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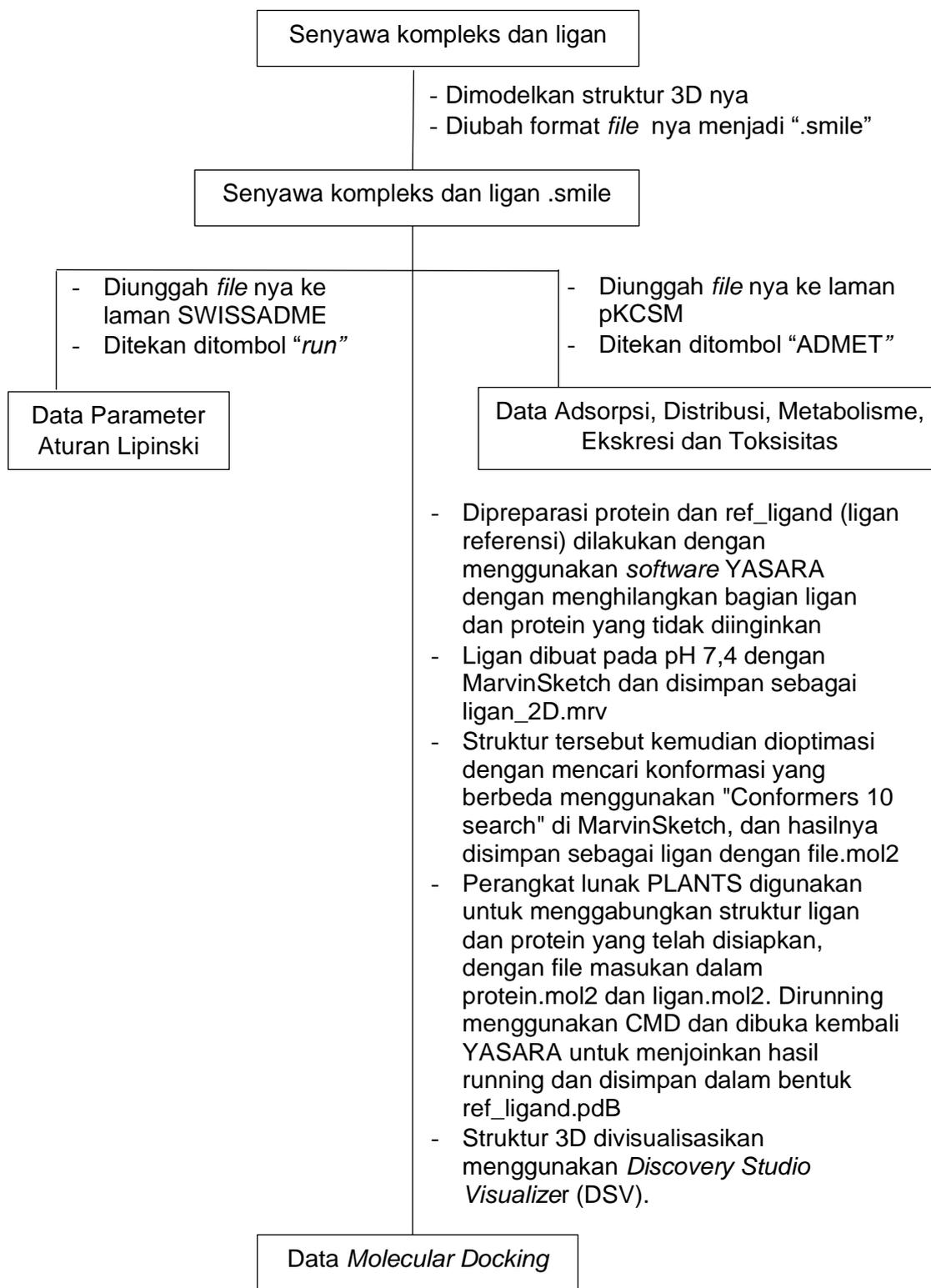
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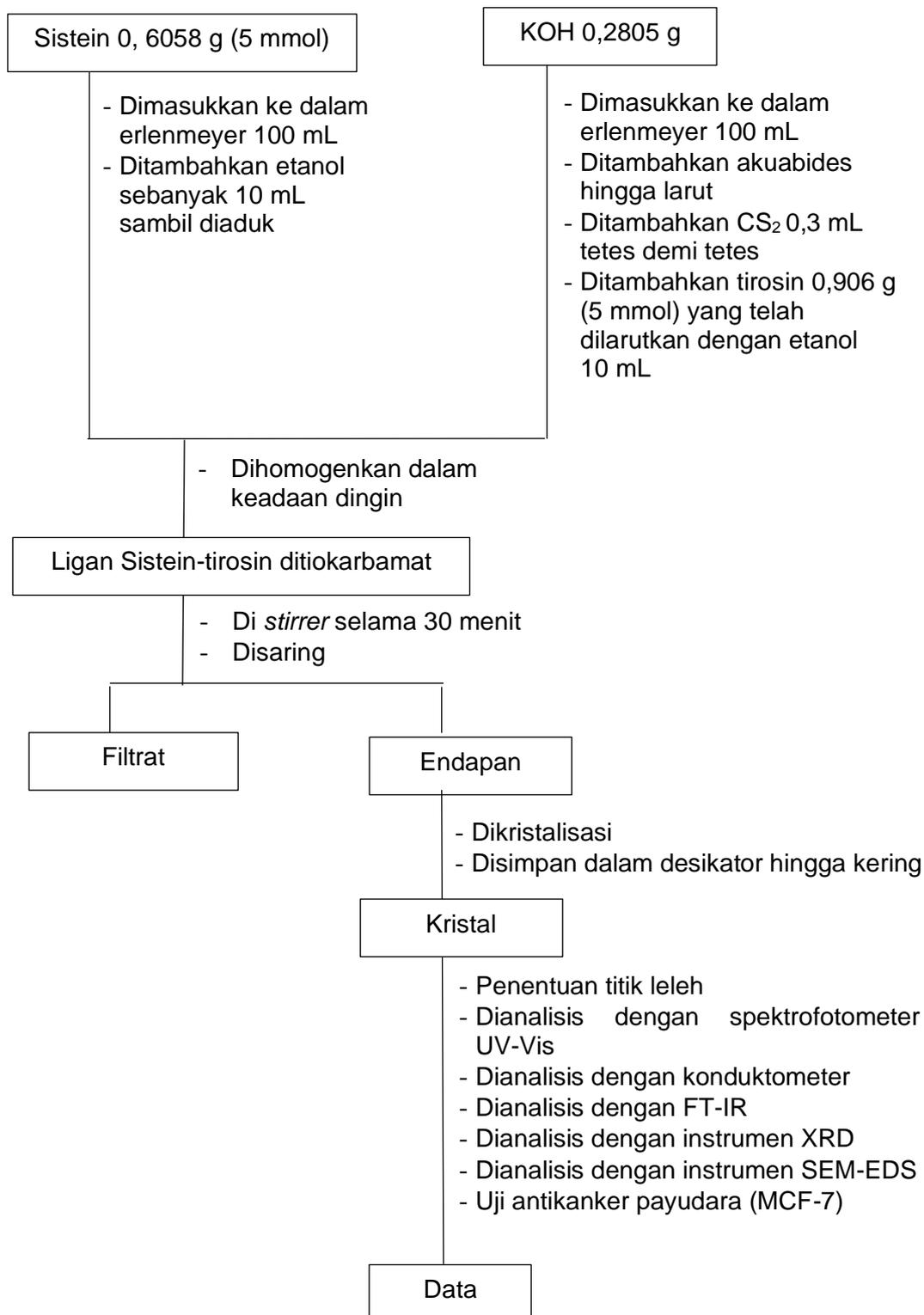
LAMPIRAN

Lampiran 1. Bagan Kerja

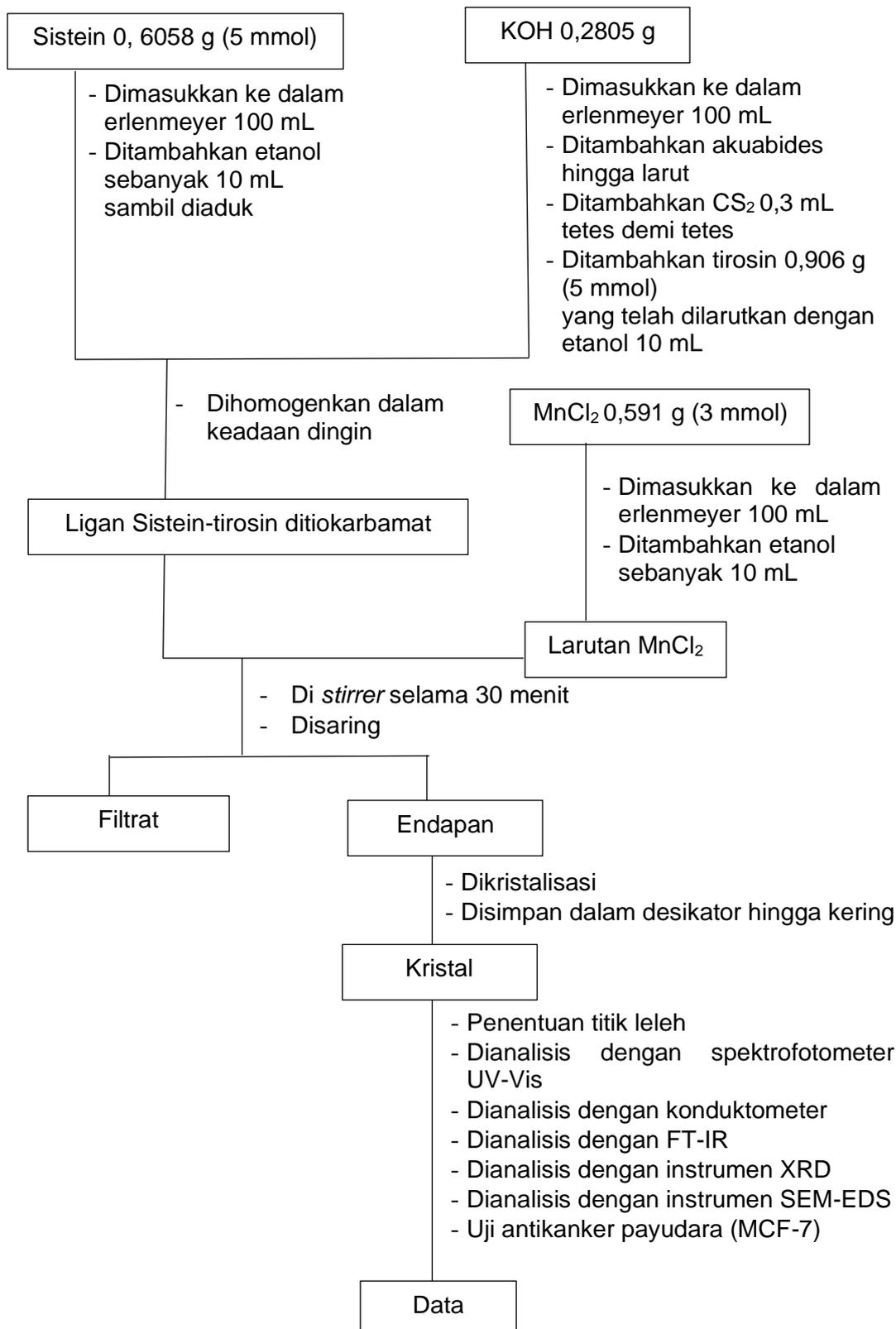
1. Bagan Kerja Desain dan Analisis Aturan Lipinski, ADMET dan *Molecular Docking*



2. Bagan Kerja Sintesis Sistein-Tirosin Ditiokarbamat



3. Bagan Kerja Sintesis, Analisis dan Uji Bioaktivitas Senyawa Kompleks Mn(II) Sis-Tir Dtc



NB: Dilakukan hal yang sama untuk logam Ni 0,711 g dan Zn 0,622 g

Lampiran 2. Perhitungan Pembuatan Larutan**1. Pembuatan Larutan $\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$ 3 mmol dalam 10 mL etanol**

$$M = \frac{n}{V} = \frac{0,003 \text{ mol}}{0,01 \text{ L}} = 0,3 \text{ mol/L}$$

$$M = \frac{g}{M_r} \times \frac{1}{L}$$

$$0,3 \text{ mol/L} = \frac{g}{197 \text{ g/mol}} \times \frac{1}{0,01 \text{ L}}$$

$$g = 0,3 \times 0,01 \times 197 \text{ g/mol}$$

$$g = 0,591 \text{ g}$$

2. Pembuatan Larutan $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$ 3 mmol dalam 10 mL etanol

$$M = \frac{n}{V} = \frac{0,003 \text{ mol}}{0,01 \text{ L}} = 0,3 \text{ mol/L}$$

$$M = \frac{g}{M_r} \times \frac{1}{L}$$

$$0,3 \text{ mol/L} = \frac{g}{237 \text{ g/mol}} \times \frac{1}{0,01 \text{ L}}$$

$$g = 0,3 \times 0,01 \times 237 \text{ g/mol}$$

$$g = 0,711 \text{ g}$$

3. Pembuatan Larutan $\text{ZnCl}_2 \cdot 4\text{H}_2\text{O}$ 3 mmol dalam 10 mL etanol

$$M = \frac{n}{V} = \frac{0,003 \text{ mol}}{0,01 \text{ L}} = 0,3 \text{ mol/L}$$

$$M = \frac{g}{M_r} \times \frac{1}{L}$$

$$0,3 \text{ mol/L} = \frac{g}{207 \text{ g/mol}} \times \frac{1}{0,01 \text{ L}}$$

$$g = 0,3 \times 0,01 \times 207 \text{ g/mol}$$

$$g = 0,622 \text{ g}$$

4. Pembuatan Sistein 5 mmol dalam 10 mL etanol

$$M = \frac{n}{V} = \frac{0,005 \text{ mol}}{0,01 \text{ L}} = 0,5 \text{ mol/L}$$

$$M = \frac{g}{M_r} \times \frac{1}{L}$$

$$0,5 \text{ mol/L} = \frac{\text{g}}{121,1583 \text{ g/mol}} \times \frac{1}{0,01 \text{ L}}$$

$$\text{g} = 0,5 \times 0,01 \times 121,1583 \text{ g}$$

$$\text{g} = 0,6058 \text{ g}$$

5. Pembuatan Tirosin 5 mmol dalam 10 mL etanol

$$M = \frac{n}{V} = \frac{0,005 \text{ mol}}{0,01 \text{ L}} = 0,5 \text{ mol/L}$$

$$M = \frac{\text{g}}{M_r} \times \frac{1}{L}$$

$$0,5 \text{ mol/L} = \frac{\text{g}}{181,2 \text{ g/mol}} \times \frac{1}{0,01 \text{ L}}$$

$$\text{g} = 0,5 \times 0,01 \times 105,093 \text{ g}$$

$$\text{g} = 0,906 \text{ g}$$

5. Pembuatan CS₂ 5 mmol

$$\text{mol} = \frac{\text{g}}{M_r}$$

$$\text{g} = \text{mol} \times M_r$$

$$\text{g} = 0,005 \text{ mol} \times 76,14 \text{ g/mol}$$

$$\text{g} = 0,3807 \text{ g}$$

$$V = \frac{m}{\rho}$$

$$V = \frac{0,3807 \text{ g}}{1,26 \text{ g/mL}}$$

$$V = 0,302 \text{ mL}$$

6. Pembuatan KOH 5 mmol

$$\text{mol} = \frac{\text{g}}{M_r}$$

$$\text{g} = \text{mol} \times M_r$$

$$\text{g} = 0,005 \text{ mol} \times 56,1 \text{ g/mol}$$

$$\text{g} = 0,2805 \text{ g}$$

Lampiran 3. Perhitungan Hasil Rendemen secara Komputasi

1. Perhitungan Hasil Rendemen senyawa kompleks Mn(II) Sis-Tir Dtc

a. Massa logam yang diperlukan:

$$\begin{aligned} m &= n \times Mr \\ &= 0,003 \text{ mol} \times 197 \text{ g/mol} \\ &= 0,591 \text{ g} \end{aligned}$$

b. Massa ligan yang diperlukan:

$$\begin{aligned} m &= n \times Mr \\ &= 0,005 \text{ mol} \times 378 \text{ g/mol} \\ &= 1,89 \text{ g} \end{aligned}$$

c. Rendemen:

	$\text{MnCl}_2 \cdot 4\text{H}_2\text{O} + \text{sistein} + \text{tirosin} + \text{CS}_2 \longrightarrow \text{Mn(II) Sis-Tir Dtc}$		
M	3 mmol	5 mmol	-
B	3 mmol	3 mmol	3 mmol
S	-	2 mmol	3 mmol

$$\begin{aligned} \text{Berat teori} &= \text{mmol Mn(II) Sis-Tir Dtc} \times \text{Mr Mn(II) Sis-Tir Dtc} \\ &= 3 \text{ mmol} \times 429,44 \text{ g/mol} \\ &= 0,003 \text{ mol} \times 429,44 \text{ g/mol} \\ &= 1,28 \text{ g} \end{aligned}$$

$$\text{Berat eksperimen} = 1,14 \text{ g}$$

$$\begin{aligned} \% \text{ Rendemen} &= \frac{\text{massa eksperimen}}{\text{massa teori}} \times 100\% \\ &= \frac{1,14 \text{ gr}}{1,28 \text{ gr}} \times 100\% \\ &= 89\% \end{aligned}$$

2. Perhitungan Hasil Rendemen senyawa kompleks Ni(II) Sis-Tir Dtc

a. Massa logam yang diperlukan:

$$\begin{aligned} m &= n \times Mr \\ &= 0,003 \text{ mol} \times 237 \text{ g/mol} \\ &= 0,711 \text{ g} \end{aligned}$$

b. Massa ligan yang diperlukan:

$$\begin{aligned} m &= n \times Mr \\ &= 0,005 \text{ mol} \times 378 \text{ g/mol} \\ &= 1,89 \text{ g} \end{aligned}$$

c. Rendemen:

	$\text{NiCl}_2 \cdot 6\text{H}_2\text{O} + \text{sistein} + \text{tirosin} + \text{CS}_2 \longrightarrow \text{Ni(II) Sis-Tir Dtc}$		
M	3 mmol	5 mmol	-
B	3 mmol	3 mmol	3 mmol
S	-	2 mmol	3 mmol

$$\begin{aligned} \text{Berat teori} &= \text{mmol Ni(II) Sis-Tir Dtc} \times \text{Mr Ni(II) Sis-Tir Dtc} \\ &= 3 \text{ mmol} \times 417,15 \text{ g/mol} \\ &= 0,003 \text{ mol} \times 417,15 \text{ g/mol} \\ &= 1,25 \text{ g} \end{aligned}$$

$$\text{Berat eksperimen} = 1,11 \text{ g}$$

$$\begin{aligned} \% \text{ Rendamen} &= \frac{\text{massa eksperimen}}{\text{massa teori}} \times 100\% \\ &= \frac{1,11 \text{ gr}}{1,25 \text{ gr}} \times 100\% \\ &= 88,8\% \end{aligned}$$

