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SUPPLEMENTARY MATERIAL TO

Dioleate and trioleate epoxides from palm oil as anticancer agents through *in vitro* and molecular docking studies

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ANALYTICAL AND SPECTRAL DATA

Fatty acid methyl esters (FAME)

Bright yellow liquid (41.09 g, 95.69 %). FTIR (NaCl, ν_max/cm^{-1}): 3008 (=C–H), 2924, 2854 (C–H), 1743 (C=O), 1658 (C=C), 1458, 1435 (CH_2), 1381 (CH_3), 1165 (C–O), 1118 (=C–H), 725 ((CH_2) n) (Fig. S-1). GC–MS (EI, 70 eV): methyl myristate (0.42 %, R_t = 30.43 min, m/z 242 $[M]^+$), methyl palmitate (36.30 %, R_t = 35.02 min, m/z 270 $[M]^+$), methyl linoleate (8.75 %, R_t = 38.40 min, m/z 294 $[M]^+$), methyl oleate (51.01 %, R_t = 38.62 min, m/z 264 $[M - CH_3OH]^+$), methyl stearate (3.27 %, R_t = 39.00 min, m/z 298 $[M]^+$), and methyl icosanoate (0.25 %, R_t = 42.70 min, m/z 326 $[M]^+$) (Fig. S-2).

Purified FAME

Pale yellow liquid (5.56 g, 88.96 %). FTIR (NaCl, ν_max/cm^{-1}): 3008 (=C–H), 2924, 2854 (C–H), 1743 (C=O), 1658 (C=C), 1458, 1435 (CH_2), 1381 (CH_3), 1165 (C–O), 1118 (=C–H), 725 ((CH_2)_n) (Fig. S-3). GC–MS (EI, 70 eV): methyl palmitate (3.26 %, R_t=29.24 min, m/z 270 $[M]^+$), methyl linoleate (9.84 %, R_t=32.47 min, m/z 294 $[M]^+$), and methyl oleate (89.90%, R_t=32.67 min, m/z 296 $[M]^+$) (Fig. S-4).

Oleic acid

Light yellow liquid (2.59 g, 92%). FTIR (NaCl, ν_max/cm^{-1}): 3100 (O–H), 2924, 2854 (C–H), 1712 (C=O), 1458 (CH_2), 1373 (CH_3), 1280 (C–O), 725 ((CH_2)$_n$) (Fig. S-5). ^{1}H NMR (500 MHz, $CDCl_3$, δ): 0.85 (t, *J* = 7.0 Hz, 3H), 1.20–1.32 (m, 20H), 1.56–1.63 (m, 2H), 1.95 (q, *J* = 7.0 Hz, 4H), 2.35 (t, *J* = 8.0 Hz, 2H), 5.30–5.35 (m, 2H) (Fig. S-6). ^{13}C NMR (125 MHz, $CDCl_3$, δ): 14.18, 22.77, 24.74, 27.23, 27.29, 29.12, 29.15, 29.24, 29.42, 29.62, 29.76, 29.85, 32.00, 34.15, 34.20, 127.79, 130.08, 180.53 (Fig. S-7).

1,2-Propanediol dioleate

Yellow liquid (6.01 g, 82.8%). FTIR (NaCl, ν_max/cm^{-1}): 3008 (=C–H), 2924, 2854 (C–H), 1736, 1712 (C=O), 1658 (C=C), 1458 (CH_2), 1381 (CH_3), 1180 (C–O), 725 ((CH_2)$_n$) (Fig. S-8). ^{1}H NMR (500 MHz, $CDCl_3$, δ): 0.81–0.84 (m, 6H), 1.14–1.32 (m, 43H), 1.54–1.61 (m,

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4H), 1.92 (q, J = 6.8 Hz, 8H), 2.25–2.30 (m, 4H), 3.95–4.05 (m, 2H), 5.08–5.12 (m, 1H), 5.28–5.32 (m, 4H) (Fig. S-9). ^{13}C NMR (125 MHz, $CDCl_3$, δ): 14.17, 16.55, 22.76, 24.80, 27.23, 27.28, 29.02, 29.11, 29.18, 29.34, 29.42, 29.47, 29.58, 29.68, 31.98, 34.19, 65.98, 68.07, 129.78, 130.06, 173.64 (Fig. S-10).

Glyceryl trioleate

Yellow liquid (7.08 g, 80 %). FTIR (NaCl, ν_max/cm^{-1}): 3008 (=C–H), 2924, 2854 (C–H), 1736 (C=O), 1658 (C=C), 1458, 1435 (CH_2), 1357 (CH_3), 1172 (C–O), 725 ($(CH_2)_n$) (Fig. S-11). ^{1}H NMR (500 MHz, $CDCl_3$, δ): 0.85 (t, J = 7.1 Hz, 9H), 1.18–1.30 (m, 60H), 1.55–1.63 (m, 6H), 1.98 (q, J = 7.2 Hz, 12H), 2.28 (t, J = 8.4 Hz, 6H), 4.09–4.16 (m, 4H), 4.73–4.77 (m, 1H), 5.28–5.33 (m, 6H) (Fig. S-12). ^{13}C NMR (125 MHz, $CDCl_3$, δ): 14.18, 24.81, 24.94, 27.24, 27.29, 29.17, 29.25, 29.41, 29.61, 29.77, 29.85, 31.68, 31.99, 34.16, 34.26, 65.09, 70.34, 129.87, 130.08, 180.03 (Fig. S-13).

Dioleate diepoxide

White solid (0.60 g, 94.49 %). FTIR (NaCl, ν_max/cm^{-1}): 2924, 2854 (C–H), 1735 (C=O), 1465 (CH_2), 1381 (CH_3), 1172 (C–O), 840 (oxirane C–O), 725 ($(CH_2)^n$) (Fig. S-14,. LC–MS (ESI, negative ion mode): purity 86.49 %, R_t=12.28 min, m/z 722 ($[M + CH_3CN + HCOO]^-$) (Fig. S-15). ^{1}H NMR (500 MHz, CD_3OD, δ/ppm): 0.80 (t, J = 7.0 Hz, 6H), 1.23–1.27 (m, 43H), 1.40 (q, J = 5.5 Hz, 4H), 1.55 (q, J = 8.0 Hz, 8H), 2.25 (t, J = 7.2 Hz, 4H), 2.85–3.32 (m, 4H), 4.04–4.07 (m, 2H), 4.84–4.90 (m, 1H) (Fig. S-16). ^{13}C NMR (125 MHz, CD_3OD, δ/ppm): 14.18, 24.81, 24.94, 27.24, 27.29, 29.17, 29.25, 29.41, 29.61, 29.73, 29.77, 29.85, 30.53, 31.88, 33.50, 34.01, 57.41, 57.50, 65.95, 68.07, 178.13 (Fig. S-17).

Trioleate triepoxide

White solid (0.81 g, 92.04 %). FTIR (NaCl, ν_max/cm^{-1}): 2924, 2854 (C–H), 1728 (C=O), 1465 (CH_2), 1373 (CH_3), 1242 (C–O), 840 (oxirane C–O), 725 ($(CH_2)_n$) (Fig. S-18). LC–MS (ESI, negative ion mode): purity 93.51 %, R_t=12.10 min, m/z 985 ($[M+ NH_4Cl]^-$) (Fig. S-19). ^{1}H NMR (500 MHz, CD_3OD, δ/ppm): 0.81 (t, J = 7.0 Hz, 9H), 1.21–1.25 (m, 60H), 1.40–1.44 (m, 6H), 1.56 (q, J = 8.3 Hz, 12H), 2.26 (t, J = 7.2 Hz, 6H), 2.87–3.34 (m, 6H), 4.06–4.08 (m, 4H), 4.81–4.87 (m, 1H) (Fig. S-20). ^{13}C NMR (125 MHz, CD_3OD, δ/ppm): 14.14, 21.06, 22.70, 24.72, 26.60, 27.79, 28.99, 29.05, 29.25, 29.35, 29.56, 29.73, 31.89, 33.49, 34.03, 57.43, 57.48, 60.53, 72.24, 171.44 (Fig. S-21).

