

Supplementary Materials: Novel NSAID-Derived Drugs for the Potential Treatment of Alzheimer's Disease

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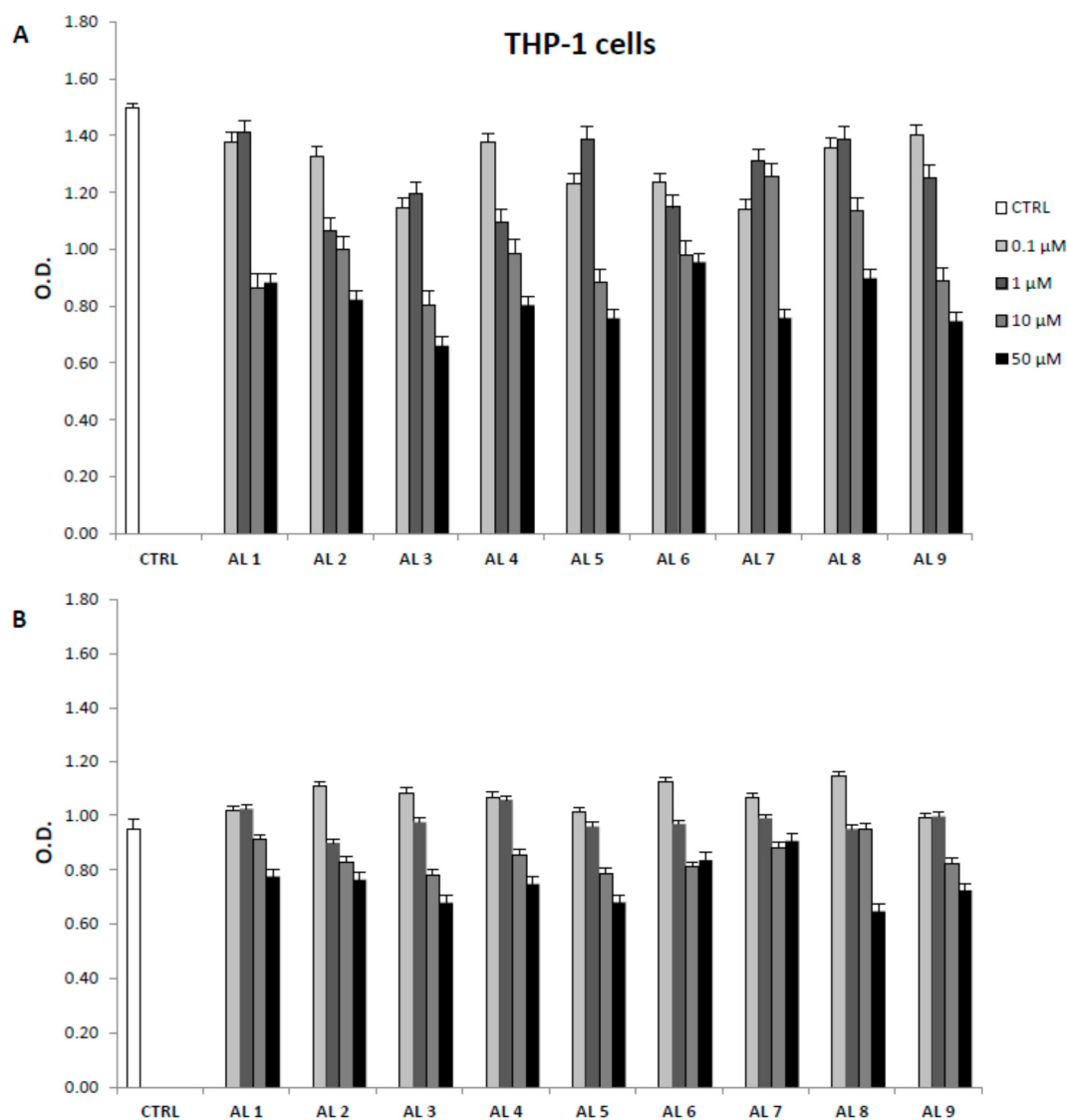


Figure S1. (A,B) Cellular vitality evaluated by MTT assay on THP-1 cell line for AL1–9.