3. Perhitungan Hasil Rendemen senyawa kompleks Zn(II) Sis-Tir Dtc

a. Massa logam yang diperlukan:

$$\begin{aligned} m &= n \times Mr \\ &= 0,003 \text{ mol} \times 207 \text{ g/mol} \\ &= 0,622 \text{ g} \end{aligned}$$

b. Massa ligan yang diperlukan:

$$\begin{aligned} m &= n \times Mr \\ &= 0,005 \text{ mol} \times 378 \text{ g/mol} \\ &= 1,89 \text{ g} \end{aligned}$$

c. Rendemen:

	$\text{ZnCl}_2 \cdot 4\text{H}_2\text{O} + \text{sistein} + \text{tirosin} + \text{CS}_2 \longrightarrow \text{Zn(II) Sis-Tir Dtc}$		
M	3 mmol	5 mmol	-
B	3 mmol	3 mmol	3 mmol
S	-	2 mmol	3 mmol

$$\begin{aligned} \text{Berat teori} &= \text{mmol Zn(II) Sis-Tir Dtc} \times \text{Mr Zn(II) Sis-Tir Dtc} \\ &= 3 \text{ mmol} \times 423,84 \text{ g/mol} \\ &= 0,003 \text{ mol} \times 423,84 \text{ g/mol} \\ &= 1,27 \text{ g} \end{aligned}$$

$$\text{Berat eksperimen} = 1,12 \text{ g}$$

$$\begin{aligned} \% \text{ Rendamen} &= \frac{\text{massa eksperimen}}{\text{massa teori}} \times 100\% \\ &= \frac{1,12 \text{ gr}}{1,27 \text{ gr}} \times 100\% \\ &= 88.1\% \end{aligned}$$

4. Perhitungan Hasil Rendemen senyawa Sis-Tir Dtc

a. Massa ligan yang diperlukan:

$$\begin{aligned} m &= n \times Mr \\ &= 0,005 \text{ mol} \times 378 \text{ g/mol} \\ &= 1,89 \text{ g} \end{aligned}$$

b. Rendemen:

	sistein + tirosin + CS ₂	→	Sis-Tir Dtc
M	5 mmol		-
B	5 mmol		5 mmol
S	-		5 mmol

$$\begin{aligned} \text{Berat teori} &= \text{mmol Sis-Tir Dtc} \times \text{Mr Sis-Tir Dtc} \\ &= 5 \text{ mmol} \times 360,47 \text{ g/mol} \\ &= 0,003 \text{ mol} \times 360,47 \text{ g/mol} \\ &= 1,80 \text{ g} \end{aligned}$$

$$\text{Berat eksperimen} = 1,08 \text{ g}$$

$$\begin{aligned} \% \text{ Rendamen} &= \frac{\text{massa eksperimen}}{\text{massa teori}} \times 100\% \\ &= \frac{1,08 \text{ gr}}{1,80 \text{ gr}} \times 100\% \\ &= 60\% \end{aligned}$$

Lampiran 4. Perhitungan Hasil Rendemen

1. Perhitungan Hasil Rendemen senyawa kompleks Mn(II) Sis-Tir Dtc

a. Massa logam yang diperlukan:

$$\begin{aligned} m &= n \times Mr \\ &= 0,003 \text{ mol} \times 197 \text{ g/mol} \\ &= 0,591 \text{ g} \end{aligned}$$

b. Massa ligan yang diperlukan:

$$\begin{aligned} m &= n \times Mr \\ &= 0,005 \text{ mol} \times 378 \text{ g/mol} \\ &= 1,89 \text{ g} \end{aligned}$$

c. Rendemen:

	$\text{MnCl}_2 \cdot 4\text{H}_2\text{O} + \text{sistein} + \text{tirosin} + \text{CS}_2 \longrightarrow \text{Mn(II) Sis-Tir Dtc}$		
m	3 mmol	5 mmol	-
b	3 mmol	3 mmol	3 mmol
s	-	2 mmol	3 mmol

$$\begin{aligned} \text{Berat teori} &= \text{mmol Mn(II) SisTirDtc} \times \text{Mr Mn(II) SisTirDtc} \\ &= 3 \text{ mmol} \times 575 \text{ g/mol} \\ &= 0,003 \text{ mol} \times 575 \text{ g/mol} \\ &= 1,725 \text{ g} \end{aligned}$$

$$\text{Berat eksperimen} = 1,14 \text{ g}$$

$$\begin{aligned} \% \text{ Rendamen} &= \frac{\text{massa eksperimen}}{\text{massa teori}} \times 100\% \\ &= \frac{1,14 \text{ gr}}{1,725 \text{ gr}} \times 100\% \\ &= 66,08\% \end{aligned}$$

2. Perhitungan Hasil Rendemen senyawa kompleks Ni(II) Sis-Tir Dtc

a. Massa logam yang diperlukan:

$$\begin{aligned} m &= n \times Mr \\ &= 0,003 \text{ mol} \times 237 \text{ g/mol} \\ &= 0,711 \text{ g} \end{aligned}$$

b. Massa ligan yang diperlukan:

$$\begin{aligned} m &= n \times Mr \\ &= 0,005 \text{ mol} \times 378 \text{ g/mol} \\ &= 1,89 \text{ g} \end{aligned}$$

c. Rendemen:

	NiCl ₂ .6H ₂ O	+ sistein	+ tirosin	+ CS ₂	→	Ni(II) Sis-Tir Dtc
m	3 mmol		5 mmol			-
b	3 mmol		3 mmol			3 mmol
s	-		2 mmol			3 mmol

$$\begin{aligned} \text{Berat teori} &= \text{mmol Ni(II) SisTirDtc} \times \text{Mr Ni(II) SisTirDtc} \\ &= 3 \text{ mmol} \times 615 \text{ g/mol} \\ &= 0,003 \text{ mol} \times 615 \text{ g/mol} \\ &= 1,845 \text{ g} \end{aligned}$$

$$\text{Berat eksperimen} = 1,11 \text{ g}$$

$$\begin{aligned} \% \text{ Rendamen} &= \frac{\text{massa eksperimen}}{\text{massa teori}} \times 100\% \\ &= \frac{1,11 \text{ gr}}{1,845 \text{ gr}} \times 100\% \\ &= 60,16\% \end{aligned}$$

3.Perhitungan Hasil Rendemen senyawa kompleks Zn(II) Sis-Tir Dtc

a. Massa logam yang diperlukan:

$$\begin{aligned} m &= n \times Mr \\ &= 0,003 \text{ mol} \times 207 \text{ g/mol} \\ &= 0,622 \text{ g} \end{aligned}$$

b. Massa ligan yang diperlukan:

$$\begin{aligned} m &= n \times Mr \\ &= 0,005 \text{ mol} \times 378 \text{ g/mol} \\ &= 1,89 \text{ g} \end{aligned}$$

c. Rendemen:

	$\text{ZnCl}_2 \cdot 4\text{H}_2\text{O} + \text{sistein} + \text{tirosin} + \text{CS}_2 \longrightarrow \text{Zn(II) Sis-Tir Dtc}$		
M	3 mmol	5 mmol	-
B	3 mmol	3 mmol	3 mmol
S	-	2 mmol	3 mmol

$$\begin{aligned} \text{Berat teori} &= \text{mmol Zn(II) SisTirDtc} \times \text{Mr Zn(II) SisTirDtc} \\ &= 3 \text{ mmol} \times 585,38 \text{ g/mol} \\ &= 0,003 \text{ mol} \times 585,38 \text{ g/mol} \\ &= 1,756 \text{ g} \end{aligned}$$

$$\text{Berat eksperimen} = 1,12 \text{ g}$$

$$\begin{aligned} \% \text{ Rendamen} &= \frac{\text{massa eksperimen}}{\text{massa teori}} \times 100\% \\ &= \frac{1,12 \text{ gr}}{1,756 \text{ gr}} \times 100\% \\ &= 63,78\% \end{aligned}$$

4. Perhitungan Hasil Rendemen senyawa Sis-Tir Dtc

a. Massa ligan yang diperlukan:

$$\begin{aligned} m &= n \times Mr \\ &= 0,005 \text{ mol} \times 378 \text{ g/mol} \\ &= 1,89 \text{ g} \end{aligned}$$

b. Rendemen:

	sistein + tirosin + CS ₂	→	Sis-Tir Dtc
m	5 mmol		-
b	5 mmol		5 mmol
s	-		5 mmol

$$\begin{aligned} \text{Berat teori} &= \text{mmol SisTirDtc} \times \text{Mr SisTirDtc} \\ &= 5 \text{ mmol} \times 378 \text{ g/mol} \\ &= 0,003 \text{ mol} \times 378 \text{ g/mol} \\ &= 1,89 \text{ g} \end{aligned}$$

$$\text{Berat eksperimen} = 1,08 \text{ g}$$

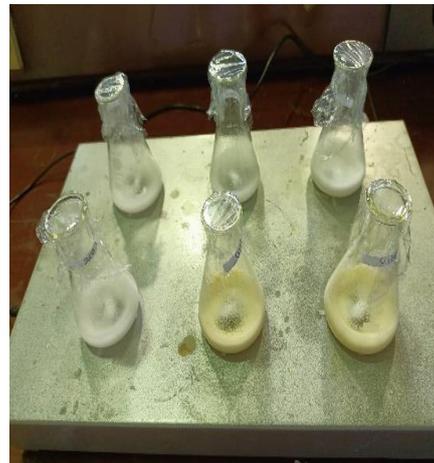
$$\begin{aligned} \% \text{ Rendamen} &= \frac{\text{massa eksperimen}}{\text{massa teori}} \times 100\% \\ &= \frac{1,08 \text{ gr}}{1,89 \text{ gr}} \times 100\% \\ &= 57,14\% \end{aligned}$$

Lampiran 5. Dokumentasi Penelitian

Penimbangan logam dan asam amino

Pemipetan CS₂

Proses sintesis senyawa kompleks



Proses pengadukkan senyawa kompleks



Penyaringan senyawa kompleks



Pendiaman senyawa kompleks



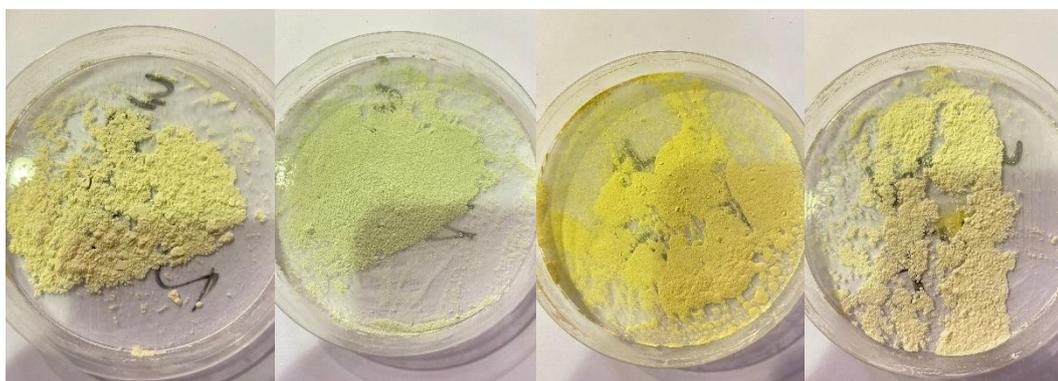
Uji melting point



Uji Uv-Vis



Uji konduktometri



Zn(II) Sis-Tir Dtc

Ni(II) Sis-Tir Dtc

Mn(II) Sis-Tir Dtc

Sis-Tir Dtc

Lampiran 6. Gambar morfologi dan hasil Uji Sitotoksitas Senyawa Kompleks terhadap sel kanker MCF-7



Gambar 25. Dokumentasi Morfologi Sel MCF-7 Hasil Uji Sis-Tir Dtc



Gambar 26. Dokumentasi Morfologi Sel MCF-7 Hasil Uji Mn(II) Sis-Tir Dtc



Gambar 27. Dokumentasi Morfologi Sel MCF-7 Hasil Uji Ni(II) Sis-Tir Dtc



Gambar 28. Dokumentasi Morfologi Sel MCF-7 Hasil Uji Zn(II) Sis-Tir Dtc

Tabel 12. Absorbansi Hasil Sis-Tir Dtc terhadap Sel MCF-7

	Media	Media + Sel	Cisplatin	Pelarut	Konsentrasi Sampel ($\mu\text{g/mL}$)							
					7,81	15,63	31,25	62,50	125,00	250,00	500,00	1000,00
Absorbansi 570nm	0,3557	0,5142	0,4306	0,4176	0,5494	0,5478	0,5466	0,5420	0,5400	0,5295	0,5110	0,4993
	0,3420	0,5317	0,4389	0,5187	0,5262	0,5300	0,5429	0,5408	0,5380	0,5167	0,5230	0,4916
Absorbansi 600nm	0,4236	0,1547	0,3384	0,3649	0,1668	0,1662	0,1649	0,1628	0,1639	0,1840	0,1913	0,2115
	0,4058	0,1650	0,3409	0,1954	0,1589	0,1614	0,1674	0,1657	0,1681	0,1825	0,2001	0,2050
Selisih Absorbansi	-0,0679	0,3595	0,0922	0,0527	0,3826	0,3816	0,3817	0,3792	0,3761	0,3455	0,3197	0,2878
	-0,0638	0,3667	0,0980	0,3233	0,3673	0,3686	0,3755	0,3751	0,3699	0,3342	0,3229	0,2866
% Sel hidup	167,56	62,26	46,70	176,66	176,27	176,30	175,32	174,10	162,04	151,88	139,31	
	170,40	64,55	153,30	170,63	171,14	173,86	173,70	171,66	157,59	153,14	138,84	
Rata-rata % sel hidup	168,98	63,40	100,00	173,65	173,70	175,08	174,51	172,88	159,82	152,51	139,08	
SEM	1,42	1,14	53,30	3,01	2,56	1,22	0,81	1,22	2,23	0,63	0,24	
Normalisasi data % Sel hidup	97,31	36,51	57,59	100,00	100,03	100,83	100,50	99,56	92,04	87,83	80,09	

Tabel 13. Absorbansi Hasil Mn(II) Sis-Tir Dtc terhadap Sel MCF-7

	Media	Media + Sel	Cisplatin	Pelarut	Konsentrasi Sampel ($\mu\text{g/mL}$)							
					7,81	15,63	31,25	62,50	125,00	250,00	500,00	1000,00
Absorbansi 570nm	0,3484	0,5524	0,4219	0,5235	0,5486	0,5385	0,5430	0,5494	0,5437	0,5293	0,4061	0,3827
	0,3475	0,5594	0,4296	0,5402	0,5630	0,5619	0,5649	0,5533	0,5539	0,5459	0,4271	0,4458
Absorbansi 600nm	0,4141	0,1913	0,3370	0,1941	0,1980	0,1947	0,1917	0,1908	0,1815	0,1840	0,3632	0,4181
	0,4119	0,1858	0,3396	0,2016	0,2017	0,1991	0,1986	0,1904	0,1872	0,2013	0,3617	0,4806
Selisih Absorbansi	-0,0657	0,3611	0,0849	0,3294	0,3506	0,3438	0,3513	0,3586	0,3622	0,3453	0,0429	-0,0354
	-0,0644	0,3736	0,0900	0,3386	0,3613	0,3628	0,3663	0,3629	0,3667	0,3446	0,0654	0,0348
% Sel hidup	106,79	37,58	98,85	104,16	102,46	104,34	106,16	107,07	102,83	27,05	7,43	
	109,92	38,85	101,15	106,84	107,22	108,09	107,24	108,19	102,66	32,69	7,58	
Rata-rata % sel hidup	108,36	38,22	100,00	105,50	104,84	106,21	106,70	107,63	102,74	29,87	7,51	
SEM	1,57	0,64	1,15	1,34	2,38	1,88	0,54	0,56	0,09	2,82	0,08	
Normalisasi data % Sel hidup	102,71	36,22	94,79	100,00	99,37	100,68	101,14	102,02	97,39	28,31	7,11	

Tabel 14. Absorbansi Hasil Ni(II) Sis-Tir Dtc terhadap Sel MCF-7

	Media	Media + Sel	Cisplatin	Pelarut	Konsentrasi Sampel ($\mu\text{g/mL}$)							
					7,81	15,63	31,25	62,50	125,00	250,00	500,00	1000,00
Absorbansi 570nm	0,4895	0,7980	0,6073	0,7897	0,8019	0,7973	0,8110	0,8113	0,8072	0,8120	0,8246	0,6076
	0,4822	0,8165	0,6294	0,8317	0,8067	0,8239	0,8199	0,8216	0,8200	0,8239	0,8382	0,6187
Absorbansi 600nm	0,6302	0,2289	0,5390	0,2031	0,2176	0,2126	0,2165	0,2094	0,2154	0,2133	0,2436	0,4736
	0,6196	0,2331	0,5446	0,2461	0,2204	0,2199	0,2225	0,2161	0,2169	0,2184	0,2581	0,4668
Selisih Absorbansi	-0,1407	0,5691	0,0683	0,5866	0,5843	0,5847	0,5945	0,6019	0,5918	0,5987	0,5810	0,1340
	-0,1374	0,5834	0,0848	0,5856	0,5863	0,6040	0,5974	0,6055	0,6031	0,6055	0,5801	0,1519
% Sel hidup	99,00	28,59	101,45	101,13	101,18	102,55	103,59	102,17	103,14	100,66	38,17	
	101,00	31,29	101,31	101,41	103,88	102,96	104,09	103,75	104,09	100,54	40,68	
Rata-rata % sel hidup	100,00	30,14	101,38	101,27	102,53	102,75	103,84	102,96	103,61	100,60	39,42	
SEM	1,00	1,15	0,07	0,14	1,35	0,20	0,25	0,79	0,48	0,06	1,25	
Normalisasi data % Sel hidup	98,75	29,76	100,11	100,00	101,25	101,47	102,54	101,68	102,32	99,34	38,93	

Tabel 15. Absorbansi Hasil Zn(II) Sis-Tir Dtc terhadap Sel MCF-7

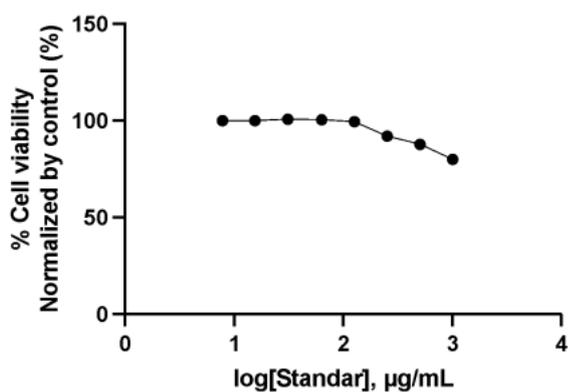
	Media	Media + Sel	Cisplatin	Pelarut	Konsentrasi Sampel ($\mu\text{g/mL}$)							
					7,81	15,63	31,25	62,50	125,00	250,00	500,00	1000,00
Absorbansi 570nm	0,4845	0,7657	0,5969	0,7708	0,7876	0,7867	0,7807	0,7868	0,7976	0,8265	0,7986	0,6605
	0,4965	0,7655	0,5851	0,7728	0,7961	0,8028	0,7892	0,8052	0,8158	0,8289	0,8016	0,6455
Absorbansi 600nm	0,6243	0,2145	0,5336	0,2218	0,2168	0,2170	0,2092	0,2122	0,2181	0,2306	0,3805	0,5302
	0,6380	0,2115	0,5321	0,3009	0,2205	0,2137	0,2145	0,2145	0,2258	0,2309	0,3804	0,5408
Selisih Absorbansi	-0,1398	0,5512	0,0633	0,5490	0,5708	0,5697	0,5715	0,5746	0,5795	0,5959	0,4181	0,1303
	-0,1415	0,5540	0,0530	0,4719	0,5756	0,5891	0,5747	0,5907	0,5900	0,5890	0,4212	0,1047
% Sel hidup		106,26	31,32	105,92	109,27	109,10	109,38	109,85	110,61	113,12	85,82	41,61
		106,69	29,74	94,08	110,01	112,08	109,87	112,33	112,22	113,45	86,29	37,68
Rata-rata % sel hidup		106,47	30,53	100,00	109,64	110,59	109,62	111,09	111,41	113,29	86,05	39,65
SEM		0,22	0,79	5,92	0,37	1,49	0,25	1,24	0,81	0,16	0,24	1,97
Normalisasi data % Sel hidup		106,47	30,53	100,00	109,64	110,59	109,62	111,09	111,41	113,29	86,05	39,65