SYNTHESIS OF FAME

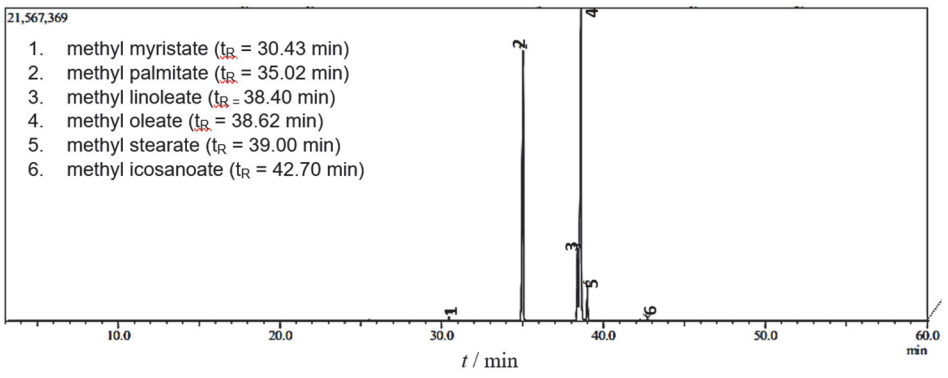

Fig. S-1. GC chromatograms of FAME

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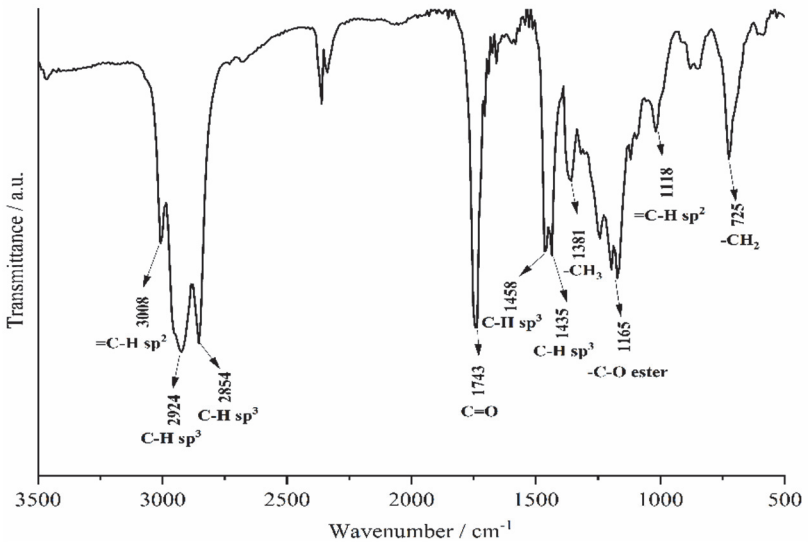

Fig. S-2. FTIR spectra of FAME

Synthesis of FAME: The FAME product was obtained as a yellow liquid (41.09 g, 95.69%). FTIR (ν, cm^{-1}): 3008 (C–H sp^2), 2924 and 2854 (C–H sp^3), 1743 (C=O), 1658 (C=C sp^2), 1458 and 1435 (–CH_2– sp^3), 1381 (–CH_3 sp^3), 1165 (C–O ester), 725 (–CH_2– sp^3). GC–MS: methyl myristate ($C_{15}H_{30}O_2$, 0.42%, retention time (t_R) 30.43 min, m/z 242 $[M]^+$), methyl palmitate ($C_{17}H_{34}O_2$, 36.30%, t_R 35.02 min, m/z 270 $[M]^+$), methyl linoleate ($C_{19}H_{34}O_2$, 8.75%, t_R 38.40 min, m/z 294 $[M]^+$), methyl oleate ($C_{19}H_{36}O_2$, 51.01%, t_R 38.62 min, m/z 264 $[M\text{-}CH_4O]^+$), methyl stearate ($C_{19}H_{38}O_2$, 3.27%, t_R 39.00 min, m/z 298 $[M]^+$), and methyl icosanoate ($C_{21}H_{42}O_2$, 0.25%, t_R 42.70 min, m/z 326 $[M]^+$).

Purified FAME

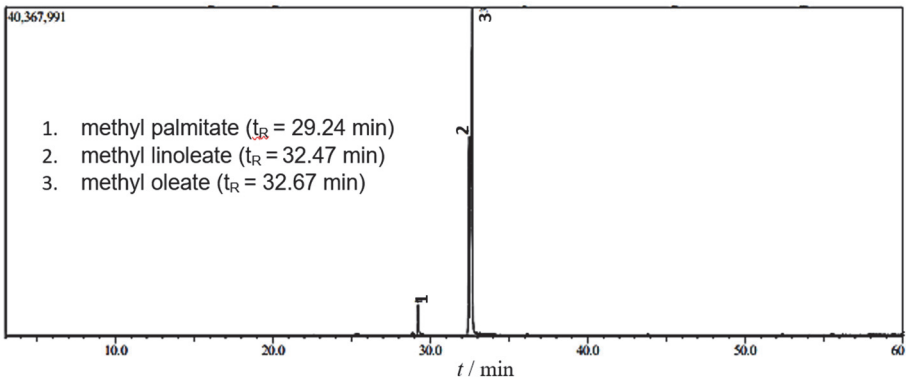

Fig. S-3. GC chromatograms of purified FAME

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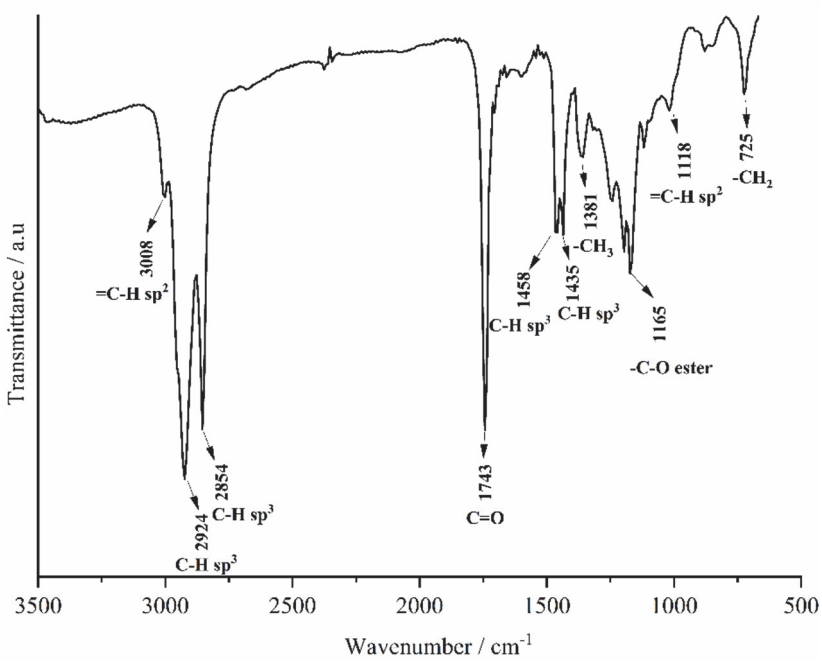

Fig. S-4. FTIR spectra of purified FAME

Purified FAME: The product was obtained as a pale yellow liquid (5.56 g, 88.96%). FTIR (ν, cm^{-1}): 3008 (C–H sp^2), 2924 and 2854 (C–H sp^3), 1743 (C=O), 1658 (C=C sp^2), 1458 and 1435 (–CH_2– sp^3), 1381 (–CH_3 sp^3), 1165 (C–O ester), 725 (–CH_2– sp^3). GC–MS: methyl palmitate ($C_{17}H_{34}O_2$, 3.26%, t_R 29.24 min, m/z 270 $[M]^+$), methyl linoleate ($C_{19}H_{34}O_2$, 9.84%, t_R 32.47 min, m/z 294 $[M]^+$), and methyl oleate ($C_{19}H_{36}O_2$, 89.90%, t_R 32.67 min, m/z 296 $[M]^+$).

