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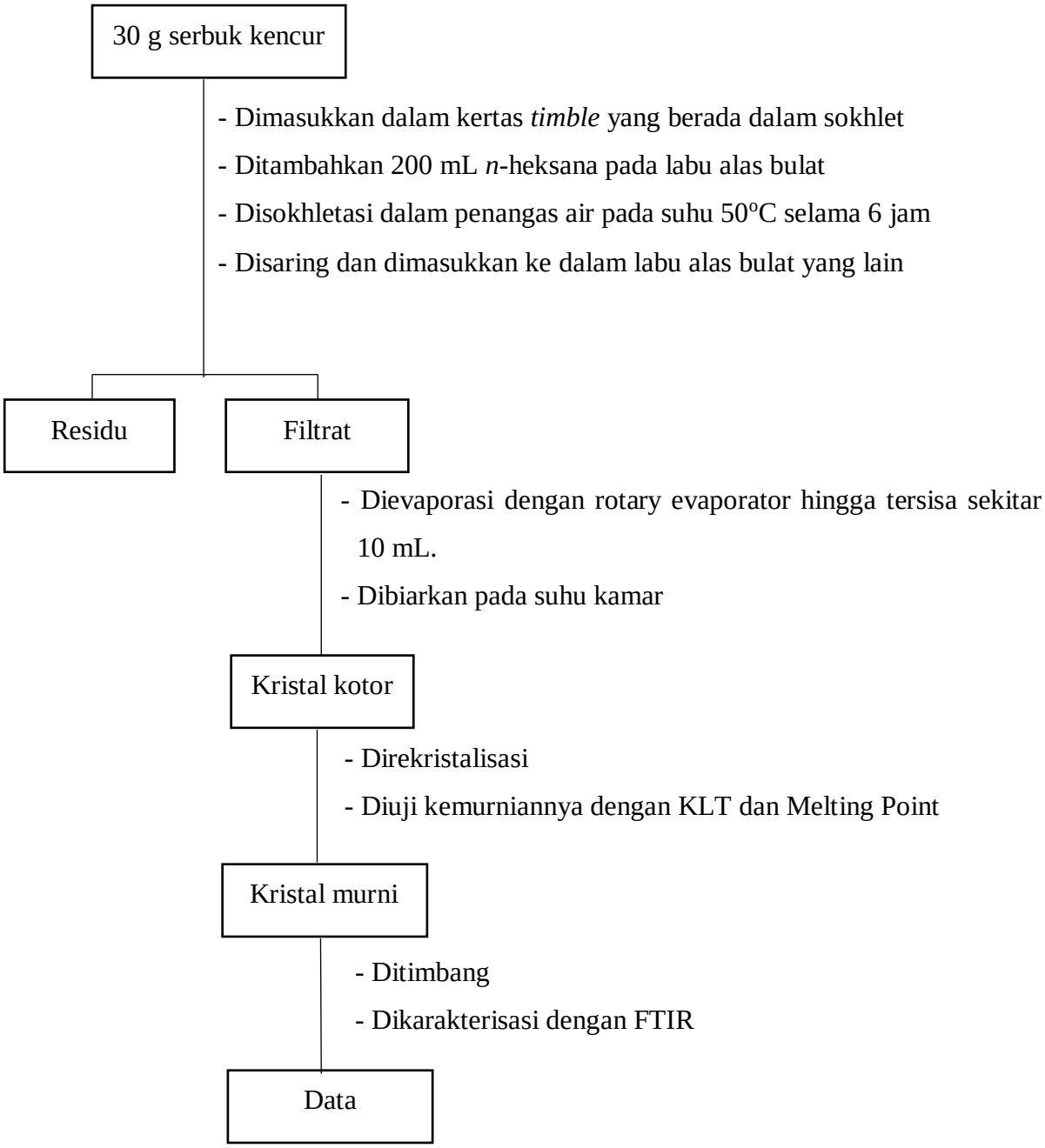
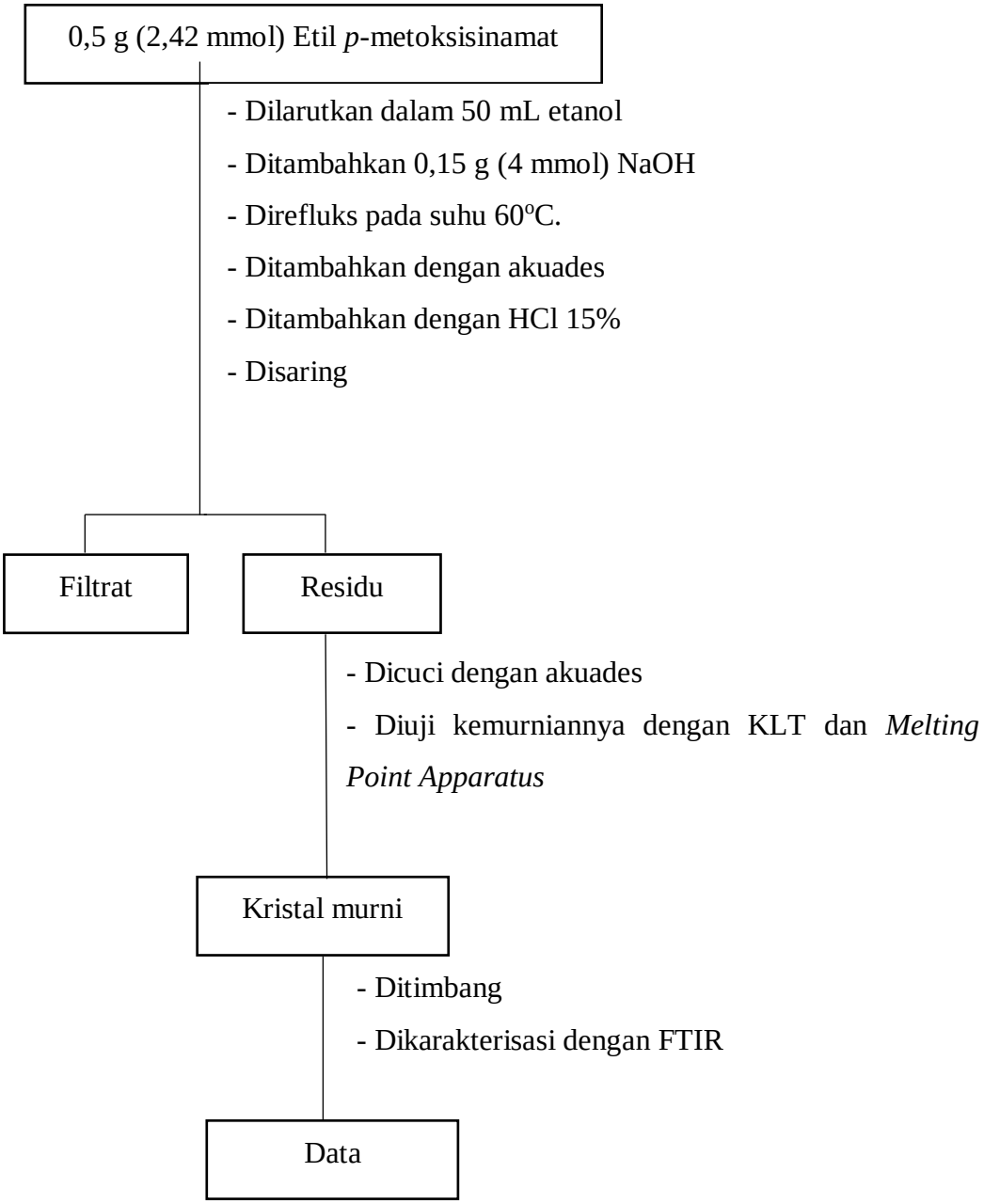
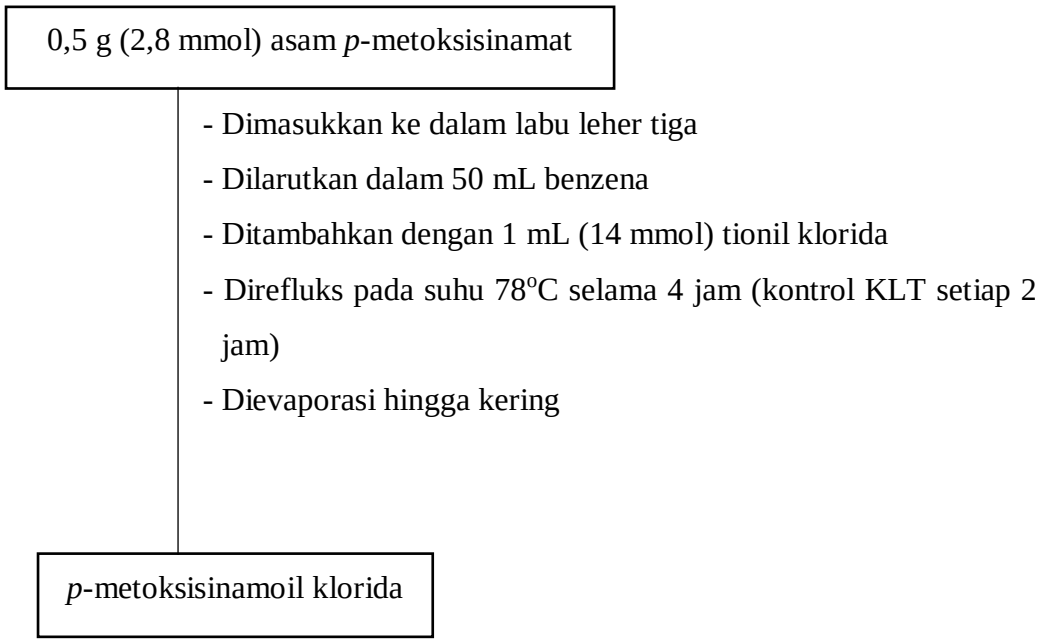
Lampiran 1. Bagan Kerja Isolasi Etil *p*-Metoksisinamat dari Kencur



