Electronic Supplementary Information

Circularly polarised luminescence from intramolecular excimer emission of bis-1,8-naphthalimide derivatives

Shiori Eguchi[1], Mami Naoe[1], Asako Kageyama[1], Yoshitane Imai[2], Norimitsu Tohnai[3], Shoko Yamazaki[4], Eiji Nakata[5], Hiroshi Takashima,[1,*]

[1]Department of Chemistry, Biology and Environmental Science, Faculty of Science, Nara Women's University, Nara 630-8506, Japan

[2] Department of Applied Chemistry, Faculty of Science and Engineering, Kindai University, Osaka 577-8502, Japan

[3] Department of Applied Chemistry, Graduate School of Engineering, Osaka University, Osaka 565-0871, Japan

[4] Department of Chemistry, Nara University of Education, Nara 630-8528, Japan

[5] Institute of Advanced Energy, Kyoto University, Kyoto 611-0011, Japan

***Correspondence**

H. Takashima

Department of Chemistry, Biology and Environmental Science, Faculty of Science,

Nara Women's University, Nara 630-8506, Japan

E-mail: hiroshi@cc.nara-wu.ac.jp

Table of contents

1. Experimental materials

1,8-Naphthalic anhydride, *D*-lysine monohydrochloride, *D*-lysine methyl ester dihydrochloride, *L*-norleucine, *D*-norleucine and diisopropylethylamine (DIEA) were from Tokyo Kasei Kogyo Co. *L*-lysine monohydrochloride, *L*-lysine methyl ester dihydrochloride, dehydrated *N*,*N*-dimethylformamide (DMF), ethyl acetate (AcOEt), dichloromethane (DCM), methanol (MeOH), ethanol (EtOH), tetrahydrofuran (THF), hexane, chloroform, 1,4-dioxane, acetonitrile (MeCN), and Wako Gel C-200 from Fuji Film Wako Pure Chemical Co. were used. KBr was used for IR absorption measurement by Fujifilm Wako Pure Chemicals Co. DMSO-d_6 for ^{1}H NMR spectra and ^{13}C NMR were used by Fujifilm Wako Pure Chemicals Co. For ESI-MS measurements, methanol for LC/MS from Fujifilm Wako Pure Chemicals Co. was used. Organic membrane filter PTFE (0.5 μm, 25 mm) was used from ADVANTEC.

2. Instrumentation

^{1}H NMR spectra (400 MHz) and ^{13}C NMR (100 MHz) in solution were recorded on a JEOL JNM-AL400 FT-NMR. ^{1}H NMR chemical shift values are reported in ppm as reference to the internal standard TMS. ESI-Mass spectra were measured with JEOL JMS-T100LC and JMS-T100LP AccuTOF. Fourier transform IR spectra (FTIR) were measured by the KBr tablet method using the JASCO FTIR-6100V spectrophotometer. X-ray crystallographic data were obtained by Rigaku R-Axis-Rapid Imaging Plate diffractometer. Elemental analysis was performed on a J-Science Lab MICRO CORDER JM10 and a Yanaco CHN corder MT-5. UV-vis electronic absorption spectra were measured using a Shimadzu UV-2550 spectrophotometer. The path length was 1 cm. Fluorescence spectrum measurements were performed using a Shimadzu RF-5300PC fluorometer using a 2 mm or a 1 cm quartz cell. The absolute quantum yields were measured by JASCO FP-6600 fluorescence spectrophotometer with an integrating sphere. Time-resolved emission spectra were measured by a single-photon counting method using a Horiba-Jobin Yvon Tempro equipped with a 430 nm cut filter. The instrumental response of the system to the excitation pulsed solid-state LED light source of 330 nm had a time width of about 100 ps and repetition rate about 1 MHz. The lifetimes were evaluated with the software attached to this equipment. All solutions were slowly and carefully purged with N_2 gas through a needle using a 1 cm quartz cell with

a septum cap. CD spectra were measured with Jasco J-720 spectrometers using a 1 cm quartz cell. CPL spectra were recorded on a JASCO CPL-300 spectrometer using a 1 cm quartz cell with two or four scan times.

3. Crystallographic data collection and structure determination

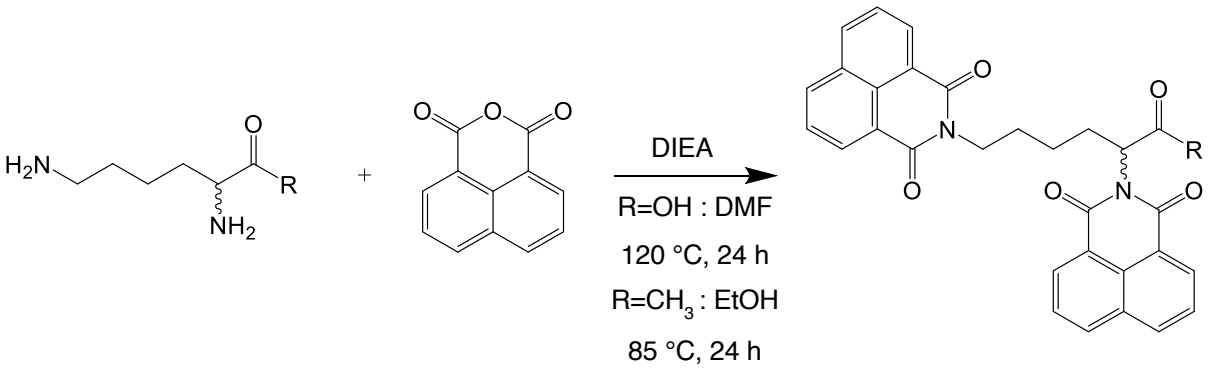
A crystal was mounted in a loop. All measurements were made on a diffractometer using multi-layer mirror monochromated Cu-Kα or Mo-Kα radiation. The data were collected at a temperature of 293 K using the ω–2θ scan technique to a maximum 2θ value of 148.9°. Data were collected and processed using CrysAlisPro (Rigaku Oxford Diffraction) [S1]. The structures were solved by direct methods and refined on F^2 by full-matrix least-squares methods, using SHELXL-97 [S2]. The non-hydrogen atoms were refined anisotropically by the full-matrix least-squares method. All hydrogen atoms were isotropically refined using olex2 [S3]. The structure was solved with the olex2solve structure solution program using Charge Flipping and refined with the olex2refine refinement package using Gauss-Newton minimization [S4].

4. Computational Methods

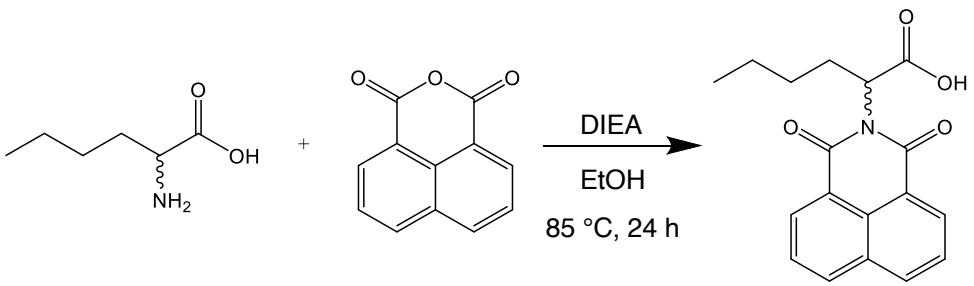
The molecular structure calculations were performed with density functional theory (DFT) using the Gaussian16 program package [S5]. The B3LYP functional [S6-S7] was used with the 6-31+G* basis set and the polarisable continuum model solvent effect (solvent = CH3CN, Chloroform, and methanol) [S8-S10].

5. Synthetic methods and characterization

Compounds *D*-LybNI, *L*-LybNI, *D*-LyMebNI, *L*-LyMebNI, *D*-NorNI, and *L*-NorNI were synthesized as the following Schemes S1 and S2.



Scheme S1. Syntheses of *D*-LybNI, *L*-LybNI, *D*-LyMebNI, and *L*-LyMebNI used in this study.



Scheme S2. Syntheses of *D*-NorNI and *L*-NorNI used in this study.

5-1. Synthesis of *L*-LybNI

L-lysine monohydrochloride 0.174 g (9.5×10^{-4} mol, 1 eq) was dissolved in 5.0 mL of dehydrated DMF and stirred in a 200 mL flask. DIEA 0.170 mL (9.4×10^{-4} mol, 1 eq) was then dissolved in 5.0 mL of dehydrated DMF and slowly added dropwise. After stirring at 120 ºC for 2 h, 0.421 g (2.1×10^{-3} mol, 2.2 eq) of 1,8-Naphthalic anhydride was added and the mixture was stirred for 24 h at 120 ºC. DMF was then distilled off, and 200 mL of AcOEt was added and stirred at room temperature for 12 h. The filtrate was collected by suction filtration through an organic membrane filter. The solvent was removed under reduced pressure using an evaporator and the resulting solid was washed with DCM. The remaining solid was collected by suction filtration through an organic membrane filter, and the resulting light orange solid was recrystallized from EtOH to give white crystals. Yield 55.2 mg (11%).

^{1}H NMR (400 MHz, DMSO-d_6, 298 K) : δ/ppm = 8.47 (dd, 2H, J = 0.80 Hz, 8.2 Hz, naphthalene-*H*), 8.40 (dd, 2H, J = 0.84 Hz, 8.2 Hz, naphthalene-*H*), 8.36 (d, 2H, J = 7.3 Hz, naphthalene-*H*), 8.24 (dd, 2H, J = 0.96 Hz, 7.3 Hz, naphthalene-*H*), 7.83 (t, 2H, J = 7.8 Hz, naphthalene-*H*), 7.76 (t, 2H, J = 7.8 Hz, naphthalene-*H*), 5.49 (dd, 1H, J = 4.9 Hz, 9.6 Hz, -CH_2-C*H*(NI)-COOH), 3.98 (m, 2H, NI-CH_2-CH_2-), 2.19 (m, 2H, -CH_2-CH_2-CH(NI)-COOH), 1.66 (m, 2H, NI-CH_2-CH_2-CH_2-), 1.29 (m, 2H,-CH_2-CH_2-CH_2-CH(NI)-). ^{13}C NMR (100 MHz, DMSO-d_6, 298 K) : δ/ppm = 171.25 (-*C*OOH), 163.53 (NI-*C*O), 163.39 (NI-*C*O), 134.90 (naphthalene-*C*H), 134.38 (naphthalene-*C*H), 131.34-131.43 (naphthalene-*C*H), 130.70 (naphthalene-*C*H), 127.39-127.53 (naphthalene-*C*), 127.28 (naphthalene-*C*), 122.08 (naphthalene-*C*), 121.65 (naphthalene-*C*), 52.85 (-*C*H(NI)-COOH), 39.52 (NI-*C*H_2-, overlapped with solvent), 28.05 (NI-CH_2-*C*H_2-), 27.38 (-*C*H_2-CH(NI)-), 23.59 (-*C*H_2-CH_2-CH(NI)-). ESI-MS (CH_3OH, negative, m/z) 505.05 ($[M-H]^-$ requires 505.15). FTIR (KBr, cm^{-1}) : 3458 (Br, m, νC=O), 3212 (Br, m, νO-H), 2961 (w, νC-H), 2920 (w, νC-H), 2862 (w, νC-H), 1745 (s, νC=O), 1692 (s, νC=O), 1654 (s, νC=O), 780 (s, δC-H). Anal. Calcd. for $C_{30}H_{22}N_2O_6$: C, 71.14; H, 4.38; N, 5.53%. Found : C, 70.92; H, 4.35; N, 5.49%.

^{1}H NMR (400 MHz, DMSO-d_6, 298 K)

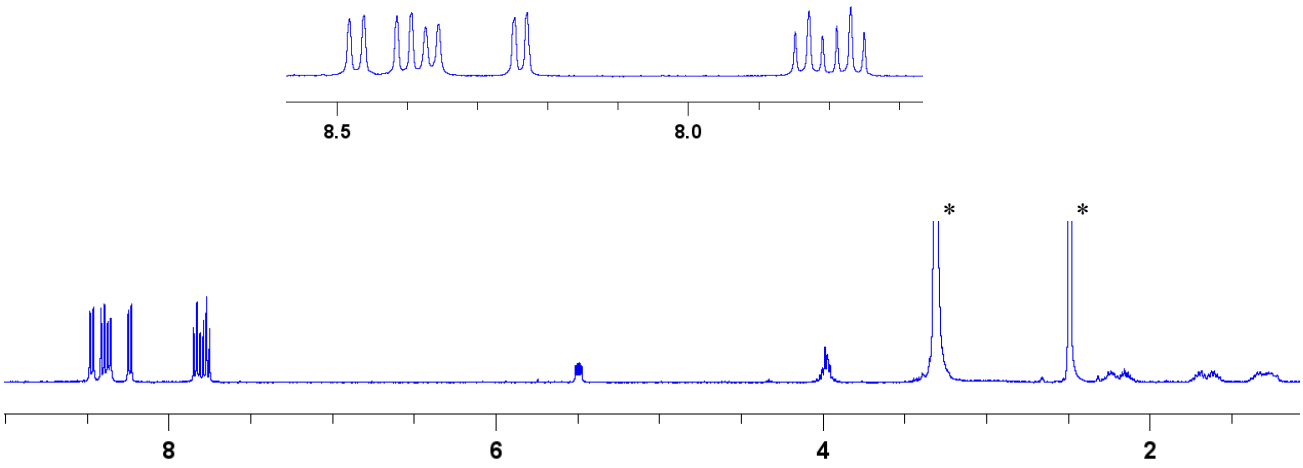


Figure S1. ^{1}H NMR (400 MHz) spectrum of *L*-LybNI (3.0×10^{-3} M) in DMSO-d_6 at 298 K.

^{13}C NMR (100 MHz, DMSO-d_6, 298 K)

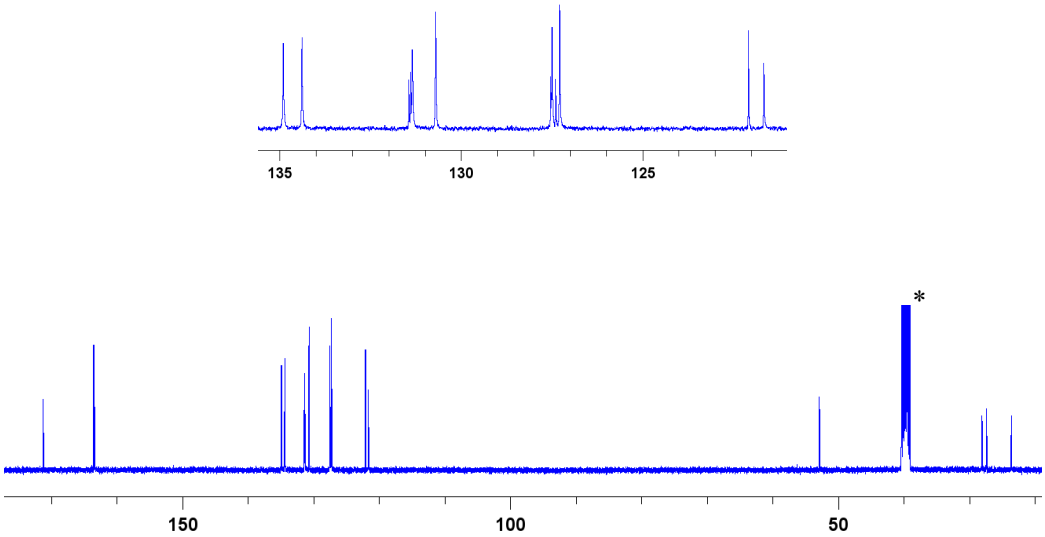


Figure S2. ^{13}C NMR (100 MHz) spectrum of *L*-LybNI (1.7×10^{-2} M) in DMSO-d_6 at 298 K.

ESI-MS (MeOH, negative)

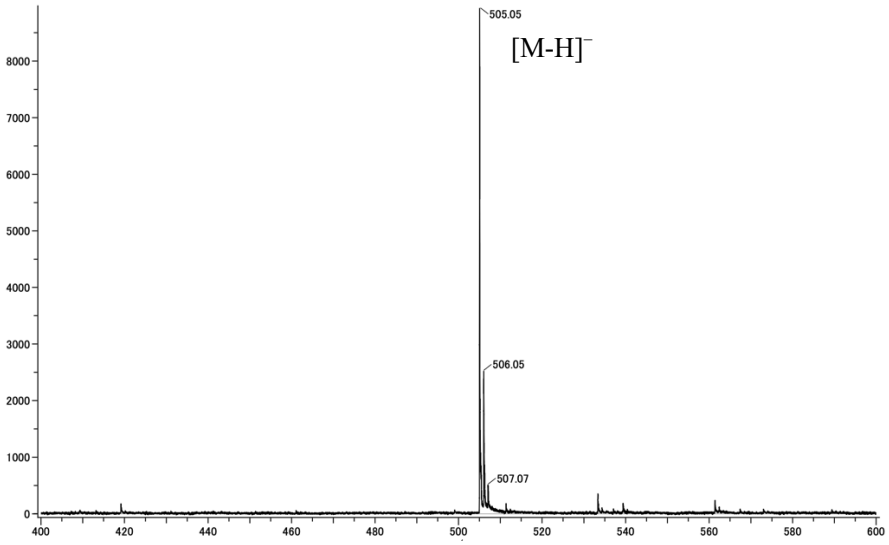


Figure S3. ESI-MS spectrum of *L*-LybNI in MeOH.

FTIR (KBr disk)

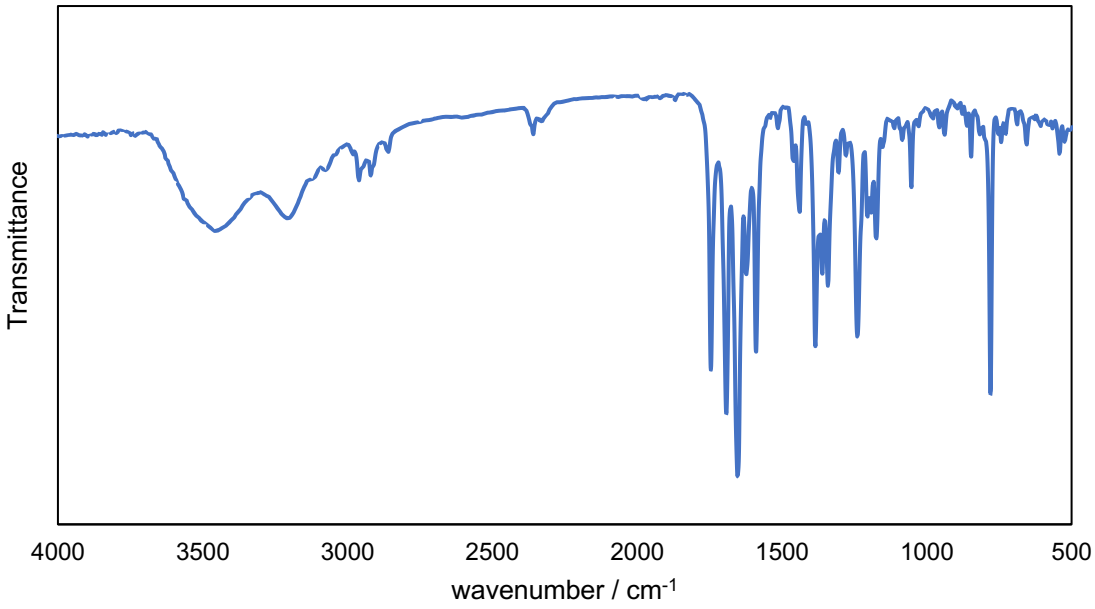


Figure S4. FTIR (KBr disk) spectrum of *L*-LybNI.

