

Lampiran

A. Perhitungan Selektivitas Lipase

$$\frac{\%mentil\ asetat}{\%mentol\ murni - \%mentol\ tidak\ bereaksi} \times 100\%$$

1. Selektivitas lipase terhadap mentil asetat pada temperatur 50⁰C dengan sumber asil asam asetat anhidrat

a) Jam ke-4

$$\frac{0\%}{100\% - 85,82\%} \times 100\% = 0\%$$

b) Jam ke-8

$$\frac{24,74\%}{100\% - 74,35\%} \times 100\% = 96,45\%$$

c) Jam ke-12

$$\frac{35,45\%}{100\% - 64,55\%} \times 100\% = 100\%$$

d) Jam ke-16

$$\frac{43,37\%}{100\% - 26,77\%} \times 100\% = 59,22\%$$

e) Jam ke-20

$$\frac{45,63\%}{100\% - 54,37\%} \times 100\% = 100\%$$

f) Jam ke-24

$$\frac{58,45\%}{100\% - 41,55\%} \times 100\% = 100\%$$

2. Selektivitas lipase terhadap mentil asetat pada temperatur 50⁰C dengan sumber asil vinil asetat
- a) Jam ke-4

$$\frac{0\%}{100\% - 97,44\%} \times 100\% = 0\%$$

- b) Jam ke-8

$$\frac{0\%}{100\% - 85,87\%} \times 100\% = 0\%$$

- c) Jam ke-12

$$\frac{0\%}{100\% - 100\%} \times 100\% = 0\%$$

- d) Jam ke-16

$$\frac{0\%}{100\% - 91,51\%} \times 100\% = 0\%$$

- e) Jam ke-20

$$\frac{0\%}{100\% - 79,46\%} \times 100\% = 0\%$$

- f) Jam ke-24

$$\frac{0,29\%}{100\% - 98,72\%} \times 100\% = 22,66\%$$

B. Perhitungan Konversi L-Menthol

$$\frac{\%mentol\ murni - \%mentol\ tidak\ bereaksi}{\%mentol\ murni} \times 100\%$$

1. **Konversi l-mentol pada temperatur 50⁰C dengan sumber asil asam asetat anhidrida**

a) **Jam ke-4**

$$\frac{100\% - 85,82\%}{100\%} \times 100\% = 14,18\%$$

b) **Jam ke-8**

$$\frac{100\% - 74,35\%}{100\%} \times 100\% = 26,65\%$$

c) **Jam ke-12**

$$\frac{100\% - 64,55\%}{100\%} \times 100\% = 35,45\%$$

d) **Jam ke-16**

$$\frac{100\% - 26,77\%}{100\%} \times 100\% = 73,23\%$$

e) **Jam ke-20**

$$\frac{100\% - 54,37\%}{100\%} \times 100\% = 45,63\%$$

f) **Jam ke-24**

$$\frac{100\% - 46,38\%}{100\%} \times 100\% = 53,62\%$$

2. **Konversi l-mentol pada temperatur 50⁰C dengan sumber asil vinil asetat**

a) **Jam ke-4**

$$\frac{100\% - 97,44\%}{100\%} \times 100\% = 2,56\%$$

b) Jam ke-8

$$\frac{100\% - 85,87\%}{100\%} \times 100\% = 14,13\%$$

c) Jam ke-12

$$\frac{100\% - 100\%}{100\%} \times 100\% = 0\%$$

d) Jam ke-16

$$\frac{100\% - 91,51\%}{100\%} \times 100\% = 8,49\%$$

e) Jam ke-20

$$\frac{100\% - 79,46\%}{100\%} \times 100\% = 20,54\%$$

f) Jam ke-24

$$\frac{100\% - 98,72\%}{100\%} \times 100\% = 1,28\%$$

C. Perhitungan harga Kd

$$\Delta G^0 = -RT \ln[k_i]$$

*Keterangan:

$$R = 1,987 \text{ kal/K.mol}$$

$$T = 50 \text{ }^\circ\text{C} = 323 \text{ K}$$

1. Docking: makromolekul, menthol, asam asetat anhidrat

a. Makromolekul-menthol

$$\Delta G^0 = -62,476 \text{ kal/mol}$$

$$-62,476 \text{ kal/mol} = -1,987 \text{ kal/K.mol} \times 323 \text{ K} \times \ln kd$$

