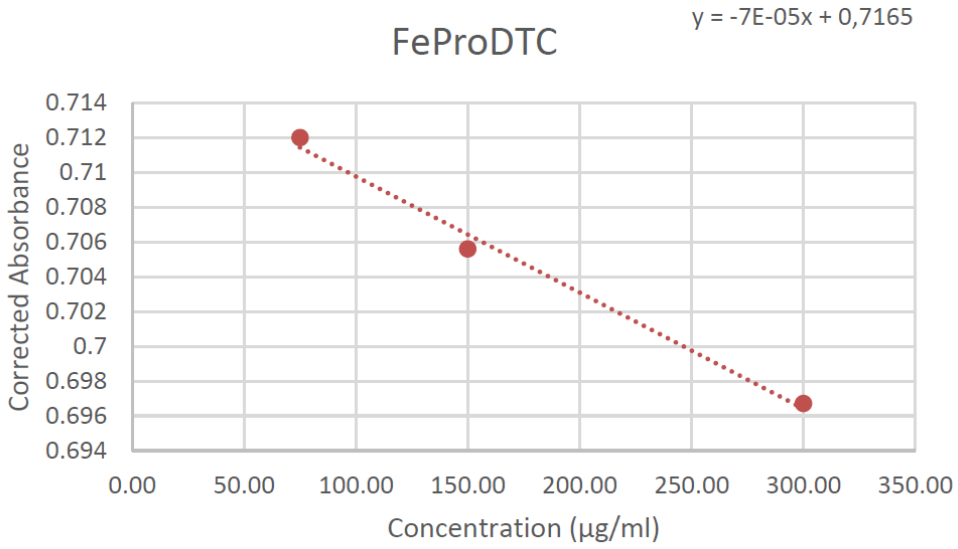
Keterangan:

a. Panjang gelombang 600 nm mengukur absorbansi Resazurin berwarna biru

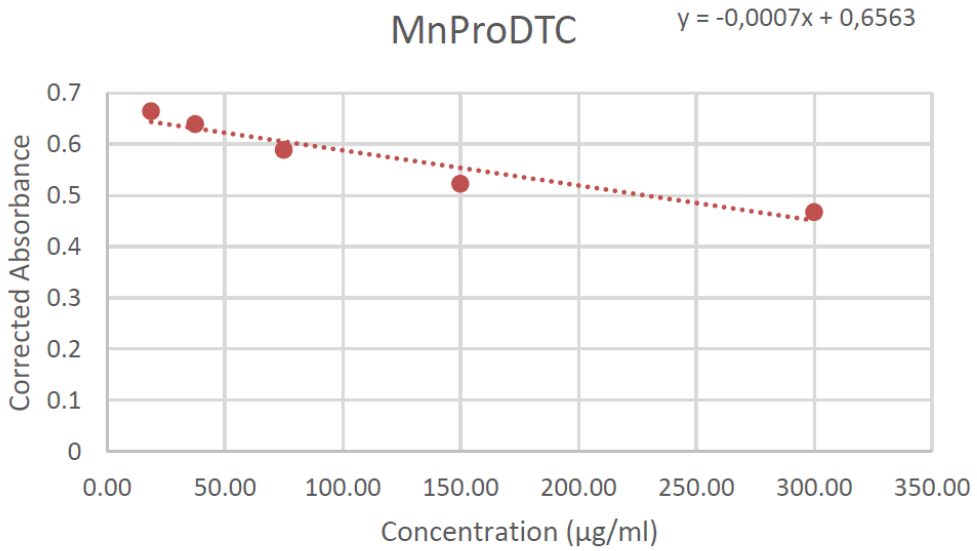
b. Panjang gelombang 570 nm mengukur absorbansi Resorufin berwarna merah

c. Corrected Absorbance: Selisih absorbansi sampel/media+Sel/Kontrol pada panjang gelombang 570 nm dan 600 nm, lalu dikurangi rata-rata selisih absorbansi media pada kedua panjang gelombang yang sama.

d. Konsentrasi cisplatin yang digunakan dalam uji sebesar 53 µM.