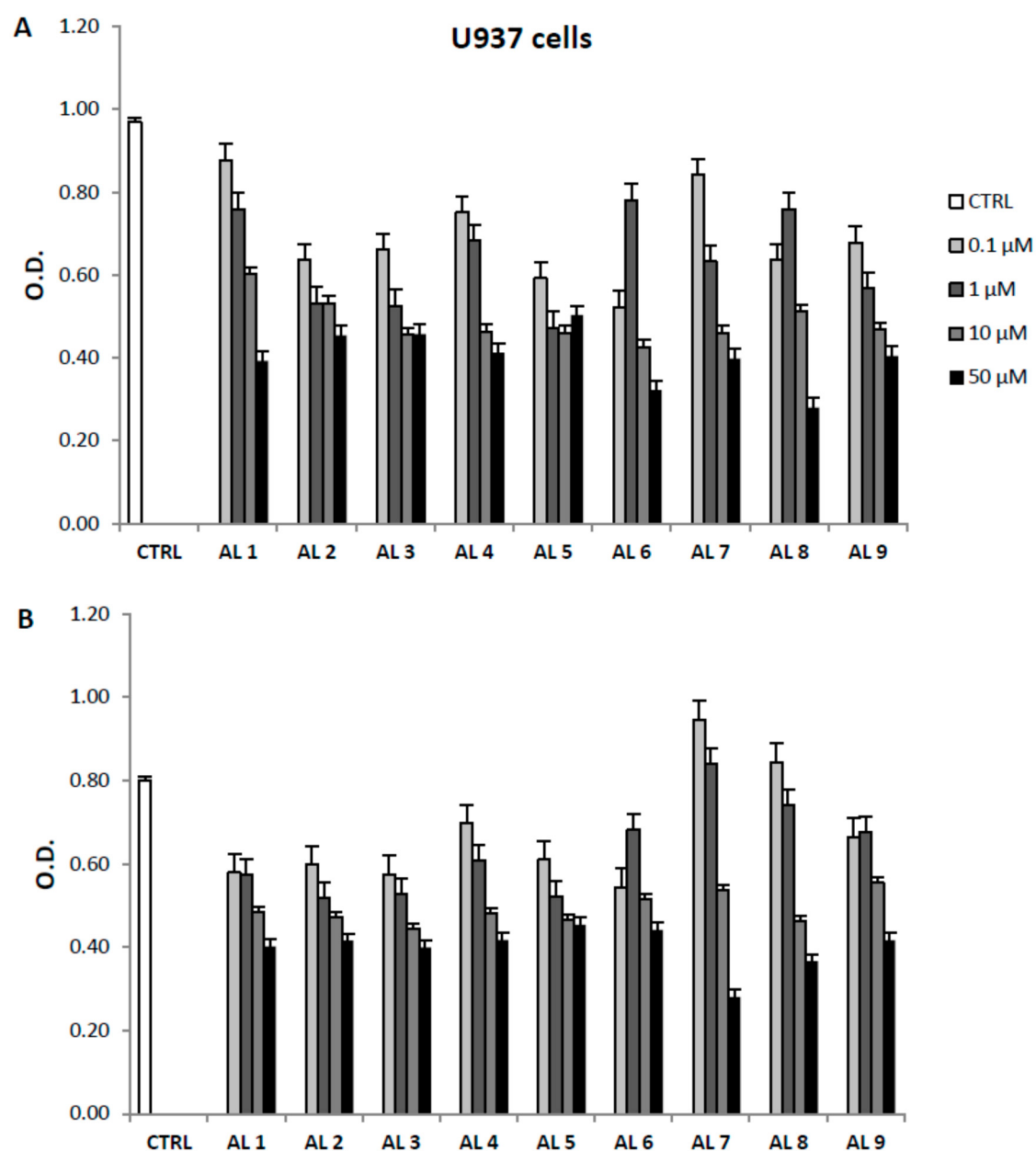
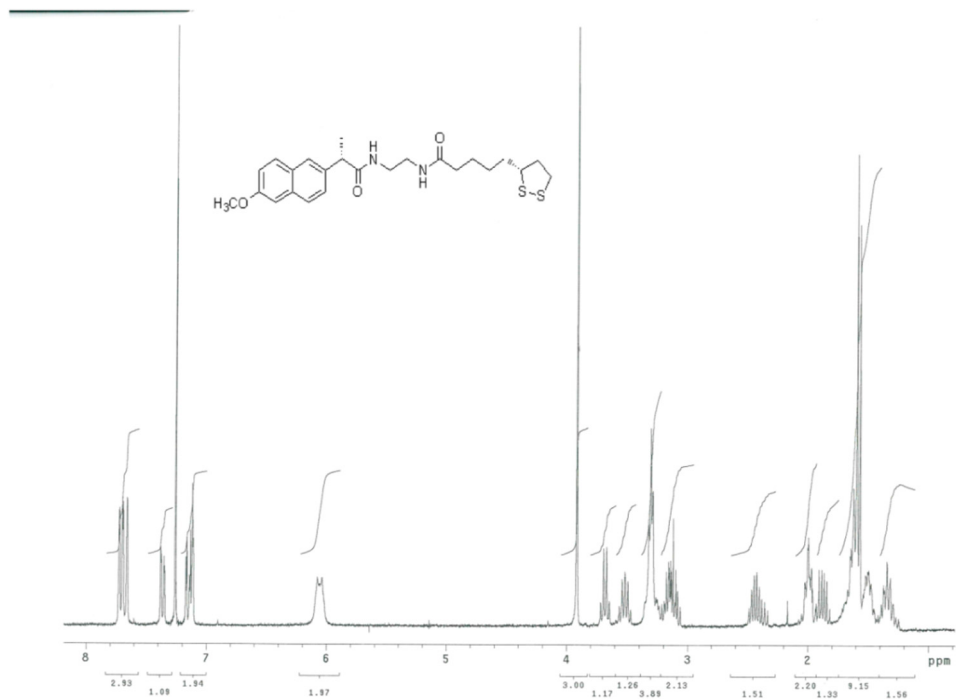