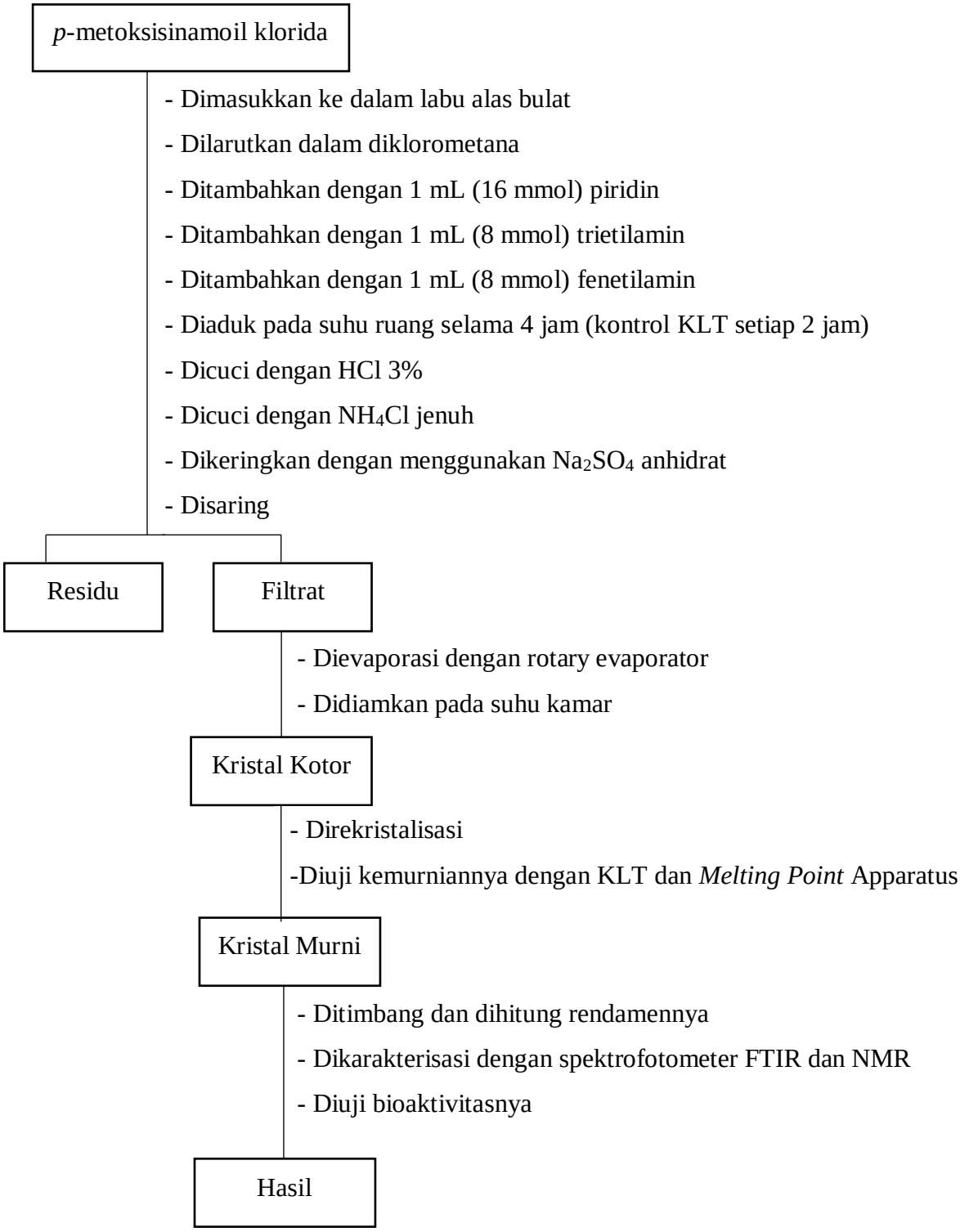
Lampiran 2. Bagan Kerja Sintesis Asam *p*-Metoksisinamat