Keterangan:

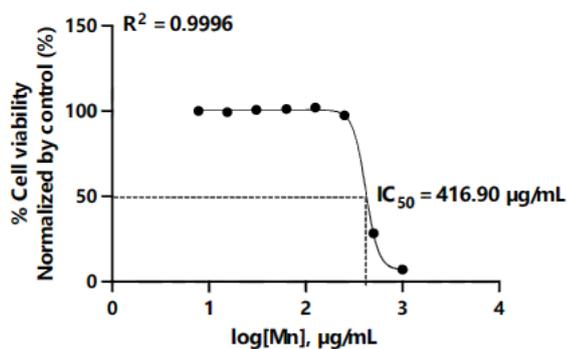
- Panjang gelombang 600 nm mengukur absorbansi Resazurin berwarna biru
- Panjang gelombang 570 nm mengukur absorbansi Resorufin berwarna merah
- Corrected Absorbance: Selisih absorbansi sampel/media+Sel/Kontrol pada panjang gelombang 570 nm dan 600 nm, lalu dikurangi rata-rata selisih absorbansi media pada kedua panjang gelombang yang sama.
- Konsentrasi Cisplatin yang digunakan pada treatment 24 jam sebesar 470 μM
- Konsentrasi Cisplatin yang digunakan pada treatment 48 jam sebesar 50 μM
- Kompleks Zn dan Cu ditreatment pada sel selama 24 jam
- Kompleks Fe dan Mg ditreatment pada sel selama 48 jam
- Semua logam ditreatment pada sel selama 48 jam

Sampel	IC ₅₀ ($\mu\text{g/mL}$)
Standar	>1.000
Mn	416,90
Ni	618,40
Zn	511,40

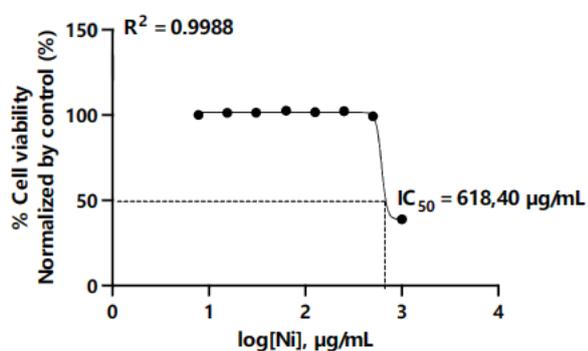
Gambar 29. Hasil Uji Antiproliferasi



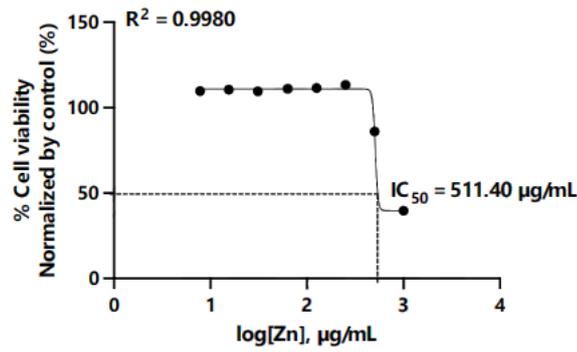
Gambar 30. Kurva Hasil Uji Sis-Tir Dtc terhadap Sel MCF-7



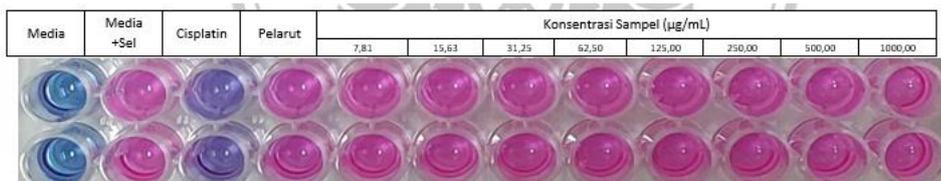
Gambar 31. Kurva Hasil Uji Mn(II) Sis-Tir Dtc terhadap Sel MCF-7



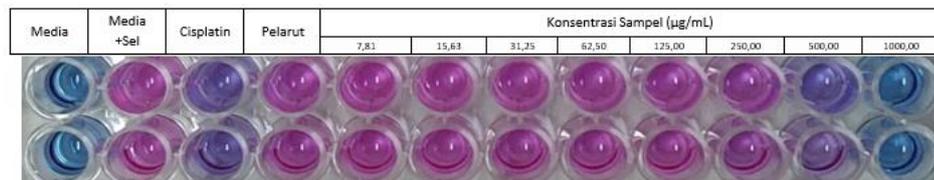
Gambar 32. Kurva Hasil Uji Ni(II) Sis-Tir Dtc terhadap Sel MCF-7



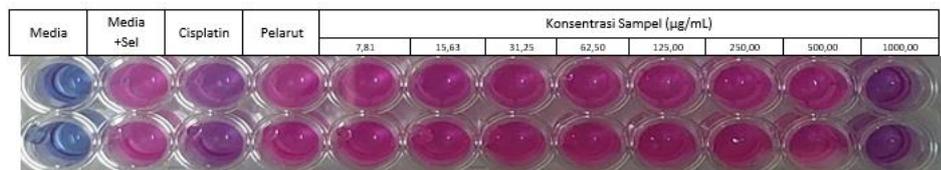
Gambar 33. Kurva Hasil Uji Zn(II) Sis-Tir Dtc terhadap Sel MCF-7



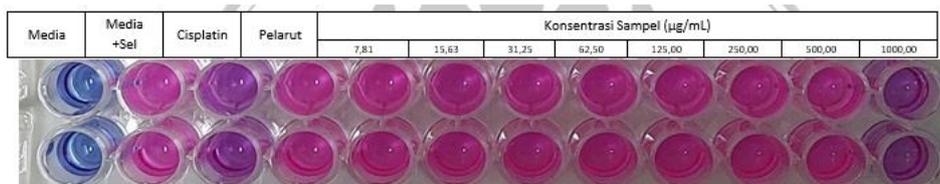
Gambar 34. Dokumentasi Well Plate Hasil Sis-Tir Dtc terhadap Sel MCF-7



Gambar 35. Dokumentasi Well Plate Hasil Mn(II) Sis-Tir Dtc terhadap Sel MCF-7

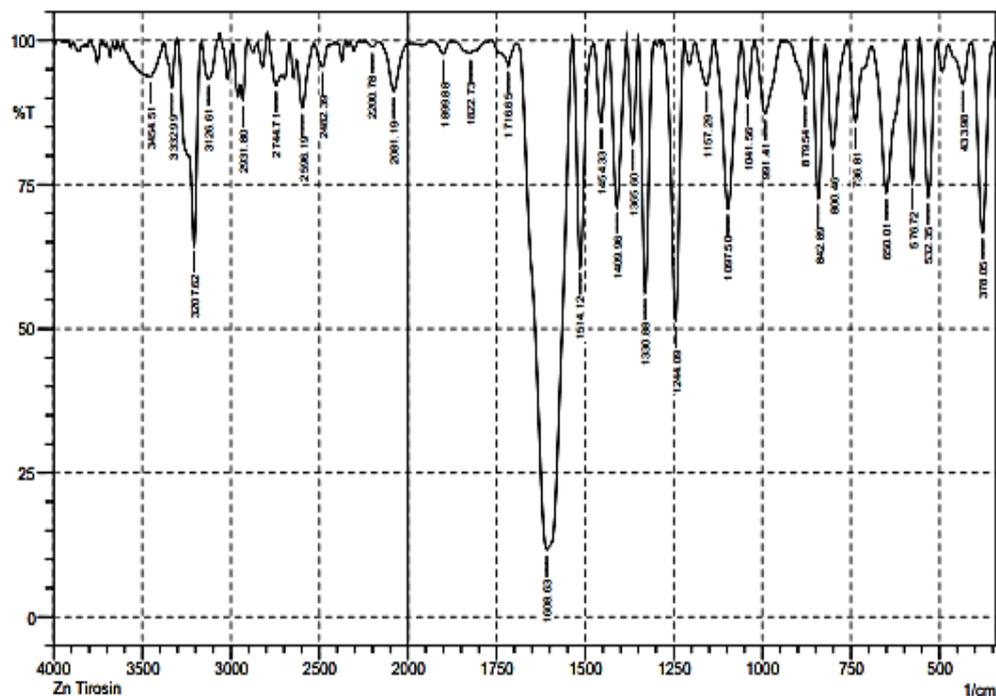


Gambar 36. Dokumentasi Well Plate Hasil Ni(II) Sis-Tir Dtc, terhadap Sel MCF-7



Gambar 37. Dokumentasi Well Plate Hasil Zn(II) Sis-Tir Dtc terhadap Sel MCF-7

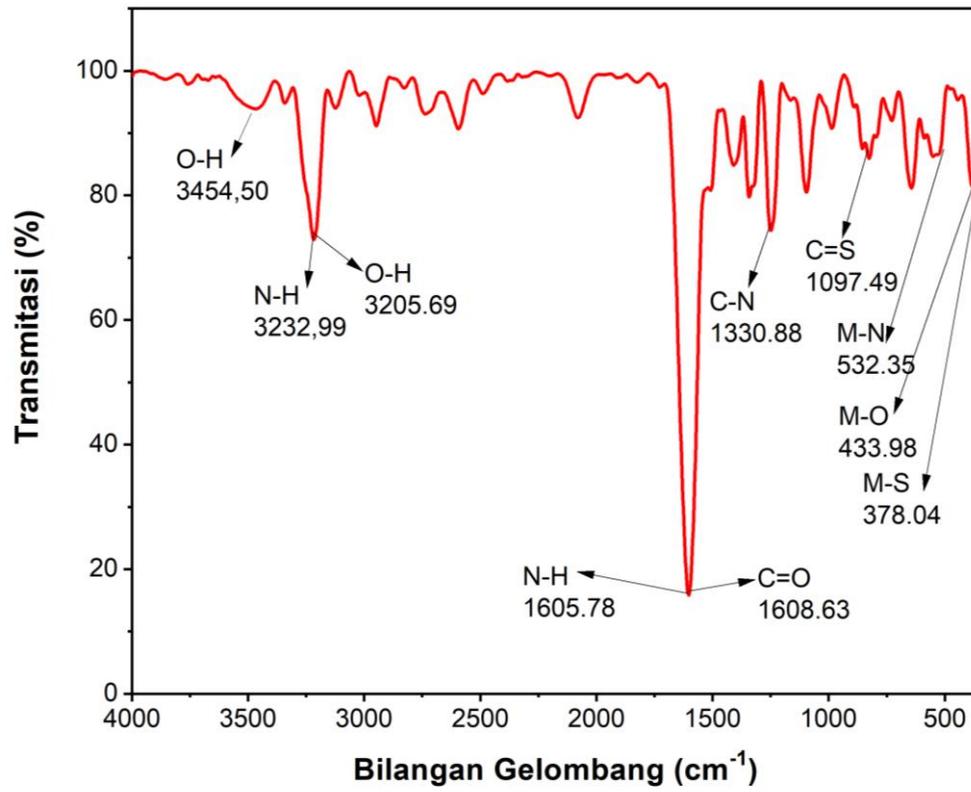
Lampiran 7. Hasil analisis FTIR Zn(II) Sis-Tir Dtc



No.	Peak	Intensity	Corr. Intensity	Base (H)	Base (L)	Area	Corr. Area
1	378.05	66.71	32.976	410.84	345.26	4.567	4.478
2	433.98	92.457	7.049	474.49	412.77	1.063	0.918
3	532.35	72.867	27.047	555.5	509.21	3.158	3.138
4	576.72	75.375	24.339	596	557.43	2.36	2.313
5	650.01	73.633	25.717	690.52	597.93	5.421	5.182
6	736.81	85.985	11.445	759.95	717.52	1.544	1.079
7	800.46	81.278	18.319	821.68	761.88	2.439	2.366
8	842.89	72.608	27.197	862.18	823.6	2.682	2.645
9	879.54	89.825	10.139	931.82	864.11	1.298	1.265
10	991.41	87.37	12.642	1022.27	947.05	2.247	2.247
11	1041.56	90.107	9.866	1058.92	1022.27	0.8	0.796
12	1097.5	70.864	29.048	1134.14	1058.92	5.036	5.007
13	1157.29	92.178	7.667	1188.15	1136.07	1.016	0.972
14	1244.09	51.475	48.399	1280.73	1222.87	6.729	6.709
15	1330.88	56.372	43.743	1350.17	1305.81	4.714	4.728
16	1365.6	82.244	17.607	1382.96	1352.1	1.435	1.418
17	1409.96	71.164	28.426	1435.04	1384.89	3.58	3.488
18	1454.33	85.869	13.77	1475.54	1436.97	1.348	1.286
19	1514.12	60.763	38.891	1533.41	1477.47	4.784	4.694
20	1608.63	11.692	88.274	1693.5	1535.34	60.588	60.546
21	1716.65	95.622	4.05	1764.87	1695.43	0.619	0.55
22	1822.73	97.761	0.836	1870.95	1811.16	0.367	0.113
23	1899.88	97.72	2.152	1936.53	1880.6	0.239	0.202
24	2081.19	91.241	8.361	2160.27	2002.11	2.658	2.383
25	2200.78	98.912	0.902	2241.28	2160.27	0.208	0.143
26	2482.39	95.48	3.928	2530.61	2447.67	0.956	0.748
27	2598.19	88.347	9.17	2627.05	2532.54	2.664	1.856
28	2744.71	92.255	4.622	2791	2713.84	1.783	0.917
29	2931.8	89.714	5.4	2945.3	2906.73	1.042	0.438
30	3126.61	93.273	7.19	3165.19	3064.89	1.62	1.891
31	3207.62	64.469	35.492	3304.06	3167.12	11.03	11.055
32	3332.99	91.899	8.167	3377.36	3305.99	1.201	1.202
33	3454.51	93.701	1.2	3469.94	3379.29	1.677	0.413

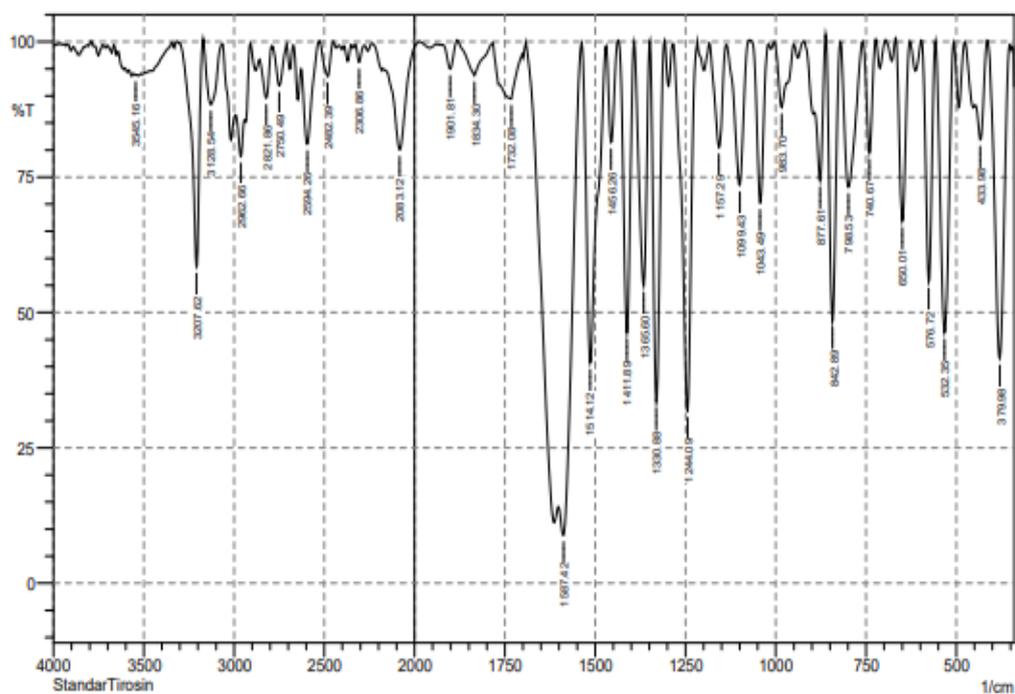
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No. of Scans;