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SYNTHESIZED OLEIC ACID

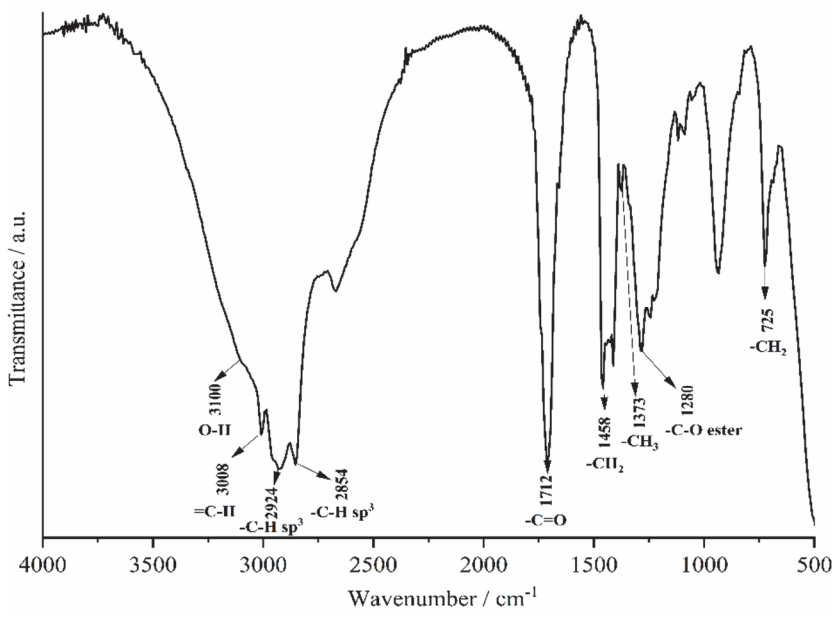

Fig. S-5. FTIR spectra of oleic acid

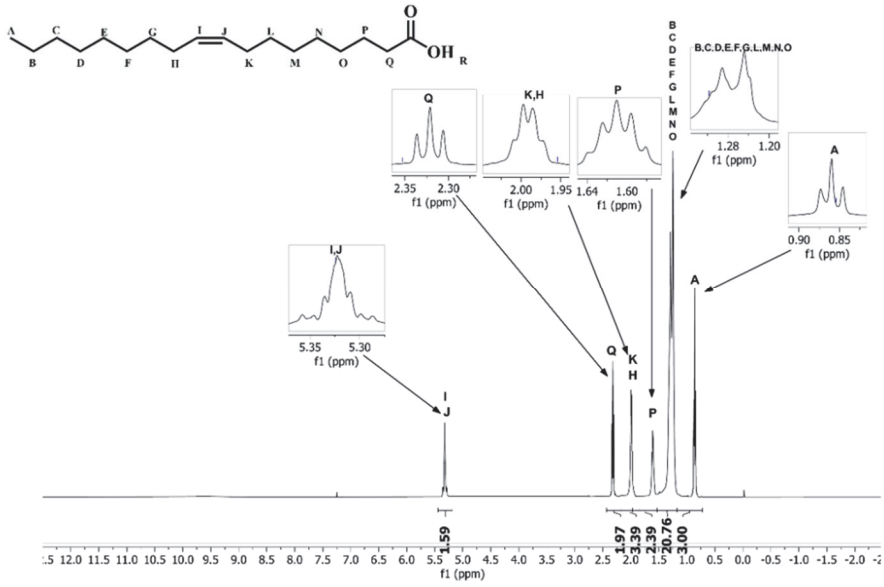

Fig. S-6. ^{1}H-NMR spectra of oleic acid

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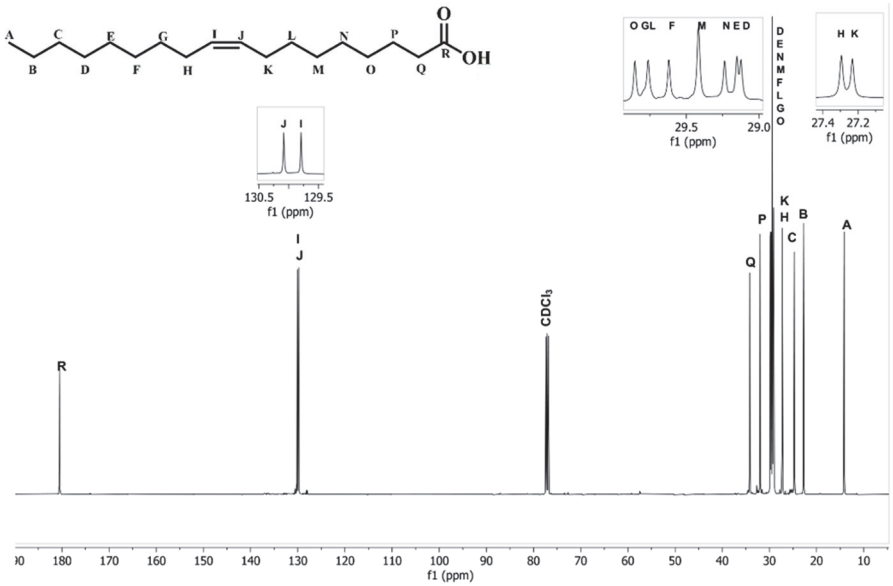

Fig. S-7. ^{13}C-NMR spectra of oleic acid

Synthesized oleic acid: Oleic acid ($C_{18}H_{34}O_2$) product was obtained as a light yellow liquid (2.59 g, 92%). FTIR (ν, cm^{-1}): 3100 (O–H), 2924 and 2854 (C–H sp^3), 1712 (C=O), 1458 (–CH_2– sp^3), 1373 (–CH_3 sp^3), 1280 (C–O ester), 725 (–CH_2– sp^3).