Lampiran 3. Bagan Kerja Sintesis *p*-metoksisinamoil klorida

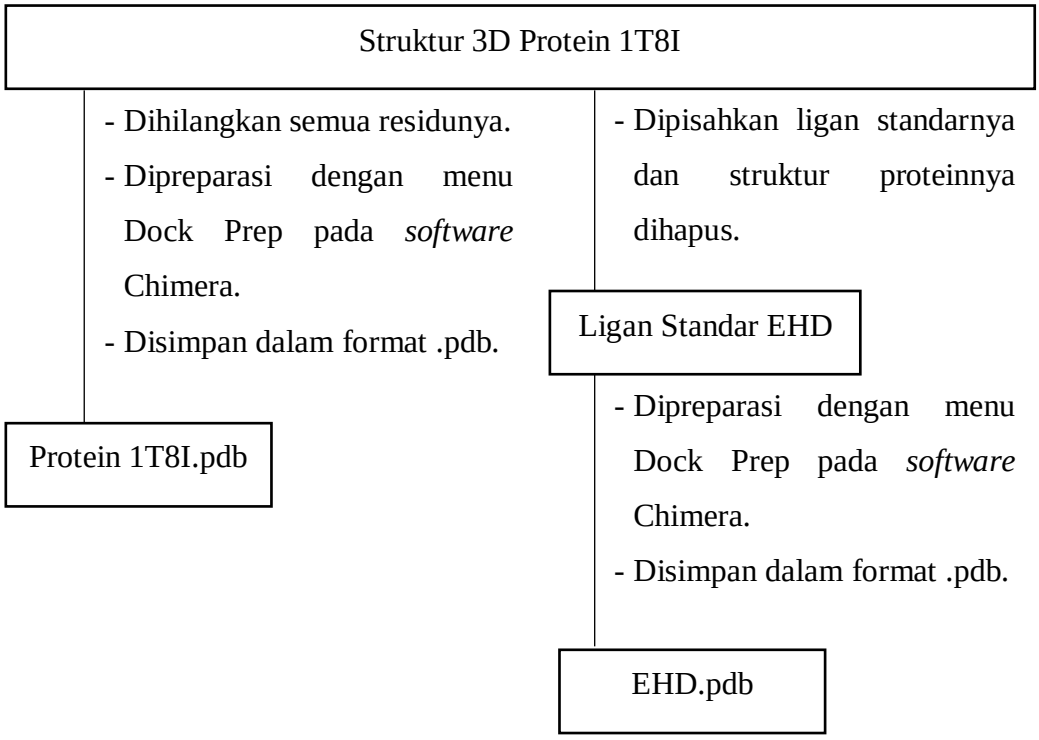


Lampiran 4. Bagan Kerja Sintesis *N*-fenetil-*p*-Metoksisinamamida

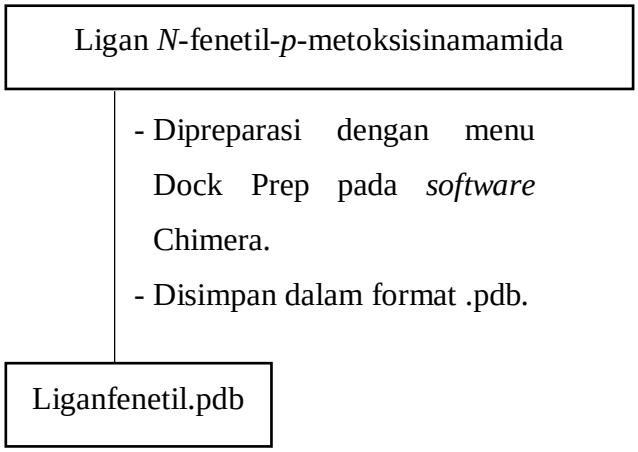


Lampiran 5. Bagan Kerja Pengujian *in silico N*-fenetil-*p*-metoksisinamamida

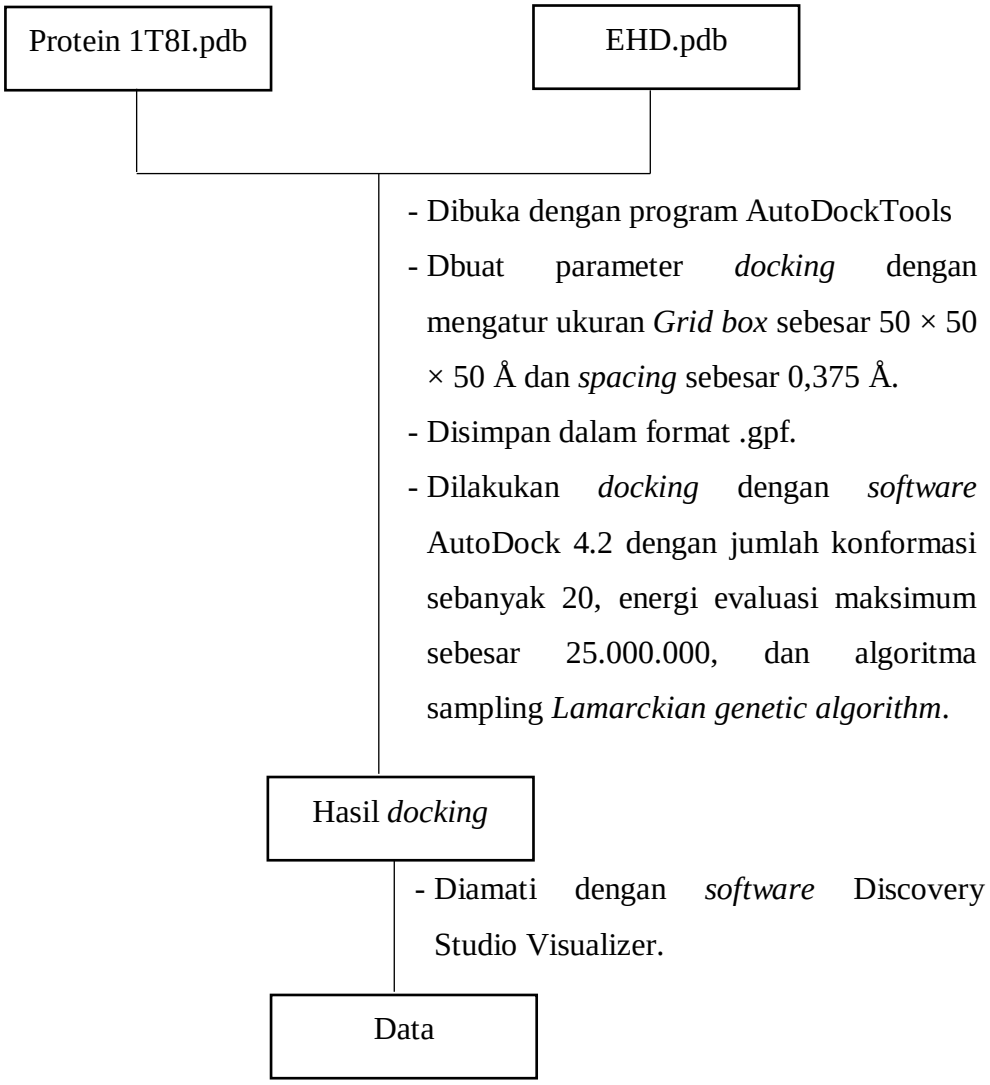
1. Preparasi Protein dan Ligan Standar



2. Preparasi Ligan *N*-fenetil-*p*-metoksisinamamida



3. Proses Penambatan Molekul



*****Dilakukan prosedur yang sama untuk *redocking* dengan mengubah ukuran Grid box 40 × 40 × 40 Å, dengan jumlah konformasi sebanyak 10, energi evaluasi maksimum sebesar 250.000