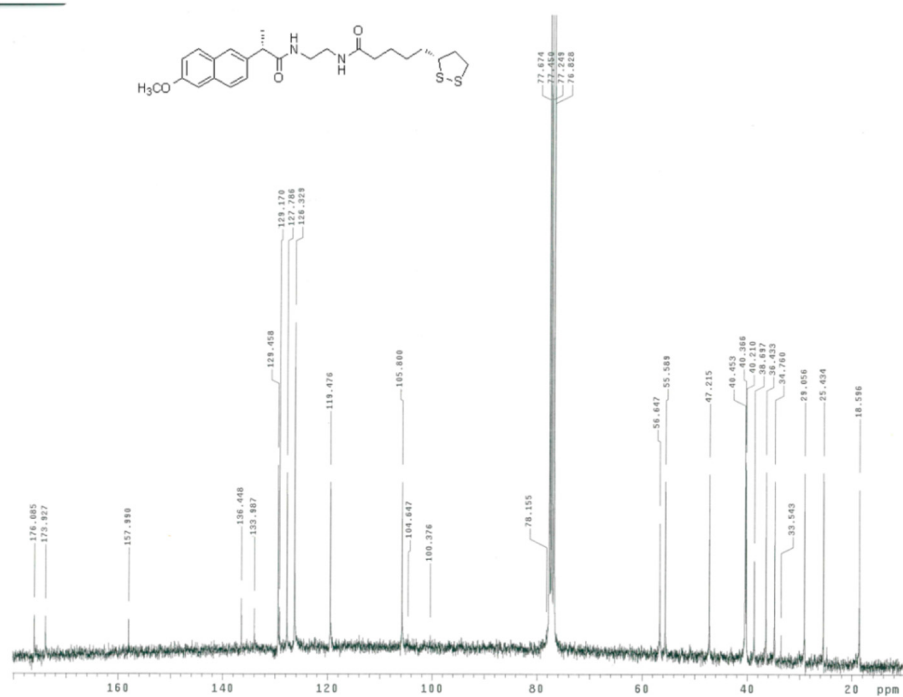