Lampiran 8. Hasil analisis FTIR Sis-Tir Dtc

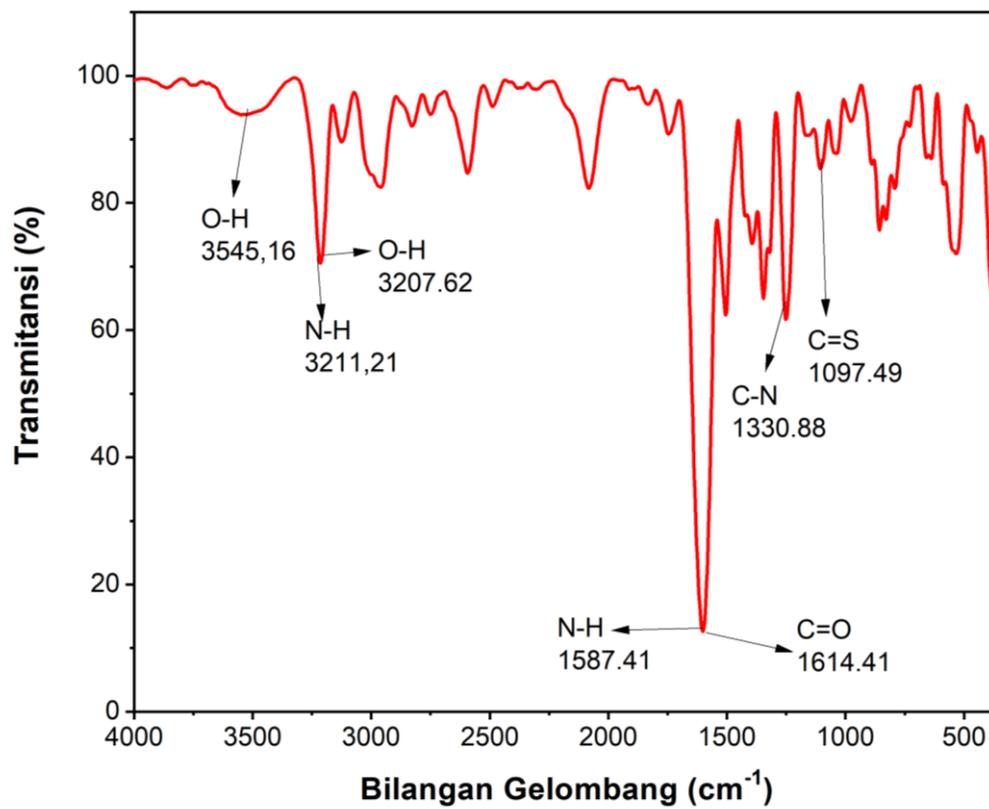
SHIMADZU



No.	Peak	Intensity	Corr. Intensity	Base (H)	Base (L)	Area	Corr. Area
1	379.98	41.51	58.25	412.77	352.97	9.7	9.64
2	433.98	81.95	10.73	445.56	414.7	1.62	0.85
3	532.35	46.3	53.41	557.43	509.21	7.59	7.53
4	576.72	55.65	44.13	596	559.36	4.24	4.21
5	650.01	66.94	33.42	667.37	628.79	3	3.05
6	740.67	79.56	20.67	759.95	723.31	1.6	1.63
7	798.53	73.2	26.62	819.75	761.88	4.24	4.19
8	842.89	48.51	51.79	860.25	821.68	5.48	5.52
9	877.61	74.42	19.1	891.11	862.18	2.16	1.41
10	983.7	87.9	7.55	1002.98	970.19	1.17	0.56
11	1043.49	70.23	29.56	1072.42	1022.27	2.87	2.83
12	1099.43	73.53	26.37	1136.07	1074.35	3.45	3.41
13	1157.29	80.52	18.96	1182.36	1138	2.1	2
14	1244.09	31.84	67.44	1282.66	1219.01	11.57	11.38
15	1330.88	33.46	66.72	1348.24	1307.74	8.04	8.07
16	1365.6	54.97	44.46	1390.68	1350.17	5.48	5.37
17	1411.89	46.29	53.7	1435.04	1392.61	5.92	5.92
18	1456.26	81.47	18.15	1469.76	1436.97	1.43	1.39
19	1514.12	40.7	58.73	1537.27	1471.69	10.91	10.7
20	1587.42	8.88	23.83	1600.92	1539.2	30.71	6.65
21	1732.08	89.47	5.46	1764.87	1703.14	2.18	0.75
22	1834.3	93.81	6.13	1880.6	1784.15	1.27	1.23
23	1901.81	95	4.86	1921.1	1882.52	0.41	0.39
24	2083.12	80.06	17.37	2173.78	1988.61	7.96	5.91
25	2306.86	96.2	3.21	2328.08	2277.93	0.45	0.32
26	2482.39	93.62	6.47	2526.75	2451.53	1.13	1.16
27	2594.26	81.1	15.49	2627.05	2528.68	4.49	3.41
28	2750.49	91.91	7.28	2785.21	2709.99	1.52	1.26
29	2821.86	89.64	8.42	2858.51	2792.93	1.94	1.35
30	2962.66	78.82	7.06	2991.59	2943.37	4.01	0.85
31	3128.54	88.41	11.74	3170.97	3066.82	3.14	3.16
32	3207.62	58.45	41.64	3302.13	3172.9	9.84	9.83
33	3545.16	93.84	0.12	3556.74	3539.38	0.47	0.01

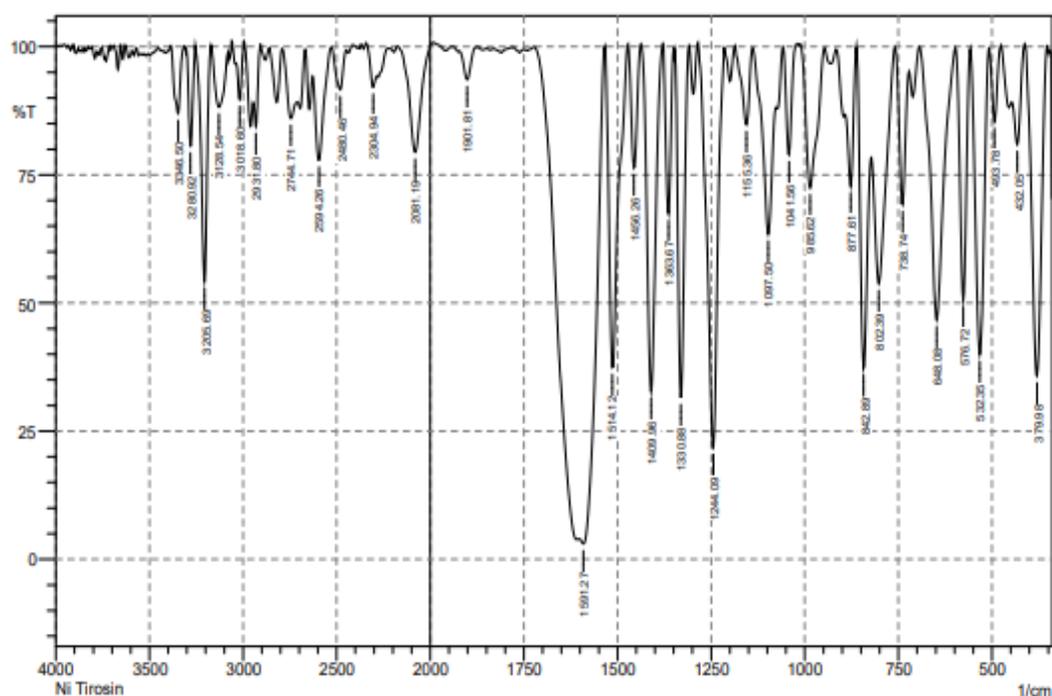
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No. of Scans;



Lampiran 9. Hasil analisis FTIR Ni(II) Sis-Tir Dtc

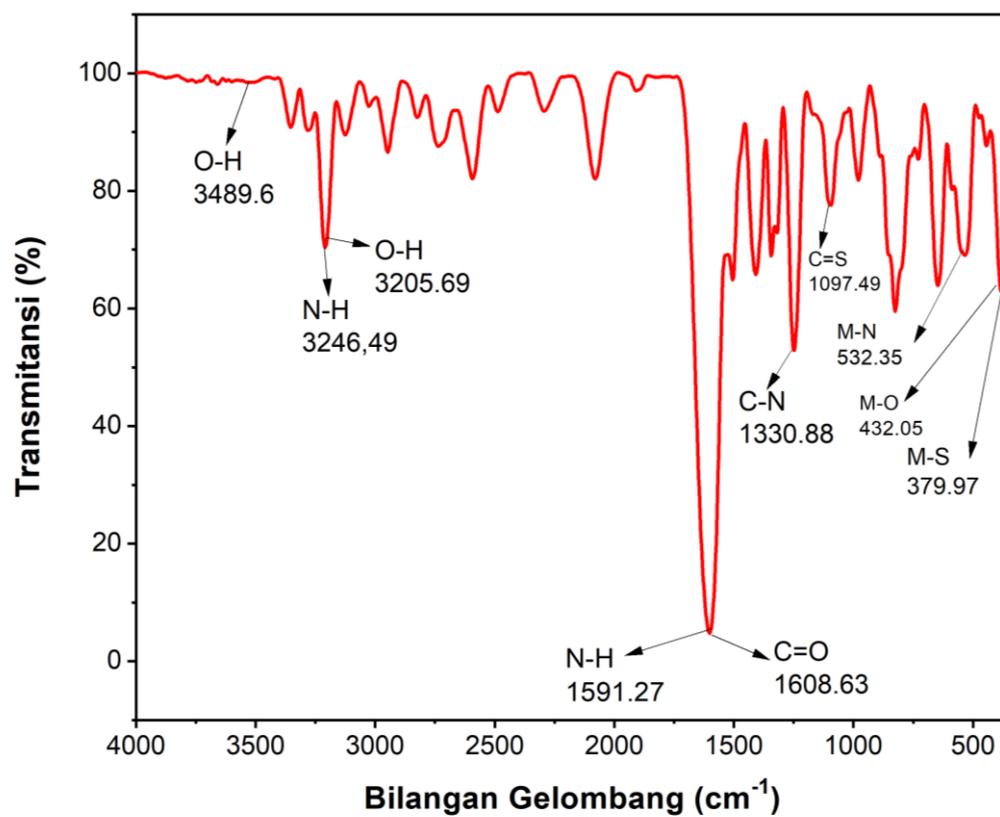
SHIMADZU



No.	Peak	Intensity	Corr. Intensity	Base (H)	Base (L)	Area	Corr. Area
1	379.98	35.755	64.514	412.77	352.97	10.868	10.94
2	432.05	80.923	12.942	445.56	414.7	1.723	0.999
3	493.78	85.396	14.394	507.28	478.35	0.995	0.971
4	532.35	39.95	59.598	557.43	509.21	8.758	8.664
5	576.72	50.56	48.652	596	559.36	4.997	4.871
6	648.08	46.786	53.068	692.44	597.93	11.438	11.368
7	738.74	69.184	27.732	758.02	723.31	2.862	2.406
8	802.39	53.783	31.271	821.68	759.95	8.799	5.613
9	842.89	37.266	51.83	862.18	823.6	8.591	6.427
10	877.61	72.849	19.904	891.11	864.11	2.304	1.452
11	985.62	72.485	27.511	1010.7	948.98	4.394	4.368
12	1041.56	78.909	21.27	1056.99	1022.27	1.544	1.58
13	1097.5	63.442	28.204	1138	1078.21	5.629	3.84
14	1155.36	84.788	15.091	1186.22	1139.93	1.542	1.53
15	1244.09	21.808	78.477	1284.59	1215.15	15.835	15.937
16	1330.88	31.522	68.559	1350.17	1309.67	7.824	7.84
17	1363.67	67.459	31.686	1377.17	1352.1	2.399	2.306
18	1409.96	32.733	67.775	1436.97	1379.1	10.138	10.266
19	1456.26	76.358	23.97	1471.69	1438.9	1.884	1.929
20	1514.12	37.438	62.705	1533.41	1473.62	10.061	10.099
21	1591.27	3.026	15.016	1600.92	1535.34	47.458	5.585
22	1901.81	93.552	5.928	1923.03	1878.67	0.608	0.511
23	2081.19	79.406	21.048	2173.78	1992.47	6.682	7.034
24	2304.94	92.085	4.689	2341.58	2281.79	1.253	0.556
25	2480.46	91.621	7.872	2524.82	2449.6	1.605	1.452
26	2594.26	77.861	18.091	2627.05	2526.75	5.351	4.013
27	2744.71	86.029	7.592	2791	2709.99	3.511	1.38
28	2931.8	84.399	8.375	2943.37	2908.65	1.488	0.688
29	3018.6	89.669	8.869	3035.96	2995.45	1.024	0.835
30	3128.54	88.213	11.307	3170.97	3082.25	3.013	2.804
31	3205.69	54.245	45.765	3253.91	3172.9	8.224	8.222
32	3280.92	80.621	19.086	3302.13	3255.84	2.184	2.137
33	3346.5	86.989	13.153	3385.07	3313.71	2.12	2.164

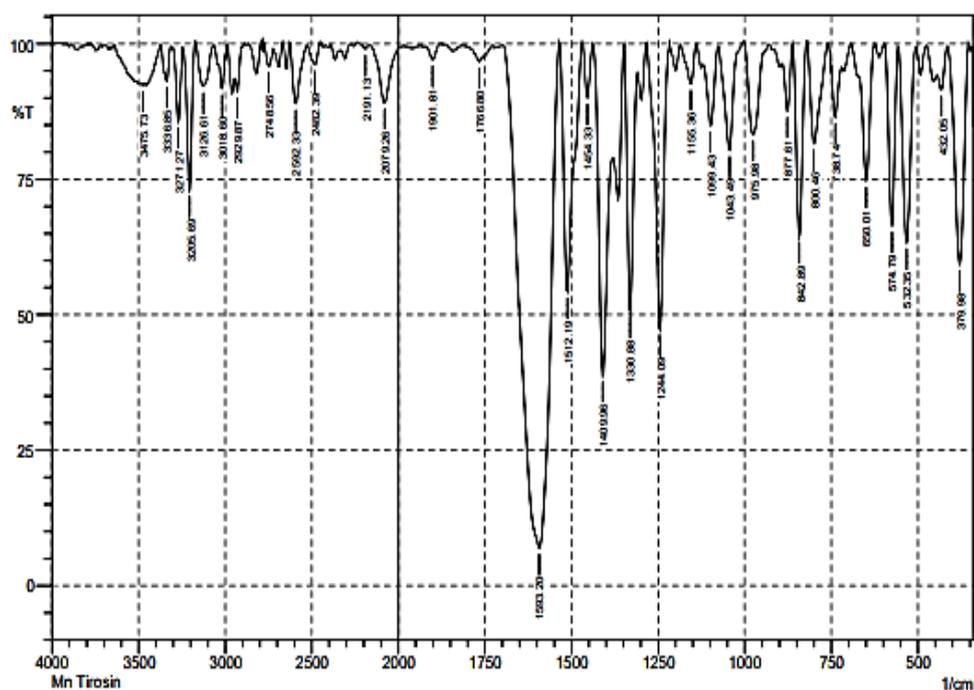
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No. of Scans;



Lampiran 10. Hasil analisis FTIR Mn(II) Sis-Tir Dtc

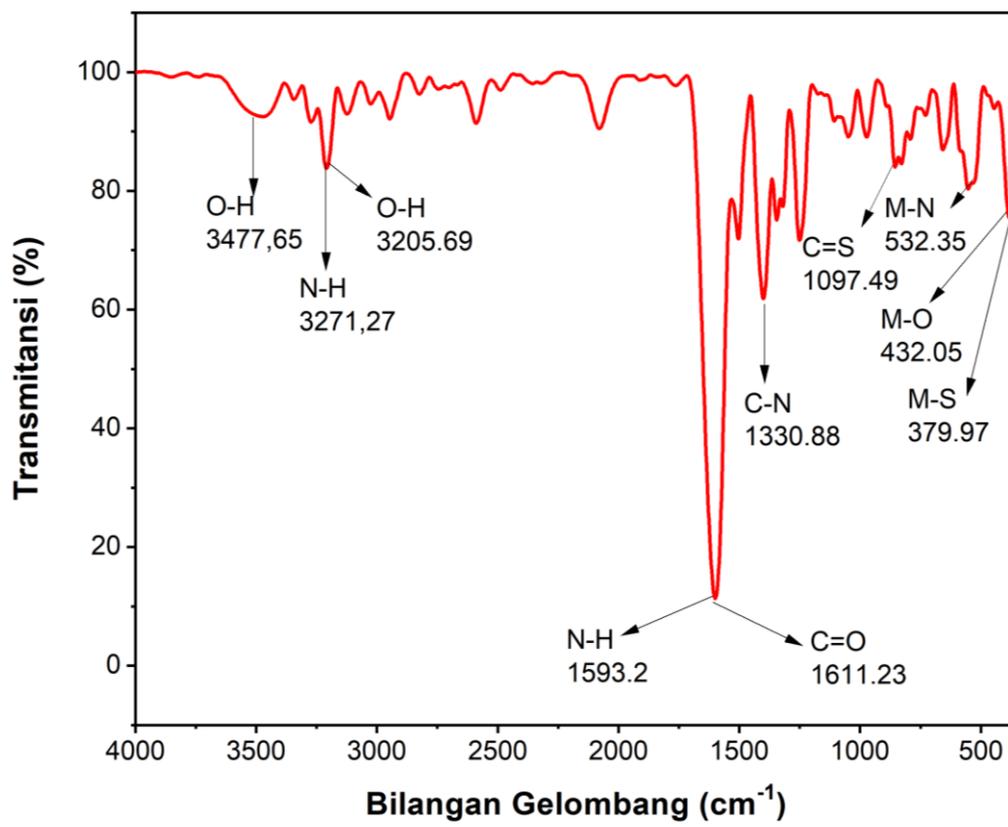
SHIMADZU



No.	Peak	Intensity	Corr. Intensity	Base (H)	Base (L)	Area	Corr. Area
1	379.98	59.379	40.469	414.7	354.9	6.239	6.19
2	432.05	91.44	5.066	445.56	414.7	0.767	0.332
3	532.35	63.43	35.905	555.5	507.28	4.59	4.451
4	574.79	66.479	33.113	596	557.43	3.182	3.115
5	650.01	74.748	25.152	692.44	624.94	3.144	3.114
6	738.74	86.425	11.188	759.95	721.38	1.323	0.934
7	800.46	81.601	18.7	819.75	761.88	2.579	2.632
8	842.89	64.55	35.275	860.25	821.68	3.472	3.459
9	877.61	87.598	10.518	893.04	862.18	0.985	0.728
10	975.98	83.256	16.81	1001.06	931.62	2.549	2.549
11	1043.49	80.423	19.474	1076.28	1002.98	2.538	2.525
12	1099.43	84.996	12.637	1118.71	1078.21	1.614	1.219
13	1155.36	92.624	7.264	1186.22	1139.93	0.747	0.723
14	1244.09	47.376	52.715	1282.66	1217.08	7.728	7.758
15	1330.88	50.77	46.638	1348.24	1309.67	5.42	4.906
16	1409.96	38.81	50.432	1436.97	1382.96	10.542	7.614
17	1454.33	90.062	10.102	1469.76	1438.9	0.665	0.687
18	1512.19	54.321	45.568	1533.41	1469.76	7.419	7.423
19	1593.2	7.018	93.016	1697.36	1535.34	74.879	74.854
20	1766.8	96.606	3.06	1815.02	1728.22	0.581	0.455
21	1901.81	97.13	2.609	1921.1	1880.6	0.258	0.214
22	2079.26	89.118	10.508	2160.27	1986.68	3.607	3.322
23	2191.13	99.116	0.733	2235.5	2167.99	0.11	0.092
24	2482.39	96.127	3.887	2526.68	2449.6	0.717	0.704
25	2592.33	88.977	10.963	2627.05	2528.68	2.398	2.343
26	2748.56	95.819	3.752	2779.42	2723.49	0.605	0.517
27	2929.87	91.103	4.077	2943.37	2889.37	0.969	0.301
28	3018.6	91.78	5.761	3037.89	2987.74	1.028	0.592
29	3126.61	92.16	7.912	3172.9	3066.82	2.088	2.094
30	3205.69	73.107	26.746	3244.27	3174.83	3.931	3.871
31	3271.27	85.588	13.715	3304.06	3246.2	1.897	1.723
32	3336.85	93.072	6.512	3371.57	3317.56	1	0.914
33	3475.73	92.44	0.468	3639.68	3466.08	4.052	0.962

Date/Time; 5/25/2023 2:45:04 PM

No. of Scans;