$$-62,476 = -641,801 \ln kd$$

$$0,097 = \ln kd$$

$$1,302 = kd$$

b. Makromolekul-asetat anhidrat

$$\Delta G^0 = -50,987 \text{ kal/mol}$$

$$-50,987 \text{ kal/mol} = -1,987 \text{ kal/K.mol} \times 323 \text{ K} \times \ln kd$$

$$-50,987 = -641,801 \ln kd$$

$$0.079 = \ln kd$$

$$1,240 = kd$$

2. Docking: makromolekul, menthol, vinil asetat

a. Makromolekul-menthol

$$\Delta G^0 = -63,445 \text{ kal/mol}$$

$$-63,445 \text{ kal/mol} = -1,987 \text{ kal/K.mol} \times 323 \text{ K} \times \ln kd$$

$$-63,445 = -641,801 \ln kd$$

$$0.099 = \ln kd$$

$$1,309 = kd$$

b. Makromolekul-asetat anhidrat

$$\Delta G^0 = -47,309 \text{ kal/mol}$$

$$-47,309 \text{ kal/mol} = -1,987 \text{ kal/K.mol} \times 323 \text{ K} \times \ln kd$$

$$-47,309 = -641,801 \ln kd$$

$$0.074 = \ln kd$$

$$1,223 = kd$$

3. Docking: makromolekul dan menthil asetat

$$\Delta G^0 = -57,938 \text{ kal/mol}$$

$$-57,938 \text{ kal/mol} = -1,987 \text{ kal/K.mol} \times 323 \text{ K} \times \ln kd$$

$$-57,938 = -641,801 \ln kd$$

$$0.090 = \ln kd$$

$$1,277 = kd$$

D. Perhitungan mol

1. Perhitungan mol menthol

$$\begin{aligned}\text{Massa menthol} &= \rho_{\text{menthol}} \times V_{\text{menthol}} \\ &= 0,89 \text{ g/mL} \times 6 \text{ mL} \\ &= 5,34 \text{ g}\end{aligned}$$

$$\begin{aligned}\text{Mol menthol} &= \frac{\text{massa menthol}}{\text{Mr menthol}} = \frac{5,34 \text{ g}}{156,27 \frac{\text{g}}{\text{mol}}} \\ &= 0.018 \text{ mol}\end{aligned}$$

2. Perhitungan mol vinil asetat

$$\begin{aligned}\text{Massa vinil asetat} &= \rho_{\text{vinil asetat}} \times V_{\text{vinil asetat}} \\ &= 0,934 \text{ g/mL} \times 5 \text{ mL} \\ &= 4,67 \text{ g}\end{aligned}$$

$$\begin{aligned}\text{Mol vinil asetat} &= \frac{\text{massa vinil asetat}}{\text{Mr vinil asetat}} = \frac{4,67 \text{ g}}{86,09 \frac{\text{g}}{\text{mol}}} \\ &= 0,054 \text{ mol}\end{aligned}$$

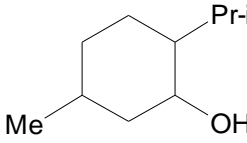
3. Perhitungan mol asetat anhidrat

$$\begin{aligned}\text{Massa asetat anhidrat} &= \rho_{\text{asetat anhidrat}} \times V_{\text{asetat anhidrat}} \\ &= 1,08 \text{ g/mL} \times 5 \text{ mL} \\ &= 5,4 \text{ g}\end{aligned}$$

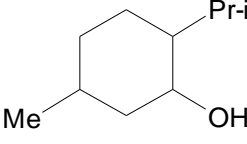
$$\begin{aligned}\text{Mol asetat anhidrat} &= \frac{\text{massa asetat anhidrat}}{\text{Mr asetat anhidrat}} \\ &= \frac{5,4 \text{ g}}{102,09 \frac{\text{g}}{\text{mol}}}\end{aligned}$$

E. Data Percobaan

E1. Menthol murni

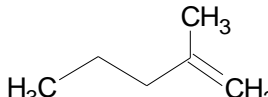
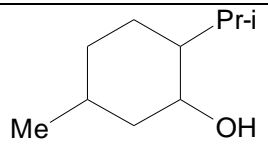
Line	t _R	%area	Fragmentasi	Kemungkinan senyawa
1	13,139	100	138, 123, 109, 95, 71, 67, 55, 41, 27	 <p>l-menthol BM = 156</p>