Figure S2. (A,B) Cellular vitality evaluated by MTT assay on U937 cell line for AL1–9.

(A)



(B)

Figure S3. (A) ¹H- and (B) ¹³C-NMR spectra of AL4.

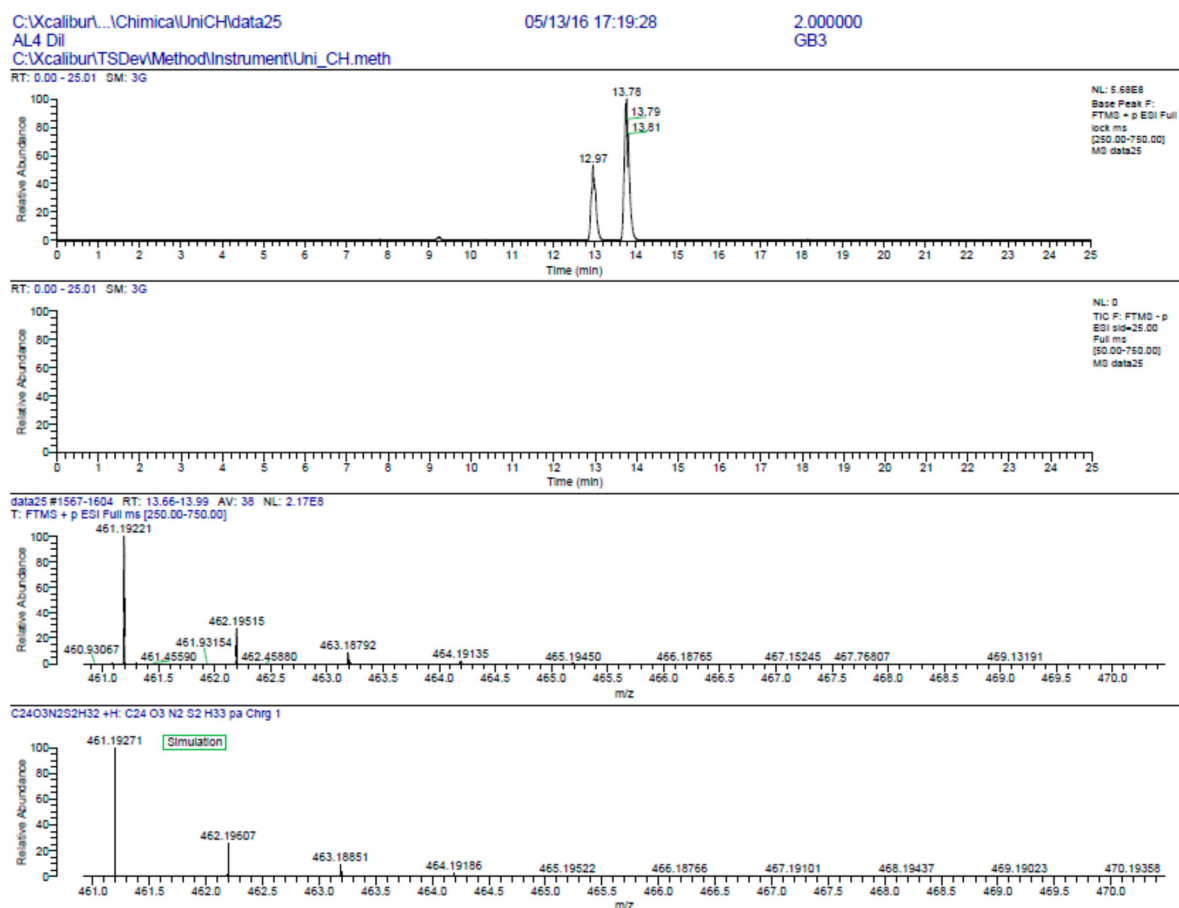
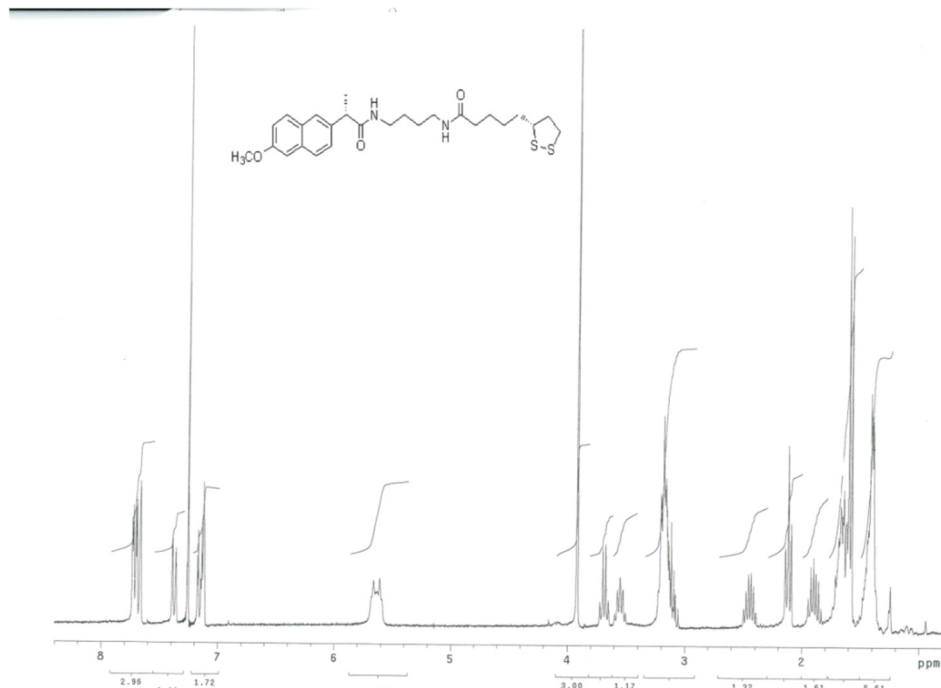
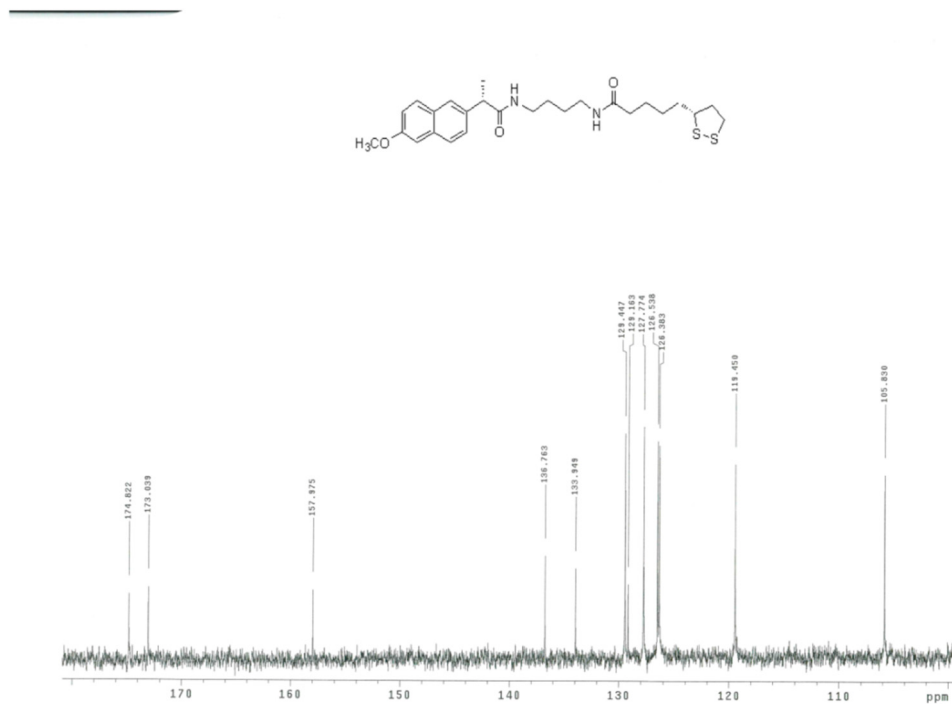