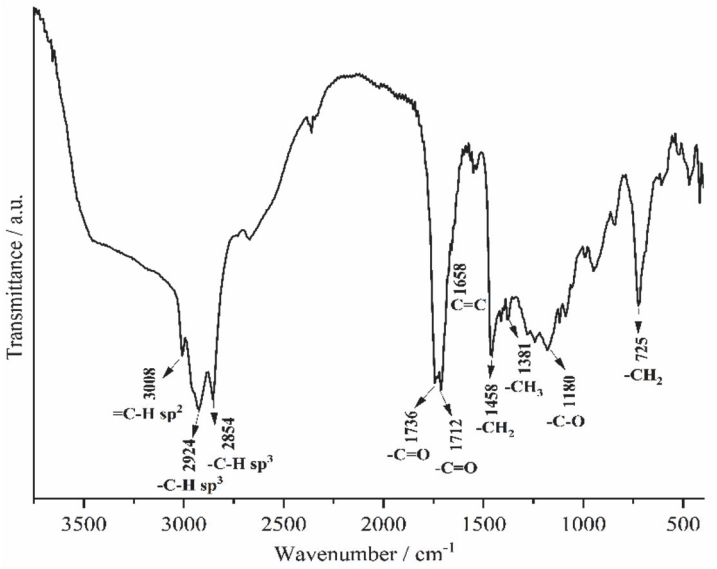

Fig. S-8. FTIR spectra of dioleate

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SYNTHESIZED DIOLEATE

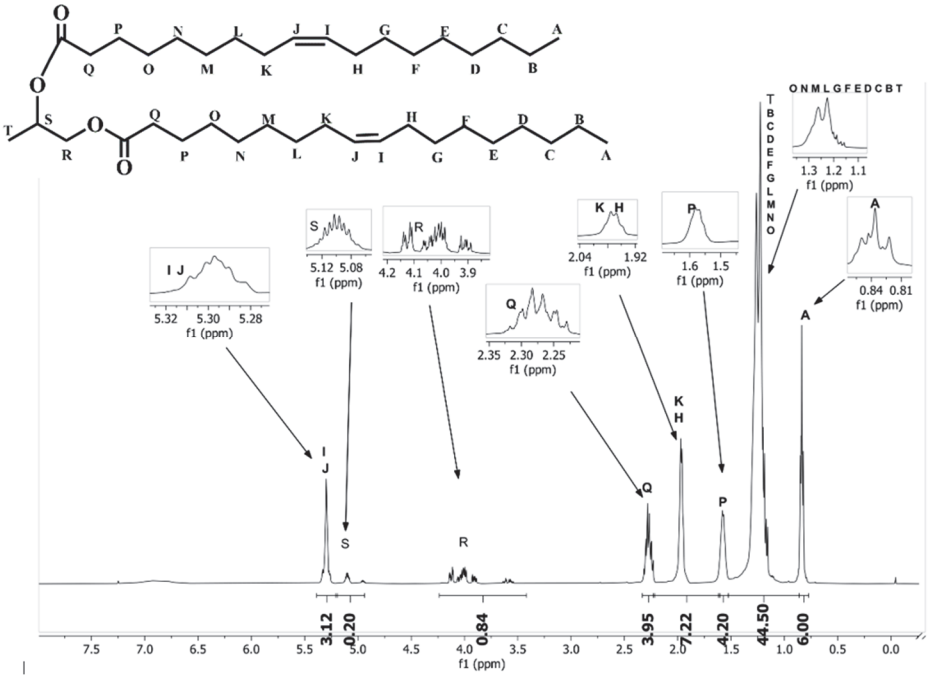

Fig. S-9. ^{1}H-NMR spectra of dioleate

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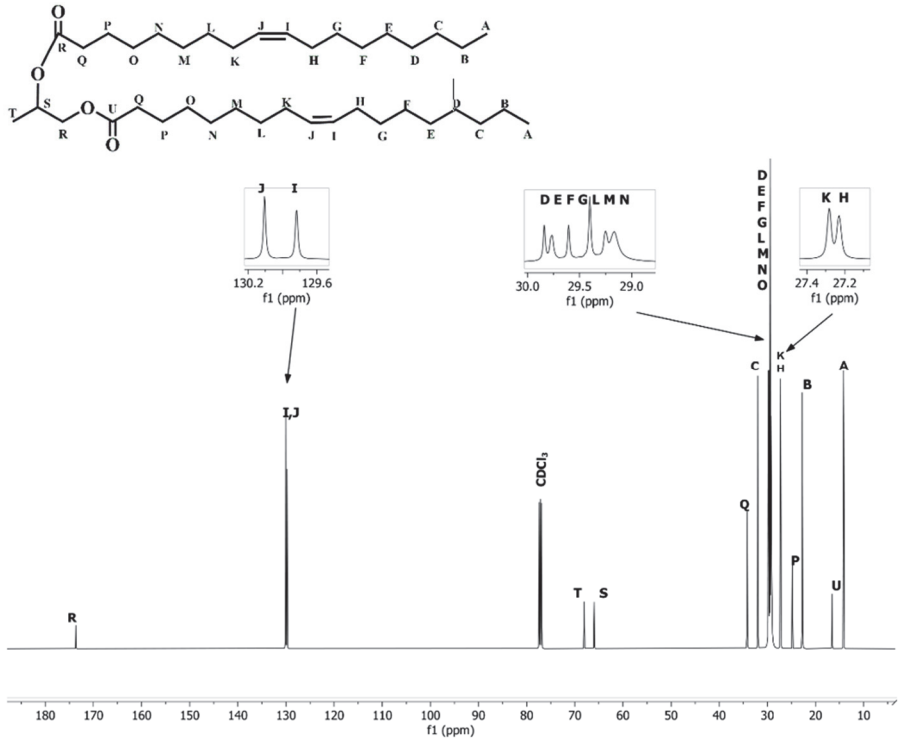

Fig. S-10. ^{13}C-NMR spectra of dioleate

Synthesized dioleate: Dioleate ($C_{39}H_{72}O_4$) product was obtained as a yellow liquid (6.01 g, 82.8%). FTIR (ν, cm^{-1}): 3008 (C–H sp^2), 2924 and 2854 (C–H sp^3), 1736 and 1712 (C=O), 1658 (C=C sp^2), 1458 (–CH_2– sp^3), 1381 (–CH_3 sp^3), 1180 (C–O ester), 725 (–CH_2– sp^3).

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SYNTHESIZED TRIOLEATE

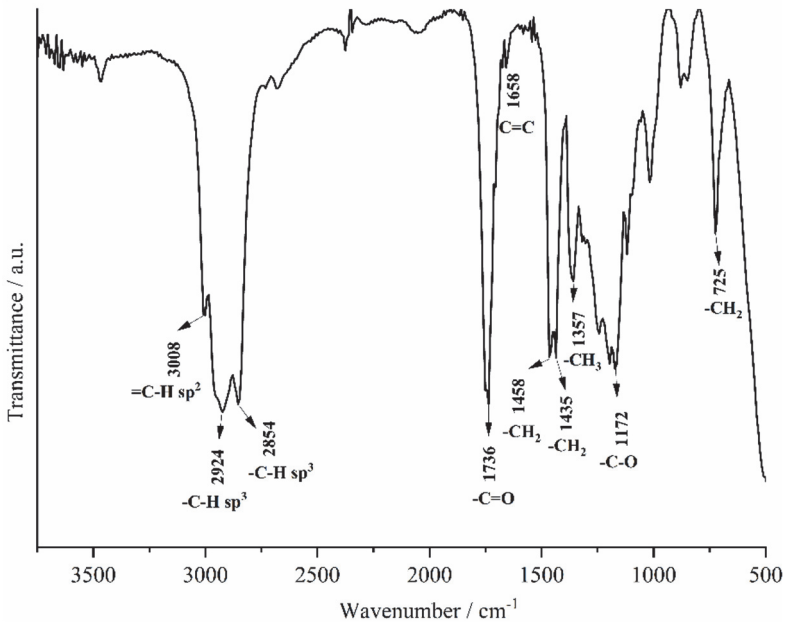

Fig. S-11. FTIR spectra of trioleate

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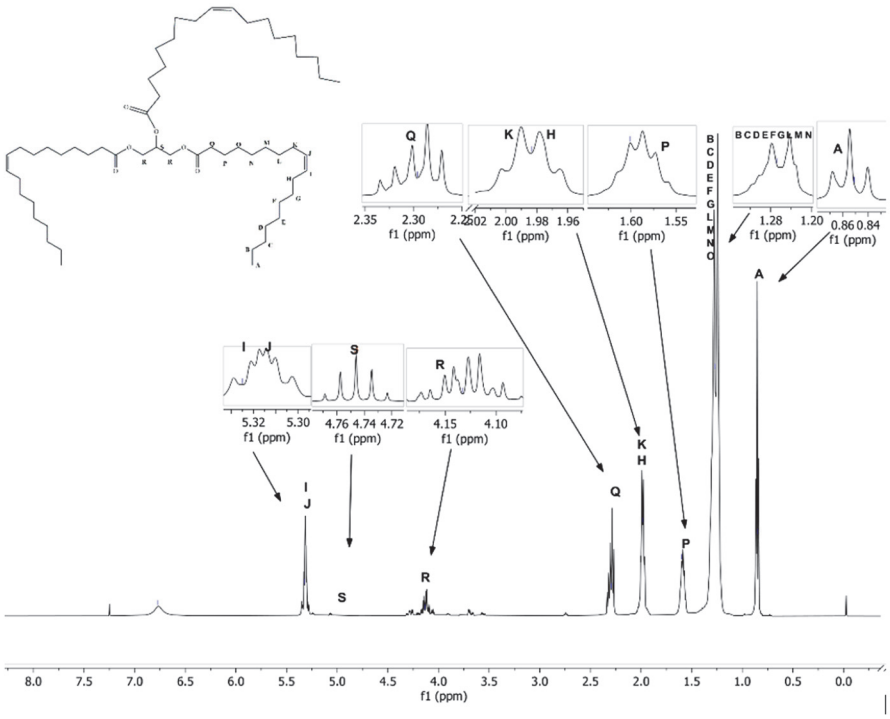

Fig. S-12. ^{1}H-NMR spectra of trioleate

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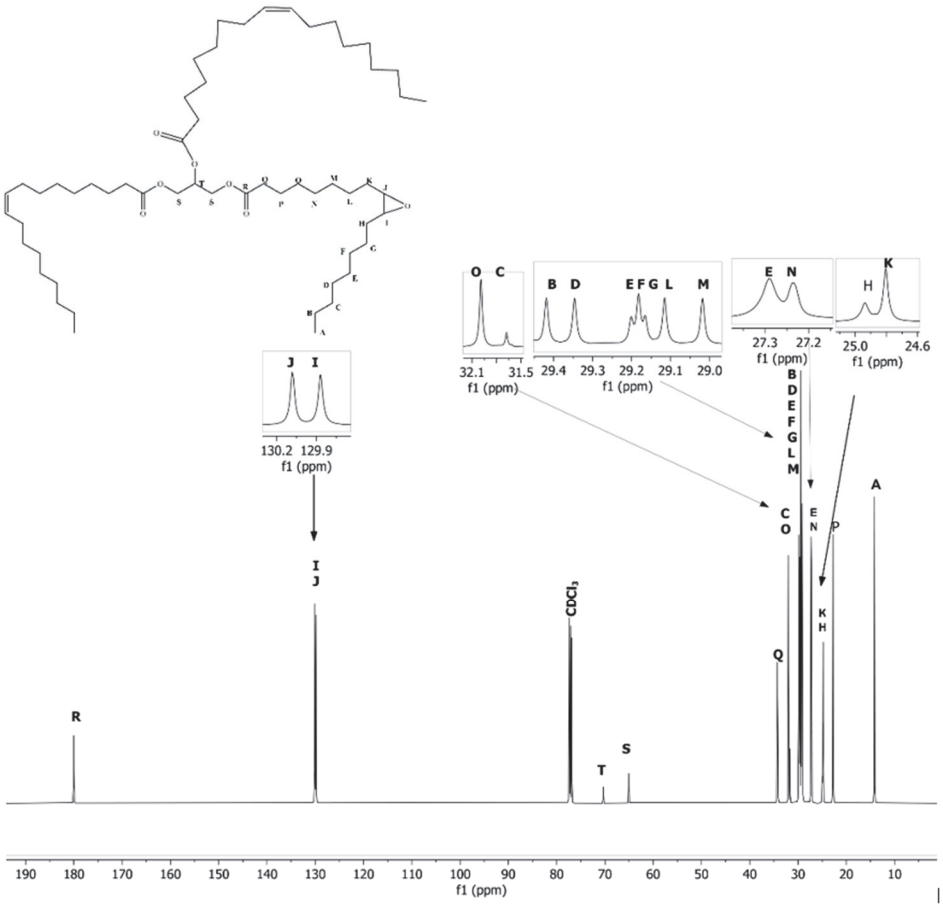

Fig. S-13. ^{13}C-NMR spectra of trioleate

Synthesized trioleate: Trioleate ($C_{57}H_{104}O_6$) product was obtained as a yellow liquid (7.08 g, 80%). FTIR (ν, cm^{-1}): 3008 (C–H sp^2), 2924 and 2854 (C–H sp^3), 1736 (C=O), 1658 (C=C sp^2), 1458 and 1435 (–CH_2– sp^3), 1357 (–CH_3 sp^3), 1172 (C–O ester), 725 (–CH_2– sp^3).