Lampiran 6. Perhitungan Reaktan

1. Sintesis senyawa asam *p*-metoksisinamat

a. Etil *p*-metoksisinamat (EPMS)

$$\text{mol EPMS} = \frac{\text{massa EPMS}}{\text{Mr EPMS}}$$

$$\text{mol EPMS} = \frac{0{,}5\ \text{g}}{206{,}24\ \text{g/mol}} = 0{,}00242\ \text{mol} = 2{,}42\ \text{mmol}$$

b. Natrium hidroksida

mol NaOH = 4 mmol

massa NaOH=mol NaOH× Mr NaOH = 4 mmol × 40 mg/mmol = 160 mg =0,16 g

2. Sintesis senyawa *p*-metoksisinamoil klorida

a. Asam *p*-metoksisinamat (APMS)

$$\text{mol APMS} = \frac{\text{massa APMS}}{\text{Mr APMS}}$$

$$\text{mol APMS} = \frac{0{,}5\ \text{g}}{178\ \text{g/mol}} = 0{,}0028\ \text{mol} = 2{,}8\ \text{mmol}$$

b. Tionil Klorida

massa tionil klorida = mol tionil klorida × Mr tionil klorida

= 14 mmol x 118.97 mg/mmol

= 1.665,5 mg = 1,6655 g

$$\text{V tionil klorida} = \frac{\text{massa tionil klorida}}{\rho\ \text{tionil klorida}} = \frac{1{,}6655\ \text{g}}{1{,}64\ \text{g/mL}} = 1\ \text{mL}$$

3. Sintesis senyawa *N*-fenetil-*p*-metoksisinamamida

a. Fenetilamin

Massa fenetilamin = mol fenetilamin × Mr fenetilamin

= 8 mmol × 121,18 mg/mmol

= 969,44 mg = 0,96944 g

$$\text{Volume fenetilamin} = \frac{\text{massa fenetilamin}}{\rho \text{ fenetilamin}} = \frac{0{,}96944 \text{ g}}{0{,}964 \text{ g/mL}} = 1 \text{ mL}$$

b. Trietilamina

Massa trietilamina = mol trietilamina × Mr trietilamina

= 8 mmol × 101,9 mg/mmol

= 815,2 mg = 0,8152 g

$$\text{Volume trietilamina} = \frac{\text{massa trietilamina}}{\rho \text{ trietilamina}} = \frac{0{,}8152 \text{ g}}{0{,}726 \text{ g/mL}} = 1 \text{ mL}$$

c. Piridin

Massa piridin = mol piridin x Mr piridin

= 16 mmol × 79,1 mg/mmol

= 1.265,6 mg = 1,2656 g

$$\text{Volume piridin} = \frac{\text{massa piridin}}{\rho \text{ piridin}} = \frac{1{,}2656 \text{ g}}{0{,}982 \text{ g/mL}} = 1 \text{ mL}$$

Lampiran 7. Perhitungan Rendemen

1. **Isolasi Etil p-metoksisinamat**

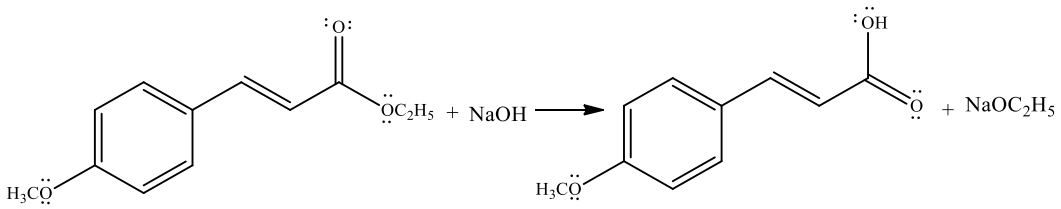
$$\% \text{ rendemen} = \frac{\text{berat hasil isolasi}}{\text{berat sampel}} \text{ x } 100\%$$

$$= \frac{0{,}099 \text{ gram}}{30 \text{ gram}} \text{ x } 100\%$$

$$= 0{,}33\%$$

2. **Sintesis Asam *p*-metoksisinamat**

Persamaan reaksi:



2,42 mmol 4 mmol 2,42 mmol

Berat teoritis = mol asam *p*-metoksisinamat x Mr asam *p*-metoksisinamat

= 0,00242 mol x 178 g/mol

= 0,43076 gram

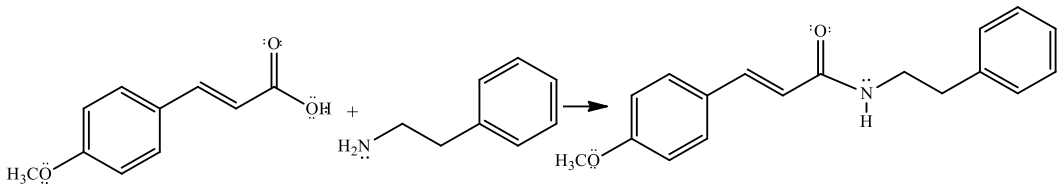
$$\% \text{ rendemen} = \frac{\text{berat praktek}}{\text{berat teoritis}} \text{ x } 100\%$$

$$= \frac{0{,}3356 \text{ gram}}{0{,}43076 \text{ gram}} \text{ x } 100\%$$

$$= 77{,}91\%$$

3. Sintesis Senyawa *N*-fenetil-*p*-metoksisinamamida

Persamaan reaksi:



2,8 mmol 8 mmol 2,8 mmol

Berat teoritis = mol produk x Mr produk

= 0,0028 mol x 282,42 g/mol

= 0,79 gram

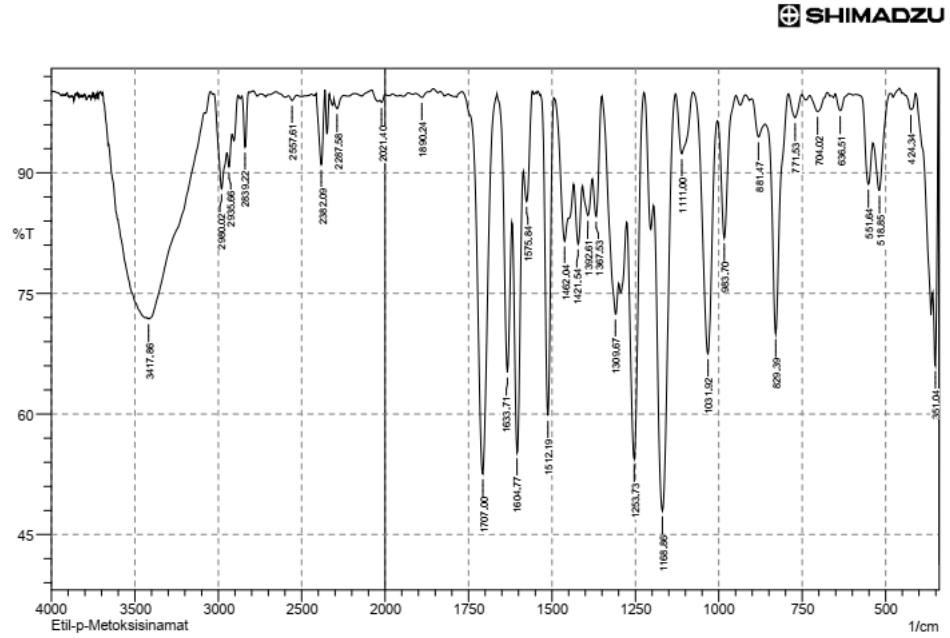
$$\% \text{ rendemen} = \frac{\text{berat praktek}}{\text{berat teoritis}} \times 100\%$$