Figure S4. HR-MS spectra of AL4.

(A)



(B)

Figure S5. (A) ¹H- and (B) ¹³C-NMR spectra of AL5.

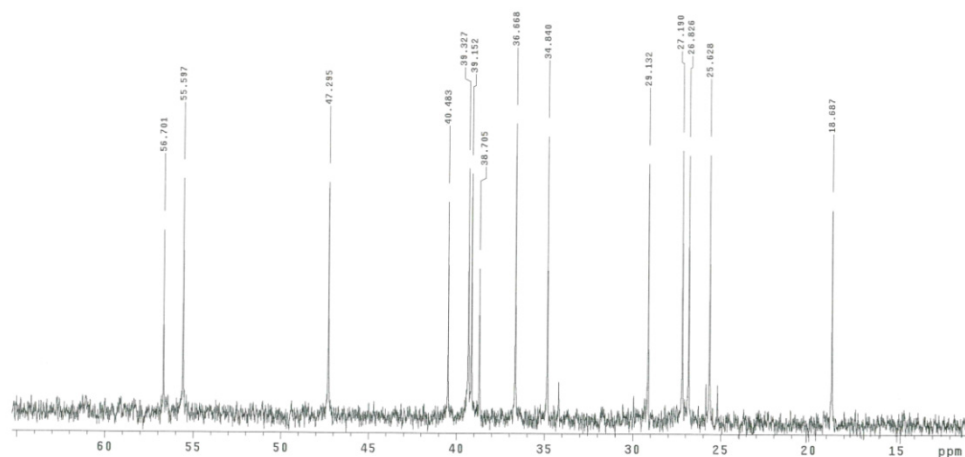