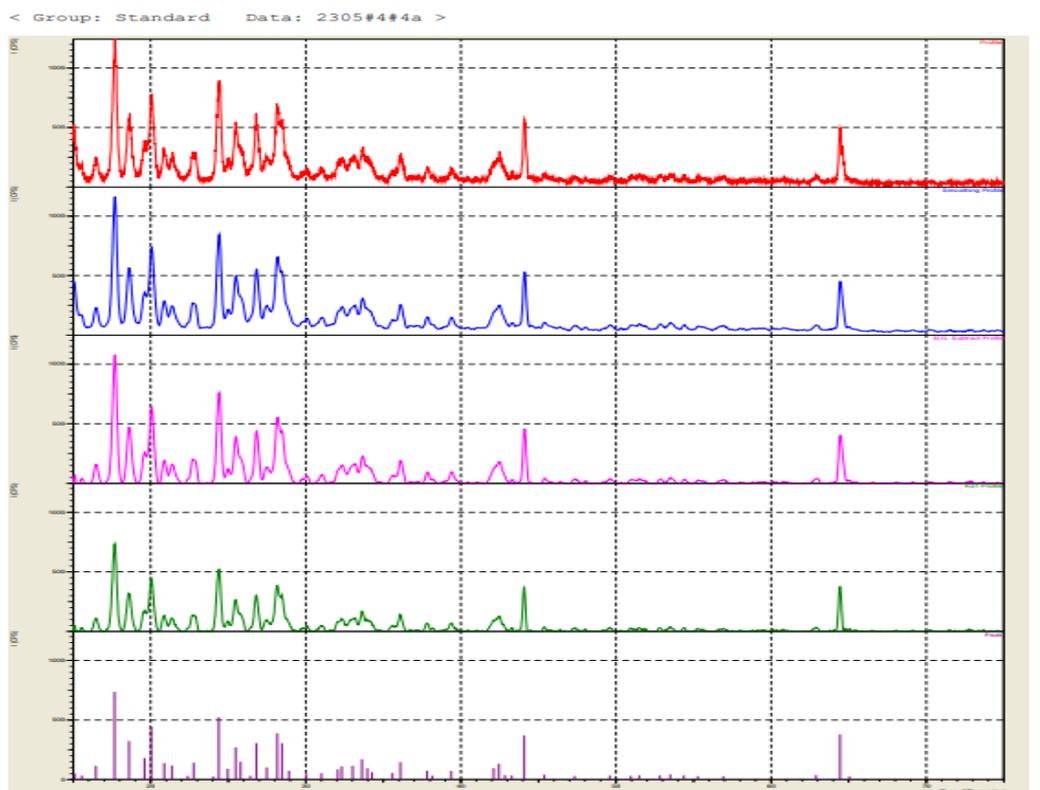
Lampiran 11. Hasil Analisa XRD Kompleks Sis-Tir Dtc

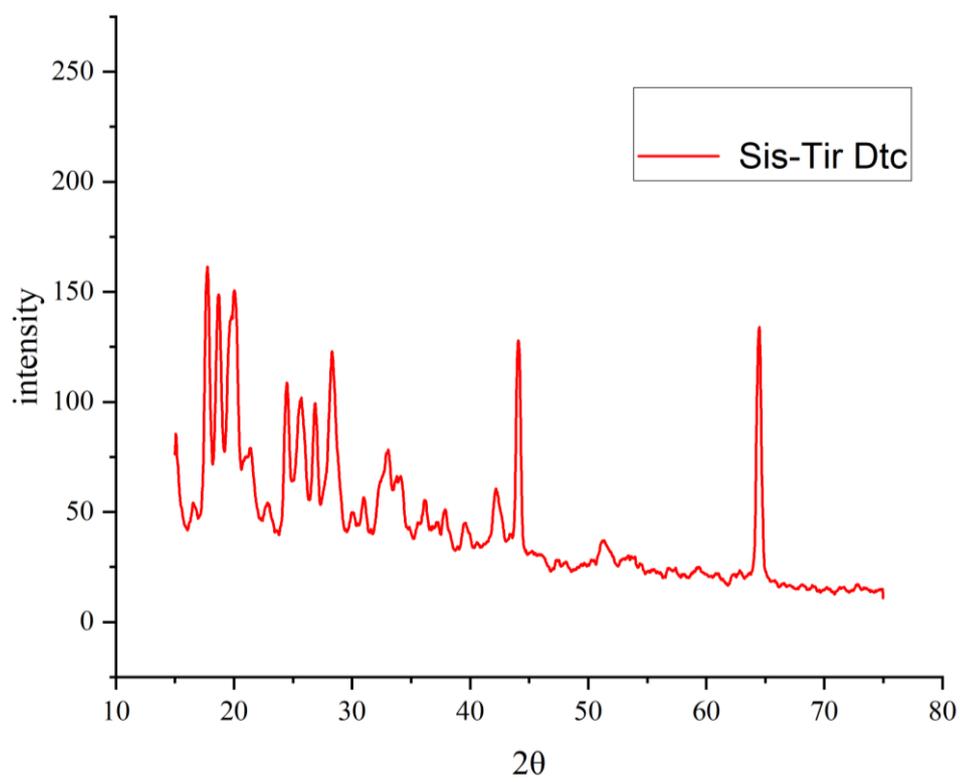
*** Basic Data Process ***

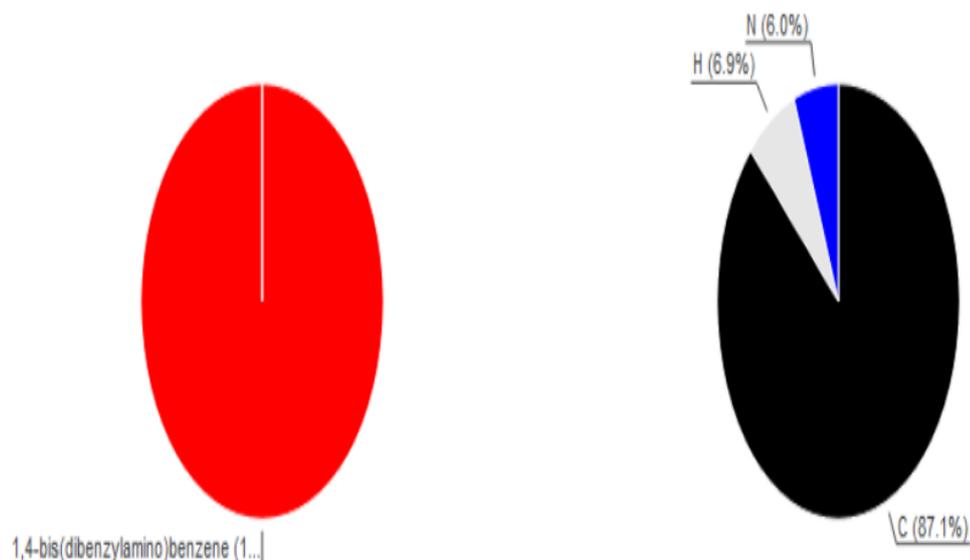
Group : Standard
Data : 2305#4#4a

# Strongest 3 peaks	no. peak	2Theta (deg)	d (Å)	I/I1	FWHM (deg)	Intensity (Counts)	Integrated Int (Counts)
1	4	17.6716	5.01487	100	0.32700	440	7793
2	13	24.3867	3.64706	71	0.32520	312	5144
3	7	20.0462	4.42586	60	0.34970	263	4638

# Peak Data List	peak no.	2Theta (deg)	d (Å)	I/I1	FWHM (deg)	Intensity (Counts)	Integrated Int (Counts)
1	15.0866	5.86782	6	0.12670	23	176	
2	15.5567	5.69154	4	0.18000	18	167	
3	16.4732	5.37689	15	0.31640	67	1086	
4	17.6716	5.01487	100	0.32700	440	7793	
5	18.6039	4.76560	44	0.36160	192	3744	
6	19.6000	4.52560	24	0.34000	106	1939	
7	20.0462	4.42586	60	0.34970	263	4638	
8	20.8809	4.25079	18	0.33530	81	1280	
9	21.3740	4.15382	15	0.37200	68	1400	
10	22.4000	3.96583	4	0.22000	16	213	
11	22.7735	3.90162	19	0.42300	83	1736	
12	24.0400	3.69886	71	0.12000	14	186	
13	24.3867	3.64706	71	0.32520	312	5144	
14	24.9800	3.56176	12	0.30000	52	932	
15	25.4800	3.49299	36	0.31700	160	2241	
16	25.8000	3.45039	20	0.41500	88	1738	
17	26.4200	3.37081	4	0.12000	17	181	
18	26.8190	3.32156	41	0.30850	181	2932	
19	27.4800	3.24315	13	0.37720	59	1364	
20	28.1600	3.16636	53	0.33460	231	3732	
21	28.4600	3.13366	41	0.34000	181	2791	
22	28.9200	3.08485	10	0.26000	42	815	
23	29.0400	3.07234	6	0.32000	28	548	
24	31.0145	2.88113	7	0.34100	30	587	
25	32.0600	2.78952	11	0.26000	49	555	
26	32.3200	2.76767	15	0.56000	64	1257	
27	33.0300	2.70978	15	0.66000	67	2027	
28	33.6200	2.66356	23	0.28000	100	1893	
29	33.9800	2.63616	13	0.00000	55	0	
30	34.2800	2.61378	8	0.29340	34	1113	
31	34.6000	2.59190	7	0.38000	31	62	
32	36.1000	2.48607	20	0.32000	86	1406	
33	37.8210	2.37680	10	0.26200	42	633	
34	38.1600	2.35646	4	0.24000	17	233	
35	39.3833	2.28604	19	0.30670	41	913	
36	41.1200	2.14362	13	0.46000	55	1265	
37	42.4600	2.12724	18	0.35600	77	1202	
38	42.8400	2.10925	5	0.16000	20	296	
39	43.2800	2.08882	4	0.16000	18	176	
40	44.0785	2.05281	50	0.21200	220	2490	
41	45.3800	1.99691	5	0.20000	22	313	
42	47.3383	1.91877	4	0.38330	16	457	
43	49.6033	1.83633	4	0.31330	18	396	
44	50.9600	1.79058	4	0.24000	17	274	
45	51.9050	1.77291	4	0.20000	19	412	
46	52.8300	1.73152	4	0.24660	19	254	
47	53.5000	1.71140	5	0.28000	23	427	
48	54.3725	1.68598	4	0.22500	18	231	
49	55.2783	1.66048	3	0.21670	15	304	







Index	Amount (%)	Name	Formula sum	Element	Amount (weight %)
A	100.0	1,4-bis(dibenzylamino)benzene	C ₃₄ H ₃₂ N ₂	C	87.1%(*)
	38.3	Unidentified peak area		H	6.9%(*)
				N	6.0%(*)
				*LE (sum)	100.0%

Details of identified phases

A: 1,4-

*bis(dibenzylamino)benzene (100.0 %)**

Formula sum	C ₃₄ H ₃₂ N ₂
Entry number	96-200-0395
Figure-of-Merit (FoM)	0.705817*
Total number of peaks	994
Peaks in range	994
Peaks matched	151
Intensity scale factor	0.51*
Space group	P 1 21/n 1
Crystal system	monoclinic
Unit cell	a= 14.7660 Å b= 5.6040 Å c= 15.8970 Å β= 97.340 °
I/c	0.66
Calc. density	1.190 g/cm ³
Reference	Rickert C., Pirota M., Müller T., "Structure of 1,4-bis(dibenzylamino)benzene", Acta Crystallographica Section C 48(12) , 2233-2235 (1992)

(*)2theta values have been shifted internally for the calculation of the amounts, the intensity scaling factors as well as the figure-of-merit (FoM), due to the active search-match option 'Automatic zero point adaption'.

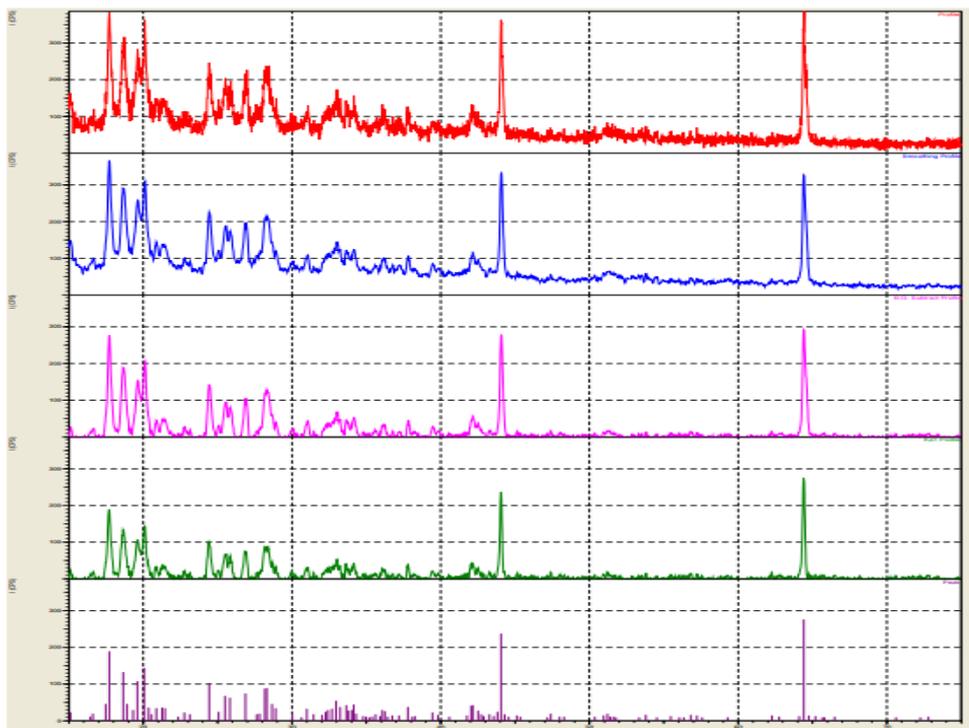
Lampiran 12. Hasil Analisa XRD Kompleks Mn(II) Sis-Tir Dtc

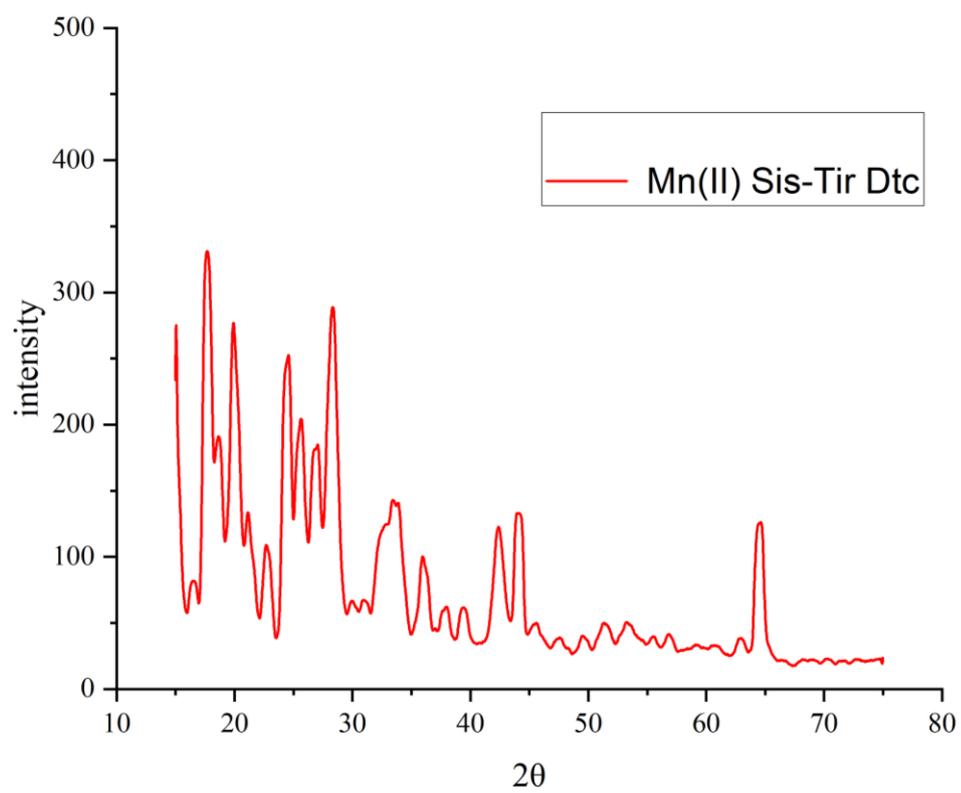
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*** Basic Data Process ***
Group      : Standard
Data       : 2305#4#4b

# Strongest 3 peaks
no. peak  2Theta      d      I/I1  FWHM      Intensity  Integrated Int
   no.    (deg)        (A)    (deg)  (deg)    (Counts)  (Counts)
1         15.1066        5.86009  8      0.13330   13         89
2         16.4400        5.38768  4      0.18000   16         49
3         16.6060        5.33419  7      0.21200   11         105
4         17.4800        5.06940  16     0.14400   27         218
5         17.7123        5.00344  68     0.25540  113        1680
6         18.6575        4.75203  48     0.35500   79         1325
7         18.9200        4.68669  16     0.16660   27         348
8         19.2200        4.59055  10     0.07340   17         81
9         19.6000        4.52560  39     0.29000   64         1046
10        20.0480        4.42547  52     0.32610   86         1295
11        20.3600        4.35835  13     0.13000   21         227
12        20.3711        4.35116  6      0.07430   10         44
13        20.8725        4.25248  12     0.23500   20         220
14        21.2800        4.17196  13     0.26000   21         212
15        21.4600        4.13737  12     0.32000   20         341
16        22.0566        3.97343  4      0.08670   6          35
17        22.7633        3.90335  8      0.16670   13         155
18        23.1350        3.84147  6      0.09000   10         58
19        24.4310        3.64054  37     0.27800   61         966
20        25.0700        3.58188  8      0.18000   14         73
21        25.5033        3.48985  24     0.31330   40         579
22        25.8312        3.44629  22     0.30250   37         453
23        26.8754        3.31472  27     0.29490   44         673
24        27.6266        3.22627  6      0.10670   10         57
25        27.8200        3.20428  7      0.12000   11         80
26        28.1800        3.16415  32     0.28800   52         324
27        28.3000        3.15101  11     0.14660   17         124
28        28.6600        3.11224  16     0.19000   27         249
29        28.9016        3.08677  12     0.14330  20         194
30        29.0266        3.07263  7      0.17330  11         136
31        29.6400        2.91502  10     0.15000  13         103
32        31.0000        2.88245  12     0.28000  19         265
33        31.4600        2.84134  6      0.08000   10         51
34        32.0400        2.79122  8      0.06670   9          30
35        32.6600        2.72668  8      0.28000  14         212
36        32.4200        2.75936  10     0.00000   17         0
37        32.6800        2.73800  12     0.20000  19         233
38        32.9653        2.71495  9      0.32270  32         420
39        33.2400        2.69314  13     0.09000   22         131
40        33.6516        2.66114  15     0.17670  25         197
41        33.7800        2.65131  10     0.15000  16         107
42        34.0000        2.63466  17     0.14660  17         103
43        34.1467        2.62368  16     0.20000  26         211
44        34.3200        2.61082  7      0.08000   11         64
45        34.7900        2.57662  4      0.14000  7          37
46        34.9866        2.56259  4      0.06670   6          26
47        35.1950        2.54789  3      0.07000   5          19
48        35.4000        2.53361  6      0.04000   16         16
49        35.6200        2.51846  6      0.22000  10         107
    