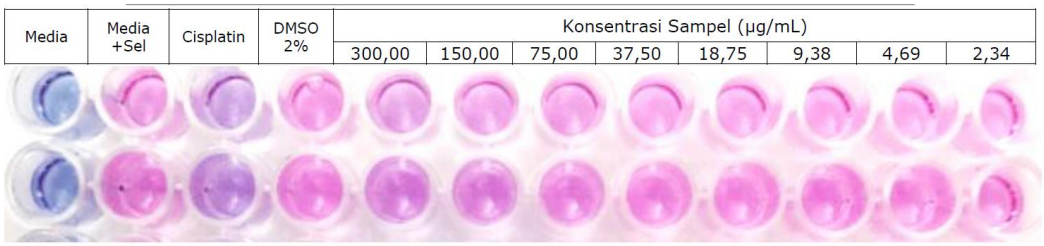
Gambar 26. Kurva Hasil Uji Fe(II)Prolindithiocarbamat terhadap sel *MCF-7*



Gambar 27. Kurva Hasil Uji Mn(II)Prolindithiocarbamat terhadap sel *MCF-7*

Media	Media +Sel	Cisplatin	DMSO 2%	Konsentrasi Sampel (µg/mL)							
				300,00	150,00	75,00	37,50	18,75	9,38	4,69	2,34

Gambar 28. Dokumentasi *Well Plate* Hasil Uji Fe(II)ProDTC terhadap Sel *MCF-7*



Gambar 29. Dokumentasi *Well Plate* Hasil Uji Mn(II)ProDTC terhadap Sel *MCF-7*

Lampiran 4. Hasil Studi Molekular Docking

Tabel 10. Kompleks senyawa dan canonical SMILES

Kompleks Senyawa	Canonical SMILES
Fe(II)Prolinedithiocarbamate	O=C2O[Fe]1SC(S1)N3CCCC23
Mn(II)Prolinedithiocarbamate	O=C2O[Mn]1SC(S1)N3CCCC23

Tabel 11. Interaksi antara Kompleks Fe(II)Prolinedithiocarbamat, dan Mn(II)Prolinedithiocarbamate terhadap protein Estrogen Receptor α.

Ligand - Protein Complex Binding energy (kJ/mol)	Interaction	Distance (A)	Category	Types	Donor
Fe(II)Prolinedithiocarbamate - Estrogen Receptor α -188,25 ± 5,3	A:ARG394:NH2 - :10:O1	2,87015	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG394:NH2
	:10:H7 - A:LEU346:O	3,01367	Hydrogen Bond	Carbon Hydrogen Bond	:10:H7
	:10:S2 - A:PHE404	5,05635	Other	Pi-Sulfur	:10:S2
	A:ALA350 - :10	4,45128	Hydrophobic	Alkyl	A:ALA350
	:10 - A:LEU387	4,92834	Hydrophobic	Alkyl	:10
	:10 - A:MET388	4,8186	Hydrophobic	Alkyl	:10
	:10 - A:LEU391	5,18461	Hydrophobic	Alkyl	:10
	:10 - A:LEU346	4,03473	Hydrophobic	Alkyl	:10
	:10 - A:LEU349	4,29863	Hydrophobic	Alkyl	:10
	A:PHE404 - :10	4,95228	Hydrophobic	Pi-Alkyl	A:PHE404
Mn(II)Prolinedithiocarbamate - Estrogen Receptor α -190,25 ± 8,5	A:ARG394:NH2 - :10:O1	2,82891	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG394:NH2
	A:ALA350 - :10	4,12256	Hydrophobic	Alkyl	A:ALA350
	:10 - A:LEU346	4,44881	Hydrophobic	Alkyl	:10
	:10 - A:LEU349	5,17795	Hydrophobic	Alkyl	:10
	:10 - A:LEU384	5,46437	Hydrophobic	Alkyl	:10
	:10 - A:LEU387	4,69449	Hydrophobic	Alkyl	:10
	:10 - A:MET388	4,2232	Hydrophobic	Alkyl	:10
	:10 - A:LEU391	4,88713	Hydrophobic	Alkyl	:10
	A:PHE404 - :10	5,32427	Hydrophobic	Pi-Alkyl	A:PHE404

Tabel 12. Interaksi antara Kompleks Fe(II)Prolinedithiocarbamat, dan Mn(II)Prolinedithiocarbamate terhadap protein Caspase-8