E2. Reaksi Asilasi dengan Sumber Asil Vinil Asetat Jam ke-4

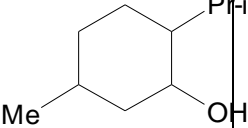
Line	t _R	%area	Fragmentasi	Kemungkinan senyawa
1	12,474	0.33	370, 355, 281, 267, 249, 147, 73	<p>2,6-dihydroxybenzoic acid 3 TMS</p> <p>BM = 370</p>
2	12,972	97,44	138, 123, 109, 95, 71, 67, 55, 41, 27	 <p>l-menthol BM = 156</p>
3	15,193	1,73	341,327, 147, 73	<p>2,3,4,4-tetrapropyl-1-(trimethylsilyl)-1-(trimethylsilyloxy)-1,3-diaza-2,4-diborabutane</p> <p>BM = 382</p>

Line	t _R	%area	Fragmentasi	Kemungkinan senyawa
4	17,657	0,49	165, 147, 73	Hexamethylborazine BM = 165

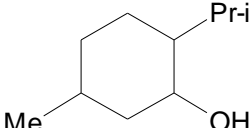
E3. Reaksi Asilasi dengan Sumber Asil Vinil Asetat Jam ke-8

Line	t _R	%area	Fragmentasi	Kemungkinan senyawa
1	3,208	14,13	84, 70, 56, 55, 41, 38	 <p>2-metilpentena BM = 84</p>
2	13,058	85,87	138, 123, 109, 95, 71, 67, 55, 41	 <p>1-menthol BM = 156</p>

E4. Reaksi Asilasi dengan Sumber Asil Vinil Asetat Jam ke-12

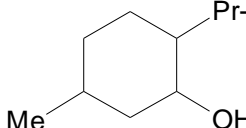
Line	t _R	%area	Fragmentasi	Kemungkinan senyawa
1	12,978	100	138, 123, 109, 95, 71, 67, 55, 41, 39	 <p>Menthol l-menthol BM = 156</p>

E5. Reaksi Asilasi dengan Sumber Asil Vinil Asetat Jam ke-16

Line	t _R	%area	Fragmentasi	Kemungkinan senyawa
1	6,129	1,30	251, 207, 44	<p>1-(pent-4-ynyl)pyrano(3,4-b)indol-3-one</p> <p>BM = 251</p>
2	9,723	0,35	402, 281	<p>(+)(-)-1-(acetoxy)-2-(1-bromoethyl)-3-methoxyanthranquinone</p> <p>BM = 402</p>
3	12,481	0,99	427, 355, 73, 69	<p>Phosponous dibromide (2,2,2-trifluoro-1(trifluoromethyl))</p> <p>BM = 428</p>
4	13,016	91,51	141, 138, 123, 109, 95, 71, 69, 55, 41, 39	 <p>Menthol</p>

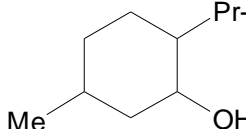
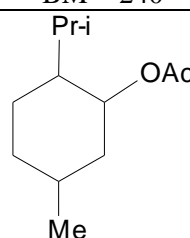
Line	t _R	%area	Fragmentasi	Kemungkinan senyawa
5	15,251	4,68	341, 327, 147, 73	2,3,4,4-tetrapropyl-1-(trimethylsilyl)-1-(trimethylsilyloxy)-1,3-diaza-2,4-diborabutane BM = 382
6	17,684	1,16	264, 147, 73, 45	2,2-bis(trimethylsilyl)styreneoxide BM = 264

E6. Reaksi Asilasi dengan Sumber Asil Vinil Asetat Jam ke-20

Line	t _R	%area	Fragmentasi	Kemungkinan senyawa
1	12,952	79,46	138, 123, 109, 95, 71, 67, 55, 41, 27	 l-menthol BM = 156
2	17,546	3,84	547, 415, 341, 327, 281, 221, 207, 147, 133, 73, 59, 45	3-ethoxy-1,1,1,7,7,7-hexamethyl-3,5,5-tris(trimethylsilyloxy)tetrasiloxane BM= 562

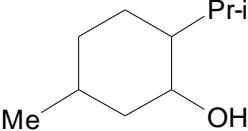
Line	t _R	%area	Fragmentasi	Kemungkinan senyawa
3	19,676	6,92	457, 429, 355, 147, 73, 45	3,4- dihydroxymandelicac id-tetra TMS BM = 472
4	21,516	3,80	401, 281, 221, 207, 147, 73, 59, 41, 28	Silicate anion tetramer BM = 888
5	23,154	1,85	401, 281, 221, 207, 147, 73, 59, 41, 28	Silicate anion tetramer BM = 888
6	25, 988	1,34	401, 281, 221, 207, 147, 73, 59, 41, 28	Silicate anion tetramer BM = 888
7	25,988	1,25	401, 281, 221, 207, 147, 73, 59, 41, 28	Silicate anion tetramer BM = 888
8	27,215	0,90	401, 281, 221, 207, 147, 73, 59, 41, 28	Silicate anion tetramer BM = 888
9	28,379	0,64	401, 281, 221, 207, 147, 73, 59, 41, 28	Silicate anion tetramer BM = 888