$$= \frac{0{,}33 \text{ gram}}{0{,}79 \text{ gram}} \times 100\%$$

= 42%

Lampiran 8. Spektrum FTIR

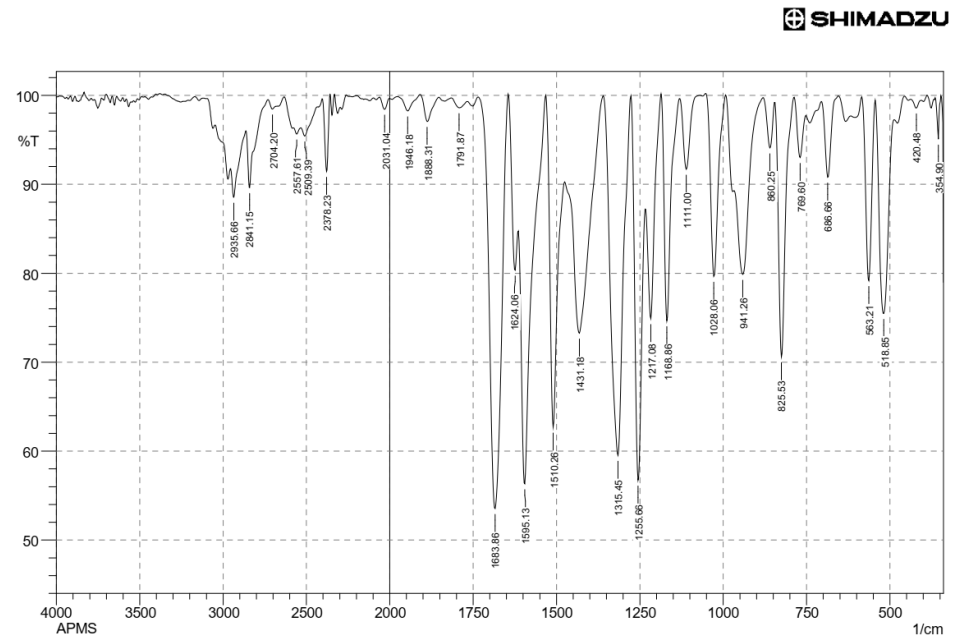
1. Spektrum FT-IR Etil *p*-metoksisinamat



No.	Peak	Intensity	Corr. Intensity	Base (H)	Base (L)	Area	Corr. Area
1	351.04	66.034	18.74	358.76	343.33	1.98	0.925
2	424.34	97.874	2.024	447.49	410.84	0.179	0.163
3	518.85	87.826	8.01	536.21	487.99	1.431	0.753
4	551.64	88.564	6.763	588.29	538.14	1.159	0.503
5	636.51	97.736	2.109	651.94	611.43	0.196	0.17
6	704.02	97.634	1.854	727.16	684.73	0.289	0.197
7	771.53	96.874	2.913	790.81	752.24	0.306	0.27
8	829.39	69.955	27.787	860.25	792.74	3.989	3.379
9	881.47	94.465	3.17	900.76	862.18	0.663	0.26
10	983.7	81.916	15.63	1002.98	948.98	1.977	1.515
11	1031.92	67.478	30.343	1076.28	1004.91	5.097	4.53
12	1111	92.378	7.524	1130.29	1078.21	1.013	0.998
13	1168.86	47.934	43.321	1193.94	1130.29	10.133	8.039
14	1253.73	54.432	36.17	1274.95	1224.8	6.774	4.914
15	1309.67	72.438	8.296	1350.17	1300.02	4.196	1.114
16	1367.53	84.595	8.971	1379.1	1352.1	1.288	0.626
17	1392.61	84.697	4.008	1408.04	1381.03	1.729	0.321
18	1421.54	81.141	7.014	1433.11	1409.96	1.742	0.474
19	1462.04	81.509	6.921	1492.9	1450.47	2.225	0.571
20	1512.19	59.806	39.834	1541.12	1494.83	3.67	3.614
21	1575.84	86.463	7.442	1585.49	1560.41	1.051	0.524
22	1604.77	55.168	31.003	1618.28	1587.42	4.95	3.039
23	1633.71	65.199	23.481	1664.57	1620.21	3.795	2.073
24	1707	52.564	47.137	1768.72	1666.5	8.561	8.455
25	1890.24	99.39	0.599	1907.6	1872.88	0.045	0.043
26	2021.4	98.76	0.509	2031.04	2002.11	0.115	0.038
27	2287.58	97.989	1.358	2306.86	2252.86	0.304	0.165
28	2382.09	91.015	9.133	2412.95	2360.87	1.129	1.152
29	2557.61	99.005	0.609	2580.76	2528.68	0.149	0.062
30	2839.22	93.199	6.614	2860.43	2816.07	0.572	0.538
31	2935.66	90.761	2.641	2947.23	2918.3	1.009	0.181
32	2980.02	88.01	7.413	3026.31	2949.16	2.622	1.257
33	3417.86	71.848	0.999	3429.43	3084.18	28.66	2.246

Date/Time; 11/16/2020 11:06:14 AM
No. of Scans;

2. Spektrum FT-IR Asam *p*-metoksisinamat



No.	Peak	Intensity	Corr. Intensity	Base (H)	Base (L)	Area	Corr. Area
1	354.9	95.071	4.791	364.55	347.19	0.148	0.137
2	420.48	98.578	0.93	437.84	405.05	0.126	0.056
3	518.85	75.469	23.004	543.93	487.99	3.644	3.231
4	563.21	79.175	20.214	584.43	545.85	1.953	1.853
5	686.66	90.812	8.728	705.95	653.87	0.837	0.751
6	769.6	93.013	5.749	786.96	752.24	0.627	0.438
7	825.53	70.595	28.811	844.82	786.96	3.333	3.207
8	860.25	94.089	5.361	879.54	844.82	0.483	0.405
9	941.26	79.868	12.501	966.34	881.47	3.885	1.858
10	1028.06	79.662	20.484	1051.2	993.34	2.319	2.351
11	1111	91.7	8.059	1130.29	1068.56	0.826	0.78
12	1168.86	74.651	25	1184.29	1132.21	2.665	2.584
13	1217.08	74.886	16.63	1232.51	1186.22	2.912	1.609
14	1255.66	56.726	36.862	1276.88	1234.44	5.624	4.303
15	1315.45	59.517	40.239	1359.82	1278.81	8.572	8.49
16	1431.18	73.259	20.755	1475.54	1361.74	7.931	5.412
17	1510.26	62.692	33.438	1531.48	1477.47	5.373	4.112
18	1595.13	56.321	32.027	1614.42	1533.41	8.507	5.64
19	1624.06	80.347	8.615	1643.35	1616.35	1.716	0.658
20	1683.86	53.542	46.443	1734.01	1645.28	9.958	9.945
21	1791.87	98.618	0.899	1815.02	1768.72	0.199	0.101
22	1888.31	97.071	2.905	1909.53	1853.59	0.332	0.317
23	1946.18	98.257	1.712	1977.04	1909.53	0.221	0.215
24	2031.04	98.432	1.294	2061.9	2002.11	0.239	0.169
25	2378.23	91.443	8.474	2405.23	2358.94	0.879	0.853
26	2509.39	95.434	1.504	2534.46	2434.17	1.407	0.313
27	2557.61	95.648	0.705	2576.9	2534.46	0.748	0.064
28	2704.2	98.458	0.725	2731.2	2673.34	0.297	0.084
29	2841.15	89.615	6.965	2862.36	2731.2	2.57	1.292
30	2935.66	88.536	4.128	2954.95	2864.29	3.167	0.692