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SYNTHESIZED DIOLEATE EPOXIDE

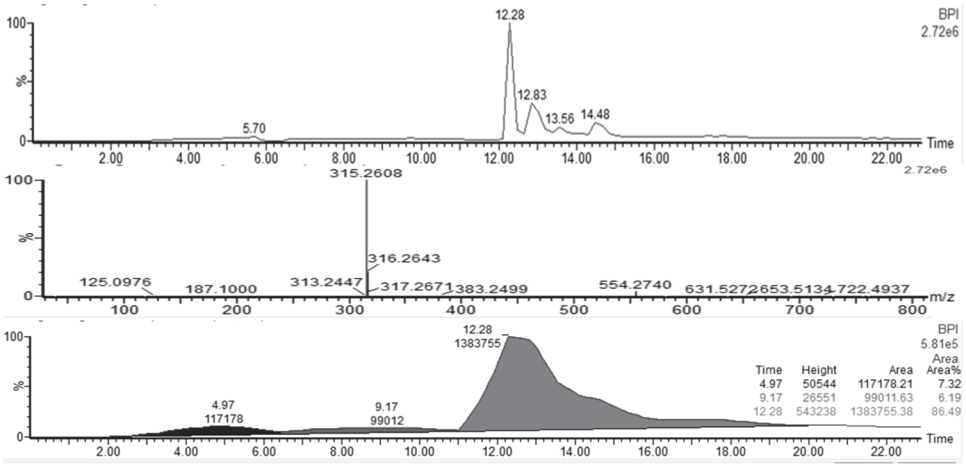

Fig. S-14. LC chromatograms and mass spectrum of dioleate epoxide

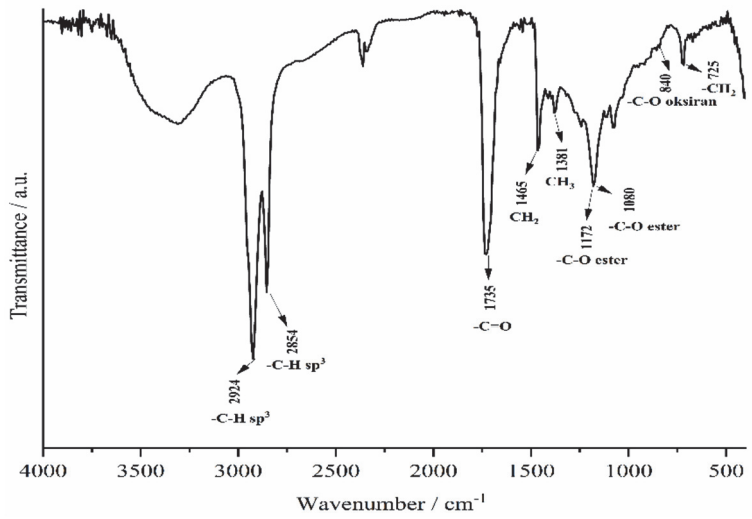

Fig. S-15. FTIR spectra of dioleate epoxide

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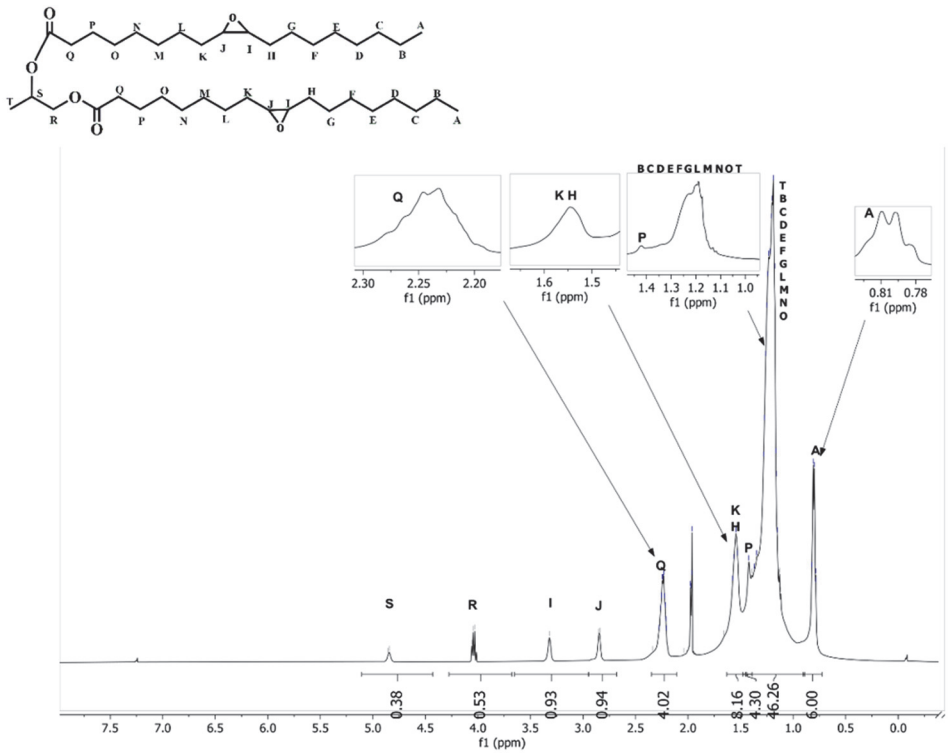