5-2. Synthesis of *D*-LybNI

D-lysine monohydrochloride 0.170 g (9.3×10^{-4} mol, 1 eq) was dissolved in 5.0 mL of dehydrated DMF and stirred in a 200 mL flask. DIEA 0.170 mL (9.4×10^{-4} mol, 1 eq) was then dissolved in 5.0 mL of dehydrated DMF and slowly added dropwise. After stirring at 120 ºC for 2 h, 0.419 g (2.1×10^{-3} mol, 2.2 eq) of 1,8-Naphthalic anhydride was added and the mixture was stirred for 24 h at 120 ºC. DMF was then distilled off, and 200 mL of AcOEt was added and stirred at room temperature for 12 h. The filtrate was collected by suction filtration through an organic membrane filter. The solvent was removed under reduced pressure using an evaporator and the resulting solid was washed with DCM. The remaining solid was collected by suction filtration through an organic membrane filter, and the resulting light orange solid was recrystallized from EtOH to give white crystals. Yield 82.9 mg (18%).

^{1}H NMR (400 MHz, DMSO-d_6, 298 K) : δ/ppm = 8.47 (dd, 2H, J = 0.80 Hz, 8.3 Hz, naphthalene-*H*), 8.40 (d, 2H, J = 8.3 Hz, naphthalene-*H*), 8.36 (d, 2H, J = 7.2 Hz, naphthalene-*H*), 8.23 (d, 2H, J = 7.2 Hz, naphthalene-*H*), 7.82 (t, 2H, J = 7.4 Hz, naphthalene-*H*), 7.77 (t, 2H, J = 7.4 Hz, naphthalene-*H*), 5.49 (dd, 1H, J = 4.8 Hz, 9.6 Hz, -CH_2-C*H*(NI)-COOH), 3.98 (m, 2H, NI-C*H*$_2$-CH_2-), 2.16 (m, 2H, -CH_2-C*H*$_2$-CH(NI)-COOH), 1.65 (m, 2H, NI-CH_2-C*H*$_2$-CH_2-), 1.29 (m, 2H,-CH_2-C*H*$_2$-CH_2-CH(NI)-). ^{13}C NMR (100 MHz, DMSO-d_6, 298 K) : δ/ppm = 171.27 (-*C*OOH), 163.54 (NI-*C*O), 163.41 (NI-*C*O), 134.92 (naphthalene-*C*H), 134.40 (naphthalene-*C*H), 131.36-131.45 (naphthalene-*C*H), 130.70 (naphthalene-*C*H), 127.51-127.54 (naphthalene-*C*), 127.30 (naphthalene-*C*), 122.09 (naphthalene-*C*), 121.66 (naphthalene-*C*), 52.85 (-*C*H(NI)-COOH), 39.52 (NI-*C*H_2-, overlapped with solvent), 28.05 (NI-CH_2-*C*H_2-), 27.38 (-*C*H_2-CH(NI)-), 23.60 (-*C*H_2-CH_2-CH(NI)-). ESI-MS (CH_3OH, negative, m/z) 505.05 ([M-H]$^-$ requires 505.15). FTIR (KBr, cm^{-1}) : 3466 (Br, m, νC=O), 3200 (Br, m, νO-H), 2961 (w, νC-H), 2920 (w, νC-H), 2862 (w, νC-H), 1745 (s, νC=O), 1692 (s, νC=O), 1655 (s, νC=O), 780 (s, δC-H). Anal. Calcd. for $C_{30}H_{22}N_2O_6$: C, 71.14; H, 4.38; N, 5.53%. Found : C, 70.94; H, 4.32; N, 5.48%.

^{1}H NMR (400 MHz, DMSO-d_6, 298 K)

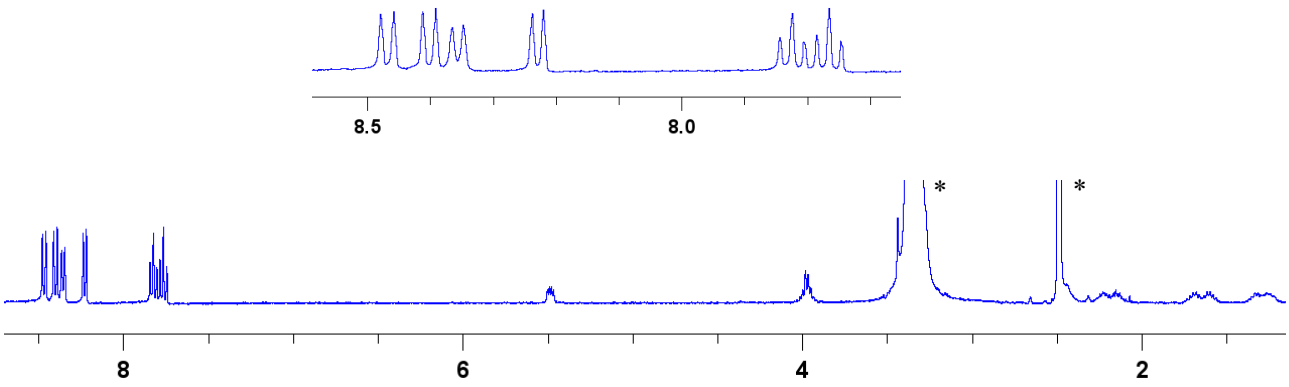


Figure S5. ^{1}H NMR (400 MHz) spectrum of *D*-LybNI (3.1×10^{-3} M) in DMSO-d_6 at 298 K.

^{13}C NMR (100 MHz, DMSO-d_6, 298 K)

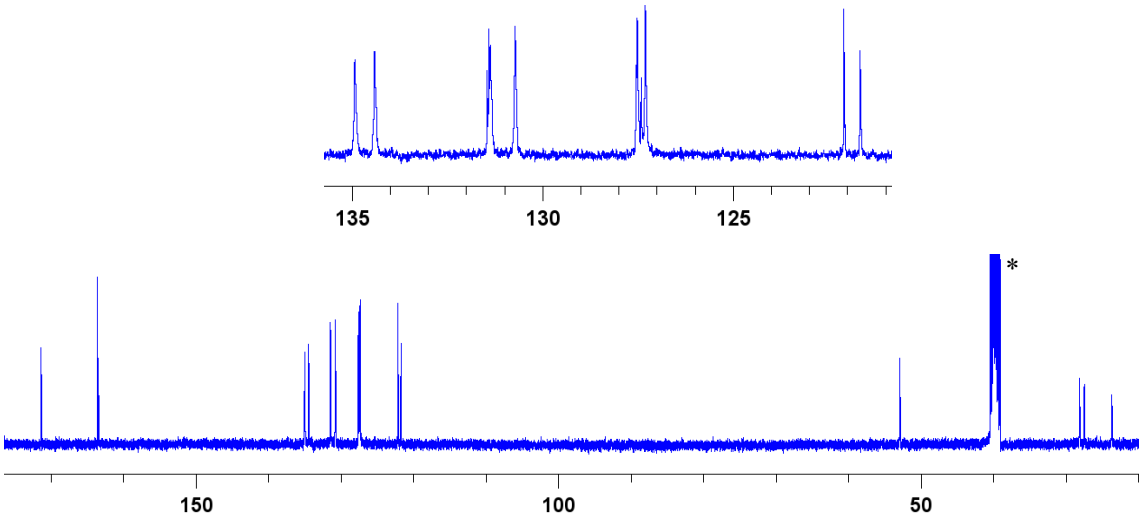


Figure S6. ^{13}C NMR (100 MHz) spectrum of *D*-LybNI (1.7×10^{-2} M) in DMSO-d_6 at 298 K.

ESI-MS (MeOH, negative)

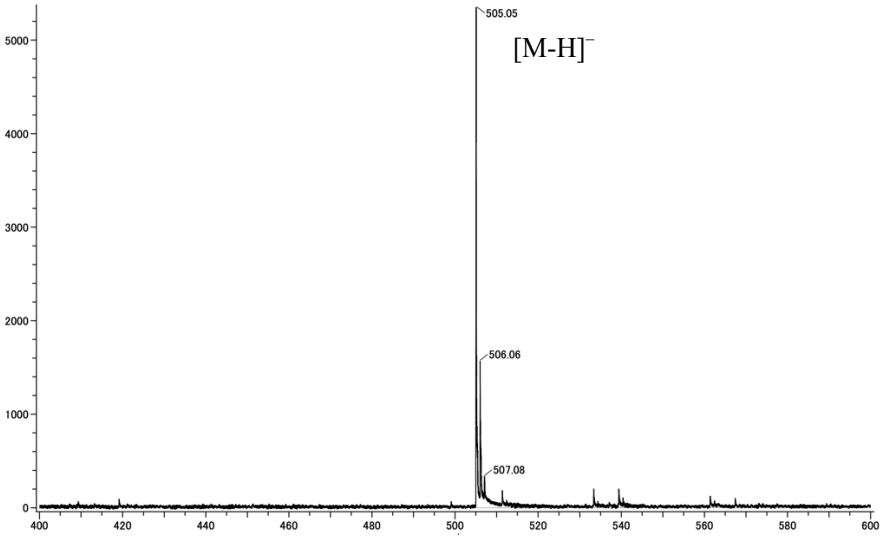


Figure S7. ESI-MS spectrum of *D*-LybNI in MeOH.

FTIR (KBr disk)

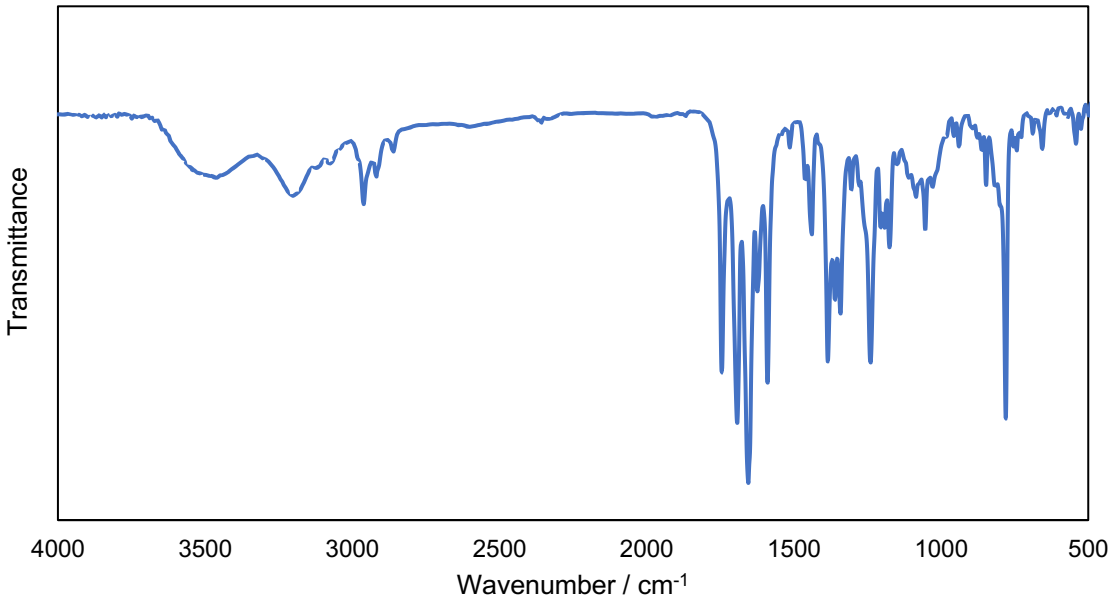


Figure S8. FTIR (KBr disk) spectrum of *D*-LybNI.

5-3. Synthesis of *L*-LyMebNI

0.115 g (4.9×10^{-4} mol) of *L*-lysine methyl ester dihydrochloride was dissolved in 10 mL of EtOH and stirred in a 200 mL flask. DIEA 0.18 mL (1.0×10^{-3} mol, 2 eq) dissolved in 5.0 mL of EtOH was then added dropwise. After stirring at 85 ºC for 2 h, 0.213 g (1.1×10^{-3} mol, 2.2 eq) of 1,8-Naphthalic anhydride was added and the mixture was stirred for 24 h at 85 ºC. The solvent was removed under reduced pressure using an evaporator and dried in vacuum. The product was purified on a column (φ 3 cm × 17 cm) using Wako Gel C-200. The eluents were separated using DCM and DCM:MeOH = 200:1 mixture. The solvent was removed under reduced pressure and the desired product was recrystallized from hexane and chloroform to give white crystals. Yield : 0.200 g (78%).

^{1}H NMR (400 MHz, DMSO-d_6, 298 K) : δ/ppm = 8.49 (d, 2H, J = 8.2 Hz, naphthalene-*H*), 8.40 (d, 2H, J = 8.2 Hz, naphthalene-*H*), 8.37 (d, 2H, J = 7.1 Hz, naphthalene-*H*), 8.21 (d, 2H, J = 7.2 Hz, naphthalene-*H*), 7.82 (t, 2H, J = 7.9 Hz, naphthalene-*H*), 7.76 (t, 2H, J = 7.9 Hz, naphthalene-*H*), 5.60 (dd, 1H, J = 4.8 Hz, 9.6 Hz, -CH_2-C*H*(NI)-COO CH_3), 3.98 (m, 2H, NI-CH_2-CH_2-), 3.58 (s, 3H, -COOCH_3), 2.20 (m, 2H, -CH_2-CH_2-CH(NI)-$COOCH_3$), 1.65 (m, 2H, NI-CH_2-CH_2-CH_2-), 1.29 (m, 2H,-CH_2-CH_2-CH_2-CH(NI)-). ^{13}C NMR (100 MHz, DMSO-d_6, 298 K) : δ/ppm = 170.30 (-*C*$OOCH_3$), 163.57 (NI-*C*O), 163.39 (NI-*C*O), 135.11 (naphthalene-*C*H), 134.43 (naphthalene-*C*H), 131.41-131.55 (naphthalene-*C*H), 130.73 (naphthalene-*C*H), 127.41-127.56 (naphthalene-*C*), 127.32 (naphthalene-*C*), 122.09 (naphthalene-*C*), 121.50 (naphthalene-*C*), 52.66 (-*C*H(NI)-$COOCH_3$), 52.36 (-COO*C*H_3), 39.52 (NI-*C*H_2-, overlapped with solvent), 28.01 (NI-CH_2-*C*H_2-), 27.35 (-*C*H_2-CH(NI)-), 23.34 (-*C*H_2-CH_2-CH(NI)-). ESI-MS (CH_3OH, positive, *m*/*z*) 543.20 ($[M+Na]^+$ requires 543.16). FTIR (KBr, cm^{-1}) : 3448 (Br, m, νC=O), 2955 (w, νC-H), 1740 (s, νC=O), 1696 (s, νC=O), 1657 (s, νC=O), 780 (s, δC-H). Anal. Calcd. for $C_{31}H_{24}N_2O_6$: C, 71.53; H, 4.55; N, 5.38%. Found : C, 71.45; H, 4.68; N, 5.30%.

^{1}H NMR (400 MHz, DMSO-d_6, 298 K)

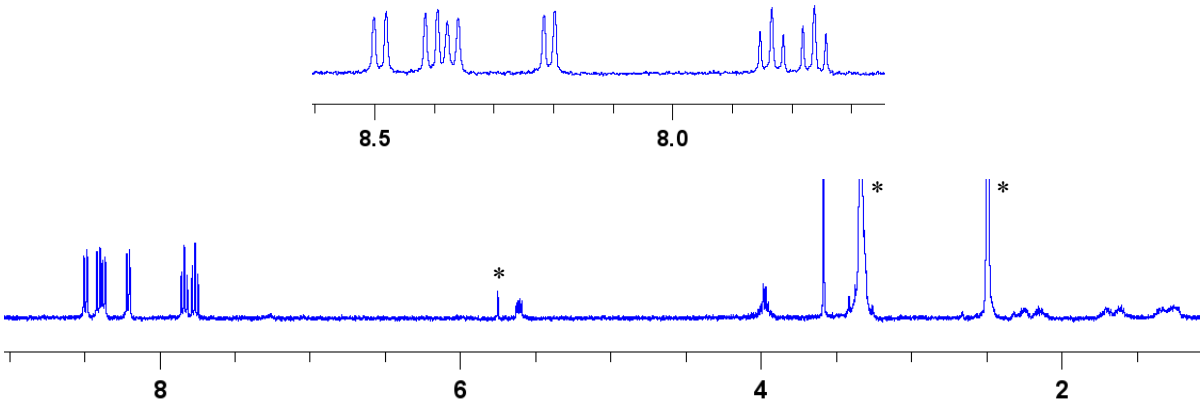


Figure S9. ^{1}H NMR (400 MHz) spectrum of *L*-LyMebNI (3.2×10^{-3} M) in DMSO-d_6 at 298 K.

^{13}C NMR (100 MHz, DMSO-d_6, 298 K)

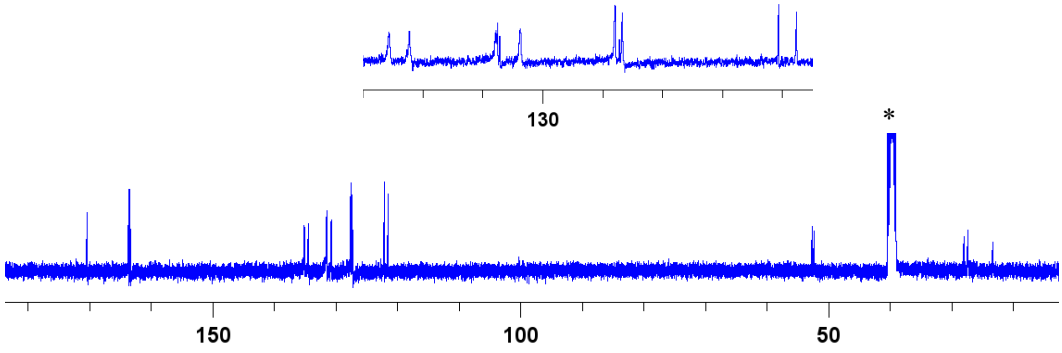


Figure S10. ^{13}C NMR (100 MHz) spectrum of *L*-LyMebNI (1.1×10^{-2} M) in DMSO-d_6 at 298 K.

ESI-MS (MeOH, positive)

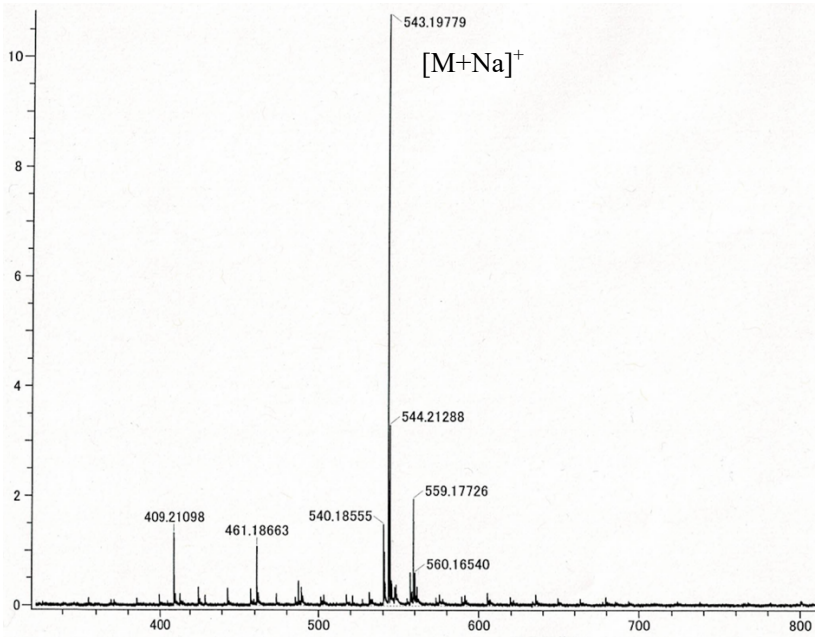


Figure S11. ESI-MS spectrum of *L*-LyMebNI in MeOH.