Comment;
APMS

Date/Time; 11/16/2020 11:00:34 AM
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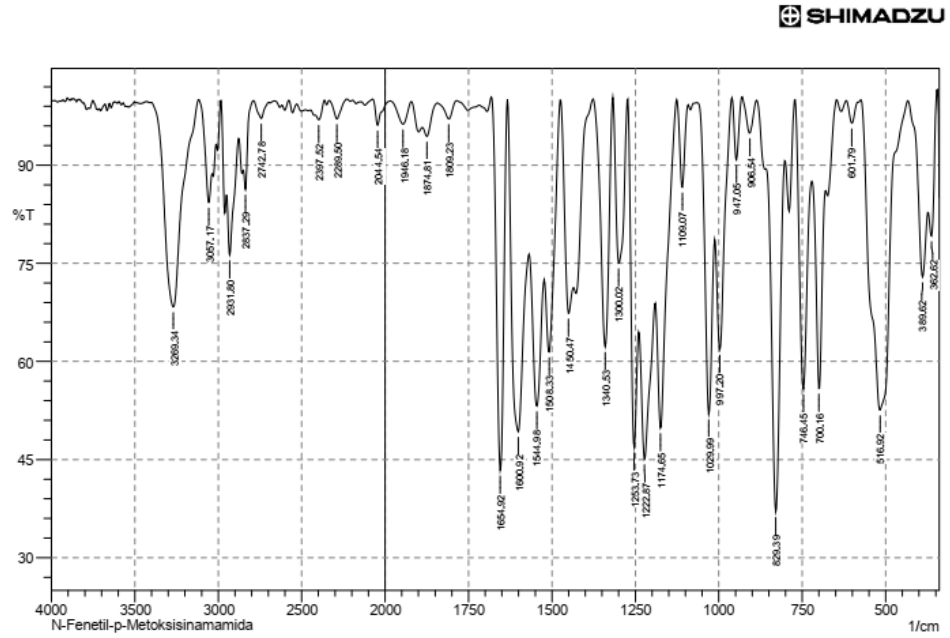
Resolution;
Apodization;

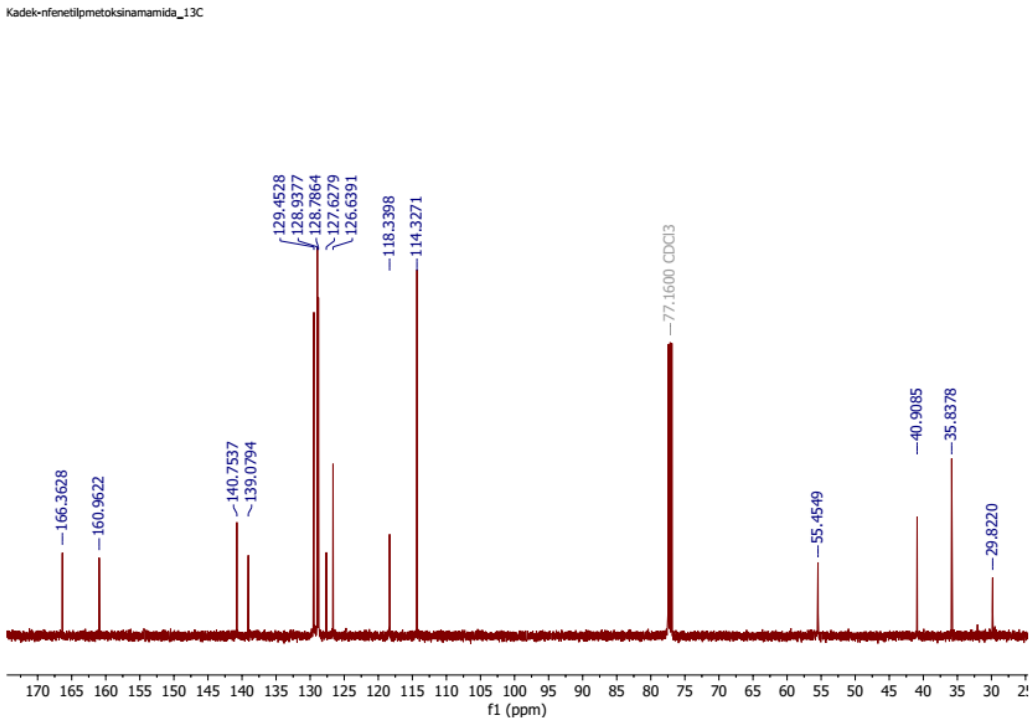
3. Spektrum FT-IR *N*-fenetil-*p*-metoksisinamamida