Fig. S-16. ^{1}H-NMR spectra of dioleate epoxide

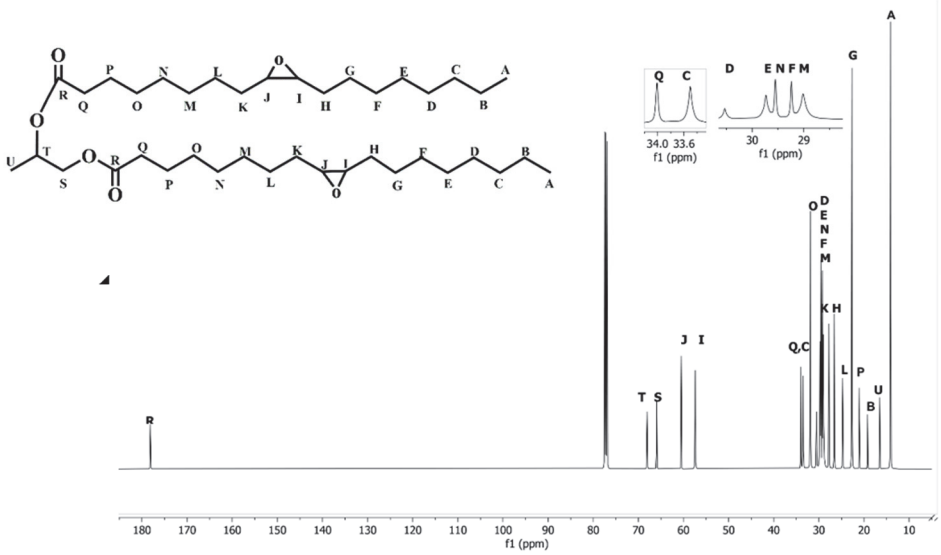

Fig. S-17. ^{13}C-NMR spectra of dioleate epoxide

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Dioleate epoxide: Dioleate epoxide ($C_{39}H_{72}O_6$) product was obtained as a white solid (0.6 g, 94.49 %). FTIR (ν, cm^{-1}): 2924 and 2854 (C–H sp^3), 1735 (C=O ester), 1465 (–CH_2– sp^3), 1381 (–CH_3 sp^3), 1172 (C–O ester), 840 (C–O oxirane), 725 (–CH_2– sp^3). LC-MS: dioleate epoxide (86.49% purity, t_R 12.28 min, MS: 722 ([M+CH_3CN+HCOO]$^-$). ^{1}H-NMR (CD_3OD, 500 MHz, δ/ppm): 0.80 (6H, 2 –CH_3 oleate, *triplet*, *J* = 7 Hz), 1.23–1.27 (43H, 20 –CH_2–, –CH_3 1,2-propanediol, *multiplet*), 1.40 (4H, –C**H$_2$**–CH_2–C=O, *quintet*, *J* = 5.5 Hz), 1.55 (8H, 2 –C**H$_2$**–CH–O–CH–C**H$_2$**–, *quartet*, *J* = 8 Hz), 2.25 (4H, 2 –CH_2–C=O, *triplet*, *J* = 7.2 Hz), 2.85 and 3.32 (4H, 2 –CH–O–CH– oxirane, *multiplet*), 4,04 (2H, –CH_2–, multiplet) and 4,84 (1H, –CH–, multiplet). ^{13}C-NMR (CD_3OD, 125 MHz, δ/ppm): 14.18 (–CH_3 oleate), 24.81 (–CH_3 propanediol), 24,94, 27.24, 27.29, 29.17, 29.25, 29.41, 29.61, 29.77, 29.85, 29.73, 30.53, 31.88, 33.50, 34.01 (–CH_2– oleate), 65.95 (–CH_2– propanediol), 57.41 and 57.50 (–CH– oxirane), 68.07 (–CH– propanediol), and 178.13 (C=O).

SYNTHESIZED TRIOLEATE EPOXIDE

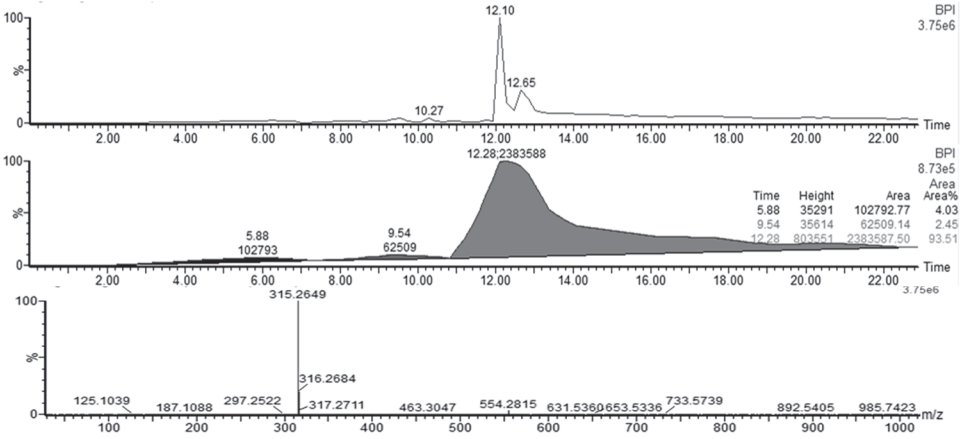

Fig. S-18. LC chromatograms and mass spectrum of trioleate epoxide

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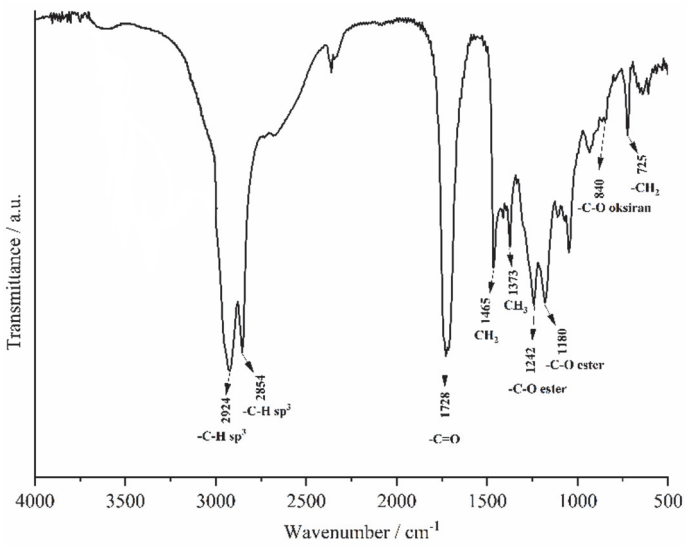
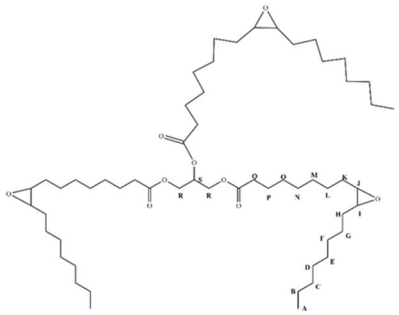


Fig. S-19. FTIR spectra of trioleate epoxide



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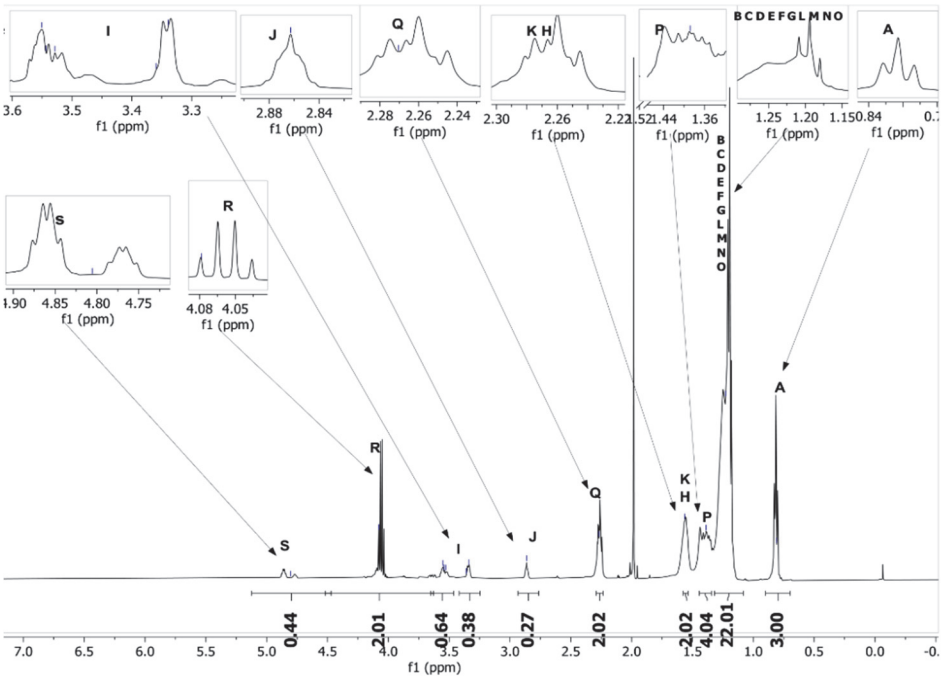

Fig. S-20. ^{13}H-NMR spectra of trioleate epoxide

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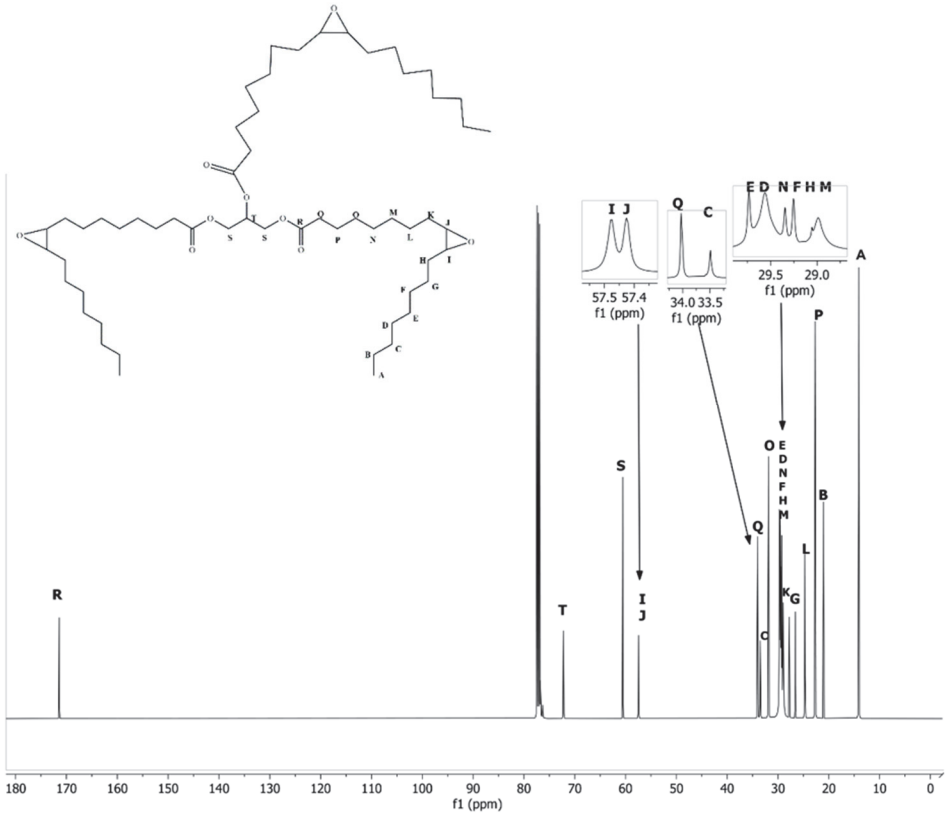