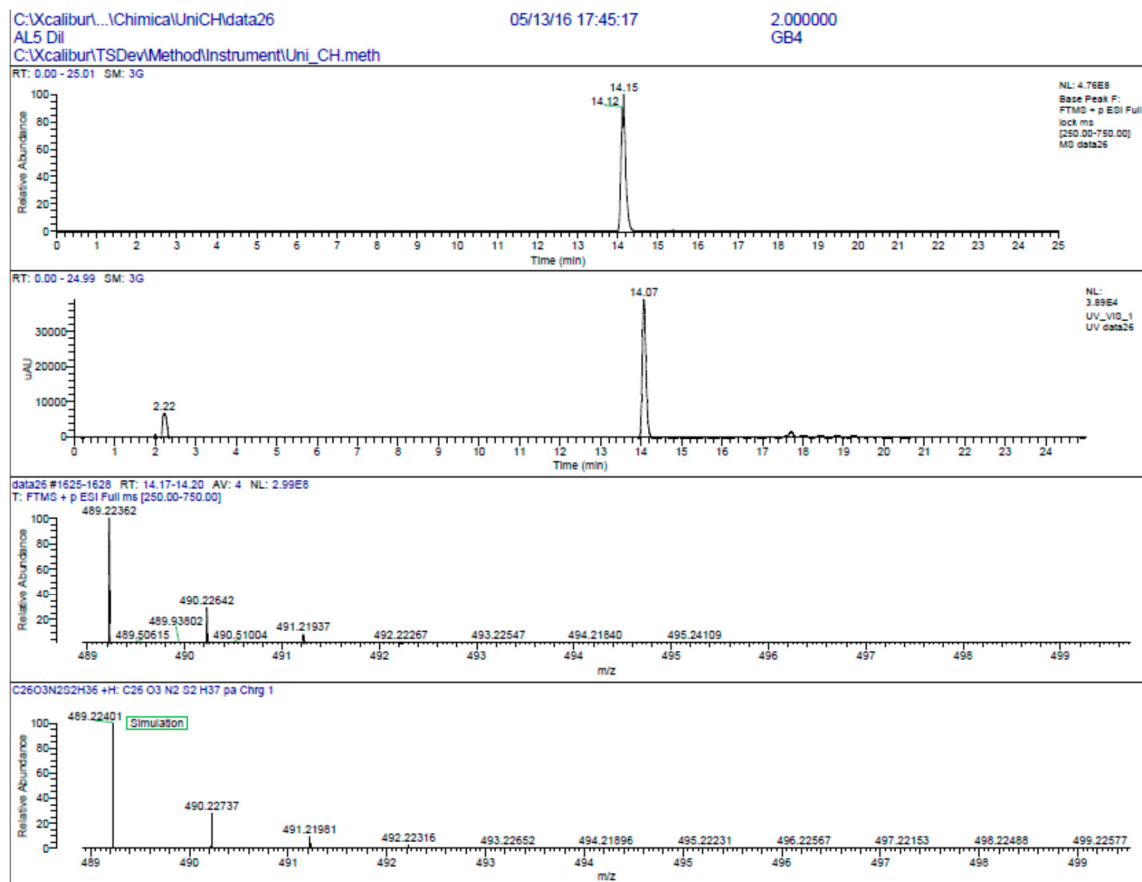
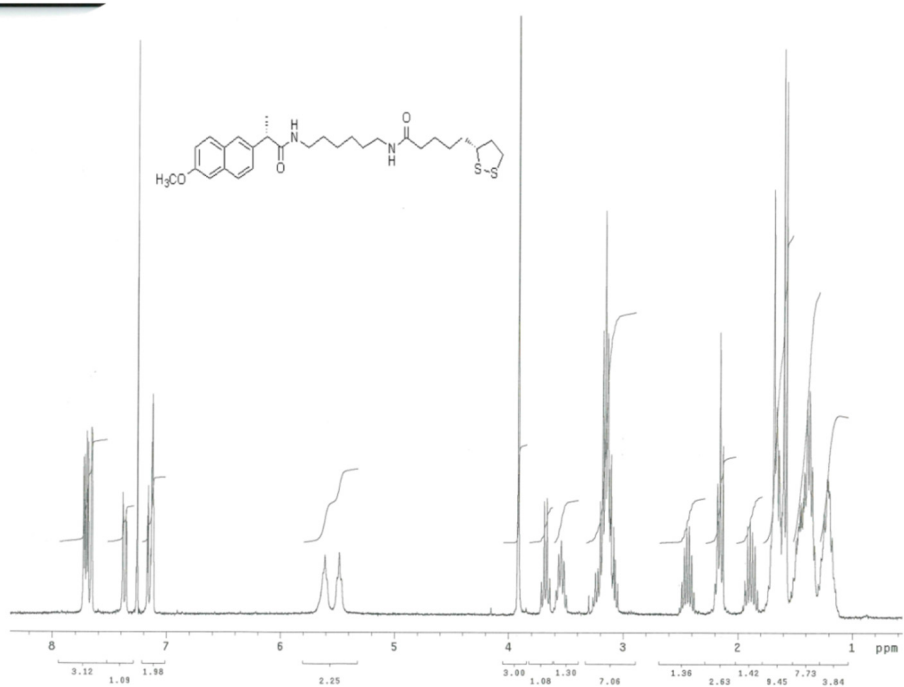
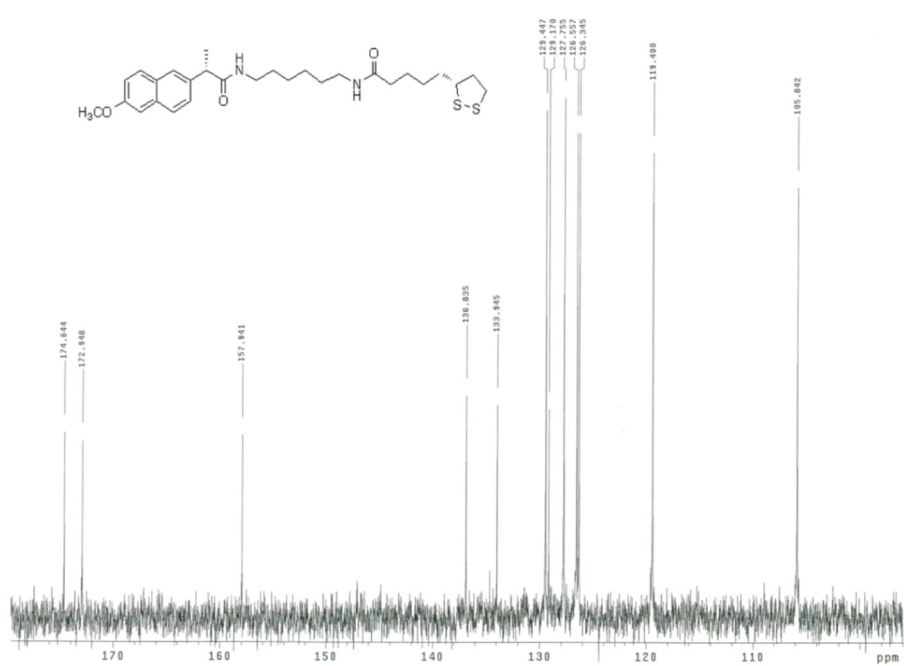
Figure S6. Expanded ^{13}C -NMR spectra of AL5.