```

< Group: Standard Data: 2305#4#4b >





Index	Amount (%)	Name	Formula sum	Element	Amount (weight %)
A	100.0	Lithium Manganese Oxide (1/2/4) - Lt	Li Mn ₂ O ₄	Mn	60.8%
	36.6	Unidentified peak area		O	35.4(*)
				Li	3.8(*)
				*LE (sum)	39.2%

Details of identified phases

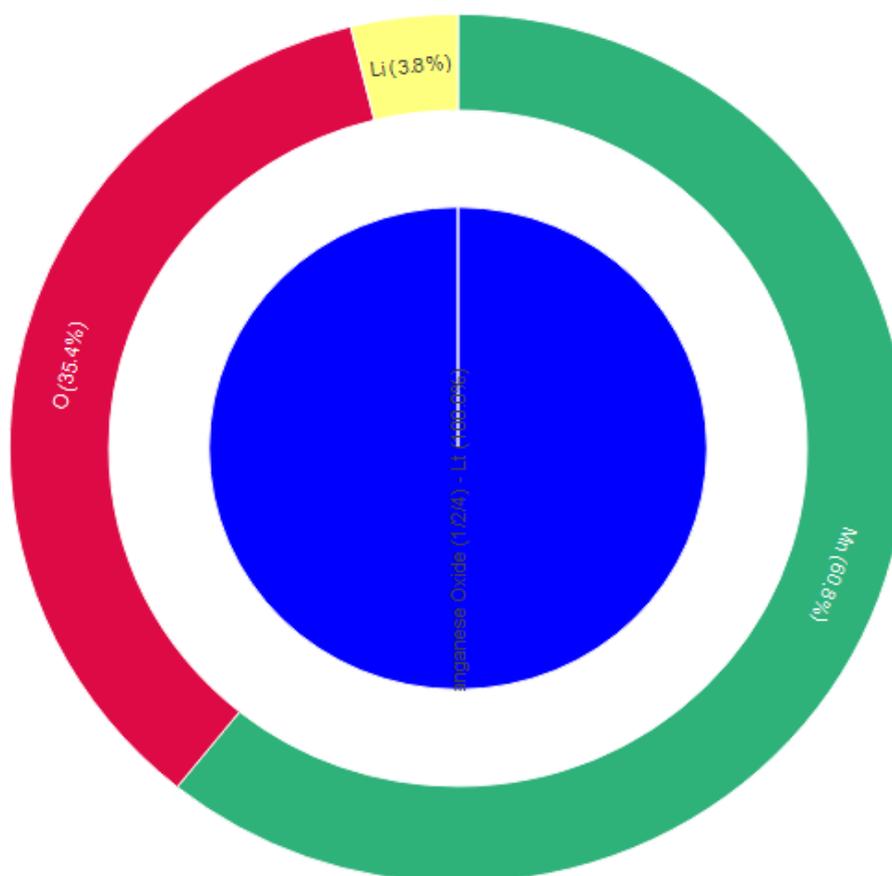
A: Lithium Manganese Oxide

(1/2/4) - Lt (100.0 %)*

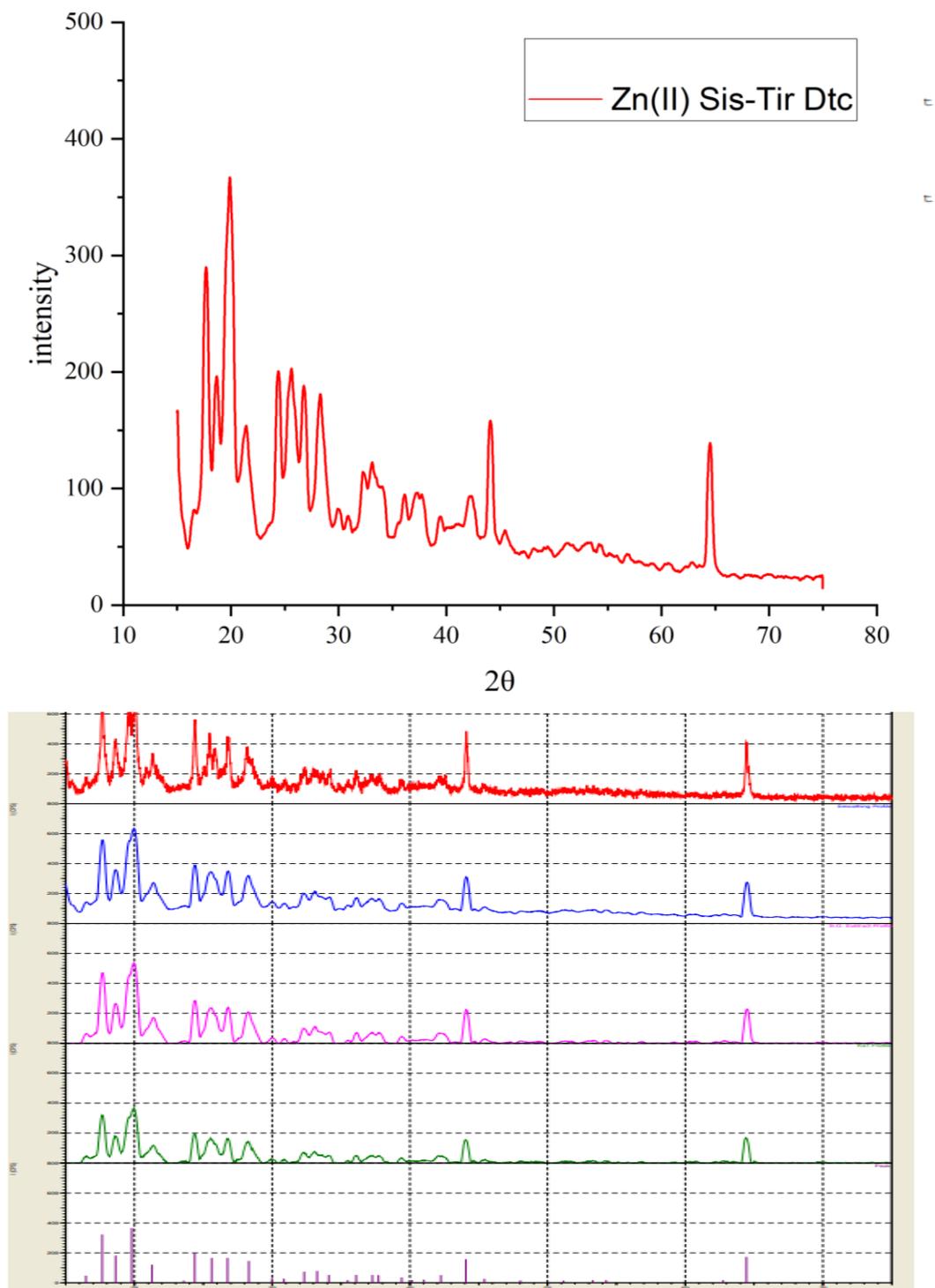
Formula sum	Li Mn ₂ O ₄
Entry number	96-151-4021
Figure-of-Merit (FoM)	0.748044*
Total number of peaks	266
Peaks in range	266
Peaks matched	84
Intensity scale factor	0.59*
Space group	F d d d
Crystal system	orthorhombic
Unit cell	a= 24.7500 Å b= 24.8010 Å c= 8.1903 Å
l/lc	5.00
Calc. density	4.300 g/cm ³
Reference	Akimoto J., Takahashi Y., Kijima N., Gotoh Y., "Single-crystal X-ray structure analysis of the low temperature form of LiMn ₂ O ₄ ", Solid State Ionics 172 , 491-494 (2004)

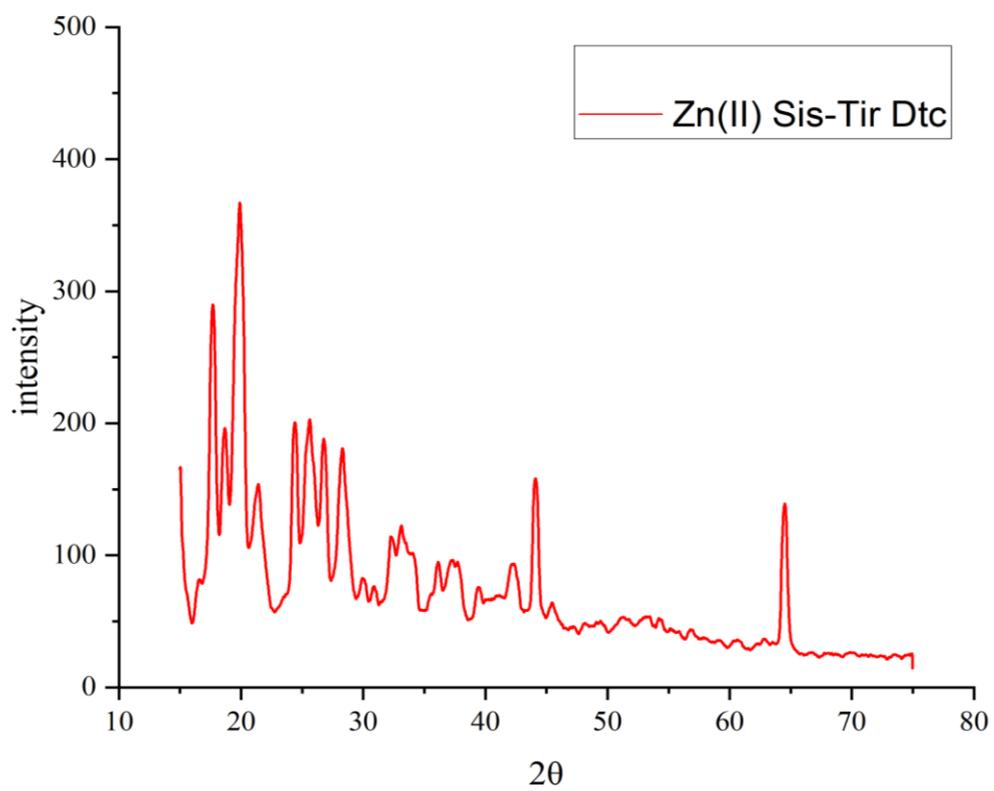
(*)2theta values have been shifted internally for the calculation of the amounts, the intensity scaling factors as well as the figure-of-merit (FoM), due to the active search-match option 'Automatic zero point adaption'.

Amounts of Phases and Elements (Weight %)



Lampiran 13. Hasil Analisa XRD Kompleks Zn(II) Sis-Tir Dtc



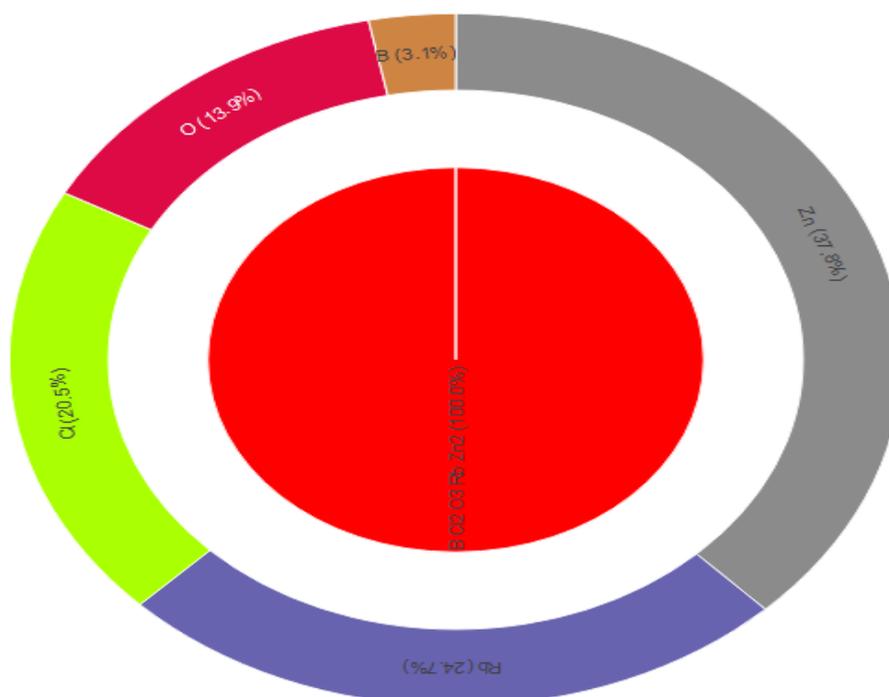


Details of identified phases

A: C₈N₄S₃ (100.0 %)[†]

Formula sum	C ₈ N ₄ S ₃
Entry number	96-210-7748
Figure-of-Merit (FoM)	0.699544 [†]
Total number of peaks	1000
Peaks in range	1000
Peaks matched	110
Intensity scale factor	0.44 [†]
Space group	P n a 21
Crystal system	orthorhombic
Unit cell	a = 8.9026 Å b = 19.9393 Å c = 6.2677 Å
I/σ	1.32
Calc. density	1.483 g/cm ³
Reference	Reilly Anthony M., Cooper Richard I., Adjiman Claire S., Bhattacharya Saswata, Boese A. Daniel, Brandenburg Jan Gerit, Bygrave Peter J., Bylsma Rita, Campbell Josh E., Car Roberto, Case David H., Chadha Renu, Cole Jason C., Cosburn Katherine, Cuppen Herma M., Curtis Farren, Day Graeme M., DiStasio Jr Robert A., Dzyabchenko Alexander, van Eijck Bouke P., Elking Dennis M., van den Ende Joost A., Facelli Julio C., Ferraro Marta B., Fusti-Molnar Laszlo, Gatsiou Christina-Anna, Gee Thomas S., de Gelder René, Ghiringhelli Luca M., Goto Hitoshi, Grimme Stefan, Guo Rui, Hofmann Detlef W. M., Hoja Johannes, Hylton Rebecca K., Iuzzolino

Amounts of Phases and Elements (Weight %)



Lampiran 14. Hasil Analisa XRD Kompleks Ni(II) Sis-Tir Dtc

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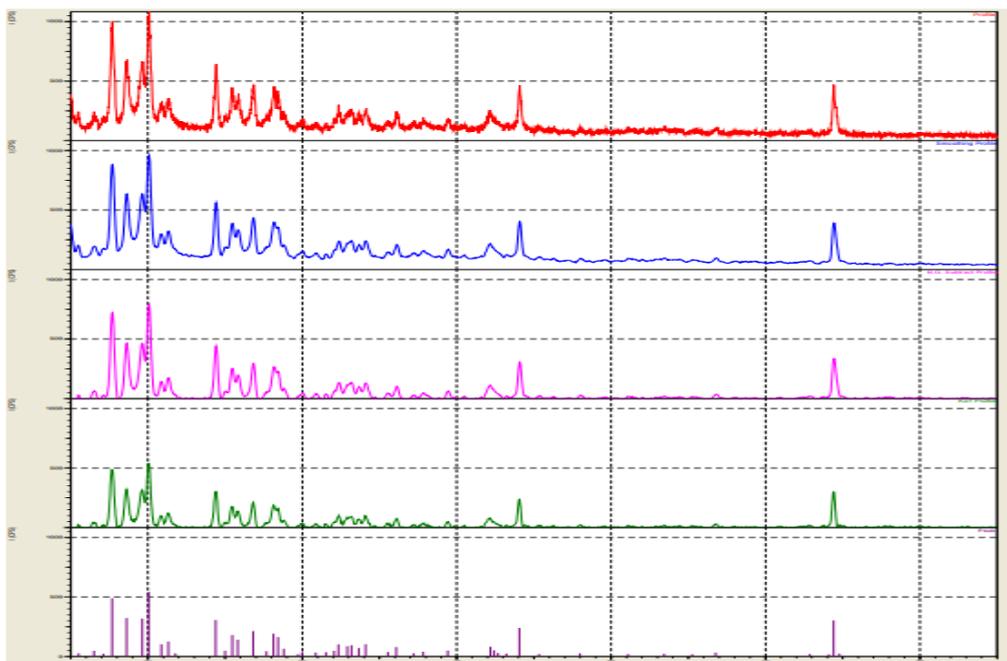
*** Basic Data Process ***
Group      : Standard
Data       : 2305#4#4c

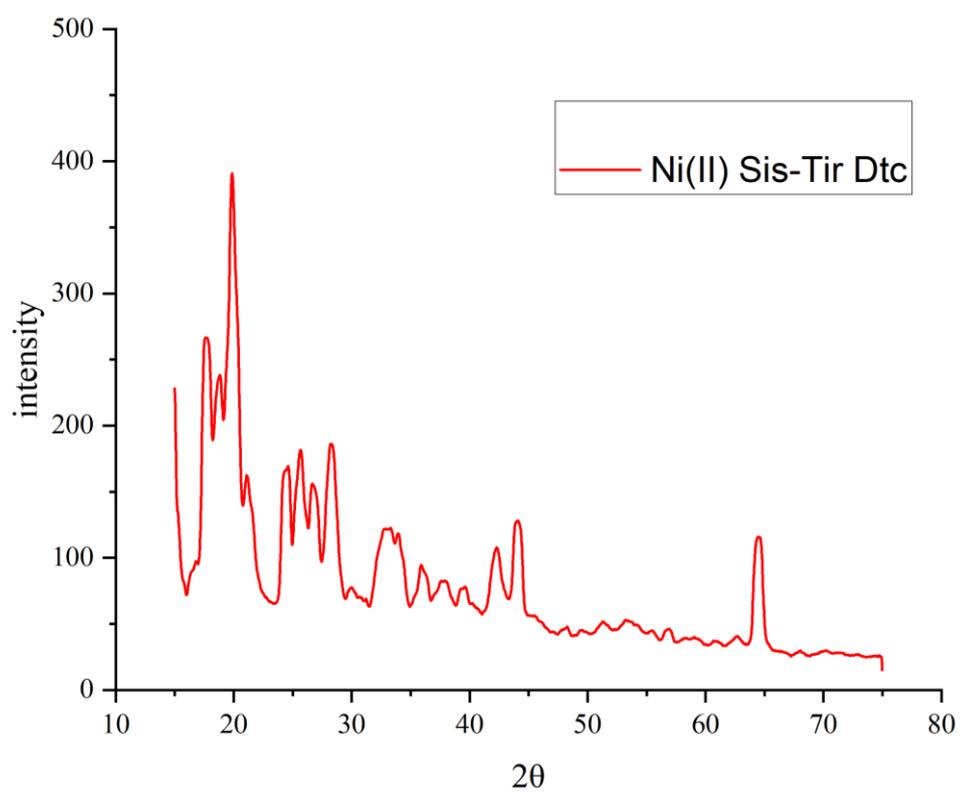
# Strongest 3 peaks
no. peak  2Theta      d          I/I1      FWHM      Intensity  Integrated Int
no.        (deg)          (A)        (deg)     (Counts)  (Counts)
1          7             20.0494    4.42516   100        324        4997
2          4             17.6860    5.01082   90         292        4686
3          5             18.6277    4.75957   59         192        3572

# Peak Data List
no.        2Theta      d          I/I1      FWHM      Intensity  Integrated Int
no.        (deg)          (A)        (deg)     (Counts)  (Counts)
1          15.5108      5.70828    5         0.12830   15         89
2          16.5100      5.36498    8         0.28000   27         390
3          17.1166      5.17620    4         0.19330   12         142
4          17.6860      5.01082    90        0.29800   292        4686
5          18.6277      4.75957    59        0.33540   192        3572
6          19.6400      4.51647    58        0.45600   189        4369
7          20.0494      4.42516    100       0.31350   324        4997
8          20.8700      4.25298    19        0.30000   60         995
9          21.3275      4.16277    23        0.31000   74         1283
10         21.7800      4.07730    4         0.07340   14         119
11         24.3987      3.64529    56        0.26410   182        2627
12         25.0000      3.55896    8         0.23200   27         358
13         25.4686      3.49453    33        0.32930   106        1579
14         25.8200      3.44776    26        0.35200   83         1459
15         26.8102      3.32263    39        0.28230   126        1988
16         27.6800      3.22016    8         0.29340   25         462
17         28.1400      3.16856    35        0.31200   113        1724
18         28.4400      3.13582    30        0.24000   96         1131
19         28.8000      3.09743    11        0.28000   37         591
20         29.7200      3.00361    3         0.12000   10         73
21         29.9866      2.97751    6         0.25330   21         274
22         30.8766      2.89368    6         0.27330   18         288
23         31.5366      2.83461    6         0.18670   20         174
24         32.0600      2.78952    8         0.24000   27         354
25         32.3500      2.76517    18        0.30000   59         803
26         32.9200      2.71859    15        0.45500   50         902
27         33.1800      2.69787    17        0.27340   55         688
28         33.6650      2.66011    13        0.31000   41         720
29         34.0983      2.62729    19        0.31670   60         1010
30         35.5466      2.52349    6         0.29330   21         330
31         36.0910      2.48667    14        0.27800   46         678
32         37.2066      2.41463    5         0.25330   15         195
33         37.8300      2.37626    7         0.30000   22         478
34         39.4208      2.28395    9         0.26830   28         440
35         42.1800      2.14071    15        0.60000   47         957
36         42.4200      2.12915    9         0.44000   29         328
37         42.6800      2.11678    5         0.32000   16         223
38         43.2200      2.09158    4         0.16000   13         141
39         44.0551      2.05385    44        0.23510   142        2033
40         45.3400      1.99858    3         0.28000   11         216
41         47.9800      1.89460    4         0.24000   14         220
42         51.1000      1.78600    3         0.20000   11         199
43         53.4400      1.71318    4         0.24000   12         300
44         55.2600      1.66099    3         0.24000   10         226
45         57.7675      1.62041    6         0.29500   18         320
46         62.8700      1.47700    8         0.34000   11         362
47         64.1000      1.45159    3         0.14660   10         188
48         64.4136      1.44528    56        0.23430   180        2170
49         64.7900      1.43779    4         0.10000   13         154