E7. Reaksi Asilasi dengan Sumber Asil Vinil Asetat Jam ke-24

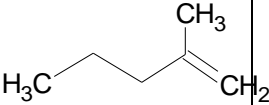
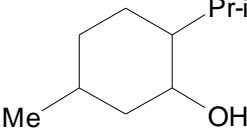
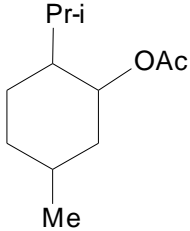
Line	t _R	%area	Fragmentasi	Kemungkinan senyawa
1	13,022	98,72	138, 123, 109, 95, 71, 67, 55, 41, 39	 <p>l-menthol BM = 156</p>
2	13,234	0,99	240, 139, 97, 83, 69, 55, 41, 27	<p>Phospine dichloromenthyl</p> <p>BM = 240</p>
3	14,848	0,29	141, 138, 123, 109, 95, 81, 67, 43, 41, 27	 <p>Menthil asetat BM = 198</p>

E8. Reaksi Asilasi dengan Sumber Asil Asetat Anhidrid Jam 4

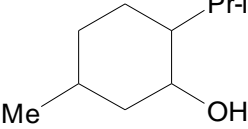
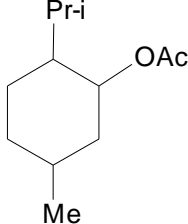
Line	t _R	%area	Fragmentasi	Kemungkinan senyawa
1	6,132	1,04	276, 207	<p>1,1,2-trifluoro-2,5- bis(trifluoromethyl) hexane BM = 276</p>
2	9,724	0,49	279, 251, 234, 213, 207, 182, 172, 155, 127, 100, 75,	<p>Phospine dichloromenthyl</p> <p>BM = 240</p>

Line	t _R	%area	Fragmentasi	Kemungkinan senyawa
			63, 50, 29, 27	2-propenoic acid, 2-cyano-3-(4-bromophenyl)-ethyl ester BM = 279
3	13,011	85,82	138, 123, 109, 95, 71, 67, 55, 41, 27	 1-menthol BM = 156
4	14,970	12,64	282, 128, 95, 82, 43	1-naphtalenemethano Idecadhydro-2-hydroxy-2,5,5,8-tetramethyl-alpha-acetate BM = 282

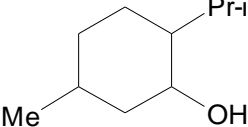
E9. Reaksi Asilasi dengan Sumber Asil Asetat Anhidrid Jam 8

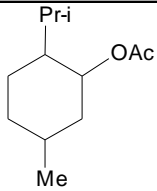
Line	t _R	%area	Fragmentasi	Kemungkinan senyawa
1	3,192	0,91	84, 70, 56, 55, 41, 38	 <p>2-metilpentena BM = 84</p>
2	13,192	74,35	138, 123, 109, 95, 71, 67, 55, 41	 <p>l-menthol BM = 156</p>
3	14,933	24,74	141, 138, 123, 109, 95, 81, 67, 43, 41, 27	 <p>Menthil asetat BM = 198</p>

E10. Reaksi Asilasi dengan Sumber Asil Asetat Anhidrid Jam 12

Line	t _R	%area	Fragmentasi	Kemungkinan senyawa
1	13,030	64,55	138, 123, 109, 95, 71, 67, 55, 41	 l-menthol BM = 156
2	14,863	35,45	141, 138, 123, 109, 95, 81, 67, 43, 41, 27	 Menthil asetat BM = 198

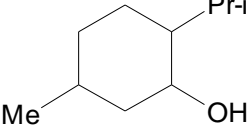
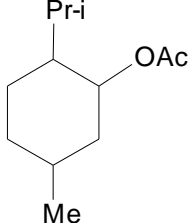
E11. Reaksi Asilasi dengan Sumber Asil Asetat Anhidrid Jam 16

Line	t _R	%area	Fragmentasi	Kemungkinan senyawa
1	13,006	26,77	138, 123, 109, 95, 71, 67, 55, 41, 39	 l-menthol BM = 156