FTIR (KBr disk)

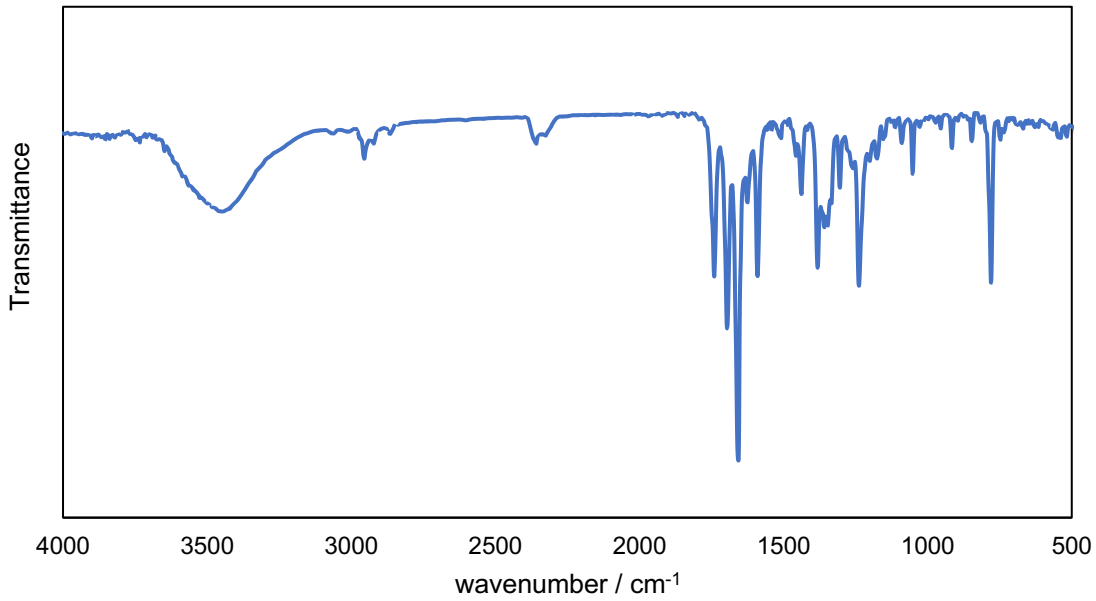


Figure S12. FTIR (KBr disk) spectrum of *L*-LyMebNI.

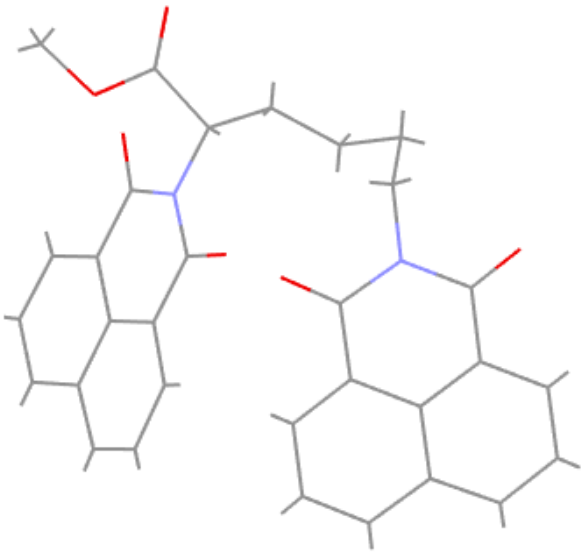


Figure S13. X-ray structure of *L*-LyMebNI.

Table S1. Crystallographic data of *L*-LyMebNI.

Formula	$C_{31}H_{24}N_2O_6$
Formula Weight	520.52
Crystal System	monoclinic
Space group	$P2_1$
a (Å)	7.4391
b (Å)	15.3129
c (Å)	10.5379
Z	2
λ (CuKα)	1.54184
$2\theta_{max}$	148.932
μ (cm^{-1})	0.834
Dc (Mgm^{-3})	1.449
T (K)	293
V ($Å^3$)	1193.17
R_1	0.0521
R_w	0.1308
GoF	1.011

5-4. Synthesis of *D*-LyMebNI

0.113 g (4.9×10^{-4} mol) of *D*-lysine methyl ester dihydrochloride was dissolved in 10 mL of EtOH and stirred in a 200 mL flask. DIEA 0.18 mL (1.0×10^{-3} mol, 2 eq) dissolved in 5.0 mL of EtOH was then added dropwise. After stirring at 85 ºC for 2 h, 0.214 g (1.1×10^{-3} mol, 2.2 eq) of 1,8-Naphthalic anhydride was added and the mixture was stirred for 24 h at 85 ºC. The solvent was removed under reduced pressure using an evaporator and dried in vacuum. The product was purified on a column (φ 3 cm × 17 cm) using Wako Gel C-200. The eluents were separated using DCM and DCM:MeOH = 200:1 mixture. The solvent was removed under reduced pressure and the desired product was recrystallized from hexane and chloroform to give white crystals. Yield：0.200 g (78%).

^{1}H NMR (400 MHz, DMSO-d_6, 298 K) : δ/ppm = 8.49 (d, 2H, J = 8.3 Hz, naphthalene-*H*), 8.40 (d, 2H, J = 8.3 Hz, naphthalene-*H*), 8.37 (d, 2H, J = 7.2 Hz, naphthalene-*H*), 8.21 (d, 2H, J = 7.3 Hz, naphthalene-*H*), 1.31 (m, 2H,-CH_2-C*H*$_2$-CH_2-CH(NI)-), 7.83 (t, 2H, J = 7.6 Hz, naphthalene-*H*), 7.76 (t, 2H, J = 7.4 Hz, naphthalene-*H*), 5.61 (dd, 1H, J = 4.8 Hz, 9.7 Hz, -CH_2-C*H*(NI)-COO CH_3), 3.98 (m, 2H, NI-C*H*$_2$-CH_2-), 3.58 (s, 3H, -COOC*H*$_3$), 2.20 (m, 2H, -CH_2-C*H*$_2$-CH(NI)-$COOCH_3$), 1.65 (m, 2H, NI-CH_2-C*H*$_2$-CH_2-). ^{13}C NMR (100 MHz, DMSO-d_6, 298 K) : δ/ppm = 170.30 (-*C*$OOCH_3$), 163.57 (NI-*C*O), 163.38 (NI-*C*O), 135.09 (naphthalene-*C*H), 134.40 (naphthalene-*C*H), 131.41-131.53 (naphthalene-*C*H), 130.71 (naphthalene-*C*H), 127.41-127.55 (naphthalene-*C*), 127.31 (naphthalene-*C*), 122.09 (naphthalene-*C*), 121.49 (naphthalene-*C*), 52.66 (-*C*H(NI)-$COOCH_3$), 52.35 (-COO*C*H_3), 39.52 (NI-*C*H_2-, overlapped with solvent), 28.01 (NI-CH_2-*C*H_2-), 27.35 (-*C*H_2-CH(NI)-), 23.33 (-*C*H_2-CH_2-CH(NI)-). ESI-MS (CH_3OH, positive, *m*/*z*) 543.23 ($[M+Na]^+$ requires 543.16). FTIR (KBr, cm^{-1}) : 3446 (Br, m, νC=O), 2955 (w, νC-H), 1740 (s, νC=O), 1696 (s, νC=O), 1658 (s, νC=O), 780 (s, δC-H). Anal. Calcd. for $C_{31}H_{24}N_2O_6$: C, 71.53; H, 4.55; N, 5.38%. Found : C, 71.26; H, 4.59; N, 5.37%.

^{1}H NMR (400 MHz, DMSO-d_6, 298 K)

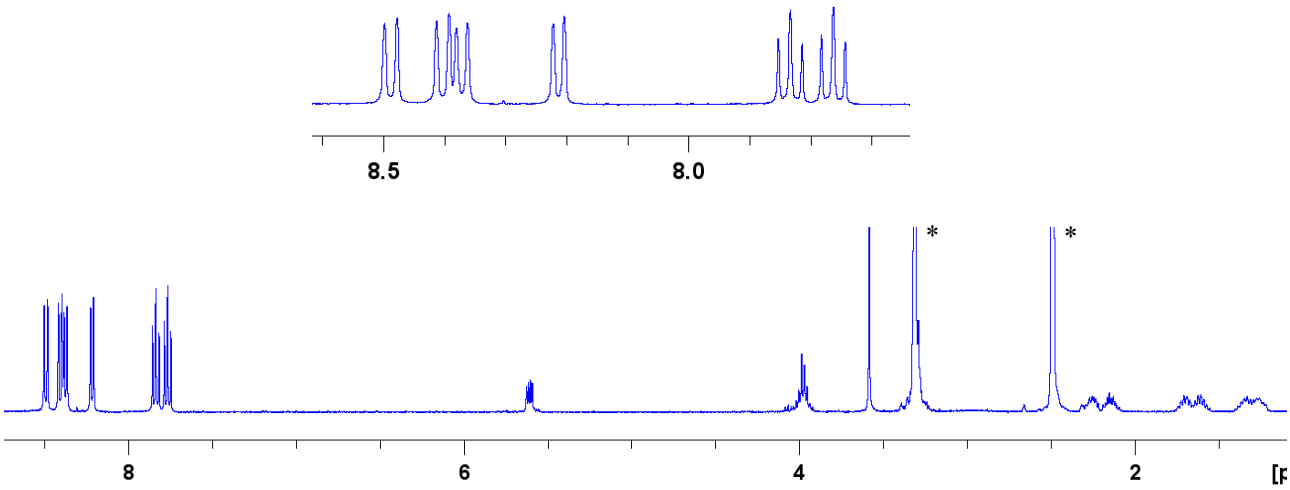


Figure S14. ^{1}H NMR (400 MHz) spectrum of *D*-LyMebNI (3.4×10^{-3} M) in DMSO-d_6 at 298 K.

^{13}C NMR (100 MHz, DMSO-d_6, 298 K)

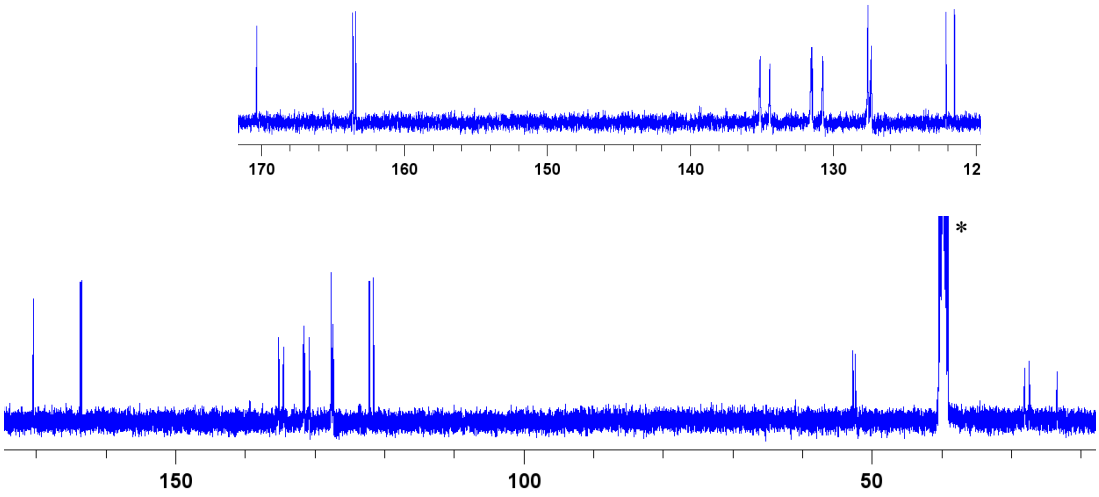


Figure S15. ^{13}C NMR (100 MHz) spectrum of *D*-LyMebNI (1.3×10^{-2} M) in DMSO-d_6 at 298 K.

ESI-MS (MeOH, positive)

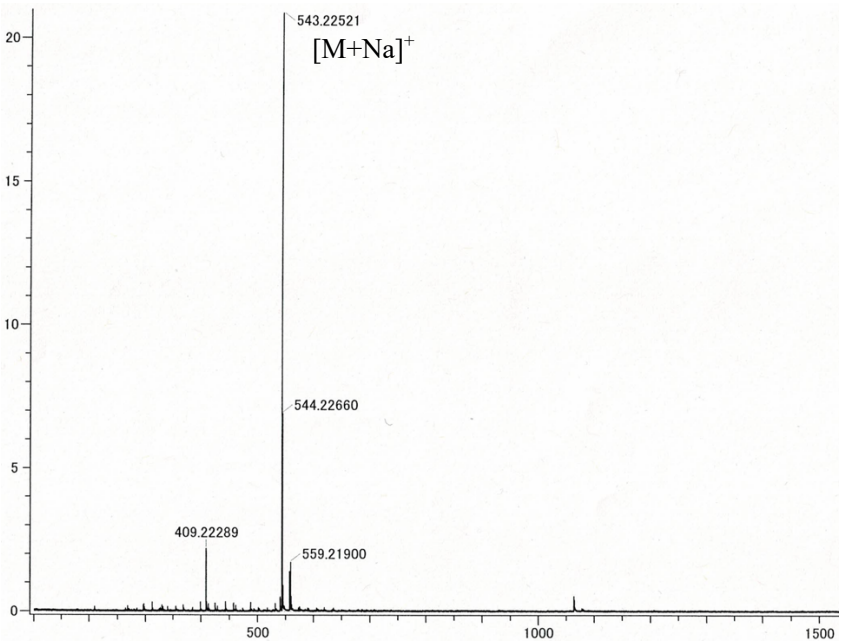


Figure S16. ESI-MS spectrum of *D*-LyMebNI in MeOH.

FTIR (KBr disk)

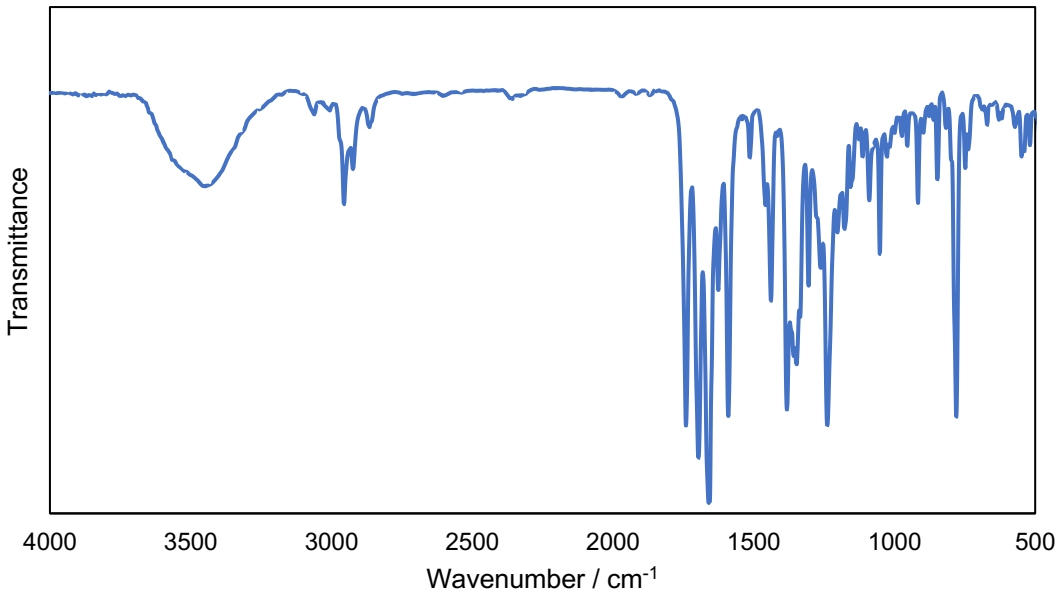


Figure S17. FTIR (KBr disk) spectrum of *D*-LyMebNI.

5-5. Synthesis of *L*-NorNI

0.068 g (5.2×10^{-4} mol) of *L*-norleucine was dissolved in 5.0 mL of EtOH and stirred in a 200 mL flask. DIEA 0.10 mL (5.2×10^{-4} mol, 1 eq) dissolved in 5.0 mL of EtOH was then added dropwise. After stirring at 85 ºC for 2 h, 0.118 g (5.9×10^{-4} mol, 1.1 eq) of 1,8-Naphthalic anhydride was added and the mixture was stirred for 24 h at 85 ºC. The solvent was removed under reduced pressure using an evaporator and dried in vacuum. The product was purified on a column (φ 3 cm × 17 cm) using Wako Gel C-200. The eluents were separated using DCM and DCM:MeOH = 100:1 – 10:3 mixtures. The solvent was removed under reduced pressure and the desired product was reprecipitated from DCM and hexane at 4 ºC to give white powders. Yield : 0.143 g (89%).

^{1}H NMR (400 MHz, DMSO-d_6, 298 K) : δ/ppm = 12.75 (br s, 1H, -COO*H*), 8.52 (d, 2H, *J* = 8.0 Hz, naphthalene-*H*), 7.90 (t, 2H, *J* = 7.8 Hz, naphthalene-*H*), 5.50 (dd, *J* = 4.4 Hz, 9.4 Hz, 1H, -CH_2-C*H*(NI)-COOH), 2.13 (m, 2H, -CH-C*H*$_2$-C_3H_7), 1.27 (m, 2H, -CH_2-C*H*$_2$-C_2H_5), 1.17 (m, 2H, -CH_2-C*H*$_2$-CH_3), 0.79 (t, 3H, *J* = 7.1 Hz, -CH_2-C*H*$_3$). ^{13}C NMR (100 MHz, DMSO-d_6, 298 K) : δ/ppm = 171.42 (-*C*OOH), 163.47 (NI-*C*O), 135.00 (naphthalene-*C*H), 131.55 (naphthalene-*C*H), 127.64 (naphthalene-*C*), 121.78 (naphthalene-*C*), 53.23 (-*C*H(NI)-COOH), 28.46 (-*C*H_2-CH_2-CH_2-CH_3), 28.31 (-*C*H_2-CH_2-CH_3), 22.14 (-*C*H_2-CH_3), 14.04 (-*C*H_3). ESI-MS (CH_3OH, positive, *m*/*z*) 334.14 ($[M+Na]^+$ requires 334.10). FTIR (KBr, cm^{-1}) : 3446 (Br, m, νC=O), 3068 (Br, m, νO-H), 2960 (m, νC-H), 2929 (m, νC-H), 2872 (m, νC-H), 1702 (s, νC=O), 1665 (s, νC=O), 1589 (s, νC=O), 779 (s, δC-H). Anal. Calcd. for $C_{18}H_{17}NO_4$: C, 69.44; H, 5.50; N, 4.50%. Found : C, 69.23; H, 5.50; N, 4.42%.