Ligand - Protein Complex Binding Energy (kJ/mol)	Interaction	Distance (A)	Category	Types	Donor
Fe(II)Prolinedithiocarbamate - Caspase-8 -216,2 ± 11,3	D:LEU328:N - :10:S2	3,39532	Hydrogen Bond	Conventional Hydrogen Bond	D:LEU328:N
	D:THR393:OG1 - :10:O1	2,97059	Hydrogen Bond	Conventional Hydrogen Bond	D:THR393:OG1
	D:THR393:OG1 - :10:O2	3,09179	Hydrogen Bond	Conventional Hydrogen Bond	D:THR393:OG1
	:10 - D:LEU329	4,40332	Hydrophobic	Alkyl	:10
	D:PHE327 - :10	4,38348	Hydrophobic	Pi-Alkyl	D:PHE327
Mn(II)Prolinedithiocarbamate - Caspase-8 -215,8 ± 4,08	B:GLN388:NE2 - :10:O1	3,13906	Hydrogen Bond	Conventional Hydrogen Bond	B:GLN388:NE2
	D:THR393:OG1 - :10:O2	2,65448	Hydrogen Bond	Conventional Hydrogen Bond	D:THR393:OG1
	D:THR390:C - :10:O1	3,74812	Hydrogen Bond	Carbon Hydrogen Bond	D:THR390:C
	:10:S1 - D:PHE327	3,7089	Other	Pi-Sulfur	:10:S1
	:10 - D:LEU329	4,30057	Hydrophobic	Alkyl	:10
	D:PHE327 - :10	4,54314	Hydrophobic	Pi-Alkyl	D:PHE327
	:10:S1 - D:PHE327	3,66558	Other	Pi-Sulfur	:10:S1
	:10 - D:LEU329	5,15993	Hydrophobic	Alkyl	:10

Tabel 13. Interaksi antara Kompleks Fe(II)Prolinedithiocarbamat, dan Mn(II)Prolinedithiocarbamate terhadap protein O(6)-methylguanine-DNA methyltransferase (MGMT)

Ligand - Protein Complex/ Binding energy (kJ/mol)	Interaction	Distance (A)	Category	Types	Donor
Fe(II)Prolinedithiocarbamate - O(6)-methylguanine-DNA methyltransferase (MGMT) -183,25 ± 10,6	A:TRP65:NE1 - :10:O1	3,01784	Hydrogen Bond	Conventional Hydrogen Bond	A:TRP65:NE1
	:10:H1 - A:GLU77:OE2	2,89471	Hydrogen Bond	Carbon Hydrogen Bond	:10:H1
	:10:S2 - A:LEU142:O	3,28874	Other	Sulfur-X	:10:S2
	:10 - A:ILE76	4,08585	Hydrophobic	Alkyl	:10
	A:TRP65 - :10	4,74783	Hydrophobic	Pi-Alkyl	A:TRP65
Mn(II)Prolinedithiocarbamate - O(6)-methylguanine-DNA methyltransferase (MGMT) -199 ± 7,07	A:PHE108:N - :10:O1	3,14316	Hydrogen Bond	Conventional Hydrogen Bond	A:PHE108:N
	A:ARG147:NH1 - :10:O1	2,88846	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG147:NH1
	A:ARG147:NH1 - :10:O2	2,80596	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG147:NH1
	A:ARG147:NH2 - :10:O1	3,08587	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG147:NH2
	A:ARG147:NH2 - :10:O2	2,89764	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG147:NH2
	:10 - A:VAL81	5,01146	Hydrophobic	Alkyl	:10
	:10 - A:LEU103	5,25018	Hydrophobic	Alkyl	:10
	:10 - A:PRO144	4,90183	Hydrophobic	Alkyl	:10
	:10 - A:ILE76	4,75311	Hydrophobic	Alkyl	:10
	A:TRP65 - :10	5,33411	Hydrophobic	Pi-Alkyl	A:TRP65
	A:TRP65 - :10	5,10318	Hydrophobic	Pi-Alkyl	A:TRP65
	A:TRP65 - :10	4,92483	Hydrophobic	Pi-Alkyl	A:TRP65