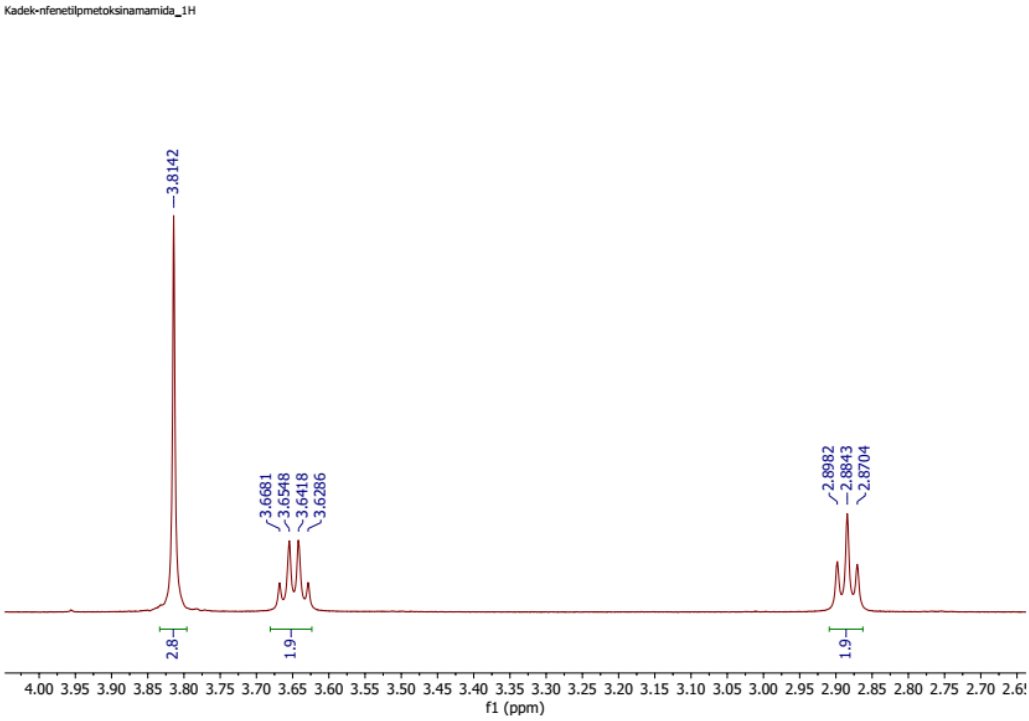
No.	Peak	Intensity	Corr. Intensity	Base (H)	Base (L)	Area	Corr. Area
1	362.62	79.198	10.753	372.26	347.19	1.599	0.733
2	389.62	72.909	14.407	432.05	374.19	3.795	1.415
3	516.92	52.561	47.344	572.86	433.98	16.775	16.712
4	601.79	96.419	3.349	617.22	582.5	0.285	0.248
5	700.16	55.896	30.822	719.45	680.87	5.623	3.228
6	746.45	55.762	37.993	771.53	721.38	6.612	5.103
7	829.39	37.034	53.055	858.32	802.39	11.369	8.833
8	906.54	94.938	5.227	929.69	887.26	0.463	0.498
9	947.05	90.844	9.538	960.55	929.69	0.574	0.626
10	997.2	61.846	22.41	1010.7	962.48	5.204	2.727
11	1029.99	51.948	33.651	1064.71	1012.63	6.681	3.923
12	1109.07	86.621	12.737	1124.5	1093.64	1.002	0.914
13	1174.65	49.848	26.596	1190.08	1126.43	9.199	4.228
14	1222.87	45.084	20.551	1238.3	1192.01	12.016	3.802
15	1253.73	46.932	32.181	1273.02	1240.23	6.722	3.419
16	1300.02	75.038	25.099	1317.38	1274.95	3.209	3.224
17	1340.53	62.276	37.448	1375.25	1319.31	5.228	5.17
18	1450.47	67.358	14.428	1473.62	1436.97	4.284	1.442
19	1508.33	61.468	18.738	1521.84	1475.54	5.747	2.591
20	1544.98	53.174	21.203	1568.13	1523.76	9.013	3.303
21	1600.92	49.261	38.361	1631.78	1570.06	12.511	8.633
22	1654.92	43.346	56.818	1680	1633.71	7.393	7.427
23	1809.23	97.079	2.655	1843.95	1786.08	0.369	0.293
24	1874.81	94.422	2.491	1888.31	1843.95	0.657	0.194
25	1946.18	96.283	3.501	1984.75	1921.1	0.529	0.472
26	2044.54	96.104	3.902	2075.41	1984.75	0.663	0.65
27	2289.5	97.073	2.905	2335.8	2229.71	0.602	0.598
28	2397.52	96.942	1.609	2418.74	2364.73	0.51	0.224
29	2742.78	97.158	2.571	2789.07	2698.41	0.596	0.491
30	2837.29	86.31	4.914	2848.86	2789.07	1.494	0.328
31	2931.8	76.297	11.233	2949.16	2877.79	5.347	2.001
32	3057.17	84.313	7.136	3116.97	3037.89	2.949	0.941
33	3269.34	68.33	31.462	3400.5	3118.9	18.425	18.191

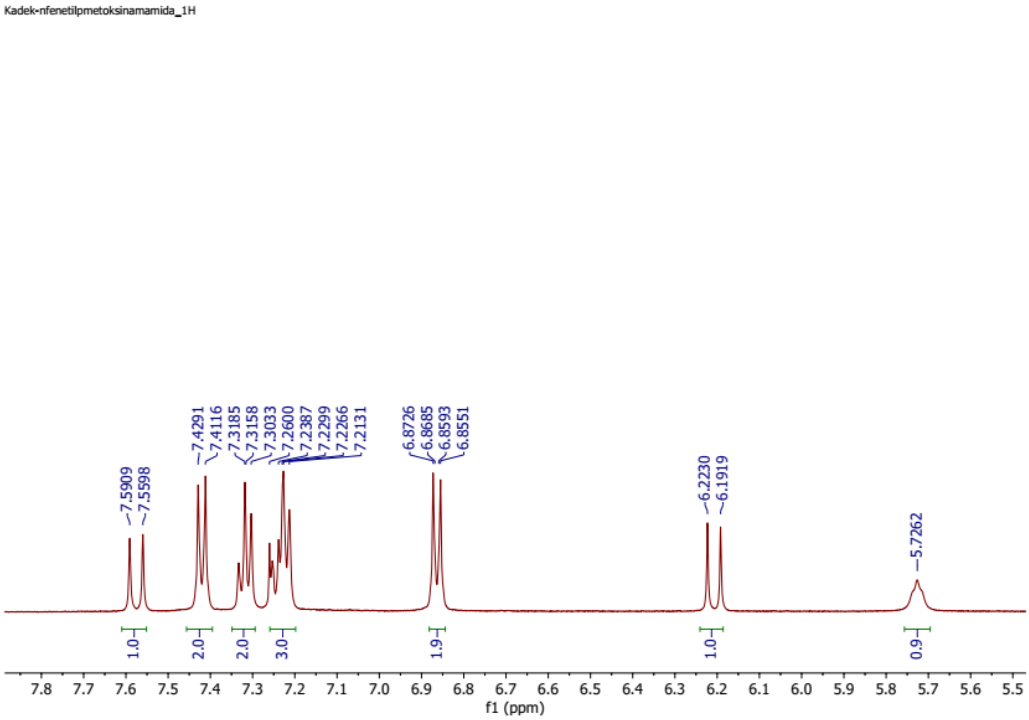
Date/Time; 11/10/2020 8:55:22 AM
No. of Scans;