^{1}H NMR (400 MHz, DMSO-d_6, 298 K)

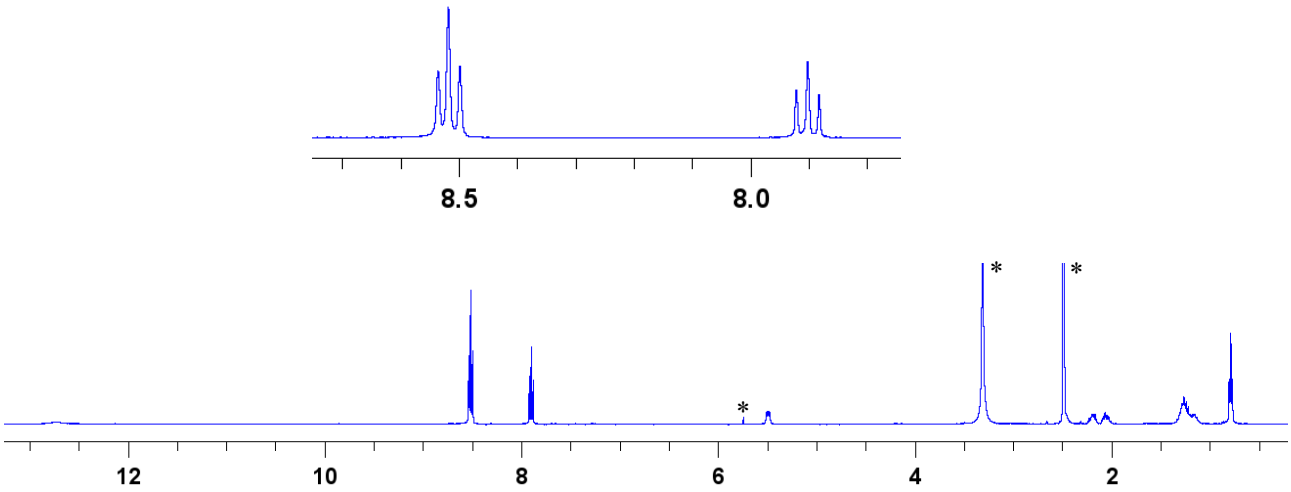


Figure S18. ^{1}H NMR (400 MHz) spectrum of *L*-NorNI (6.1×10^{-3} M) in DMSO-d_6 at 298 K.

^{13}C NMR (100 MHz, DMSO-d_6, 298 K)

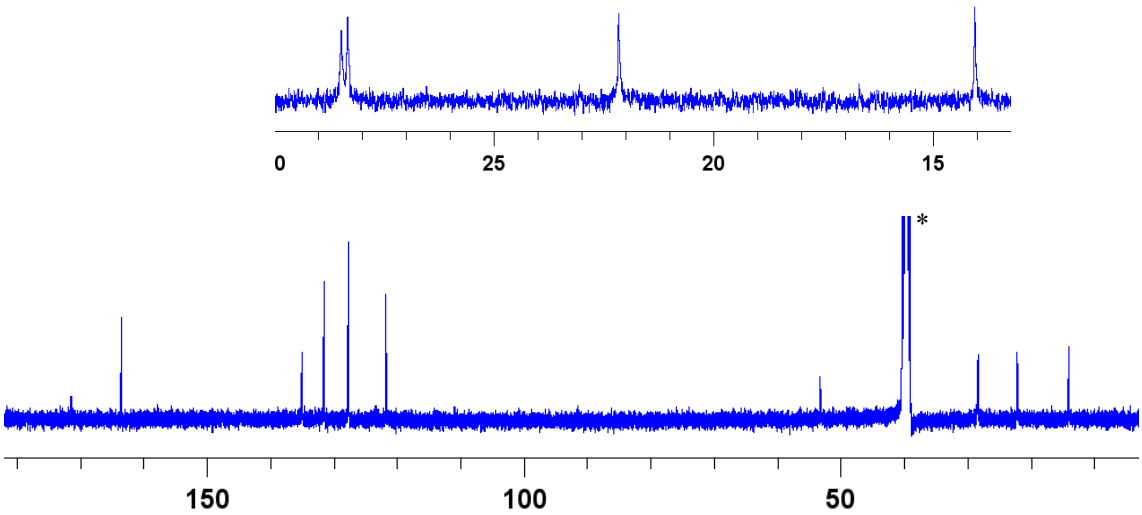


Figure S19. ^{13}C NMR (100 MHz) spectrum of *L*-NorNI (1.1×10^{-2} M) in DMSO-d_6 at 298 K.

ESI-MS (MeOH, positive)

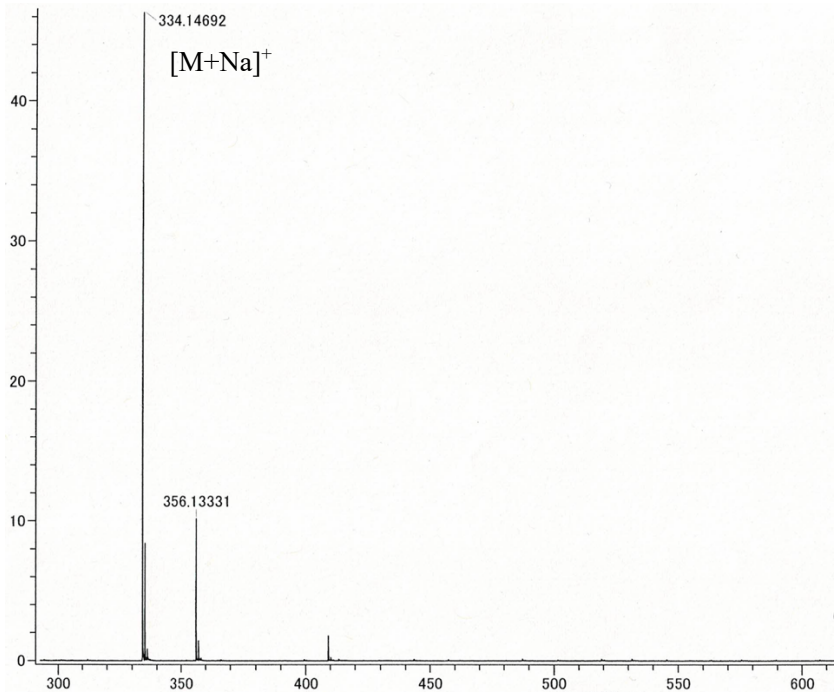


Figure S20. ESI-MS spectrum of *L*-NorNI in MeOH.

FTIR (KBr disk)

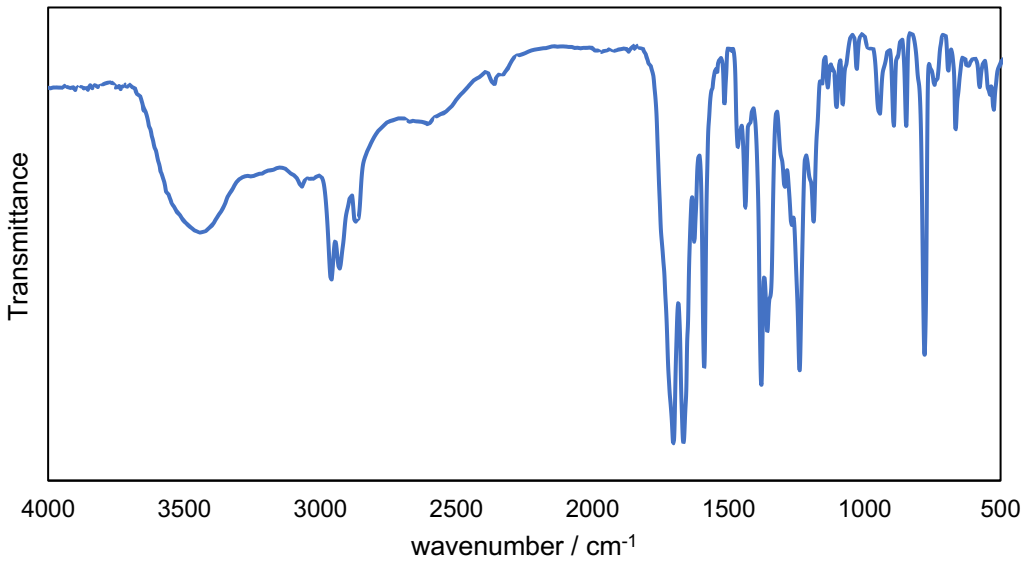


Figure S21. FTIR (KBr disk) spectrum of *L*-NorNI.

5-6. Synthesis of *D*-NorNI

0.065 g (4.9×10^{-4} mol) of *D*-norleucine was dissolved in 10 mL of EtOH and stirred in a 200 mL flask. DIEA 0.10 mL (5.2×10^{-4} mol, 1.1 eq) dissolved in 5.0 mL of EtOH was then added dropwise. After stirring at 85 ºC for 2 h, 0.112 g (5.6×10^{-4} mol, 1.1 eq) of 1,8-Naphthalic anhydride was added and the mixture was stirred for 24 h at 85 ºC. The solvent was removed under reduced pressure using an evaporator and dried in vacuum. The product was purified on a column (φ 3 cm × 17 cm) using Wako Gel C-200. The eluents were separated using DCM and DCM:MeOH = 100:1 – 10:3 mixtures. The solvent was removed under reduced pressure and the desired product was reprecipitated from DCM and hexane at 4 ºC to give white powders. Yield : 0.113 g (73%).

^{1}H NMR (400 MHz, DMSO-d_6, 298 K) : δ/ppm = 12.75 (br s, 1H, -COO*H*), 8.52 (d, 2H, *J* = 8.0 Hz, naphthalene-*H*), 8.51 (d, 2H, *J* = 8.0 Hz, naphthalene-*H*), 7.90 (t, 2H, *J* = 7.8 Hz, naphthalene-*H*), 5.50 (dd, *J* = 4.4 Hz, 9.4 Hz, 1H, -CH_2-C*H*(NI)-COOH), 2.13 (m, 2H, -CH-C*H*$_2$-C_3H_7), 1.27 (m, 2H, -CH_2-C*H*$_2$-C_2H_5), 1.17 (m, 2H, -CH_2-C*H*$_2$-CH_3), 0.79 (t, 3H, *J* = 7.1 Hz, -CH_2-C*H*$_3$). ^{13}C NMR (100 MHz, DMSO-d_6, 298 K) : δ/ppm = 171.43 (-*C*OOH), 163.46 (NI-*C*O), 134.99 (naphthalene-*CH*), 131.52 (naphthalene-*CH*), 127.63 (naphthalene-*C*), 121.77 (naphthalene-*C*), 53.22 (-*C*H(NI)-COOH), 28.45 (-*C*H$_2$-CH_2-CH_2-CH_3), 28.31 (-*C*H$_2$-CH_2-CH_3), 22.13 (-*C*H$_2$-CH_3), 14.02 (-*C*H$_3$). ESI-MS (CH_3OH, negative, *m*/*z*) 310.06 ($[M-H]^-$ requires 310.12). FTIR (KBr, cm^{-1}) : 3446 (Br, m, νC=O), 3068 (Br, m, νO-H), 2960 (m, νC-H), 2929 (m, νC-H), 2872 (m, νC-H), 1702 (s, νC=O), 1665 (s, νC=O), 1589 (s, νC=O), 779 (s, δC-H). Anal. Calcd. for $C_{18}H_{17}NO_4$・0.5 H_2O : C, 67.48; H, 5.66; N, 4.37%. Found : C, 68.24; H, 5.66; N, 4.37%.

^{1}H NMR (400 MHz, DMSO-d_6, 298 K)

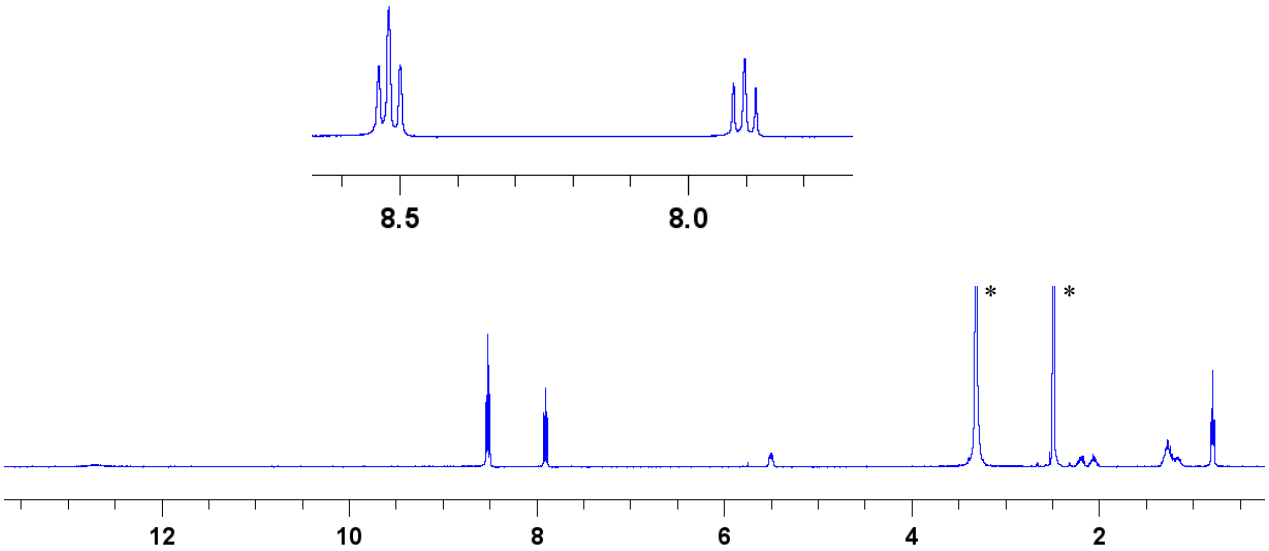


Figure S22. ^{1}H NMR (400 MHz) spectrum of *D*-NorNI (3.6×10^{-3} M) in DMSO-d_6 at 298 K.

^{13}C NMR (100 MHz, DMSO-d_6, 298 K)

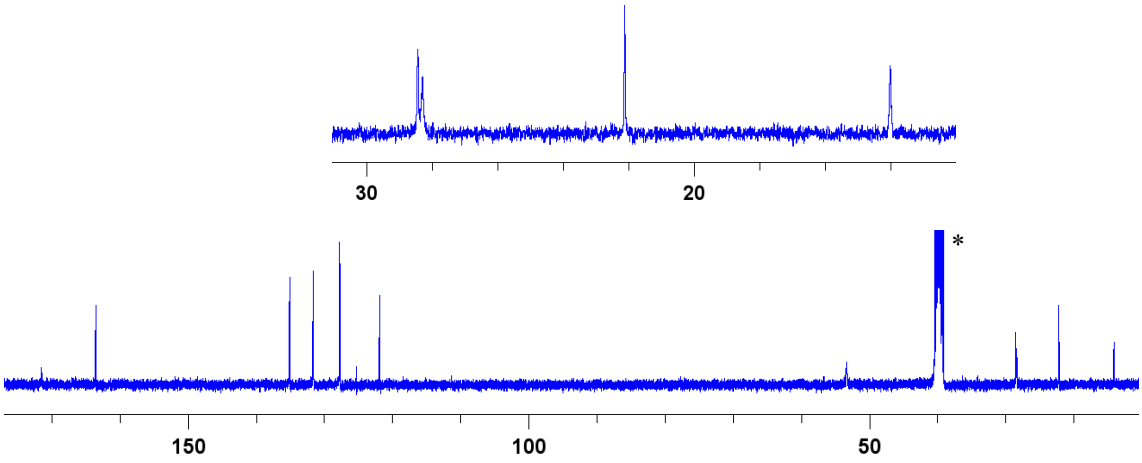


Figure S23. ^{13}C NMR (100 MHz) spectrum of *D*-NorNI (1.3×10^{-2} M) in DMSO-d_6 at 298 K.

ESI-MS (MeOH, negative)

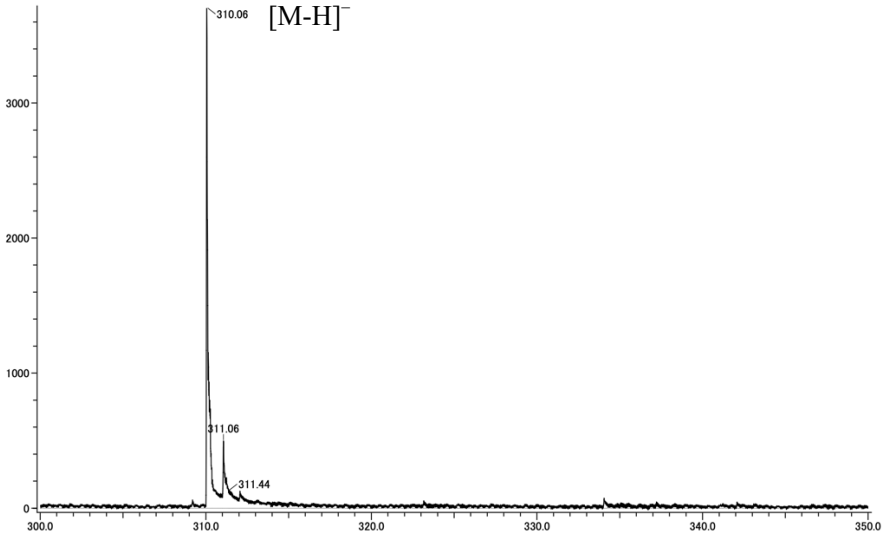


Figure S24. ESI-MS spectrum of *D*-NorNI in MeOH.

FTIR (KBr disk)

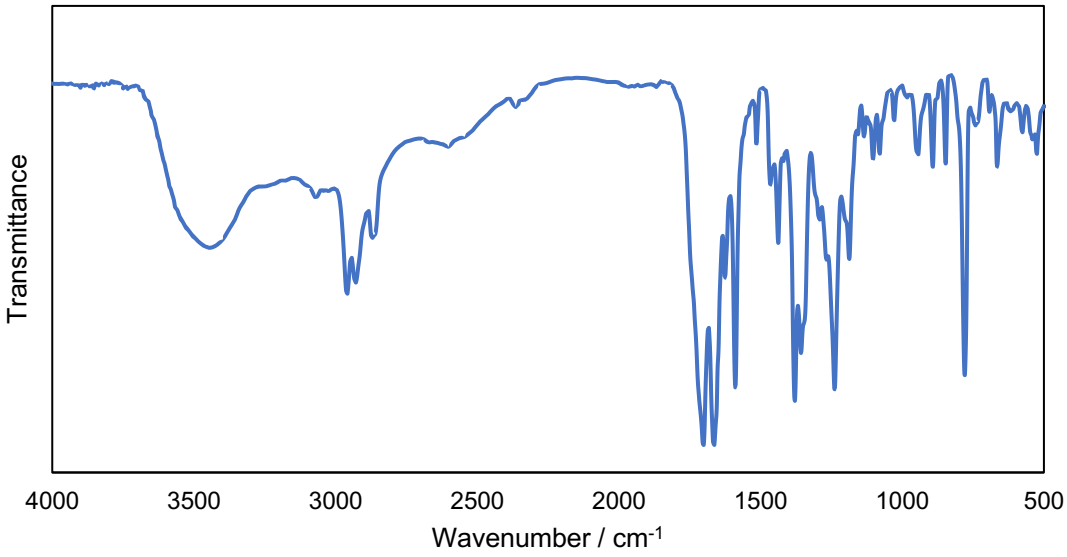


Figure S25. FTIR (KBr disk) spectrum of *D*-NorNI.

6. UV-vis spectra

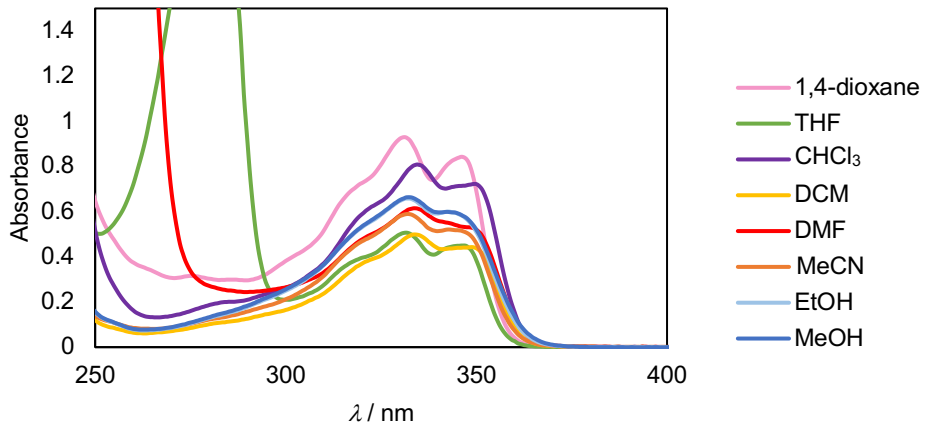


Figure S26. UV-vis spectra of *L*-LybNI in 1,4-dioxane, THF, $CHCl_3$, DCM, DMF, MeCN, EtOH, and MeOH (2.5×10^{-5} M) at room temperature.