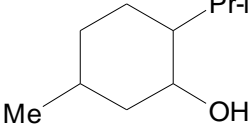
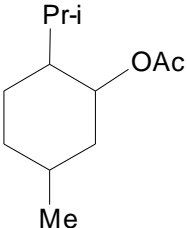
Line	t _R	%area	Fragmentasi	Kemungkinan senyawa
2	14,864	43,37	138, 123, 109, 95, 81, 67, 43, 41, 39	 <p>Menthil asetat BM = 198</p>
3	17,567	17,22	517, 415, 341, 327, 281, 221, 147, 73, 43	3-isopropyl- 1,1,1,7,7,7- hexamethyl-3,5,5- tris(trimethylsilox y)tetrasiloxane BM = 576
4	19,709	8,74	355, 281, 267, 147, 73	2,5- dihydroxybenzoic acid BM=370
5	21,566	2,01	245, 147, 73	2,2,4,4,5,8,8- heptamethyl-3,7- dioxo-2,8- disilanonane BM = 262
6	23,238	0,86	165, 147, 73	Hexamethylbora- zine BM = 165
7	24,725	0,51	73, 58, 40, 30	Trans-2-buten-3- ol-1-ol BM=72
8	26,093	0,52	298, 73	(4-fluorobenzoyl)

Line	t _R	%area	Fragmentasi	Kemungkinan senyawa
				(tert-butyl)dimethylsilane BM = 298

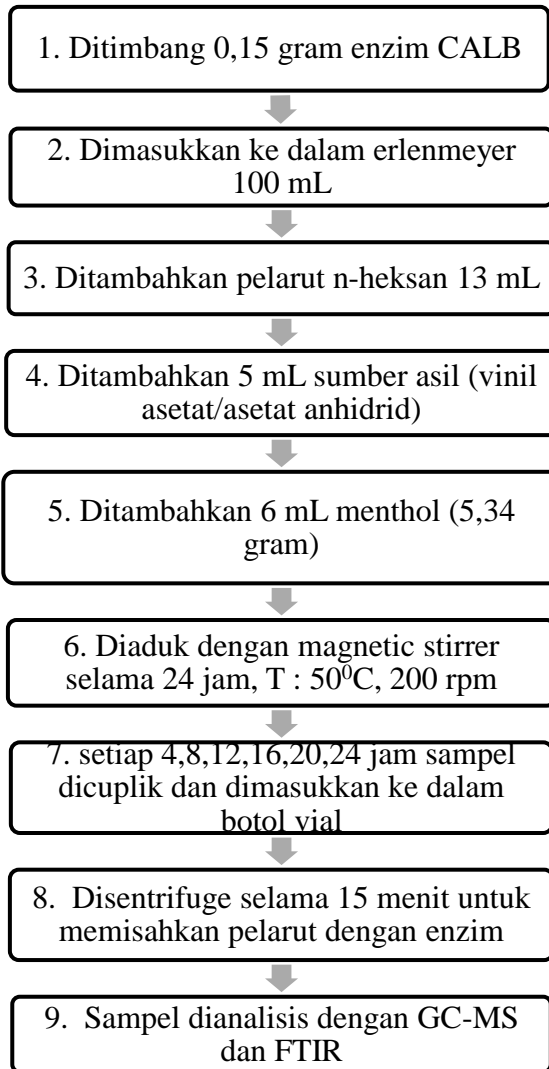
E12. Reaksi Asilasi dengan Sumber Asil Asetat Anhidrid Jam 20

Line	t _R	%area	Fragmentasi	Kemungkinan senyawa
1	12,992	54,37	138, 123, 109, 95, 71, 67, 55, 41, 39	 <p>l-menthol BM = 156</p>
2	14,850	45,63	138, 123, 109, 95, 71, 67, 55, 43, 41, 39	 <p>Menthil asetat BM = 198</p>

E12. Reaksi Asilasi dengan Sumber Asil Asetat Anhidrid Jam 24

Line	t _R	%area	Fragmentasi	Kemungkinan senyawa
1	12,966	41,55	138, 123, 109, 95, 71, 67, 55, 41, 27	 <p>l-menthol BM = 156</p>
2	14,837	58,45	141, 138, 123, 109, 95, 81, 69, 43, 41, 27	 <p>Menthil asetat BM = 198</p>

F. DIAGRAM ALIR REAKSI ASILASI MENTHOL DENGAN ENZIM CALB



G. DIAGRAM ALIR PROSES DOCKING MENTHOL, SUMBER ASIL, DAN ENZIM CALB