```

< Group: Standard Data: 2305#4#4c >



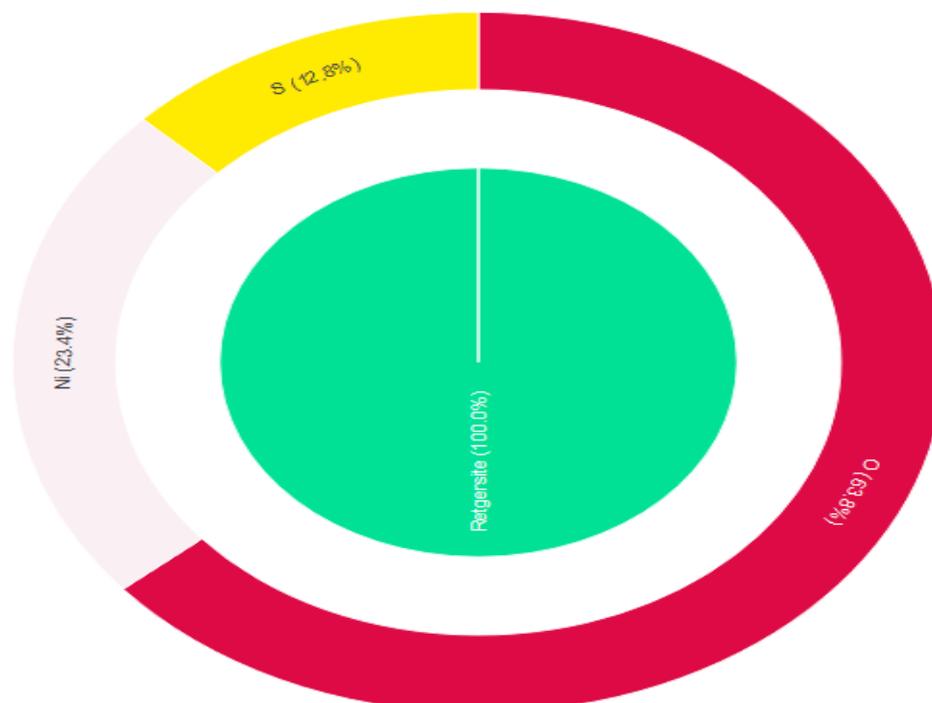


Details of identified phases

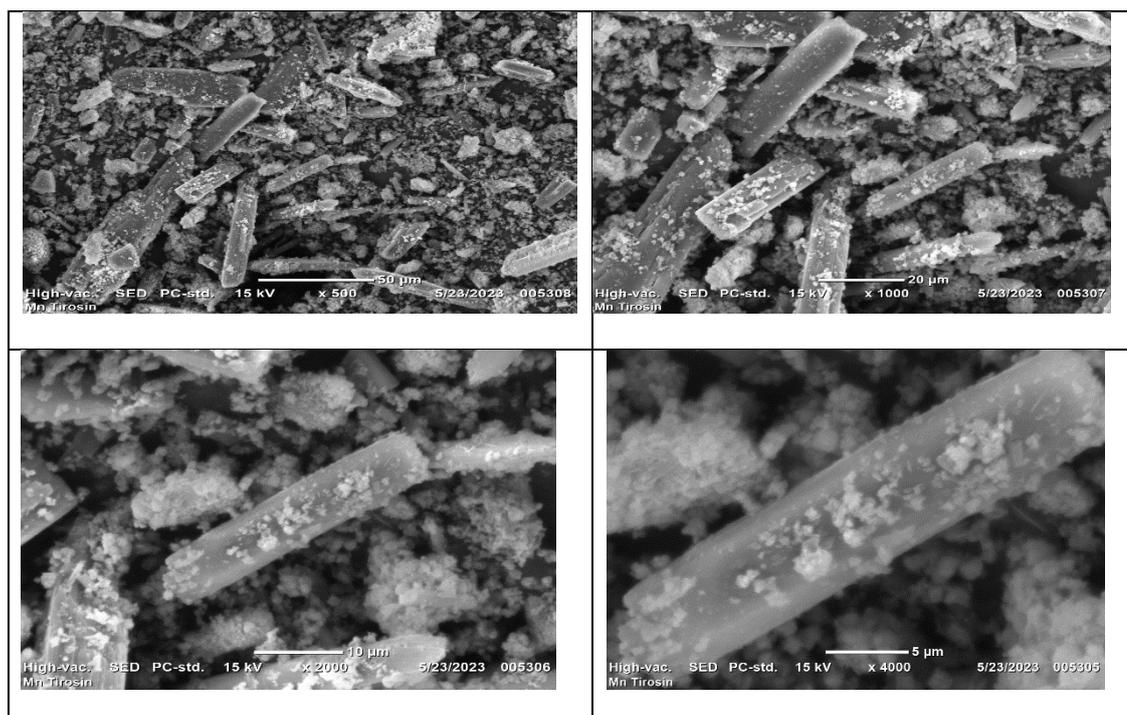
A: C8 N4 S3 (100.0 %)*

Formula sum	C8 N4 S3
Entry number	96-210-7748
Figure-of-Merit (FoM)	0.722159*
Total number of peaks	1000
Peaks in range	1000
Peaks matched	114
Intensity scale factor	0.45*
Space group	P n a 21
Crystal system	orthorhombic
Unit cell	a= 8.9026 Å b= 19.9393 Å c= 6.2677 Å
I/c	1.32
Calc. density	1.483 g/cm ³
Reference	Reilly Anthony M., Cooper Richard I., Adjiman Claire S., Bhattacharya Saswata, Boese A. Daniel, Brandenburg Jan Gerit, Bygrave Peter J., Bylisma Rita, Campbell Josh E., Car Roberto, Case David H., Chadha Renu, Cole Jason C., Cosburn Katherine, Cuppen Herma M., Curtis Farren, Day Graeme M., DiStasio Jr Robert A., Dzyabchenko Alexander, van Eijck Bouke P., Elking Dennis M., van den Ende Joost A., Facelli Julio C., Ferraro Marta B., Fusti-Molnar Laszlo, Gatsiou Christina-Anna, Gee Thomas S., de Gelder René, Ghiringhelli Luca M., Goto Hitoshi, Grimme Stefan, Guo Rui, Hofmann Detlef W. M., Hoja Johannes, Hylton Rebecca K., Iuzzolino Luca, Jankiewicz Wojciech, de Jong Daniël T., Kendrick John, de Klerk Niek J. J., Ko Hsin-Yu, Kuleshova

Amounts of Phases and Elements (Weight %)



Lampiran 15. Hasil Analisis SEM EDS Mn(II) Sis-Tir Dtc

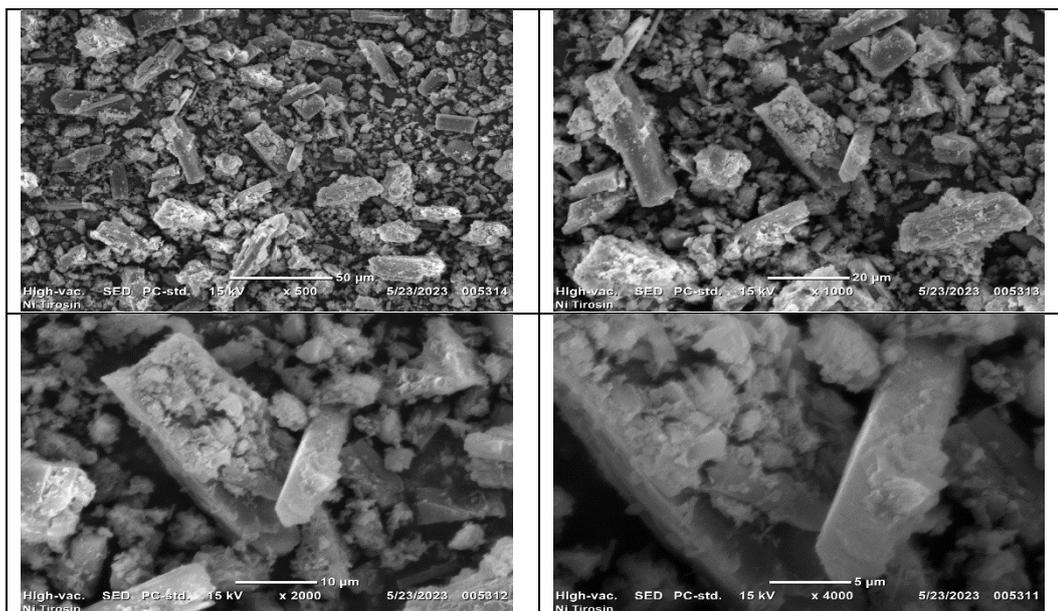


Deskripsi Energy (E_c) Tegangan Emisi Minimum, persentase massa, persentase atom, dan persentase mol masing-masing unsur

N o	Elemen t	Ec Tegangan Emisi Minimum (keV)	Massa %	Atom %	Mol %	Senyaw a
1	C K	0.277	12.55	26.24	34.34	C
2	N K	0.392	2.98	5.35	7.00	N
3	O K	0.525	15.03	23.59	-	-
4	S K	2.307	40.05	31.38	41.07	SO ₃
5	Mn K	5.894	29.39	13.44	17.59	MnO
TOTAL		9.395	100	100	100	

KET:		Huruf kulit electron (memiliki bilangan kuantum n = 1)
	K :	
	C	Carbon
	N	Nitrogen
	O	Oxygen
	S	Sulphur
	Mn	Manganese

Lampiran 16. Hasil Analisis SEM EDS Ni(II) Sis-Tir Dtc

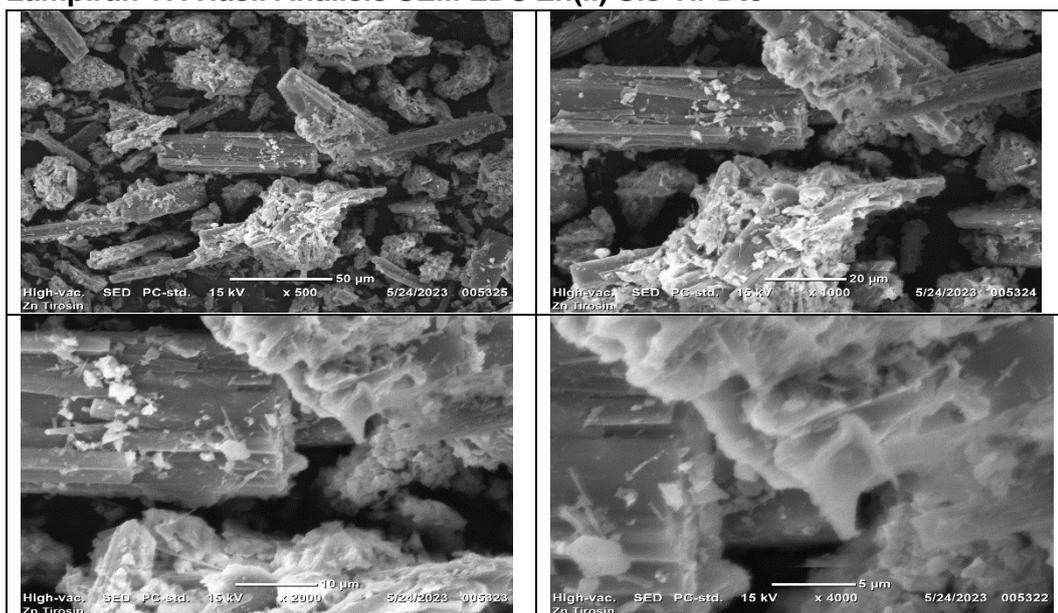


Deskripsi Energy (E_C) Tegangan Emisi Minimum, persentase massa, persentase atom, dan persentase mol masing-masing unsur

No	Element	Ec Tegangan Emisi Minimum (keV)	Massa %	Atom %	Mol %	Senyawa
1	CK	0.277	8.88	19.90	24.98	C
2	NK	0.392	2.72	5.23	6.57	N
3	OK	0.525	12.11	20.37	-	-
4	SK	2.307	51.33	43.07	54.08	SO ₃
5	Ni K	7.471	24.96	11.44	14.37	NiO
TOTAL		10.972	100	100	100	

KET:	K :	Huruf kulit electron (memiliki bilangan kuantum n = 1)
	C	Carbon
	N	Nitrogen
	O	Oxygen
	S	Sulphur
	Ni	Nickel

Lampiran 17. Hasil Analisis SEM EDS Zn(II) Sis-Tir Dtc

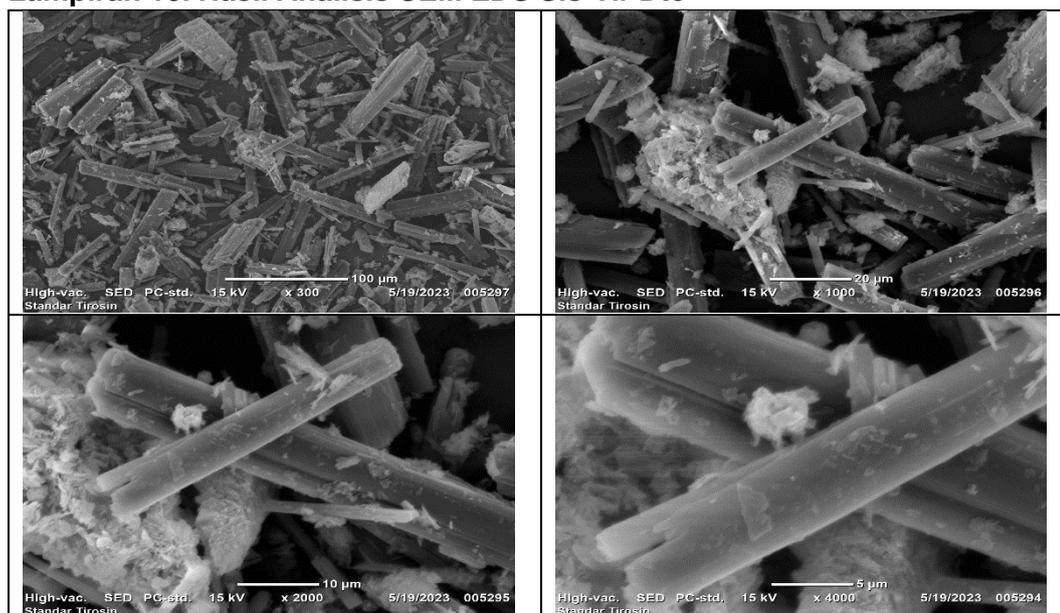


Deskripsi Energy (E_C) Tegangan Emisi Minimum, persentase massa, persentase atom, dan persentase mol masing-masing unsur

No	Element	Ec Tegangan Emisi Minimum (keV)	Massa %	Atom %	Mol %	Senyawa
1	C K	0.277	8.27	20.28	25.58	C
2	N K	0.392	2.48	5.22	6.58	N
3	O K	0.525	11.25	20.71	-	-
4	S K	2.307	39.88	36.63	46.20	SO ₃
5	Zn K	8.630	38.11	17.16	21.64	ZnO
TOTAL		12.131	100	100	100	

KET:	K :	Huruf kulit electron (memiliki bilangan kuantum n = 1)
	C	Carbon
	N	Nitrogen
	O	Oxygen
	S	Sulphur
	Zn	Zinc

Lampiran 18. Hasil Analisis SEM EDS Sis-Tir Dtc

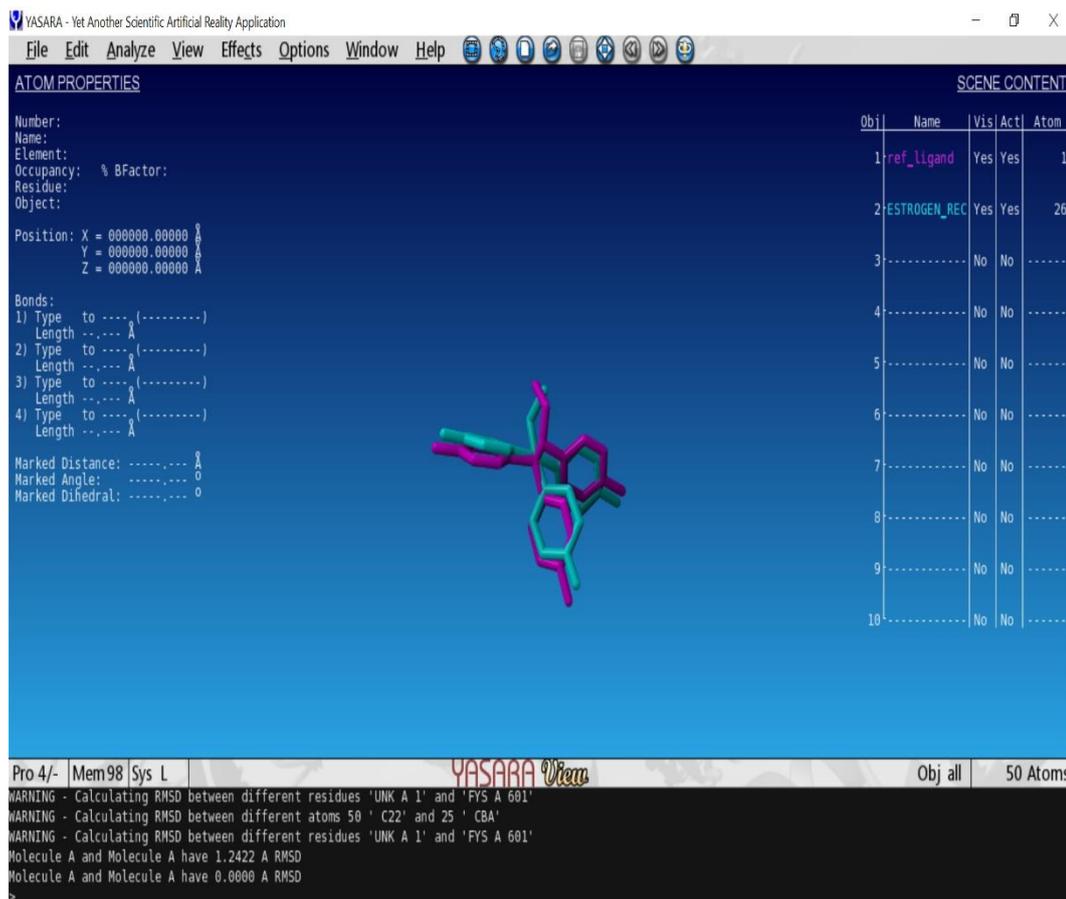


Deskripsi Energy (E_C) Tegangan Emisi Minimum, persentase massa, persentase atom, dan persentase mol masing-masing unsur