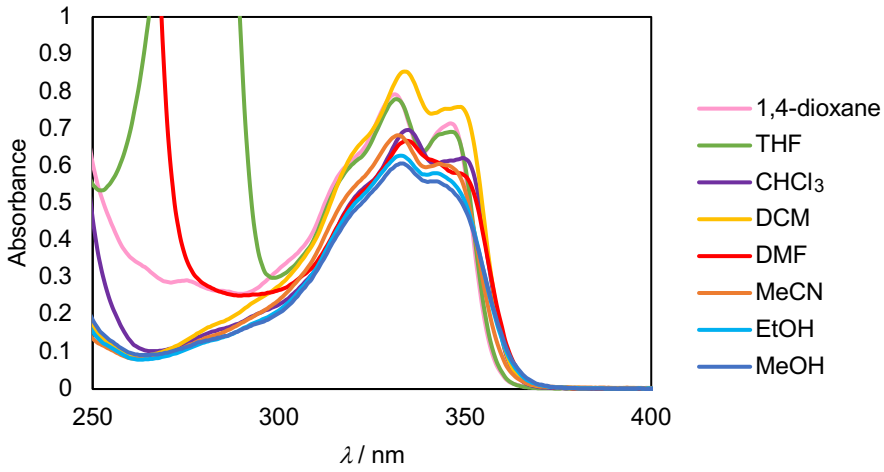


Figure S27. UV-vis spectra of *L*-LyMebNI in 1,4-dioxane, THF, $CHCl_3$, DCM, DMF, MeCN, EtOH, and MeOH (2.5×10^{-5} M) at room temperature.

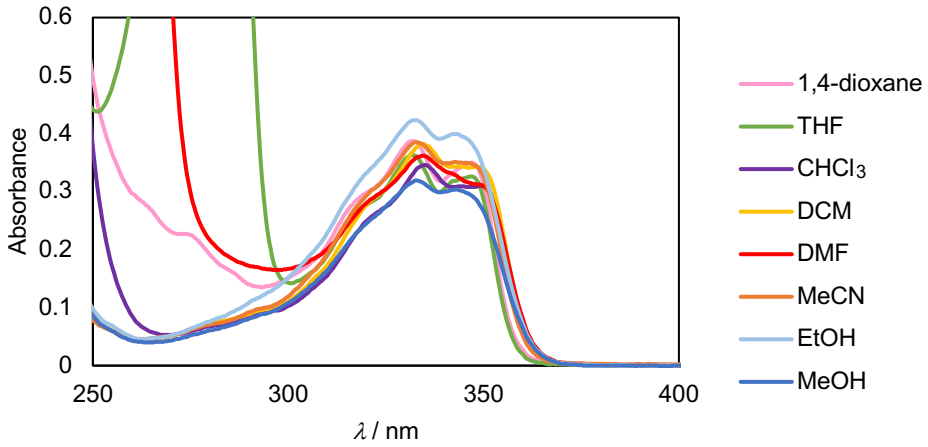


Figure S28. UV-vis spectra of *L*-NorNI in1,4-dioxane, THF, $CHCl_3$, DCM, DMF, MeCN, EtOH, and MeOH (2.5×10^{-5} M) at room temperature.

Table S2. Absorption properties of *L*-LyMebNI, *L*-LybNI, and *L*-NorNI in 1,4-Dioxane, THF, $CHCl_3$, DCM, DMF, MeCN, EtOH, and MeOH at room temperature.

		***L*-LyMebNI**		***L*-LybNI**		***L*-NorNI**	
Solvent	$E_T(30)$	λ_{max} / nm	ε / M^{-1} cm^{-1}	λ_{max} / nm	ε / M^{-1} cm^{-1}	λ_{max} / nm	ε / M^{-1} cm^{-1}
1,4-dioxane	36.0	331	3.2×10^4	331	3.7×10^4	332	1.5×10^4
THF	37.4	332	3.1×10^4	332	2.0×10^4	332	1.5×10^4
$CHCl_3$	39.1	335	2.8×10^4	334	3.2×10^4	335	1.4×10^4
DCM	40.7	334	3.4×10^4	334	2.0×10^4	335	1.5×10^4
DMF	43.2	334	2.7×10^4	334	2.5×10^4	334	1.4×10^4
ACN	45.6	332	2.7×10^4	332	2.4×10^4	333	1.5×10^4
EtOH	51.9	333	2.5×10^4	332	2.6×10^4	333	1.7×10^4
MeOH	55.4	333	2.4×10^4	332	2.7×10^4	333	1.3×10^4

7. Fluorescence spectra

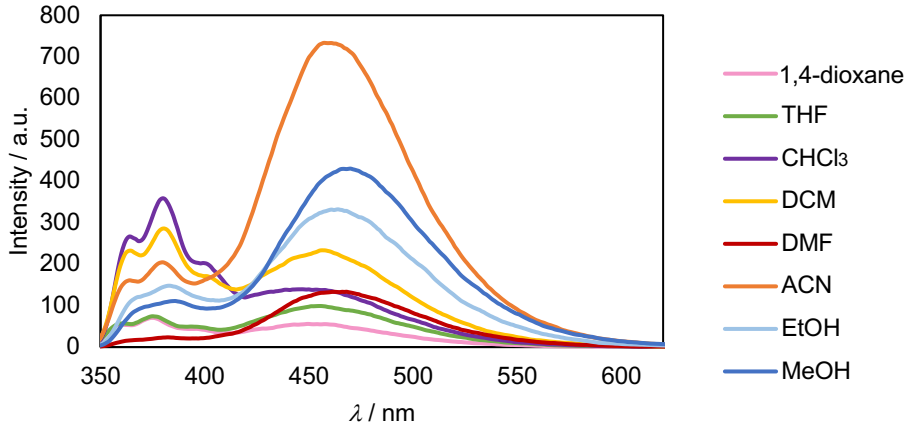


Figure S29. Fluorescence spectra of *L*-LybNI in N_2-saturated 1,4-dioxane (pink), THF (green), $CHCl_3$ (purple), DCM (light orange), DMF (red), MeCN (orange), EtOH (light blue), and MeOH (blue) (2.5×10^{-5} M) at room temperature. The path length was 1 cm.

Table S3. Fluorescence properties of *L*-LybNI in 1,4-dioxane, THF, $CHCl_3$, DCM, DMF, MeCN, EtOH, and MeOH at room temperature.

Solvent	$\lambda_{em\_monomer}$ / nm	$\lambda_{em\_excimer}$ / nm	I_{LW}/I_{SW}	Φ
1,4-dioxane	375	450	0.79	0.032
THF	375	455	1.3	0.036
$CHCl_3$	380	447	0.39	0.068
DCM	380	456	0.82	0.075
DMF	382	468	5.7	0.039
MeCN	380	457	3.6	0.122
EtOH	383	464	2.2	0.059
MeOH	386	470	3.9	0.052

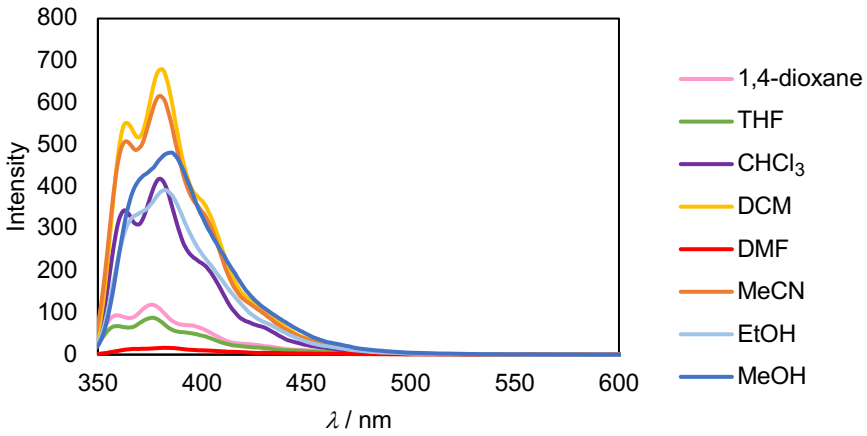


Figure S30. Emission spectra of *L*-NorNI in N_2-saturated 1,4-dioxane, THF, $CHCl_3$, DCM, DMF, MeCN, EtOH, and MeOH (2.5×10^{-5} M) at room temperature. The path length was 1 cm.

Table S4. Emission properties of *L*-NorNI in 1,4-dioxane, THF, $CHCl_3$, DCM, DMF, MeCN, EtOH, and MeOH.

Solvent	λ_{em} / nm	ϕ_f
1,4-dioxane	376	0.007
THF	376	0.009
$CHCl_3$	380	0.052
DCM	381	0.066
DMF	382	0.004
MeCN	380	0.044
EtOH	383	0.048
MeOH	385	0.056

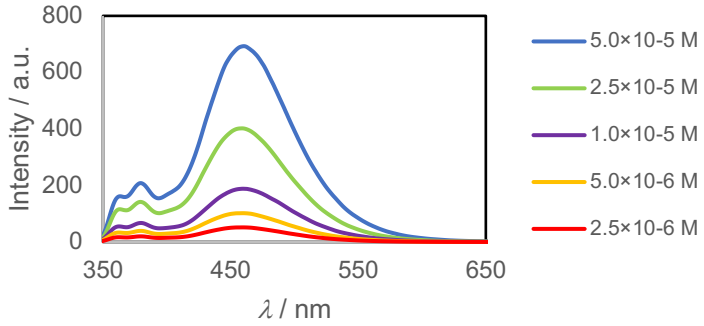


Figure S31. Fluorescence spectra of *L*-LyMebNI in N_2-saturated MeCN (5.0×10^{-5}, 2.5×10^{-5}, 1.0×10^{-5}, 5.0×10^{-6}, and 2.5×10^{-6} M) at room temperature (λ_{ex} = 332 nm). The path length was 2 mm.

8. Fluorescence lifetimes

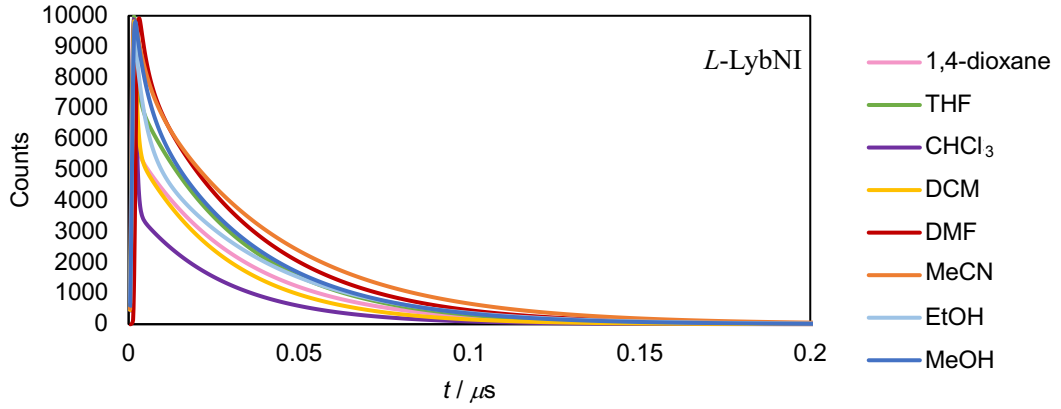


Figure S32. Emission decay of *L*-LybNI in N_2-saturated 1,4-dioxane, THF, $CHCl_3$, DCM, DMF, MeCN, EtOH, and MeOH (2.5×10^{-5} M) at room temperature (λ_{ex} = 330 nm, λ_{em} > 430 nm).

Table S5. Lifetimes and kinetic parameters of *L*-LybNI in N_2-saturated 1,4-dioxane, THF, $CHCl_3$, DCM, DMF, MeCN, EtOH, and MeOH (2.5×10^{-5} M) at room temperature (λ_{ex} = 330 nm, λ_{em} > 430 nm).

Solvent	Lifetime / ns (*A* / %)			χ^2	k_r / 10^6 s^{-1}	k_{nr} / 10^7 s^{-1}
	τ_1	τ_2	τ_{ave}			
1,4-dioxane	0.46 (5)	31.2 (95)	29.7	1.00	1.1	3.3
THF	0.80 (3)	30.8 (97)	29.9	1.00	1.2	3.2
$CHCl_3$	0.48 (11)	26.4 (89)	23.5	1.00	2.9	4.0
DCM	0.64 (5)	27.3 (95)	26.0	1.00	2.9	3.6
DMF	2.25 (3)	33.4 (97)	32.5	1.00	1.2	3.0
MeCN	3.38 (2)	39.4 (98)	38.6	1.00	3.2	2.3
EtOH	2.92 (6)	35.3 (94)	33.3	1.00	1.8	2.8
MeOH	3.36 (4)	32.0 (96)	30.9	1.00	1.7	3.0

Table S6. Lifetimes and kinetic parameters of *L*-NorNI in N_2-saturated 1,4-dioxane, THF, $CHCl_3$, DCM, DMF, MeCN, EtOH, and MeOH (2.5×10^{-5} M) at room temperature (λ_{ex} = 330 nm, λ_{em} > 430 nm).

Solvent	Lifetime / ns (*A* / %)			χ^2	k_r / 10^6 s^{-1}	k_{nr} / 10^7 s^{-1}
	τ_1	τ_2	τ_{ave}			
1,4-dioxane	0.30 (53)	1.43 (47)	0.83	1.00	8.4	120
THF	0.89 (96)	14.6 (4)	1.44	1.00	6.1	69
$CHCl_3$	20.8 (4)	0.63 (96)	1.43	1.00	36	66
DCM	0.64 (100)		0.64	1.00	102	146
DMF	0.34 (67)	22.6 (33)	7.68	1.00	0.55	13
MeCN	0.79 (98)	18.5 (2)	1.14	1.00	39	84
EtOH	0.78 (98)	25.6 (2)	1.27	1.00	38	75
MeOH	26.9 (3)	1.00 (97)	1.77	1.00	32	53

9. DFT calculations

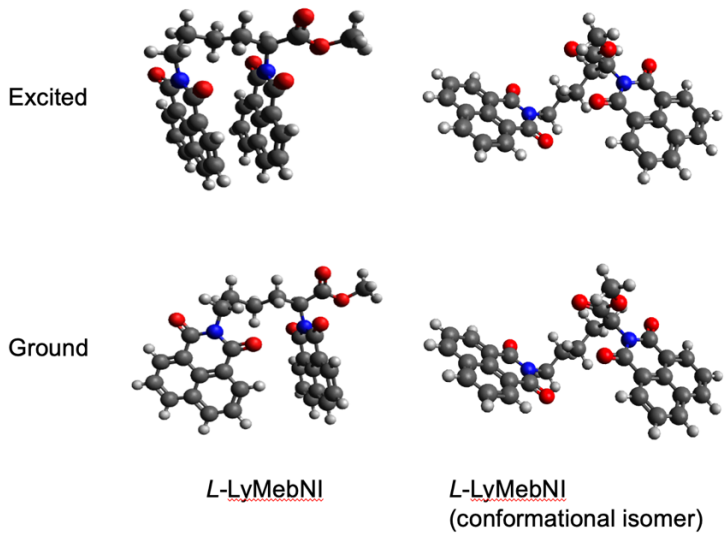


Figure S33. Calculated structures for the ground and excited states of *L*-LyMebNI (left), obtained by optimising the X-ray structure, and its linear conformational isomer (right) with solvent MeCN.

Table S7. Calculated absorption energies in eV, absorption wavelengths, fluorescence energies, and fluorescence wavelengths of *L*-LyMebNI and its linear conformational isomer with solvents $CHCl_3$, MeCN, and MeOH.

	L-LyMebNI[a]				*L*-LyMebNI (conformational isomer)			
	absorption		fluorescence		absorption		fluorescence	
Solvent	energy/eV	λ_{max} / nm	energy/eV	λ_{max} / nm	energy/eV	λ_{max} / nm	energy/eV	λ_{max} / nm
$CHCl_3$	3.61	344	2.97	417	3.57	348	3.17	391
MeCN	3.59	345	2.91	425	3.55	349	3.17	391
MeOH	3.59	345	2.91	425	3.56	349	3.17	391

[a] The ground state geometries were obtained by optimizing the X-ray structure.

10. CD spectra

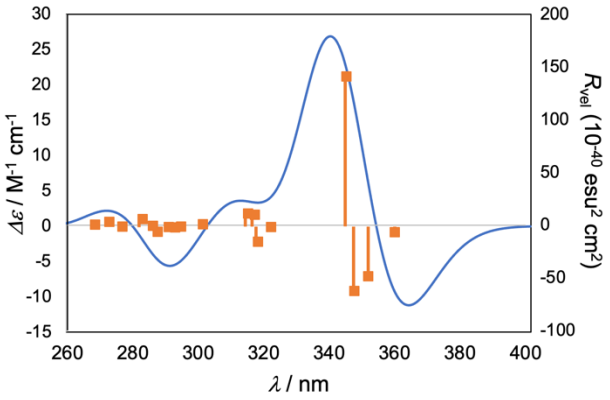


Figure S34. Calculated CD spectrum and rotatory strengths of *L*-LyMebNI from DFT calculation with SCRF = (pcm, solvent = CH3CN).

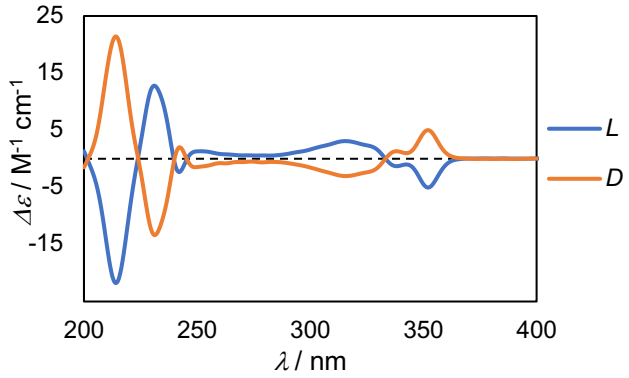


Figure S35. CD spectra of *D*-LyMebNI (orange line) and *L*-LyMebNI (blue line) in MeCN (2.5×10^{-5} M) at room temperature.

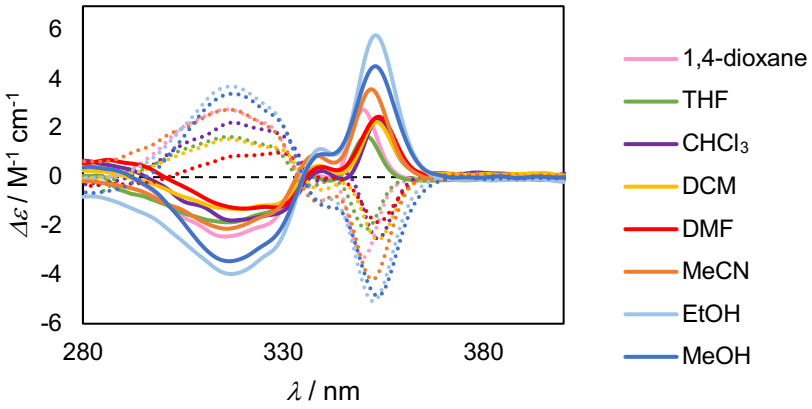


Figure S36. CD spectra of *D*-LybNI (solid line) and *L*-LybNI (dotted line) in 1,4-dioxane, THF, $CHCl_3$, DCM, DMF, MeCN, EtOH, and MeOH (2.5×10^{-5} M) at room temperature.