Fig. S-21. ^{13}C-NMR spectra of trioleate epoxide

Trioleate epoxide: Trioleate epoxide ($C_{57}H_{104}O_9$) product was obtained as a white solid (0.81 g, 92.04%). FTIR (ν, cm^{-1}): 2924 and 2854 (C–H sp^3), 1728 (C=O ester), 1465 (–CH_2– sp^3), 1373 (–CH_3 sp^3), 1242 (C–O ester), 840 (C–O oxirane), 725 (–CH_2– sp^3). LC-MS: trioleate epoxide (93.51% purity, t_R 12.10 min, MS: 985 $[M+NH_4Cl]^-$). ^{1}H-NMR (CD_3OD, 500 MHz, δ/ppm): 0.81 (9H, 3 –CH_3 oleate, *triplet*, J = 7 Hz), 1.21–1.25 (60H, 30 –CH_2–, *multiplet*), 1.40 (6H, 3 –C**H$_2$**–CH_2–C=O, *multiplet*), 1.56 (12H, 3 –C**H$_2$**–CH–O–CH–C**H$_2$**–, *quartet*, J = 8.3 Hz), 2.26 (6H, 3 –CH_2–C=O, *triplet*, J = 7.2 Hz), 2.87 and 3.34 (6H, 3 –CH–O–CH– oxirane, *multiplet*), 4,06 (4H, –CH_2– glycerol, multiplet), and 4,81 (1H, –CH– glycerol, multiplet). ^{13}C-NMR (CD_3OD, 125 MHz, δ/ppm): 14.14 (–CH_3), 21.06, 22.70, 24.72, 26.60, 27.79, 28.99, 29.05, 29.25, 29.35, 29.56, 29.73, 31.89, 33.49, and 34.03 (–CH_2– oleate), 57.43 and 57.48 (–CH– oxirane), 60.53 (–CH_2– glycerol), 72.24 (–CH– glycerol), and 171.44 (C=O).

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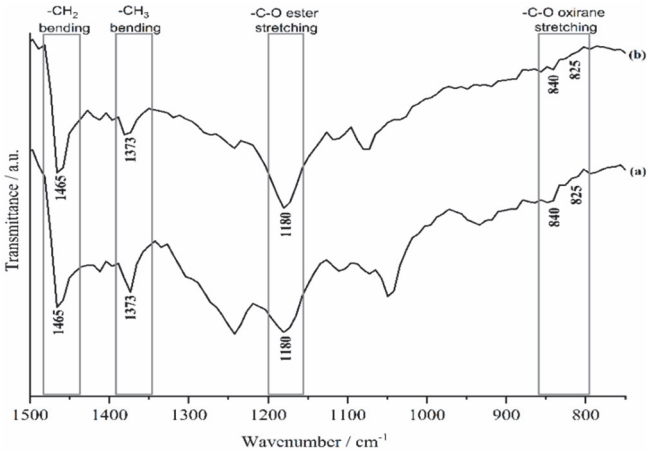

Fig S-22. FTIR profile spectra at 1500–750 cm^{-1} of (a) dioleate epoxide and (b) trioleate epoxide

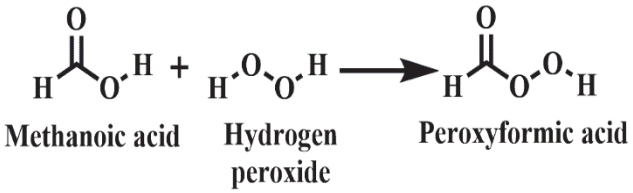

Fig S-23. Reaction scheme of performic acid

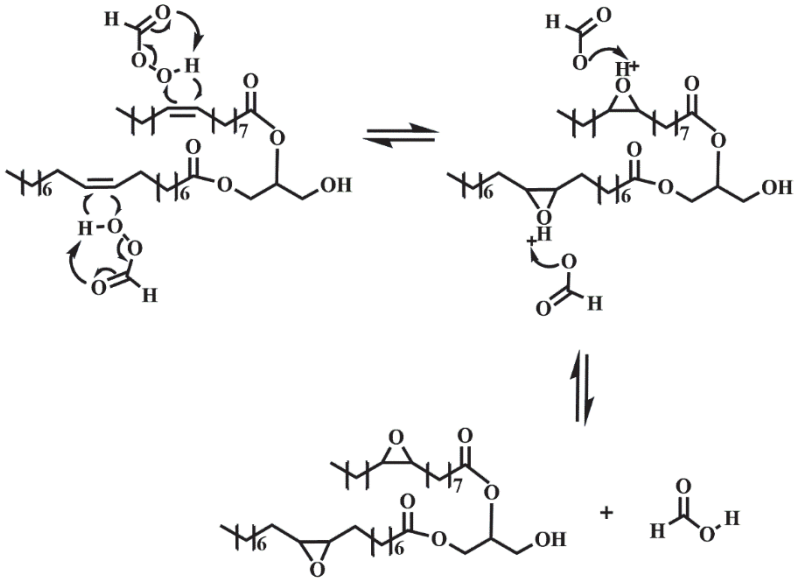

Fig S-24. Reaction scheme of the synthesis of dioleate

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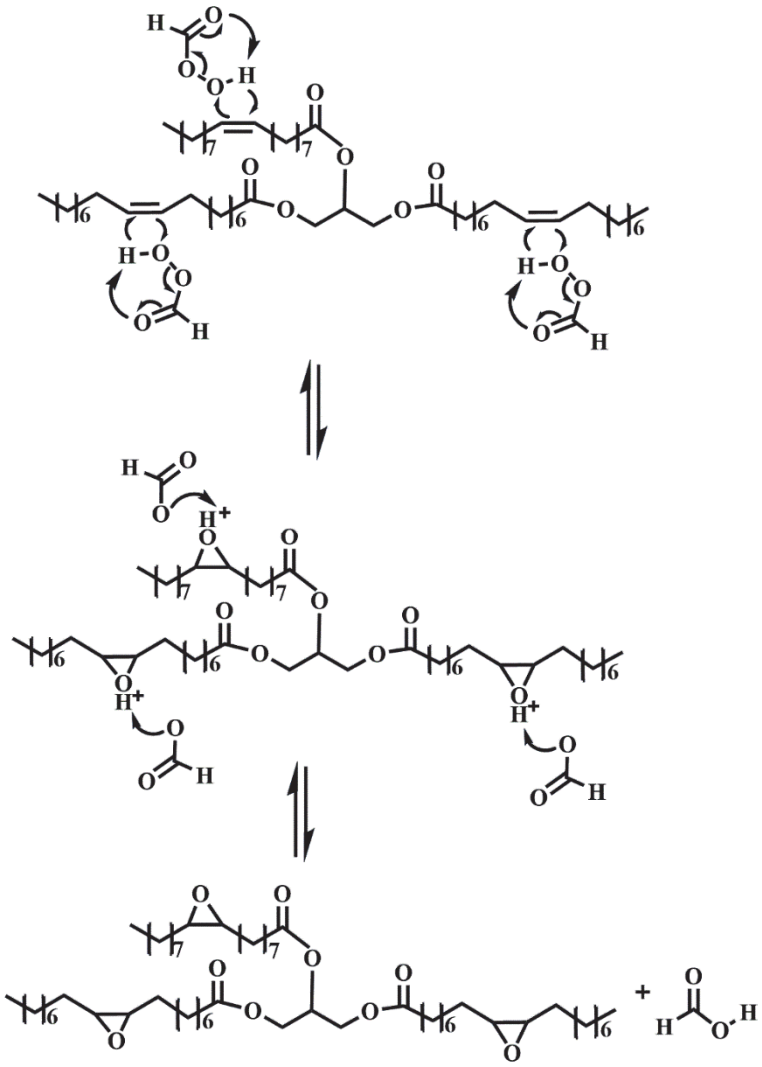