No	Element	Ec Tegangan Emisi Minimum (keV)	Massa %	Atom %	Mol %	Senyawa
1	CK	0.277	15.90	28.57	37.60	C
2	NK	0.392	3.22	4.96	6.53	N
3	OK	0.525	17.81	24.02	-	-
4	SK	2.307	63.07	42.44	55.87	SO ₃
TOTAL		3.501	100	100	100	

KET:	K :	Huruf kulit electron (memiliki bilangan kuantum n = 1)
	C	Carbon
	N	Nitrogen
	O	Oxygen
	S	Sulphur

Lampiran 19. Data Hasil Analisis *Docking*, ADMET, Lipinski



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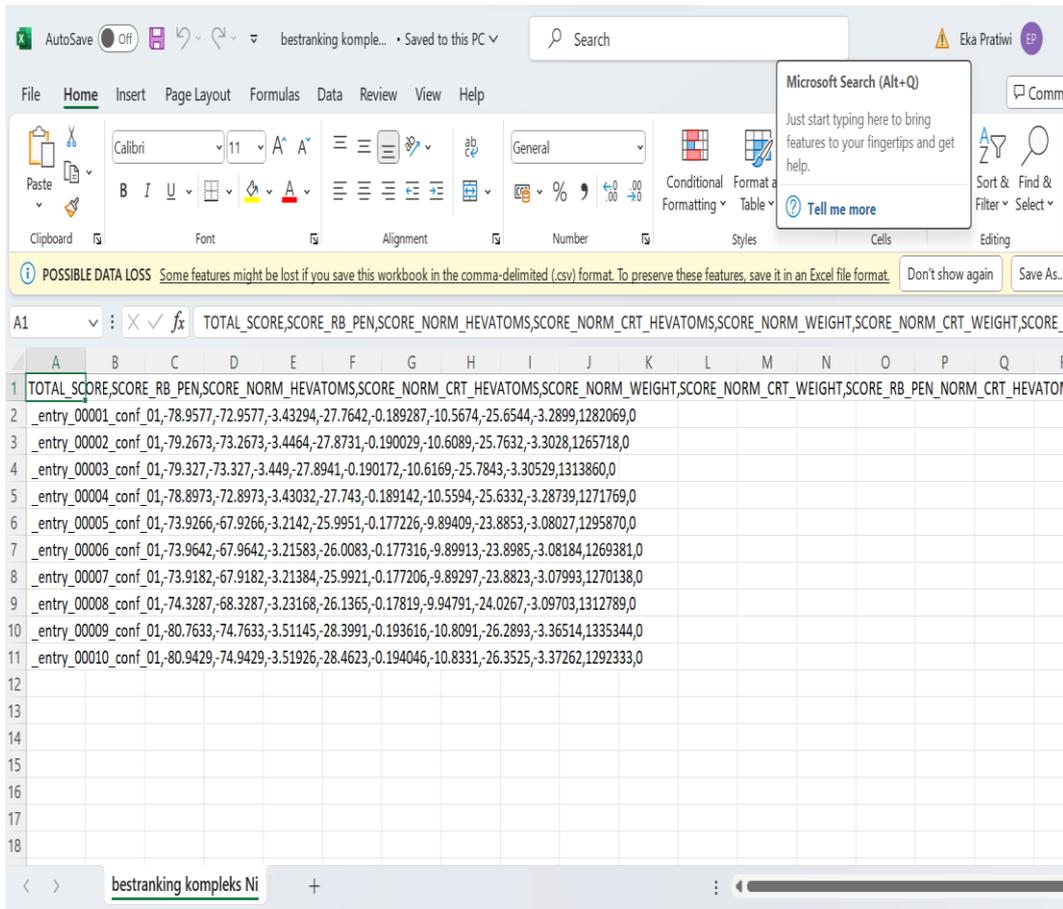
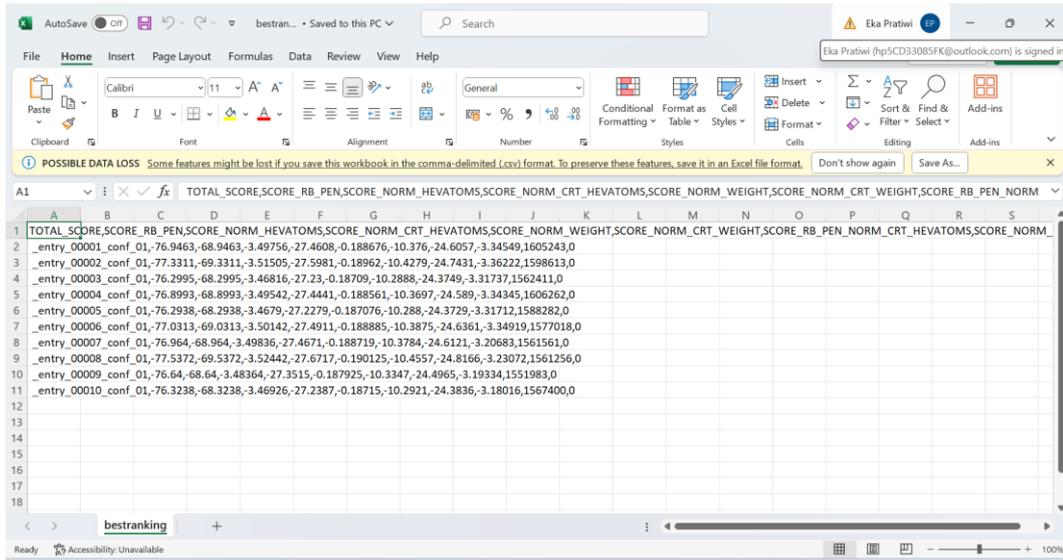
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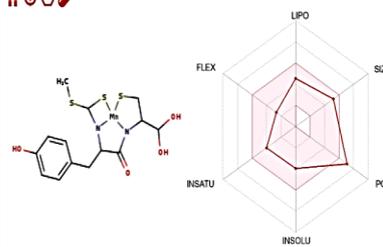
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	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S
1	TOTAL SC																		
2	ESTROGEN RECEPTOR_entry_00001_conf_01,-102.766,-86.7664,-4.11065,-35.1456,-0.307319,-14.8058,-29.6737,-3.80616,3375608,0																		
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11	ESTROGEN RECEPTOR_entry_00010_conf_01,-102.553,-86.5533,-4.10213,-35.0727,-0.306682,-14.7751,-29.6008,-3.79827,3225908,0																		
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molecule 1



SMILES CSC1S[Mn]23N1C(Cc1ccc(cc1)O)C(=O)N3C(CS2)C(O)O

Physicochemical Properties

Formula	C14H18MnN2O4S3
Molecular weight	429.44 g/mol
Num. heavy atoms	24
Num. arom. heavy atoms	6
Fraction Csp3	0.50
Num. rotatable bonds	4
Num. H-bond acceptors	5
Num. H-bond donors	3
Molar Refractivity	101.77
TPSA	160.14 Å²

Lipophilicity

Log P _{ow} (LOGP)	0.00
Log P _{ow} (XLOGP3)	2.43
Log P _{ow} (WLOGP)	0.32

Water Solubility

Log S (ESOL)	-3.95
Solubility	4.77e-02 mg/ml ; 1.11e-04 mol/l
Class	Soluble
Log S (All)	-5.44
Solubility	1.57e-03 mg/ml ; 3.67e-06 mol/l
Class	Moderately soluble
Log S (SILICOS-IT)	-1.18
Solubility	2.83e+01 mg/ml ; 6.59e-02 mol/l
Class	Soluble

Pharmacokinetics

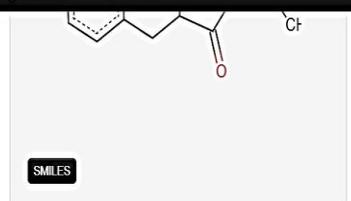
GI absorption	Low
BBB permeant	No
P-gp substrate	Yes
CYP1A2 inhibitor	No
CYP2C19 inhibitor	Yes
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K _p (skin permeation)	-7.19 cm/s

Druglikeness

Lipinski	Yes; 0 violation
Ghose	Yes
Veber	No; 1 violation: TPSA>140
Egan	No; 1 violation: TPSA>131.6
Muegge	No; 1 violation: TPSA>150
Rinacallability Score	0.55

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Molecule properties:

Descriptor	Value
Molecular Weight	429.447
LogP	1.0809
#Rotatable Bonds	4
#Acceptors	8
#Donors	3
Surface Area	153.296

Absorption	P-glycoprotein I inhibitor	No	Categorical (Yes/No)
Absorption	P-glycoprotein II inhibitor	No	Categorical (Yes/No)
Distribution	VDss (human)	-0.321	Numeric (log L/kg)
Distribution	Fraction unbound (human)	0.351	Numeric (Fu)
Distribution	BBB permeability	-1.088	Numeric (log BB)
Distribution	CNS permeability	-3.545	Numeric (log PS)
Metabolism	CYP2D6 substrate	No	Categorical (Yes/No)
Metabolism	CYP3A4 substrate	No	Categorical (Yes/No)
Metabolism	CYP1A2 inhibitor	No	Categorical (Yes/No)
Metabolism	CYP2C19 inhibitor	No	Categorical (Yes/No)
Metabolism	CYP2C9 inhibitor	No	Categorical (Yes/No)
Metabolism	CYP2D6 inhibitor	No	Categorical (Yes/No)
Metabolism	CYP3A4 inhibitor	No	Categorical (Yes/No)
Excretion	Total Clearance	-0.055	Numeric (log ml/min/kg)
Excretion	Renal OCT2 substrate	ChemDraw Pro 12.0	Categorical (Yes/No)

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SMILES: O=C1NC(CS[Ni]23N(C1Cc1ccc(cc1)O)C(S2)S3)C(=O)O

Physicochemical Properties

Formula	C13H14N2NiO4S3
Molecular weight	417.15 g/mol
Num. heavy atoms	23
Num. arom. heavy atoms	6
Fraction Csp3	0.38
Num. rotatable bonds	3
Num. H-bond acceptors	5
Num. H-bond donors	3
Molar Refractivity	96.32
TPSA	165.77 Å²

Lipophilicity

Log P _{ow} (LOGP)	0.00
Log P _{ow} (XLOGP3)	0.74
Log P _{ow} (WLOGP)	0.75
Log P _{ow} (MLOGP)	-0.05
Log P _{ow} (SILICOS-IT)	-0.54
Consensus Log P _{ow}	0.18

Pharmacokinetics

GI absorption	Low
BBB permeant	No
P-gp substrate	Yes
CYP1A2 inhibitor	No
CYP2C19 inhibitor	Yes
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K _p (skin permeation)	-8.32 cm/s

Druglikeness

Lipinski	Yes; 0 violation
Ghose	Yes
Veber	No; 1 violation: TPSA>140
Egan	No; 1 violation: TPSA>131.6
Muegge	No; 1 violation: TPSA>150
Bioavailability Score	0.11

Medicinal Chemistry

PAINS	0 alert
Brenk	0 alert
Leadlikeness	No; 1 violation: MW>350

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SMILES

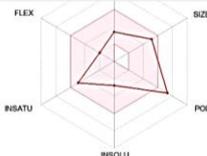
Molecule properties:

Descriptor	Value
Molecular Weight	417.159
LogP	1.5126
#Rotatable Bonds	3
#Acceptors	7
#Donors	3
Surface Area	144.946

Category	Property	Value	Unit
Absorption	P-glycoprotein substrate	Yes	Categorical (Yes/No)
Absorption	P-glycoprotein I inhibitor	No	Categorical (Yes/No)
Absorption	P-glycoprotein II inhibitor	No	Categorical (Yes/No)
Distribution	VDs (human)	-0.493	Numeric (log L/kg)
Distribution	Fraction unbound (human)	0.392	Numeric (Fu)
Distribution	BBB permeability	-1.079	Numeric (log BB)
Distribution	CNS permeability	-3.581	Numeric (log PS)
Metabolism	CYP2D6 substrate	No	Categorical (Yes/No)
Metabolism	CYP3A4 substrate	No	Categorical (Yes/No)
Metabolism	CYP1A2 inhibitor	No	Categorical (Yes/No)
Metabolism	CYP2C19 inhibitor	No	Categorical (Yes/No)
Metabolism	CYP2C9 inhibitor	No	Categorical (Yes/No)
Metabolism	CYP2D6 inhibitor	No	Categorical (Yes/No)
Metabolism	CYP3A4 inhibitor	No	Categorical (Yes/No)
Excretion	Total Clearance	-0.218	Numeric (log ml/min/kg)

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SMILES OC(=O)C1CS[Zn]23N1C(=O)C(NC(S2)S3)C1ccc(cc1)O

Physicochemical Properties	
Formula	C13H14N2O4S3Zn
Molecular weight	423.84 g/mol
Num. heavy atoms	23
Num. arom. heavy atoms	6
Fraction Csp3	0.38
Num. rotatable bonds	3
Num. H-bond acceptors	5
Num. H-bond donors	3
Molar Refractivity	96.32
TPSA	165.77 Å²
Lipophilicity	
Log P_{ow} (ILOGP)	0.00
Log P_{ow} (XLOGP3)	0.45
Log P_{ow} (WLOGP)	0.75
Log P_{ow} (MLOGP)	-0.05
Log P_{ow} (SILICOS-IT)	-0.50
Consensus Log P_{ow}	0.13

Class	Soluble
Log S (All)	-3.50
Solubility	1.34e-01 mg/ml ; 3.17e-04 mol/l
Class	Soluble
Log S (SILICOS-IT)	-2.03
Solubility	3.99e+00 mg/ml ; 9.42e-03 mol/l
Class	Soluble
Pharmacokinetics	
GI absorption	Low
BBB permeant	No
P-gp substrate	Yes
CYP1A2 inhibitor	No
CYP2C19 inhibitor	Yes
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-8.57 cm/s
Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	No; 1 violation: TPSA>140
Egan	No; 1 violation: TPSA>131.6
Muegge	No; 1 violation: TPSA>150
Bioavailability Score	0.55
Medicinal Chemistry	
PAINS	0 alert
Brenk	1 alert: heavy_metal

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SMILES

Molecule properties:	
Descriptor	Value
Molecular Weight	423.856
LogP	1.5126
#Rotatable Bonds	3
#Acceptors	7
#Donors	3
Surface Area	144.929

Absorption	P-glycoprotein I inhibitor	No	Categorical (Yes/No)
Absorption	P-glycoprotein II inhibitor	No	Categorical (Yes/No)
Distribution	VDss (human)	-0.103	Numeric (log L/kg)
Distribution	Fraction unbound (human)	0.525	Numeric (Fu)
Distribution	BBB permeability	-1.047	Numeric (log BB)
Distribution	CNS permeability	-3.2	Numeric (log PS)
Metabolism	CYP2D6 substrate	No	Categorical (Yes/No)
Metabolism	CYP3A4 substrate	No	Categorical (Yes/No)
Metabolism	CYP1A2 inhibitor	No	Categorical (Yes/No)
Metabolism	CYP2C19 inhibitor	No	Categorical (Yes/No)
Metabolism	CYP2C9 inhibitor	No	Categorical (Yes/No)
Metabolism	CYP2D6 inhibitor	No	Categorical (Yes/No)
Metabolism	CYP3A4 inhibitor	No	Categorical (Yes/No)
Excretion	Total Clearance	-6.594	Numeric (log ml/min/kg)
Excretion	Renal OCT2 substrate	No	Categorical (Yes/No)

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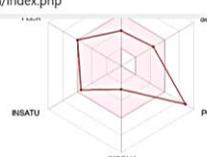
SMILES

Molecule properties:

Descriptor	Value
Molecular Weight	360.482
LogP	0.6068
#Rotatable Bonds	7
#Acceptors	5
#Donors	6
Surface Area	143.666

Category	Property	Value	Unit
Absorption	Skin Permeability	-2.735	Numeric (log Kp)
Absorption	P-glycoprotein substrate	Yes	Categorical (Yes/No)
Absorption	P-glycoprotein I inhibitor	No	Categorical (Yes/No)
Absorption	P-glycoprotein II inhibitor	No	Categorical (Yes/No)
Distribution	VDss (human)	-0.634	Numeric (log L/kg)
Distribution	Fraction unbound (human)	0.53	Numeric (Fu)
Distribution	BBB permeability	-1.3	Numeric (log BB)
Distribution	CNS permeability	-3.554	Numeric (log PS)
Metabolism	CYP2D6 substrate	No	Categorical (Yes/No)
Metabolism	CYP3A4 substrate	No	Categorical (Yes/No)
Metabolism	CYP1A2 inhibitor	No	Categorical (Yes/No)
Metabolism	CYP2C19 inhibitor	No	Categorical (Yes/No)
Metabolism	CYP2C9 inhibitor	No	Categorical (Yes/No)
Metabolism	CYP2D6 inhibitor	No	Categorical (Yes/No)
Metabolism	CYP3A4 inhibitor	No	Categorical (Yes/No)

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SMILES SCC(C(=O)O)NC(=O)C(Cc1ccc(cc1)O)NC(=S)S

Formula C₁₃H₁₆N₂O₄S₃

Molecular weight 360.47 g/mol

Num. heavy atoms 22

Num. arom. heavy atoms 6

Fraction Csp³ 0.31

Num. rotatable bonds 9

Num. H-bond acceptors 4

Num. H-bond donors 4

Molar Refractivity 93.50

TPSA 208.35 Å²

Lipophilicity

Log P _{ow} (LOGP)	1.58
Log P _{ow} (XLOGP3)	1.62
Log P _{ow} (WLOGP)	0.61
Log P _{ow} (MLOGP)	0.26
Log P _{ow} (SILICOS-IT)	2.02
Consensus Log P _{ow}	1.22

Pharmacokinetics

GI absorption	Low
BBB permeant	No
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K _p (skin permeation)	-7.35 cm/s

Druglikeness

Lipinski	Yes; 0 violation
Ghose	Yes
Veber	No; 1 violation: TPSA>140
Egan	No; 1 violation: TPSA>131.6
Muegge	No; 1 violation: TPSA>150
Bioavailability Score	0.11

Medicinal Chemistry

PAINS	0 alert
Brenk	2 alerts: thiocarbonyl_group, thiol_2
Leadlikeness	No; 2 violations: MW>350, Rotors>7

Lampiran 20. Data Hasil Analisis UV Vis