Table S8. CD properties of *D*-LybNI (solid line) in 1,4-dioxane, THF, $CHCl_3$, DCM, DMF, MeCN, EtOH, and MeOH (2.5×10^{-5} M) at room temperature.

solvent	λ_1 / nm	$\Delta\varepsilon$ / $M^{-1}cm^{-1}$	$\lvert g_{abs}\rvert$	λ_2 / nm	$\Delta\varepsilon$ / $M^{-1}cm^{-1}$	$\lvert g_{abs}\rvert$
1,4-dioxane	350	2.76	1.0×10^{-4}	315	−2.43	0.9×10^{-4}
THF	351	1.67	1.2×10^{-4}	316	−1.85	1.3×10^{-4}
$CHCl_3$	354	2.35	1.0×10^{-4}	317	−1.77	0.8×10^{-4}
DCM	353	2.25	1.5×10^{-4}	319	−1.31	0.9×10^{-4}
DMF	354	2.47	1.6×10^{-4}	321	−1.29	0.7×10^{-4}
MeCN	352	3.60	2.3×10^{-4}	316	−2.11	1.3×10^{-4}
EtOH	353	5.81	3.7×10^{-4}	317	−3.97	2.0×10^{-4}
MeOH	353	4.54	2.7×10^{-4}	316	−3.44	1.8×10^{-4}

Table S9. CD properties of *L*-LybNI (dotted line) in 1,4-dioxane, THF, $CHCl_3$, DCM, DMF, MeCN, EtOH, and MeOH (2.5×10^{-5} M) at room temperature.

solvent	λ_1 / nm	$\Delta\varepsilon$ / $M^{-1}cm^{-1}$	$\lvert g_{abs}\rvert$	λ_2 / nm	$\Delta\varepsilon$ / $M^{-1}cm^{-1}$	$\lvert g_{abs}\rvert$
1,4-dioxane	350	−3.30	1.2×10^{-4}	316	2.78	1.0×10^{-4}
THF	351	−2.12	1.6×10^{-4}	316	1.65	1.1×10^{-4}
$CHCl_3$	354	−2.51	1.1×10^{-4}	318	2.23	1.2×10^{-4}
DCM	354	−2.55	1.9×10^{-4}	317	1.56	1.2×10^{-4}
DMF	354	−1.84	1.2×10^{-4}	321	1.00	0.5×10^{-4}
MeCN	352	−4.19	2.3×10^{-4}	317	2.76	1.6×10^{-4}
EtOH	352	−5.06	2.9×10^{-4}	317	3.72	1.9×10^{-4}
MeOH	354	−4.85	3.2×10^{-4}	317	3.41	1.7×10^{-4}

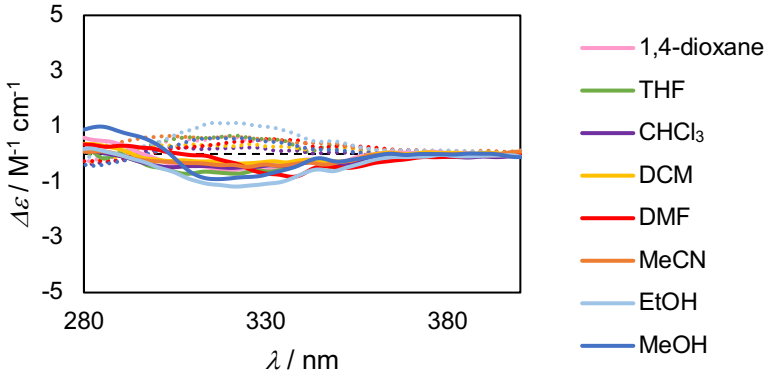


Figure S37. CD spectra of *D*-NorNI (solid line) and *L*-NorNI (dotted line) in 1,4-dioxane, THF, $CHCl_3$, DCM, DMF, MeCN, EtOH, and MeOH (2.5×10^{-5} M) at room temperature.

Table S10. CD properties of *D*-NorNI (solid line) and *L*-NorNI (dotted line) in 1,4-dioxane, THF, $CHCl_3$, DCM, DMF, MeCN, EtOH, and MeOH (2.5×10^{-5} M) at room temperature.

	D-NorNI			*L*-NorNI		
solvent	λ / nm	$\Delta\varepsilon$ / $M^{-1}cm^{-1}$	$\lvert g_{abs}\rvert$	λ / nm	$\Delta\varepsilon$ / $M^{-1}cm^{-1}$	$\lvert g_{abs}\rvert$
1,4-dioxane	319	−0.62	0.5×10^{-4}	320	0.64	0.5×10^{-4}
THF	308	−0.72	1.0×10^{-4}	321	0.66	0.6×10^{-4}
$CHCl_3$	320	−0.50	0.5×10^{-4}	324	0.23	0.2×10^{-4}
DCM	323	−0.35	0.3×10^{-4}	326	0.36	0.3×10^{-4}
DMF	337	−0.82	0.6×10^{-4}	331	0.54	0.4×10^{-4}
MeCN	325	−0.47	0.4×10^{-4}	324	0.60	0.5×10^{-4}
EtOH	322	−1.18	0.9×10^{-4}	316	1.12	0.9×10^{-4}
MeOH	317	−0.91	1.0×10^{-4}	324	0.58	0.5×10^{-4}

11. CPL spectra

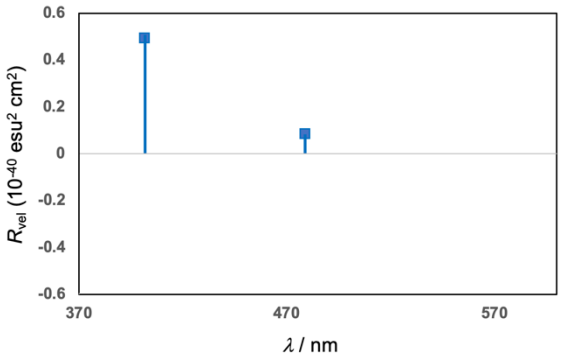


Figure S38. Calculated CPL rotatory strengths of *L*-LyMebNI from DFT calculations with SCRF = (pcm, solvent = CH3CN).

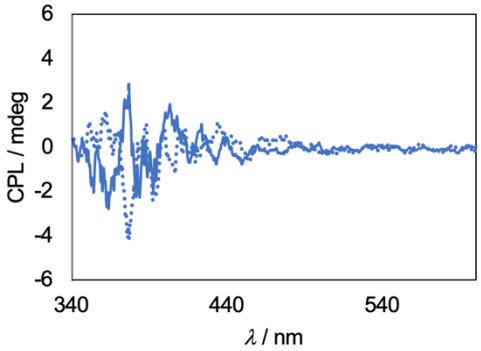


Figure S39. CPL spectra of *D* (solid line) and *L* (dotted line) forms of NorNI (2.5×10^{-5} M) in MeCN at room temperature (λ_{ex} = 310 nm). The $|g_{lum}|$ value is 9.0×10^{-4} at 377 nm.

12. Cartesian coordinates and energies of the optimized geometries

L-LyMebNI (ground state (solvent=CH3CN) in Figure 6) LysMebNIRpcnh.out

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.894047	-0.589817	-1.790677
2	8	0	5.077154	-1.366225	0.185272
3	8	0	2.319996	-0.343280	2.731581
4	8	0	-0.824417	-0.710893	-1.621207
5	8	0	-3.954883	-3.401021	0.342333
6	7	0	2.529405	-0.475820	0.453912
7	8	0	4.371614	-3.343794	-0.645083
8	7	0	-2.370869	-2.050013	-0.596041
9	6	0	2.288797	0.233785	1.645243
10	6	0	-4.071805	0.191789	-0.241016
11	6	0	-4.497271	-1.088428	0.197378
12	6	0	-4.923708	1.323538	-0.051543
13	6	0	-1.919781	-0.807022	-1.068305
14	6	0	2.590310	0.105840	-0.822216
15	6	0	-2.810138	0.358845	-0.867737
16	6	0	1.996417	1.677401	1.518331
17	6	0	-3.621871	-2.265168	0.001809
18	6	0	2.292315	1.547726	-0.927681
19	6	0	2.002597	2.296809	0.241607
20	6	0	-3.244993	2.737022	-1.110432
21	6	0	1.720012	3.693319	0.132512
22	6	0	1.736616	4.294121	-1.155051
23	6	0	-2.407763	1.616147	-1.294548
24	6	0	-1.508361	-3.238109	-0.798152
25	6	0	-4.477876	2.595462	-0.501464
26	6	0	2.794117	-1.927167	0.552548
27	6	0	2.303186	2.167709	-2.168880
28	6	0	4.143304	-2.293682	-0.073741
29	6	0	1.717714	2.425843	2.653294
30	6	0	2.022485	3.545640	-2.281791
31	6	0	-0.746452	-3.662182	0.468037
32	6	0	1.632879	-2.793039	0.036261
33	6	0	-5.734616	-1.239345	0.806311
34	6	0	1.436552	3.804467	2.550531
35	6	0	-6.579422	-0.125159	0.996635
36	6	0	-6.183585	1.131066	0.576832
37	6	0	1.437553	4.426882	1.316092
38	6	0	0.383841	-2.724450	0.927848
39	6	0	6.410192	-1.633762	-0.304975
40	1	0	1.995231	-3.826628	0.006825
41	1	0	-0.330447	-4.660744	0.272963
42	1	0	1.219803	4.374367	3.448912
43	1	0	0.009924	-1.694229	0.986861
44	1	0	7.004769	-0.772277	-0.003309
45	1	0	-7.544223	-0.261376	1.475842
46	1	0	-0.828833	-2.995093	-1.614056
47	1	0	-1.470112	-3.786078	1.281417
48	1	0	2.528194	1.579626	-3.052650
49	1	0	-6.834821	1.989045	0.723138
50	1	0	6.396931	-1.730359	-1.393075
51	1	0	-5.122621	3.459140	-0.360075
52	1	0	-2.163144	-4.050374	-1.118401
53	1	0	-6.045410	-2.225406	1.135811
54	1	0	-2.913548	3.713387	-1.450959
55	1	0	2.915991	-2.111490	1.624977
56	1	0	1.717574	1.937468	3.622211
57	1	0	1.521516	5.356080	-1.241870
58	1	0	1.396925	-2.506331	-0.992376
59	1	0	-1.439646	1.728149	-1.771486
60	1	0	0.664349	-3.007120	1.951404
61	1	0	1.222526	5.489515	1.237118
62	1	0	2.032902	4.015196	-3.260730
63	1	0	6.800885	-2.548771	0.146248

```
 ---------------------------------------------------------------------
SCF Done:  E(RB3LYP) =  -1756.81467161    A.U. after   1 cycles
Zero-point correction=                       0.493248 (Hartree/Particle)
 Thermal correction to Energy=                 0.524860
 Thermal correction to Enthalpy=               0.525805
 Thermal correction to Gibbs Free Energy=        0.427272
 Sum of electronic and zero-point Energies=         -1756.321424
 Sum of electronic and thermal Energies=           -1756.289811
 Sum of electronic and thermal Enthalpies=         -1756.288867
 Sum of electronic and thermal Free Energies=       -1756.387400
```

L-LyMebNI (excited state (solvent=CH3CN) in Figure 6) LysMebNI2R.tdoptpcmh.out

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.800466	-0.541873	-2.182839
2	6	0	-4.091161	-1.100774	-0.925637
3	6	0	-3.626098	-0.486885	0.263024
4	6	0	-2.831018	0.698502	0.156688
5	6	0	-2.518693	1.223951	-1.120930
6	6	0	-3.015878	0.602918	-2.283606
7	6	0	-3.903503	-1.004554	1.550714
8	6	0	-3.441133	-0.346867	2.703560
9	6	0	-2.683720	0.815998	2.597663
10	6	0	-2.367450	1.340376	1.328807
11	6	0	-1.552548	2.566651	1.226799
12	7	0	-1.202157	3.005738	-0.055095
13	6	0	-1.662917	2.420512	-1.243368
14	6	0	-0.257764	4.145283	-0.150433
15	6	0	1.182103	3.750150	0.222706
16	6	0	1.726602	2.552484	-0.569625
17	6	0	3.005552	1.964353	0.043892
18	6	0	3.342631	0.564083	-0.505326
19	6	0	4.643687	0.005412	0.070804
20	8	0	4.769084	-1.310697	-0.155616
21	8	0	5.508591	0.688523	0.589075
22	7	0	2.223978	-0.390634	-0.365557
23	6	0	1.567292	-0.808229	-1.538739
24	6	0	0.398077	-1.675025	-1.371853
25	6	0	-0.025305	-2.060128	-0.072559
26	6	0	0.688100	-1.638081	1.077913
27	6	0	1.879365	-0.800072	0.930700
28	6	0	-0.303206	-2.127604	-2.510977
29	6	0	-1.421539	-2.942144	-2.363650
30	6	0	-1.875615	-3.311343	-1.086362
31	6	0	-1.183885	-2.893432	0.078578
32	6	0	-1.595957	-3.252564	1.385679
33	6	0	-0.868327	-2.831401	2.510668
34	6	0	0.263170	-2.034622	2.365015
35	8	0	-1.350101	2.884523	-2.344356
36	8	0	-1.171671	3.185003	2.225620
37	8	0	1.970899	-0.435441	-2.651202
38	8	0	2.580088	-0.442861	1.890495
39	1	0	0.046303	-1.832504	-3.494000
40	1	0	-1.955002	-3.291471	-3.242715
41	1	0	-2.739180	-3.962433	-0.983955
42	1	0	-2.463482	-3.894819	1.508564
43	1	0	-1.194024	-3.131657	3.502258
44	1	0	0.830987	-1.708127	3.229317
45	1	0	-2.325458	1.330441	3.482378
46	1	0	-3.677820	-0.751805	3.682263
47	1	0	-4.512736	-1.898480	1.644074
48	1	0	-4.715591	-1.986297	-0.856932
49	1	0	-4.185231	-1.015172	-3.080342
50	1	0	-2.777002	1.031212	-3.250457
51	6	0	5.994092	-1.931113	0.294521
52	1	0	-0.617945	4.930289	0.517837
53	1	0	-0.315293	4.503075	-1.177371
54	1	0	1.813266	4.635298	0.067617
55	1	0	1.217295	3.522963	1.294135
56	1	0	1.900429	2.834692	-1.616471
57	1	0	0.957950	1.771997	-0.583746
58	1	0	2.902683	1.902191	1.131440
59	1	0	3.863526	2.614130	-0.158883
60	1	0	3.504284	0.636240	-1.585748
61	1	0	6.095464	-1.819876	1.376614
62	1	0	6.852401	-1.479654	-0.208553
63	1	0	5.899392	-2.982162	0.024151

SCF Done: E(RB3LYP) = -1756.79965523 A.U. after 1 cycles
Zero-point correction= 0.490030 (Hartree/Particle)
Thermal correction to Energy= 0.521585
Thermal correction to Enthalpy= 0.522529

Thermal correction to Gibbs Free Energy= 0.428350
Sum of electronic and zero-point Energies= -1756.214349
Sum of electronic and thermal Energies= -1756.182795
Sum of electronic and thermal Enthalpies= -1756.181851
Sum of electronic and thermal Free Energies= -1756.276030

L-LyMebNI (conformational isomer, ground state (solvent=CH3CN) in Table S7) LysMebNIA2pcmh.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.621604	3.265709	1.103949
2	6	0	5.752114	2.527021	1.399156
3	6	0	5.949992	1.242118	0.825846
4	6	0	4.956167	0.726763	-0.062376
5	6	0	3.803183	1.500781	-0.352047
6	6	0	3.644069	2.752335	0.225243
7	6	0	7.097537	0.449945	1.098795
8	6	0	7.252018	-0.794432	0.516719
9	6	0	6.267935	-1.298158	-0.360372
10	6	0	5.133964	-0.552721	-0.648451
11	6	0	4.109333	-1.091891	-1.569709
12	7	0	2.969832	-0.307684	-1.802175
13	6	0	2.768046	0.977266	-1.272015
14	6	0	1.949778	-0.858074	-2.724947
15	6	0	1.025430	-1.898229	-2.075750
16	6	0	0.121557	-1.351846	-0.960987
17	6	0	-0.777600	-2.459444	-0.395908
18	6	0	-1.735153	-2.108608	0.757819
19	6	0	-1.046079	-1.832460	2.094528
20	8	0	-1.931049	-1.470251	3.036731
21	8	0	0.131292	-2.046814	2.315686
22	7	0	-2.738709	-1.075261	0.413524
23	6	0	-3.976456	-1.535920	-0.076218
24	6	0	-4.980290	-0.515016	-0.440902
25	6	0	-4.682622	0.863171	-0.284369
26	6	0	-3.425298	1.280964	0.222381
27	6	0	-2.407429	0.277241	0.593804
28	6	0	-6.215104	-0.908720	-0.937249
29	6	0	-7.184216	0.053843	-1.289612
30	6	0	-6.913890	1.401931	-1.144966
31	6	0	-5.660537	1.842102	-0.640992
32	6	0	-5.341182	3.216853	-0.476720
33	6	0	-4.109317	3.602704	0.018255
34	6	0	-3.147381	2.632565	0.369652
35	8	0	1.765398	1.626074	-1.570323
36	8	0	4.227902	-2.185597	-2.123691
37	8	0	-4.185770	-2.743248	-0.189867
38	8	0	-1.306345	0.579627	1.050142
39	1	0	-6.426932	-1.966749	-1.051282
40	1	0	-8.145230	-0.271644	-1.676120
41	1	0	-7.660831	2.143371	-1.416570
42	1	0	-6.082425	3.964486	-0.747132
43	1	0	-3.875193	4.656017	0.138835
44	1	0	-2.180195	2.934967	0.757571
45	1	0	6.388800	-2.275231	-0.816689
46	1	0	8.132742	-1.391976	0.732020
47	1	0	7.855778	0.838088	1.774189
48	1	0	6.505494	2.922610	2.075531
49	1	0	4.479423	4.246605	1.547455
50	1	0	2.756624	3.332316	-0.005847
51	6	0	-1.406849	-1.241303	4.363052
52	1	0	2.487688	-1.310867	-3.559967
53	1	0	1.375092	-0.008856	-3.094045
54	1	0	0.402966	-2.310574	-2.882803
55	1	0	1.630411	-2.730123	-1.694802
56	1	0	-0.490194	-0.535444	-1.363211
57	1	0	0.729991	-0.924597	-0.157723
58	1	0	-0.153873	-3.287943	-0.037917
59	1	0	-1.398495	-2.868412	-1.203305
60	1	0	-2.334261	-3.006434	0.940462
61	1	0	-0.662123	-0.442214	4.339084
62	1	0	-0.958424	-2.157223	4.755101
63	1	0	-2.266062	-0.946844	4.964634

SCF Done: E(RB3LYP) = -1756.81307325   A.U. after   5 cycles
Zero-point correction=   0.493325 (Hartree/Particle)
 Thermal correction to Energy=   0.524918
 Thermal correction to Enthalpy=   0.525862

Thermal correction to Gibbs Free Energy=	0.427307
Sum of electronic and zero-point Energies=	-1756.319748
Sum of electronic and thermal Energies=	-1756.288155
Sum of electronic and thermal Enthalpies=	-1756.287211
Sum of electronic and thermal Free Energies=	-1756.385766