Fig S-25. Reaction scheme of the synthesis of trioleate

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LINEAR REGRESSION OF DIOLEATE EPOXIDE CYTOTOXIC EVALUATION

Table S-I. Table concentration of dioleate epoxide versus cell viability

Concentration (ppm)	Log concentration	Cell viability (%)		
		T47D	WiDr	Vero
6.25	0.796	64.18	60.39	86.54
12.5	1.097	55.74	52.17	78.02
25	1.398	51.48	54.11	86.71
50	1.699	43.57	45.41	75.98
100	2.000	32.85	39.13	78.88
200	2.301	27.83	31.40	66.95
400	2.602	16.58	26.81	32.88

Table S-II. IC_{50} and SI values of dioleate epoxide

Cells	Linear regression equation	IC_{50} (ppm)	SI
T47D	y = -0.1062x + 53.787 R^2 = 0.8159	35.66	8.16
WiDr	y = -0.0777x + 52.953 R^2 = 0.8006	38.25	7.60
Vero	y = -0.1062x + 53.787 R^2 = 0.8159	291,04	

Linear Regression of Trioleate Epoxide Cytotoxic Evaluation

Table S-III. The concentration of trioleate epoxide versus cell viability

Concentration (ppm)	Log conc.	Cell viability (%)		
		T47D	WiDr	Vero
6.25	0.796	62.36	62.08	89.27
12.5	1.097	56.73	56.04	79.05
25	1.398	51.56	53.62	73.25
50	1.699	39.47	43.96	73.25
100	2.000	34.60	32.61	79.90
200	2.301	25.48	23.19	64.40
400	2.602	16.81	17.15	39.95

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Table S-IV. IC_{50} and SI values of trioleate epoxide

Cells	Linear regression equation	IC_{50} (ppm)	SI
T47D	y = -0.1046x + 52.866 R^2 = 0.8016	27.40	10.87
WiDr	y = -0.0977x + 50.585 R^2 = 0.8148	38.41	9.19
Vero	y = -0.1123x + 83.458 R^2 = 0.8839	297.93	

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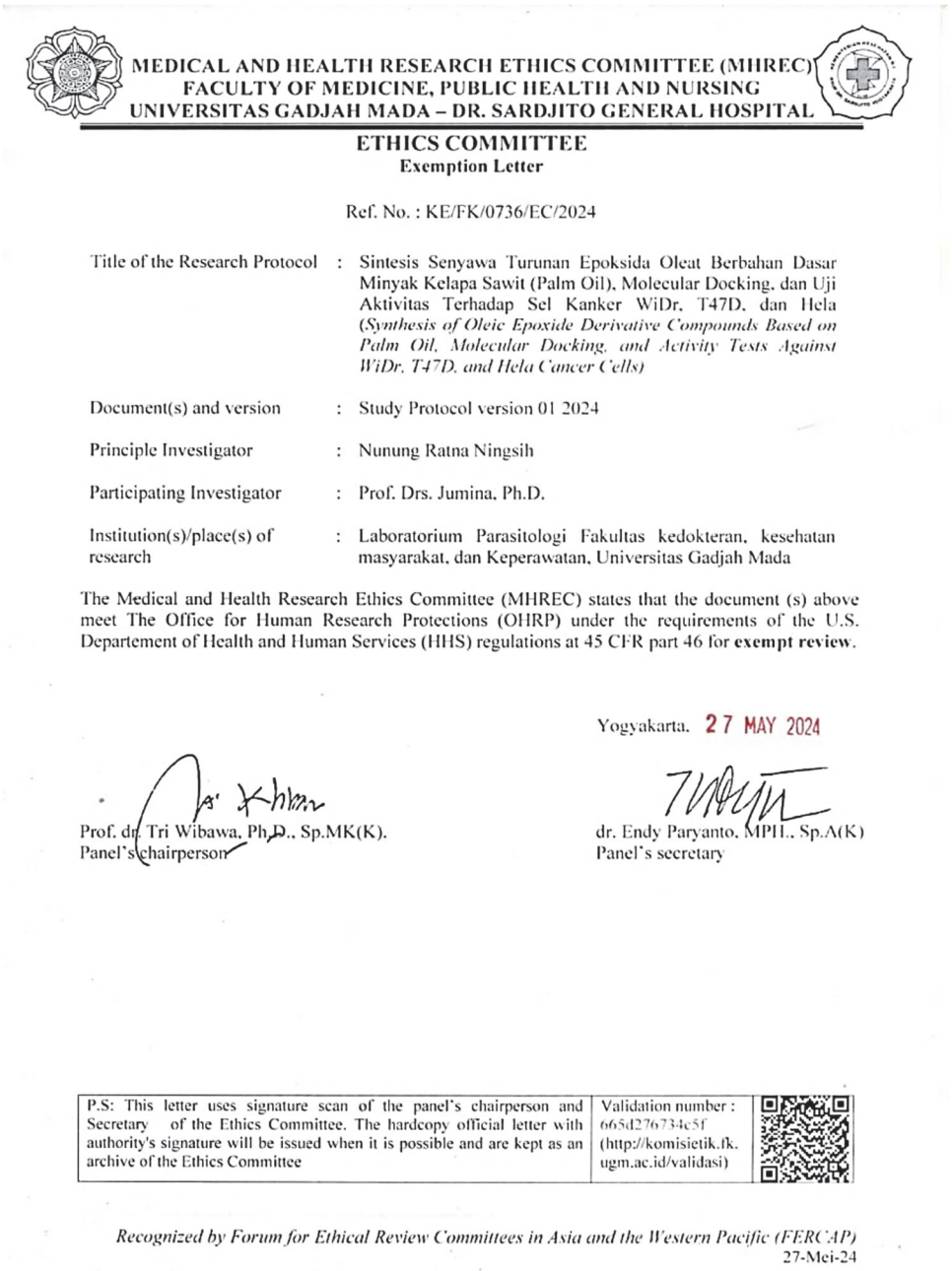

MEDICAL AND HEALTH RESEARCH ETHICS COMMITTEE (MHREC)
FACULTY OF MEDICINE, PUBLIC HEALTH AND NURSING
UNIVERSITAS GADJAH MADA – DR. SARDJITO GENERAL HOSPITAL

ETHICS COMMITTEE
Exemption Letter

Ref. No. : KE/FK/0736/EC/2024

Title of the Research Protocol	:	Sintesis Senyawa Turunan Epoksida Oleat Berbahan Dasar Minyak Kelapa Sawit (Palm Oil), Molecular Docking, dan Uji Aktivitas Terhadap Sel Kanker WiDr, T47D, dan Hela (*Synthesis of Oleic Epoxide Derivative Compounds Based on Palm Oil, Molecular Docking, and Activity Tests Against WiDr, T47D, and Hela Cancer Cells*)
Document(s) and version	:	Study Protocol version 01 2024
Principle Investigator	:	Nunung Ratna Ningsih
Participating Investigator	:	Prof. Drs. Jumina, Ph.D.
Institution(s)/place(s) of research	:	Laboratorium Parasitologi Fakultas kedokteran, kesehatan masyarakat, dan Keperawatan, Universitas Gadjah Mada

The Medical and Health Research Ethics Committee (MHREC) states that the document (s) above meet The Office for Human Research Protections (OHRP) under the requirements of the U.S. Departement of Health and Human Services (HHS) regulations at 45 CFR part 46 for **exempt review**.

Yogyakarta, 27 MAY 2024

Prof. dr. Tri Wibawa, Ph.D., Sp.MK(K).
Panel's chairperson

dr. Endy Paryanto, MPH., Sp.A(K)
Panel's secretary

P.S: This letter uses signature scan of the panel's chairperson and Secretary of the Ethics Committee. The hardcopy official letter with authority's signature will be issued when it is possible and are kept as an archive of the Ethics Committee	Validation number : 665d276734c5f (http://komisietik.fk.ugm.ac.id/validasi)

Recognized by Forum for Ethical Review Committees in Asia and the Western Pacific (FERCAP)
27-Mei-24

Fig S-26. Ethical clearance approval letter for cytotoxic evaluation

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