Lampiran 9. Spektrum ^{13}C-NMR Senyawa *N*-fenetil-*p*-metoksisinamamida



Lampiran 10. Spektrum ^{1}H-NMR Senyawa *N*-fenetil-*p*-metoksisinamamida



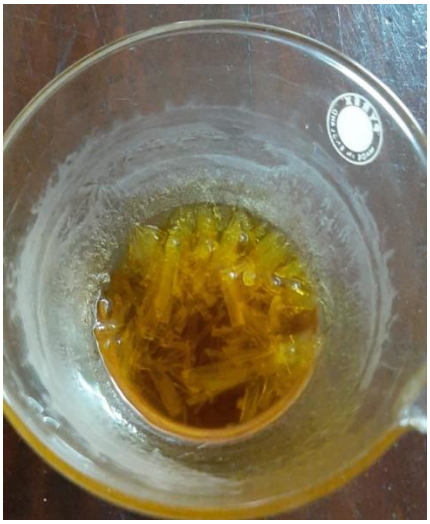


Lampiran 11. Dokumentasi Hasil Penelitian

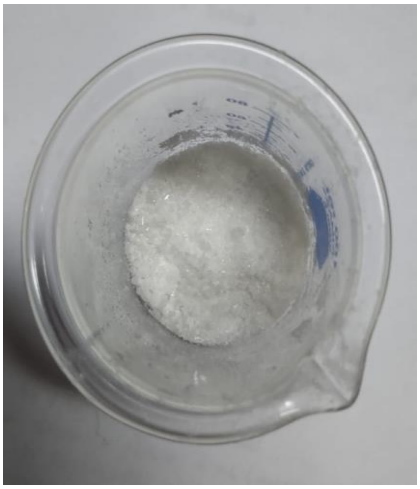
Rimpang kencur

Bubuk kencur

Proses sokhletasi sampel kencur



Kristal kotor hasil isolasi

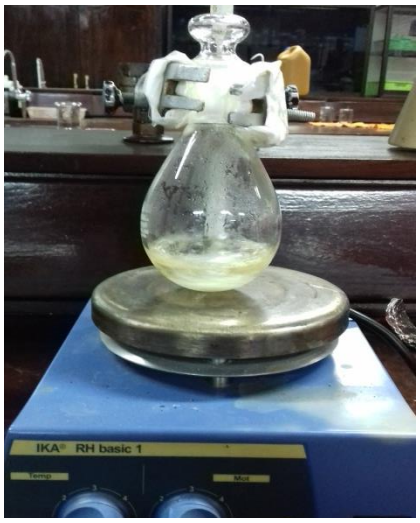


Kristal murni hasil isolasi

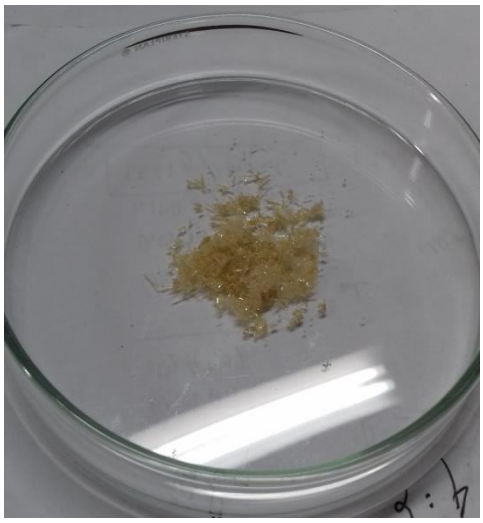
Proses hidrolisis

Kristal murni APMS

Proses klorinasi



Proses Amidasi



Kristal kotor hasil amidasi

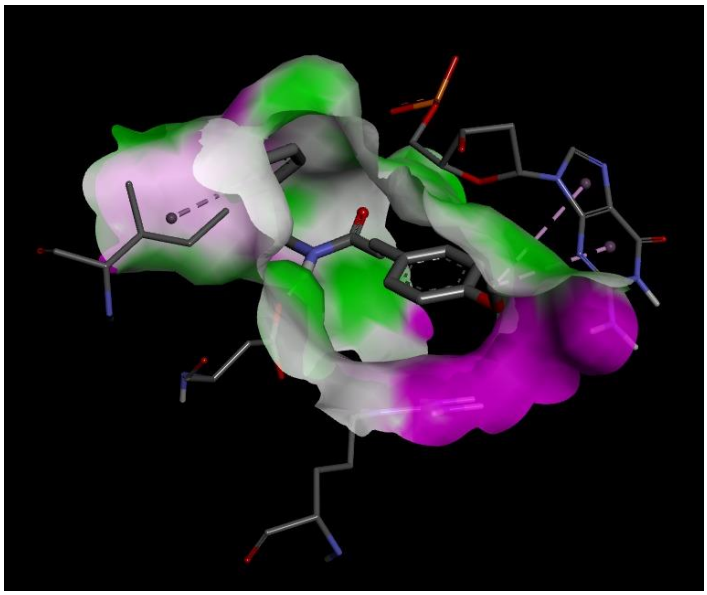
Kristal murni hasil amidasi

Lampiran 12. Hasil *Docking* Senyawa Hasil Sintesis Terhadap Protein Top1

RMSD TABLE

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
1	1	11	-7.70	0.00	5.70	RANKING
1	2	18	-6.94	0.75	5.69	RANKING
1	3	9	-6.93	1.10	5.76	RANKING
2	1	15	-7.54	0.00	3.22	RANKING
3	1	10	-7.43	0.00	5.43	RANKING
3	2	12	-7.12	0.85	4.96	RANKING
4	1	17	-7.25	0.00	3.70	RANKING
4	2	20	-7.25	0.11	3.67	RANKING
5	1	4	-7.23	0.00	3.36	RANKING
5	2	1	-7.12	1.61	3.79	RANKING
5	3	5	-7.07	0.92	3.71	RANKING
5	4	3	-7.06	0.75	3.68	RANKING
5	5	2	-7.06	1.10	3.06	RANKING
5	6	14	-7.05	1.15	3.79	RANKING
5	7	6	-6.95	0.58	3.31	RANKING
6	1	13	-7.20	0.00	2.62	RANKING
7	1	8	-6.99	0.00	4.77	RANKING
8	1	19	-6.79	0.00	4.25	RANKING
8	2	16	-6.63	0.25	4.30	RANKING
9	1	7	-6.29	0.00	5.39	RANKING

Tabel RMSD *docking* senyawa hasil sintesis terhadap protein Top1



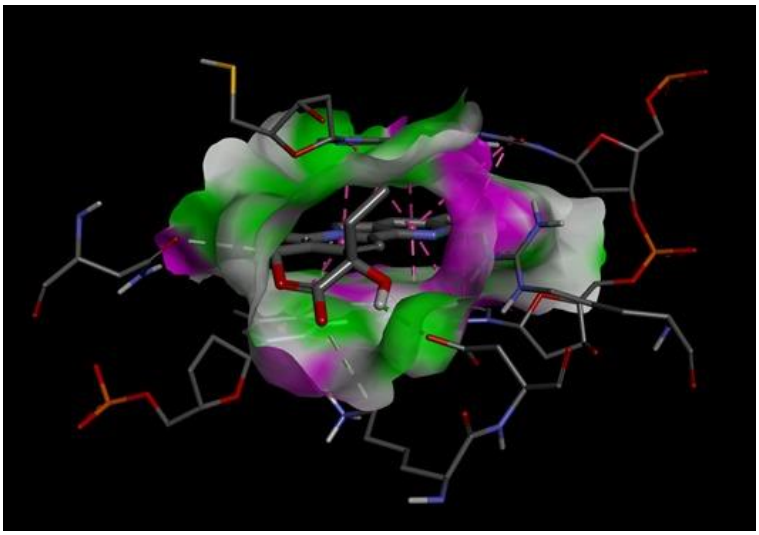
Visualisasi 3D konformasi 11 interaksi senyawa hasil sintesis terhadap protein Top1

Lampiran 13. Hasil *Redocking* Ligan EHDTerhadap Protein Top1

RMSD TABLE

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
1	1	5	-10.62	0.00	0.66	RANKING
1	2	6	-10.60	0.11	0.62	RANKING
1	3	10	-10.56	0.16	0.60	RANKING
1	4	8	-10.51	0.26	0.67	RANKING
1	5	3	-10.50	0.28	0.67	RANKING
1	6	1	-10.48	0.35	0.59	RANKING
1	7	9	-10.48	0.35	0.60	RANKING
1	8	7	-10.47	0.35	0.58	RANKING
1	9	2	-10.47	0.33	0.54	RANKING
1	10	4	-10.46	0.33	0.58	RANKING

Tabel RMSD *redocking* ligan EHD terhadap protein Top1



Visualisasi 3D konformasi 2 interaksi ligan EHD terhadap protein Top1