L-LyMebNI (conformational isomer, excited state (solvent=CH3CN) in Table S7)
LysMebNIA2Rtdoptpcmh.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.611639	3.275059	1.069589
2	6	0	5.738130	2.535788	1.378445
3	6	0	5.934675	1.244185	0.819952
4	6	0	4.943511	0.722606	-0.067679
5	6	0	3.794624	1.497366	-0.371497
6	6	0	3.636785	2.755557	0.191470
7	6	0	7.078232	0.451186	1.107103
8	6	0	7.231578	-0.799769	0.539038
9	6	0	6.250209	-1.309573	-0.337569
10	6	0	5.120059	-0.563629	-0.639029
11	6	0	4.098384	-1.109424	-1.559583
12	7	0	2.962580	-0.324170	-1.806013
13	6	0	2.762518	0.967335	-1.291269
14	6	0	1.944886	-0.881805	-2.727039
15	6	0	1.016836	-1.914169	-2.070676
16	6	0	0.114098	-1.359103	-0.959279
17	6	0	-0.781141	-2.463235	-0.381353
18	6	0	-1.737069	-2.100906	0.770229
19	6	0	-1.045675	-1.815936	2.103754
20	8	0	-1.929936	-1.449794	3.045668
21	8	0	0.131394	-2.032018	2.326322
22	7	0	-2.735486	-1.066829	0.418448
23	6	0	-3.970297	-1.523316	-0.070110
24	6	0	-4.960539	-0.512939	-0.436506
25	6	0	-4.665068	0.863774	-0.285626
26	6	0	-3.408888	1.275478	0.220755
27	6	0	-2.403762	0.280555	0.591683
28	6	0	-6.234589	-0.928329	-0.948990
29	6	0	-7.172884	0.023926	-1.294806
30	6	0	-6.891871	1.407193	-1.149144
31	6	0	-5.644782	1.847640	-0.646735
32	6	0	-5.320335	3.215264	-0.483783
33	6	0	-4.056650	3.611484	0.025946
34	6	0	-3.109772	2.669569	0.376318
35	8	0	1.763593	1.616216	-1.601757
36	8	0	4.216267	-2.209318	-2.101379
37	8	0	-4.198908	-2.742188	-0.184695
38	8	0	-1.294242	0.601312	1.053724
39	1	0	-6.433349	-1.988113	-1.054862
40	1	0	-8.139625	-0.280359	-1.684305
41	1	0	-7.642868	2.141435	-1.426947
42	1	0	-6.052440	3.971336	-0.753867
43	1	0	-3.840414	4.669502	0.138155
44	1	0	-2.139997	2.954247	0.766657
45	1	0	6.370152	-2.291596	-0.783339
46	1	0	8.109273	-1.397781	0.765109
47	1	0	7.834241	0.844108	1.782222
48	1	0	6.489351	2.935939	2.054542
49	1	0	4.470579	4.261028	1.502035
50	1	0	2.752472	3.335784	-0.050637
51	6	0	-1.404331	-1.217226	4.370421
52	1	0	2.485067	-1.344134	-3.555398
53	1	0	1.373782	-0.034951	-3.106918
54	1	0	0.393519	-2.330853	-2.874928
55	1	0	1.619574	-2.744966	-1.683720
56	1	0	-0.501843	-0.548437	-1.366880
57	1	0	0.723070	-0.922204	-0.161774
58	1	0	-0.155334	-3.286987	-0.016144
59	1	0	-1.403211	-2.880982	-1.183352
60	1	0	-2.340270	-2.995016	0.959118
61	1	0	-0.660179	-0.417615	4.343884
62	1	0	-0.954699	-2.131788	4.764436
63	1	0	-2.262889	-0.921925	4.972611

Zero-point correction= 0.489448 (Hartree/Particle)
Thermal correction to Energy= 0.521568
Thermal correction to Enthalpy= 0.522512

Thermal correction to Gibbs Free Energy= 0.422587
Sum of electronic and zero-point Energies= -1756.203306
Sum of electronic and thermal Energies= -1756.171186
Sum of electronic and thermal Enthalpies= -1756.170242
Sum of electronic and thermal Free Energies= -1756.270167

L-LyMebNI (ground state (solvent= Chloroform) in Table S7) LysMebNIXCpcmh.out

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.903780	-0.616307	1.784777
2	8	0	-5.063056	-1.364860	-0.210403
3	8	0	-2.271839	-0.331717	-2.729127
4	8	0	0.795020	-0.654491	1.552015
5	8	0	3.969593	-3.404208	-0.255201
6	7	0	-2.515865	-0.485179	-0.455852
7	8	0	-4.383465	-3.379159	0.551333
8	7	0	2.367170	-2.028110	0.614256
9	6	0	-2.264269	0.234223	-1.637762
10	6	0	4.075180	0.204127	0.222200
11	6	0	4.507055	-1.088112	-0.172128
12	6	0	4.931592	1.329769	0.017050
13	6	0	1.903733	-0.770668	1.033930
14	6	0	-2.592547	0.084887	0.825797
15	6	0	2.802332	0.388763	0.820584
16	6	0	-1.989283	1.682137	-1.496170
17	6	0	3.628742	-2.261049	0.044328
18	6	0	-2.302946	1.529609	0.945305
19	6	0	-2.012326	2.291723	-0.214978
20	6	0	3.236184	2.771051	1.009285
21	6	0	-1.745310	3.690364	-0.092568
22	6	0	-1.776578	4.279154	1.200326
23	6	0	2.393757	1.656156	1.207531
24	6	0	1.504000	-3.211095	0.842902
25	6	0	4.478955	2.613069	0.425542
26	6	0	-2.777833	-1.935557	-0.569810
27	6	0	-2.326980	2.136945	2.191393
28	6	0	-4.138772	-2.311012	0.025305
29	6	0	-1.710654	2.441329	-2.622928
30	6	0	-2.060554	3.517114	2.318090
31	6	0	0.757333	-3.675550	-0.418141
32	6	0	-1.627048	-2.803021	-0.033165
33	6	0	5.753809	-1.257205	-0.755037
34	6	0	-1.446687	3.822821	-2.507475
35	6	0	6.602766	-0.148750	-0.962066
36	6	0	6.201684	1.118709	-0.584053
37	6	0	-1.463506	4.435823	-1.268802
38	6	0	-0.370619	-2.754293	-0.915236
39	6	0	-6.398752	-1.641482	0.262430
40	1	0	-1.997562	-3.833180	0.009560
41	1	0	0.341457	-4.668921	-0.197279
42	1	0	-1.230917	4.402267	-3.400207
43	1	0	0.000874	-1.724810	-0.997741
44	1	0	-6.987941	-0.767592	-0.014281
45	1	0	7.575631	-0.298875	-1.420694
46	1	0	0.814689	-2.943462	1.643025
47	1	0	1.490894	-3.823393	-1.218628
48	1	0	-2.550497	1.535958	3.066819
49	1	0	6.856765	1.971872	-0.742512
50	1	0	-6.392132	-1.774840	1.346842
51	1	0	5.127128	3.472504	0.272841
52	1	0	2.157772	-4.011458	1.193946
53	1	0	6.067298	-2.253396	-1.049850
54	1	0	2.900570	3.756341	1.319235
55	1	0	-2.876547	-2.111707	-1.646208
56	1	0	-1.698408	1.957866	-3.594270
57	1	0	-1.574618	5.343067	1.297885
58	1	0	-1.399308	-2.502258	0.993123
59	1	0	1.417356	1.778084	1.664919
60	1	0	-0.640490	-3.063067	-1.934258
61	1	0	-1.262057	5.500624	-1.180556
62	1	0	-2.081839	3.977590	3.301388
63	1	0	-6.791797	-2.540136	-0.219159

SCF Done: E(RB3LYP) = -1756.80714974 A.U. after 1 cycles
Zero-point correction= 0.493472 (Hartree/Particle)
Thermal correction to Energy= 0.525073
Thermal correction to Enthalpy= 0.526017

Thermal correction to Gibbs Free Energy= 0.427496
Sum of electronic and zero-point Energies= -1756.313678
Sum of electronic and thermal Energies= -1756.282077
Sum of electronic and thermal Enthalpies= -1756.281132
Sum of electronic and thermal Free Energies= -1756.379653

L-LyMebNI (excited state (solvent=Chloroform) in Table S7) LysMebNICR.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.792396	-0.546402	-2.173470
2	6	0	-4.077121	-1.105970	-0.915406
3	6	0	-3.612751	-0.489650	0.272114
4	6	0	-2.825278	0.700387	0.162547
5	6	0	-2.521106	1.228307	-1.115554
6	6	0	-3.016094	0.603810	-2.276938
7	6	0	-3.884888	-1.005013	1.561795
8	6	0	-3.421607	-0.344122	2.712284
9	6	0	-2.669611	0.821877	2.602755
10	6	0	-2.361486	1.346034	1.332176
11	6	0	-1.554142	2.579910	1.228005
12	7	0	-1.210659	3.019872	-0.055422
13	6	0	-1.676733	2.435408	-1.242542
14	6	0	-0.265526	4.158939	-0.154841
15	6	0	1.173550	3.761012	0.219016
16	6	0	1.713689	2.558731	-0.569283
17	6	0	2.994328	1.971851	0.041551
18	6	0	3.331289	0.572427	-0.510962
19	6	0	4.637020	0.019574	0.060141
20	8	0	4.749623	-1.305328	-0.128831
21	8	0	5.514482	0.710905	0.541835
22	7	0	2.214844	-0.383992	-0.369047
23	6	0	1.565115	-0.810290	-1.543789
24	6	0	0.400102	-1.685121	-1.376155
25	6	0	-0.020377	-2.075020	-0.077568
26	6	0	0.688084	-1.645420	1.073176
27	6	0	1.871626	-0.793408	0.928163
28	6	0	-0.294379	-2.144265	-2.516451
29	6	0	-1.403915	-2.971041	-2.370457
30	6	0	-1.854703	-3.346654	-1.094038
31	6	0	-1.169482	-2.922446	0.072546
32	6	0	-1.573659	-3.290111	1.379792
33	6	0	-0.849877	-2.862302	2.504643
34	6	0	0.270366	-2.049408	2.359877
35	8	0	-1.382270	2.903889	-2.343661
36	8	0	-1.178384	3.198522	2.225636
37	8	0	1.966892	-0.440355	-2.655431
38	8	0	2.561285	-0.426389	1.889509
39	1	0	0.056621	-1.844190	-3.497431
40	1	0	-1.930393	-3.328258	-3.250983
41	1	0	-2.709576	-4.010144	-0.993157
42	1	0	-2.430401	-3.947594	1.502139
43	1	0	-1.167549	-3.172315	3.496165
44	1	0	0.837843	-1.716757	3.222061
45	1	0	-2.308439	1.340828	3.483701
46	1	0	-3.653466	-0.748345	3.692561
47	1	0	-4.490742	-1.901041	1.659103
48	1	0	-4.694839	-1.996319	-0.844616
49	1	0	-4.175303	-1.022787	-3.070280
50	1	0	-2.779497	1.034987	-3.243093
51	6	0	5.974212	-1.916006	0.329567
52	1	0	-0.624432	4.945622	0.512329
53	1	0	-0.324417	4.512122	-1.183483
54	1	0	1.806940	4.643864	0.058902
55	1	0	1.209677	3.540006	1.291661
56	1	0	1.880007	2.833154	-1.619367
57	1	0	0.944609	1.778180	-0.576159
58	1	0	2.895312	1.906984	1.129277
59	1	0	3.852339	2.621633	-0.160952
60	1	0	3.487803	0.645226	-1.592332
61	1	0	6.087622	-1.767515	1.406100
62	1	0	6.830930	-1.486685	-0.195723
63	1	0	5.871540	-2.975482	0.096220

SCF Done: E(RB3LYP) = -1756.79161212 A.U. after 1 cycles
Zero-point correction= 0.490070 (Hartree/Particle)
Thermal correction to Energy= 0.521680
Thermal correction to Enthalpy= 0.522624

Thermal correction to Gibbs Free Energy=	0.428176
Sum of electronic and zero-point Energies=	-1756.204423
Sum of electronic and thermal Energies=	-1756.172813
Sum of electronic and thermal Enthalpies=	-1756.171869
Sum of electronic and thermal Free Energies=	-1756.266317

L-LyMebNI (conformational isomer, ground state (solvent=Chloroform) in Table S7)
LysMebNIC2pcmh.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.525879	3.300815	-1.090266
2	6	0	-5.642486	2.561140	-1.431023
3	6	0	-5.856368	1.271181	-0.875329
4	6	0	-4.892180	0.752253	0.043034
5	6	0	-3.753619	1.528361	0.380082
6	6	0	-3.578123	2.784194	-0.180947
7	6	0	-6.990186	0.476391	-1.193923
8	6	0	-7.159104	-0.773115	-0.627829
9	6	0	-6.203510	-1.280864	0.278394
10	6	0	-5.084334	-0.533101	0.611334
11	6	0	-4.087996	-1.078919	1.561725
12	7	0	-2.958779	-0.293265	1.836370
13	6	0	-2.748401	1.002296	1.333647
14	6	0	-1.960805	-0.853324	2.776260
15	6	0	-1.032594	-1.897810	2.139530
16	6	0	-0.131063	-1.365292	1.015984
17	6	0	0.777505	-2.479264	0.478164
18	6	0	1.723046	-2.152889	-0.692461
19	6	0	1.018237	-1.926027	-2.030433
20	8	0	1.890997	-1.573144	-2.990530
21	8	0	-0.154757	-2.168693	-2.236409
22	7	0	2.715624	-1.097282	-0.386329
23	6	0	3.963314	-1.528051	0.104168
24	6	0	4.957623	-0.482456	0.430430
25	6	0	4.639451	0.887071	0.241813
26	6	0	3.372059	1.273580	-0.264330
27	6	0	2.364974	0.245649	-0.605231
28	6	0	6.201444	-0.846871	0.924688
29	6	0	7.160153	0.137933	1.243798
30	6	0	6.869673	1.477956	1.068931
31	6	0	5.606029	1.888505	0.565868
32	6	0	5.263838	3.253801	0.371631
33	6	0	4.021876	3.608654	-0.120351
34	6	0	3.071455	2.616021	-0.440552
35	8	0	-1.767992	1.657428	1.680555
36	8	0	-4.222867	-2.175965	2.101823
37	8	0	4.191830	-2.726965	0.251833
38	8	0	1.261167	0.521970	-1.065734
39	1	0	6.426637	-1.899288	1.062879
40	1	0	8.129194	-0.164447	1.629488
41	1	0	7.608645	2.236060	1.316026
42	1	0	5.995692	4.019234	0.617695
43	1	0	3.770077	4.655381	-0.262225
44	1	0	2.094877	2.891702	-0.824948
45	1	0	-6.332812	-2.262721	0.722071
46	1	0	-8.029125	-1.372700	-0.878865
47	1	0	-7.726479	0.866733	-1.892312
48	1	0	-6.372484	2.959439	-2.131418
49	1	0	-4.370996	4.285211	-1.522038
50	1	0	-2.699671	3.362243	0.086538
51	6	0	1.345098	-1.378411	-4.311853
52	1	0	-2.516083	-1.306743	3.599980
53	1	0	-1.387617	-0.007967	3.156646
54	1	0	-0.409091	-2.297920	2.952407
55	1	0	-1.635431	-2.736298	1.770345
56	1	0	0.472328	-0.533412	1.399276
57	1	0	-0.740389	-0.962230	0.201203
58	1	0	0.159282	-3.323181	0.147986
59	1	0	1.408201	-2.859131	1.292435
60	1	0	2.332909	-3.048098	-0.851695
61	1	0	0.590689	-0.588252	-4.292395
62	1	0	0.900174	-2.306667	-4.678648
63	1	0	2.191797	-1.086608	-4.932750

SCF Done: E(RB3LYP) = -1756.80549944 A.U. after 5 cycles
Zero-point correction= 0.493409 (Hartree/Particle)
Thermal correction to Energy= 0.525038

Thermal correction to Enthalpy= 0.525983
Thermal correction to Gibbs Free Energy= 0.426730
Sum of electronic and zero-point Energies= -1756.312091
Sum of electronic and thermal Energies= -1756.280461
Sum of electronic and thermal Enthalpies= -1756.279517
Sum of electronic and thermal Free Energies= -1756.378769

L-LyMebNI (conformational isomer, excited state (solvent=Chloroform) in Table S7)
LysMebNIC2Rtdoptpcmh.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.203474	3.616957	0.602827
2	6	0	4.268816	3.056986	1.329835
3	6	0	4.738017	1.755610	1.036914
4	6	0	4.105805	1.022067	-0.009293
5	6	0	3.038270	1.596866	-0.728655
6	6	0	2.592629	2.897597	-0.419122
7	6	0	5.802223	1.150700	1.740739
8	6	0	6.229640	-0.148953	1.413945
9	6	0	5.608208	-0.860394	0.392260
10	6	0	4.542041	-0.281015	-0.322447
11	6	0	3.870214	-1.065058	-1.402282
12	7	0	2.788651	-0.475804	-2.050653
13	6	0	2.361274	0.833819	-1.819819
14	6	0	2.035318	-1.305302	-3.030208
15	6	0	1.128052	-2.341691	-2.347637
16	6	0	0.203939	-1.755617	-1.271286
17	6	0	-0.727963	-2.819894	-0.679175
18	6	0	-1.558963	-2.411205	0.551704
19	6	0	-0.746088	-2.333591	1.842164
20	8	0	-1.524664	-1.997103	2.888223
21	8	0	0.413752	-2.691438	1.959643
22	7	0	-2.400788	-1.220996	0.342455
23	6	0	-3.703396	-1.457175	-0.144970
24	6	0	-4.536148	-0.291639	-0.366208
25	6	0	-4.032967	1.008238	-0.079077
26	6	0	-2.711642	1.189841	0.423740
27	6	0	-1.860517	0.044299	0.640844
28	6	0	-5.850500	-0.450787	-0.865853
29	6	0	-6.656912	0.665797	-1.075848
30	6	0	-6.185878	1.952633	-0.799234
31	6	0	-4.874498	2.158942	-0.297822
32	6	0	-4.353987	3.447592	0.000730
33	6	0	-3.056570	3.599543	0.497618
34	6	0	-2.235681	2.493924	0.710444
35	8	0	1.467644	1.353362	-2.471669
36	8	0	4.260493	-2.187943	-1.692741
37	8	0	-4.075824	-2.632021	-0.366252
38	8	0	-0.686731	0.111756	1.081594
39	1	0	-6.210235	-1.451645	-1.077322
40	1	0	-7.666340	0.535241	-1.459569
41	1	0	-6.825181	2.816798	-0.965313
42	1	0	-4.985053	4.318351	-0.161180
43	1	0	-2.683770	4.596723	0.722440
44	1	0	-1.229744	2.608294	1.098610
45	1	0	5.924320	-1.864946	0.136032
46	1	0	7.046386	-0.598625	1.967164
47	1	0	6.291552	1.694953	2.542520
48	1	0	4.736576	3.625894	2.127125
49	1	0	2.855097	4.614299	0.845831
50	1	0	1.766445	3.313876	-0.983281
51	6	0	-0.875445	-1.911596	4.168281
52	1	0	2.769623	-1.793461	-3.673972
53	1	0	1.452028	-0.605843	-3.627311
54	1	0	0.535981	-2.807943	-3.147317
55	1	0	1.745365	-3.136692	-1.912351
56	1	0	-0.391560	-0.938705	-1.697951
57	1	0	0.800473	-1.318481	-0.465922
58	1	0	-0.141800	-3.700918	-0.388959
59	1	0	-1.437321	-3.152339	-1.447000
60	1	0	-2.277541	-3.221038	0.718106
61	1	0	-0.088429	-1.153090	4.139625
62	1	0	-0.446704	-2.877984	4.447168
63	1	0	-1.657152	-1.623009	4.871187

SCF Done: E(RB3LYP) = -1756.79624240 A.U. after 1 cycles
Zero-point correction= 0.489935 (Hartree/Particle)
Thermal correction to Energy= 0.521959

Thermal correction to Enthalpy= 0.522903
Thermal correction to Gibbs Free Energy= 0.423032
Sum of electronic and zero-point Energies= -1756.195646
Sum of electronic and thermal Energies= -1756.163622
Sum of electronic and thermal Enthalpies= -1756.162678
Sum of electronic and thermal Free Energies= -1756.262550

L-LyMebNI (ground state (solvent=methanol) in Table S7) LysMebNIRXMeOHpcmh.out

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.895287	-0.590294	1.790348
2	8	0	-5.077106	-1.366172	-0.187206
3	8	0	-2.317638	-0.342990	-2.731455
4	8	0	0.823821	-0.709030	1.620098
5	8	0	3.954897	-3.401461	-0.339366
6	7	0	-2.529121	-0.475901	-0.453998
7	8	0	-4.372431	-3.344385	0.642310
8	7	0	2.370622	-2.049391	0.597074
9	6	0	-2.287657	0.233901	-1.645011
10	6	0	4.071934	0.191910	0.240459
11	6	0	4.497406	-1.088779	-0.196558
12	6	0	4.924024	1.323384	0.050191
13	6	0	1.919409	-0.805870	1.067833
14	6	0	-2.590952	0.105501	0.822228
15	6	0	2.810067	0.359693	0.866574
16	6	0	-1.995584	1.677575	-1.517618
17	6	0	3.621867	-2.265287	-0.000026
18	6	0	-2.293043	1.547401	0.928168
19	6	0	-2.002651	2.296741	-0.240779
20	6	0	3.245174	2.738011	1.107321
21	6	0	-1.720293	3.693269	-0.131241
22	6	0	-1.737788	4.293810	1.156433
23	6	0	2.407723	1.617414	1.292150
24	6	0	1.507989	-3.237221	0.800143
25	6	0	4.478217	2.595759	0.498842
26	6	0	-2.793793	-1.927235	-0.553105
27	6	0	-2.304728	2.167107	2.169477
28	6	0	-4.143533	-2.293923	0.071911
29	6	0	-1.716278	2.426256	-2.652258
30	6	0	-2.024238	3.545054	2.282839
31	6	0	0.746521	-3.662619	-0.465865
32	6	0	-1.633007	-2.793190	-0.035942
33	6	0	5.734896	-1.240416	-0.804990
34	6	0	-1.435350	3.804901	-2.549061
35	6	0	6.579866	-0.126489	-0.996149
36	6	0	6.184056	1.130172	-0.577652
37	6	0	-1.437179	4.427083	-1.314512
38	6	0	-0.383553	-2.725238	-0.926972
39	6	0	-6.410440	-1.633888	0.302067
40	1	0	-1.995617	-3.826672	-0.006172
41	1	0	0.330370	-4.660935	-0.269815
42	1	0	-1.218145	4.375001	-3.447203
43	1	0	-0.009612	-1.695035	-0.986486
44	1	0	-7.004670	-0.771991	0.000866
45	1	0	7.544791	-0.263267	-1.474953
46	1	0	0.828148	-2.993310	1.615525
47	1	0	1.470425	-3.787458	-1.278867
48	1	0	-2.530215	1.578770	3.052955
49	1	0	6.835432	1.987942	-0.724578
50	1	0	-6.397768	-1.731514	1.390080
51	1	0	5.123122	3.459230	0.356881
52	1	0	2.162653	-4.049174	1.121480
53	1	0	6.045662	-2.226846	-1.133401
54	1	0	2.913780	3.714716	1.446939
55	1	0	-2.914737	-2.111357	-1.625674
56	1	0	-1.715520	1.938021	-3.621247
57	1	0	-1.522927	5.355797	1.243599
58	1	0	-1.397499	-2.506042	0.992668
59	1	0	1.439450	1.729919	1.768664
60	1	0	-0.663534	-3.008536	-1.950502
61	1	0	-1.222291	5.489726	-1.235204
62	1	0	-2.035276	4.014398	3.261880
63	1	0	-6.801083	-2.548406	-0.150196

SCF Done: E(RB3LYP) = -1756.81454236   A.U. after   1 cycles
Zero-point correction=   0.493253 (Hartree/Particle)
 Thermal correction to Energy=   0.524865
 Thermal correction to Enthalpy=   0.525809

Thermal correction to Gibbs Free Energy= 0.427295
Sum of electronic and zero-point Energies= -1756.321290
Sum of electronic and thermal Energies= -1756.289678
Sum of electronic and thermal Enthalpies= -1756.288734
Sum of electronic and thermal Free Energies= -1756.387248

L-LyMebNI (excited state (solvent=methanol) in Table S7) LysMebNI2RMeOH.tdoptpcmh.out

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.799923	-0.542181	-2.182516
2	6	0	-4.090318	-1.101147	-0.925280
3	6	0	-3.625340	-0.487104	0.263339
4	6	0	-2.830690	0.698568	0.156886
5	6	0	-2.518675	1.224107	-1.120779
6	6	0	-3.015746	0.602884	-2.283393
7	6	0	-3.902427	-1.004805	1.551095
8	6	0	-3.440151	-0.346917	2.703865
9	6	0	-2.683146	0.816194	2.597851
10	6	0	-2.367198	1.340629	1.328930
11	6	0	-1.552686	2.567186	1.226831
12	7	0	-1.202419	3.006223	-0.055118
13	6	0	-1.663342	2.421006	-1.243353
14	6	0	-0.257984	4.145738	-0.150560
15	6	0	1.181801	3.750474	0.222755
16	6	0	1.726240	2.552717	-0.569464
17	6	0	3.005072	1.964447	0.044195
18	6	0	3.342251	0.564304	-0.505307
19	6	0	4.643475	0.005730	0.070543
20	8	0	4.768639	-1.310537	-0.155196
21	8	0	5.508608	0.689024	0.588140
22	7	0	2.223670	-0.390518	-0.365585
23	6	0	1.567273	-0.808354	-1.538845
24	6	0	0.398101	-1.675310	-1.372031
25	6	0	-0.025322	-2.060518	-0.072785
26	6	0	0.687904	-1.638337	1.077742
27	6	0	1.879016	-0.799979	0.930673
28	6	0	-0.302974	-2.127988	-2.511223
29	6	0	-1.421188	-2.942718	-2.364019
30	6	0	-1.875307	-3.312040	-1.086775
31	6	0	-1.183750	-2.894058	0.078243
32	6	0	-1.595801	-3.253323	1.385312
33	6	0	-0.868275	-2.832116	2.510355
34	6	0	0.263052	-2.035061	2.364797
35	8	0	-1.350927	2.885109	-2.344375
36	8	0	-1.172036	3.185716	2.225583
37	8	0	1.971098	-0.435869	-2.651264
38	8	0	2.579459	-0.442647	1.890542
39	1	0	0.046631	-1.832770	-3.494176
40	1	0	-1.954477	-3.292140	-3.243154
41	1	0	-2.738728	-3.963353	-0.984475
42	1	0	-2.463180	-3.895810	1.508106
43	1	0	-1.193886	-3.132555	3.501923
44	1	0	0.830825	-1.708477	3.229090
45	1	0	-2.324907	1.330828	3.482465
46	1	0	-3.676591	-0.751893	3.682624
47	1	0	-4.511338	-1.898943	1.644585
48	1	0	-4.714412	-1.986913	-0.856487
49	1	0	-4.184583	-1.015659	-3.079976
50	1	0	-2.777047	1.031269	-3.250246
51	6	0	5.993632	-1.930780	0.295131
52	1	0	-0.618150	4.930821	0.517637
53	1	0	-0.315463	4.503385	-1.177555
54	1	0	1.813081	4.635542	0.067658
55	1	0	1.216878	3.523390	1.294213
56	1	0	1.900147	2.834814	-1.616324
57	1	0	0.957507	1.772298	-0.583643
58	1	0	2.902046	1.902011	1.131711
59	1	0	3.863091	2.614270	-0.158250
60	1	0	3.503750	0.636637	-1.585743
61	1	0	6.095399	-1.818488	1.377075
62	1	0	6.851887	-1.479988	-0.208653
63	1	0	5.898612	-2.982074	0.025805

SCF Done: E(RB3LYP) = -1756.79950182   A.U. after   1 cycles
Zero-point correction=   0.490035 (Hartree/Particle)
 Thermal correction to Energy=   0.521589
 Thermal correction to Enthalpy=   0.522533

Thermal correction to Gibbs Free Energy= 0.428361
Sum of electronic and zero-point Energies= -1756.214170
Sum of electronic and thermal Energies= -1756.182616
Sum of electronic and thermal Enthalpies= -1756.181672
Sum of electronic and thermal Free Energies= -1756.275844

L-LyMebNI (conformational isomer, ground state (solvent=methanol) in Table S7)
LysMebNIMeOH2pcmh.out

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.576897	3.285002	1.092476
2	6	0	5.704763	2.549752	1.405847
3	6	0	5.911519	1.261696	0.842853
4	6	0	4.929115	0.739420	-0.054053
5	6	0	3.778576	1.509979	-0.362273
6	6	0	3.610671	2.764795	0.205284
7	6	0	7.056927	0.472922	1.134290
8	6	0	7.220296	-0.774627	0.561578
9	6	0	6.247545	-1.285115	-0.324201
10	6	0	5.115921	-0.543266	-0.630133
11	6	0	4.103427	-1.089699	-1.560468
12	7	0	2.965716	-0.308665	-1.811493
13	6	0	2.755394	0.979166	-1.291552
14	6	0	1.957688	-0.866247	-2.743121
15	6	0	1.029999	-1.907311	-2.100092
16	6	0	0.123086	-1.365217	-0.985811
17	6	0	-0.778667	-2.474617	-0.428105
18	6	0	-1.733306	-2.129661	0.730050
19	6	0	-1.041673	-1.874532	2.069809
20	8	0	-1.923913	-1.516852	3.016364
21	8	0	0.133964	-2.100446	2.288519
22	7	0	-2.728882	-1.084584	0.398652
23	6	0	-3.971942	-1.529747	-0.091997
24	6	0	-4.968901	-0.496686	-0.441415
25	6	0	-4.660041	0.877203	-0.269529
26	6	0	-3.397942	1.279135	0.238055
27	6	0	-2.386656	0.263158	0.594066
28	6	0	-6.208187	-0.874827	-0.938719
29	6	0	-7.170910	0.099341	-1.276503
30	6	0	-6.889722	1.443464	-1.116487
31	6	0	-5.631544	1.867851	-0.610984
32	6	0	-5.301133	3.237976	-0.430617
33	6	0	-4.064894	3.608278	0.065323
34	6	0	-3.109136	2.626606	0.401212
35	8	0	1.755418	1.624580	-1.605764
36	8	0	4.230306	-2.186495	-2.106393
37	8	0	-4.191493	-2.733958	-0.218545
38	8	0	-1.282009	0.551628	1.050599
39	1	0	-6.428373	-1.929731	-1.065047
40	1	0	-8.135518	-0.214055	-1.664011
41	1	0	-7.631659	2.193929	-1.376717
42	1	0	-6.037475	3.994617	-0.689159
43	1	0	-3.822610	4.658201	0.198697
44	1	0	-2.138449	2.916534	0.789841
45	1	0	6.375362	-2.264452	-0.773672
46	1	0	8.099320	-1.369419	0.790970
47	1	0	7.806375	0.866363	1.816389
48	1	0	6.449286	2.950497	2.088965
49	1	0	4.428084	4.268326	1.528338
50	1	0	2.725230	3.341816	-0.040383
51	6	0	-1.398018	-1.306863	4.345168
52	1	0	2.506174	-1.320871	-3.570294
53	1	0	1.384931	-0.020080	-3.122045
54	1	0	0.410057	-2.316821	-2.910589
55	1	0	1.633064	-2.740803	-1.719577
56	1	0	-0.487373	-0.546369	-1.385149
57	1	0	0.729902	-0.942441	-0.179085
58	1	0	-0.157082	-3.307816	-0.077659
59	1	0	-1.402131	-2.874898	-1.237863
60	1	0	-2.339191	-3.024943	0.902629
61	1	0	-0.649116	-0.511414	4.330753
62	1	0	-0.954267	-2.229777	4.725937
63	1	0	-2.255459	-1.015275	4.950666

SCF Done: E(RB3LYP) = -1756.81290623 A.U. after 1 cycles
Zero-point correction= 0.493144 (Hartree/Particle)
Thermal correction to Energy= 0.524814

Thermal correction to Enthalpy= 0.525758
Thermal correction to Gibbs Free Energy= 0.426322
Sum of electronic and zero-point Energies= -1756.319762
Sum of electronic and thermal Energies= -1756.288093
Sum of electronic and thermal Enthalpies= -1756.287148
Sum of electronic and thermal Free Energies= -1756.386584

L-LyMebNI (conformational isomer, excited state (solvent=methanol) in Table S7)
LysMebNIMeOH2Rtdoptpcmh.out

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.608948	3.276489	1.068190
2	6	0	5.735038	2.537303	1.378678
3	6	0	5.932080	1.245369	0.821128
4	6	0	4.941816	0.723379	-0.067267
5	6	0	3.793351	1.498088	-0.372795
6	6	0	3.635001	2.756594	0.189288
7	6	0	7.075243	0.452412	1.109947
8	6	0	7.229055	-0.798887	0.542780
9	6	0	6.248554	-1.309112	-0.334562
10	6	0	5.118824	-0.563220	-0.637657
11	6	0	4.098013	-1.109517	-1.558920
12	7	0	2.962511	-0.324328	-1.806918
13	6	0	2.762186	0.967665	-1.293441
14	6	0	1.945510	-0.882551	-2.728333
15	6	0	1.017236	-1.914764	-2.072052
16	6	0	0.114255	-1.359634	-0.960872
17	6	0	-0.781091	-2.463862	-0.383266
18	6	0	-1.736697	-2.101934	0.768697
19	6	0	-1.044887	-1.818032	2.102241
20	8	0	-1.928805	-1.451992	3.044572
21	8	0	0.132095	-2.034810	2.324433
22	7	0	-2.734843	-1.067317	0.417751
23	6	0	-3.969914	-1.523116	-0.070844
24	6	0	-4.959948	-0.512179	-0.436283
25	6	0	-4.664046	0.864348	-0.284534
26	6	0	-3.407617	1.275331	0.221797
27	6	0	-2.402648	0.279851	0.591815
28	6	0	-6.234244	-0.926849	-0.948745
29	6	0	-7.172341	0.025930	-1.293685
30	6	0	-6.890893	1.409010	-1.147135
31	6	0	-5.643556	1.848752	-0.644711
32	6	0	-5.318629	3.216161	-0.480858
33	6	0	-4.054693	3.611656	0.028800
34	6	0	-3.108001	2.669209	0.378252
35	8	0	1.763879	1.616598	-1.605646
36	8	0	4.216404	-2.209700	-2.099962
37	8	0	-4.198913	-2.741809	-0.186238
38	8	0	-1.292996	0.600011	1.053789
39	1	0	-6.433300	-1.986513	-1.055271
40	1	0	-8.139261	-0.277811	-1.683172
41	1	0	-7.641742	2.143663	-1.424256
42	1	0	-6.050581	3.972648	-0.750214
43	1	0	-3.838101	4.669533	0.141666
44	1	0	-2.137988	2.953238	0.768477
45	1	0	6.368797	-2.291426	-0.779608
46	1	0	8.106438	-1.396871	0.770142
47	1	0	7.830578	0.845642	1.785648
48	1	0	6.485551	2.937759	2.055388
49	1	0	4.467487	4.262699	1.499965
50	1	0	2.750963	3.336705	-0.054093
51	6	0	-1.402685	-1.220262	4.369242
52	1	0	2.486257	-1.345207	-3.556152
53	1	0	1.374514	-0.035942	-3.108918
54	1	0	0.394103	-2.331511	-2.876423
55	1	0	1.619849	-2.745545	-1.684881
56	1	0	-0.501592	-0.548917	-1.368537
57	1	0	0.723015	-0.922765	-0.163190
58	1	0	-0.155335	-3.287865	-0.018545
59	1	0	-1.403390	-2.881162	-1.185324
60	1	0	-2.340173	-2.995956	0.957141
61	1	0	-0.658160	-0.420997	4.342813
62	1	0	-0.953327	-2.135195	4.762718
63	1	0	-2.260920	-0.924835	4.971841

SCF Done: E(RB3LYP) = -1756.80634937 A.U. after 1 cycles
Zero-point correction= 0.489449 (Hartree/Particle)
Thermal correction to Energy= 0.521569

Thermal correction to Enthalpy= 0.522513
Thermal correction to Gibbs Free Energy= 0.422572
Sum of electronic and zero-point Energies= -1756.203129
Sum of electronic and thermal Energies= -1756.171009
Sum of electronic and thermal Enthalpies= -1756.170065
Sum of electronic and thermal Free Energies= -1756.270006

13. References

S1 CrysAlisPro Data Collection and Processing Software, Rigaku Corporation, Japan (2015).

S2. SHELXL 97, Sheldrick, G. M. University of Göttingen, Germany (1997).

S3. Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K., Puschmann, H.: J. Appl. Cryst. **42**, 339–341 (2009).

S4. Bourhis, L. J., Dolomanov, O. V., Gildea, R. J., Howard, J. A. K., Puschmann, H.: Acta Cryst. **A71**, 59–75 (2015).

S5. Gaussian 16, Revision C.01, Frisch, M. J., Trucks, G. W., Schlegel, H. B., Scuseria, G. E., Robb, M. A., Cheeseman, J. R., Scalmani, G., Barone, V., Petersson, G. A., Nakatsuji, H., Li, X., Caricato, M., Marenich, A., Bloino, J., Janesko, B. G., Gomperts, R., Mennucci, B., Hratchian, H. P., Ortiz, J. V., Izmaylov, A. F., Sonnenberg, J. L., Williams-Young, D., Ding, F., Lipparini, F., Egidi, F., Goings, J., Peng, B., Petrone, A., Henderson, T., Ranasinghe, D., Zakrzewski, V. G., Gao, J., Rega, N., Zheng, G., Liang, W., Hada, M., Ehara, M., Toyota, K., Fukuda, R., Hasegawa, J., Ishida, M., Nakajima, T., Honda, Y., Kitao, O., Nakai, H., Vreven, T., Throssell, K., Montgomery, Jr., J. A., Peralta, J. E., Ogliaro, F., Bearpark, M., Heyd, J. J., Brothers, E., Kudin, K. N., Staroverov, V. N., Keith, T., Kobayashi, R., Normand, J., Raghavachari, K., Rendell, A., Burant, J. C., Iyengar, S. S., Tomasi, J., Cossi, M., Millam, J. M., Klene, M., Adamo, C., Cammi, R., Ochterski, J. W., Martin, R. L., Morokuma, K., Farkas, O., Foresman, J. B., Fox, D. J.: Gaussian, Inc., Wallingford CT (2016).

S6. Becke, A. D.: J. Chem. Phys. **98**, 5648–5652 (1993).

S7. Lee, C., Yang, W., Parr, R. G.: Phys. Rev. **B37**, 785–789 (1988).

S8. Cancès, E., Mennucci, B., Tomasi, J.: J. Chem. Phys. **107**, 3032–3041 (1997).

S9. Cossi, M., Barone, V., Mennucci, B., Tomasi,: J. Chem. Phys. Lett. **286**, 253–260 (1998).

S10. Mennucci, B., Tomasi, J.: J. Chem. Phys. **106**, 5151–5158 (1997).