Figure S7. HR-MS spectra of AL5.

(A)



(B)

**Figure S8.** (A) ^1H - and (B) ^{13}C -NMR spectra of AL6.

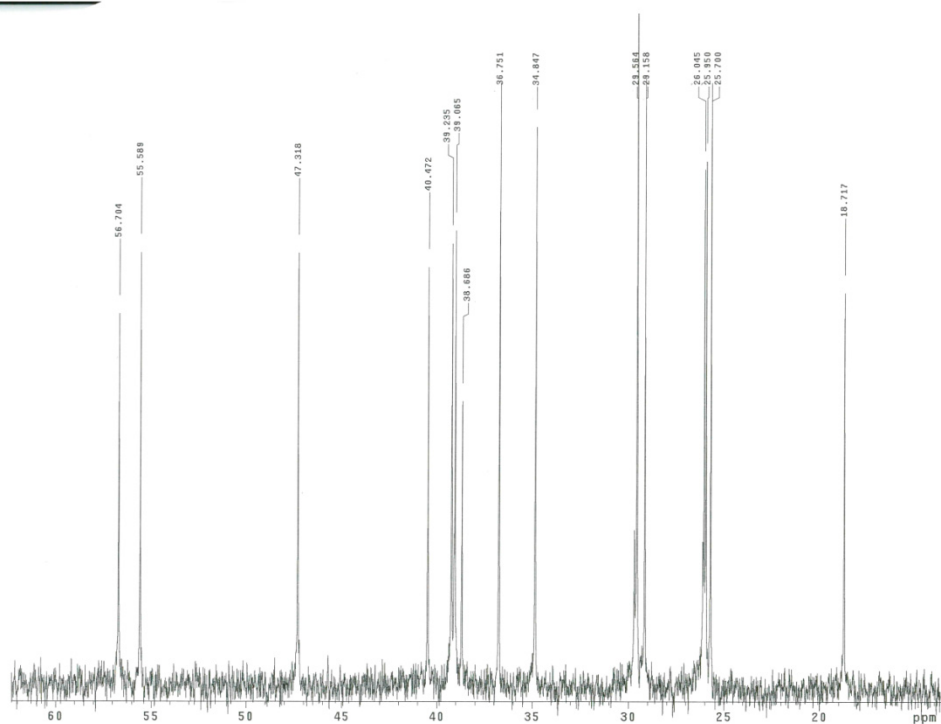
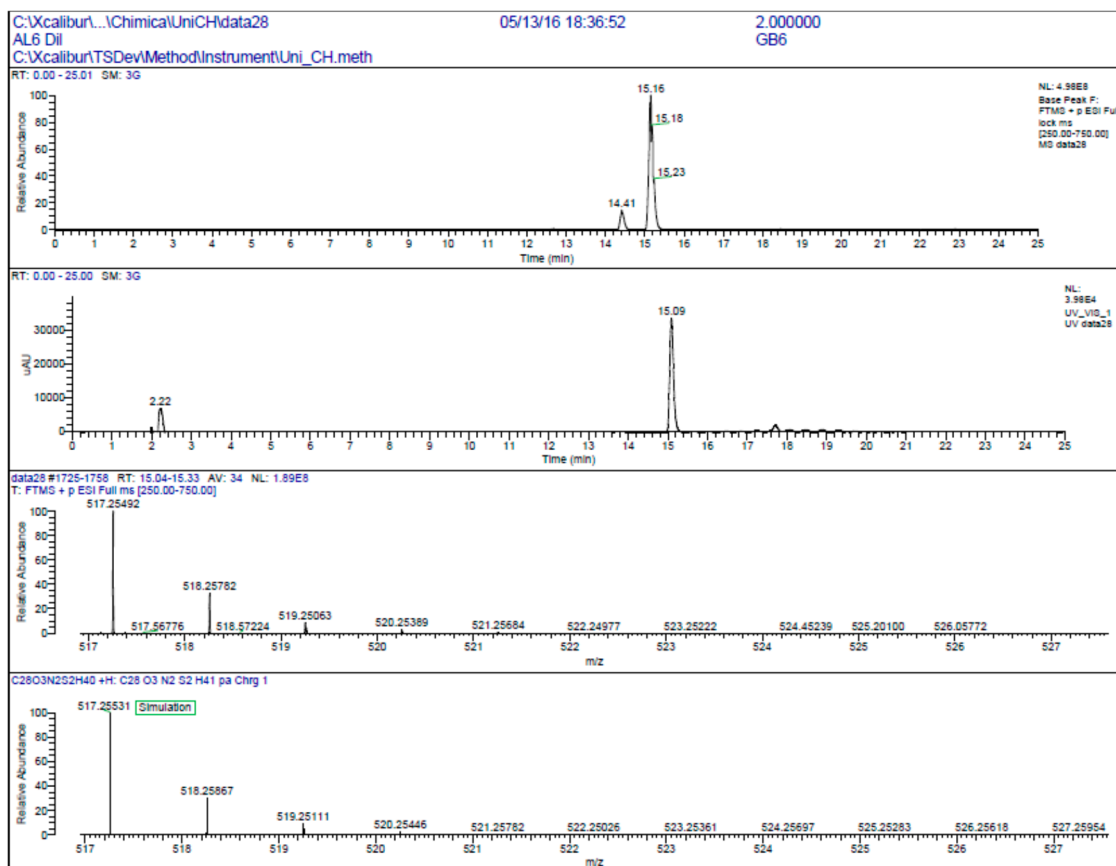
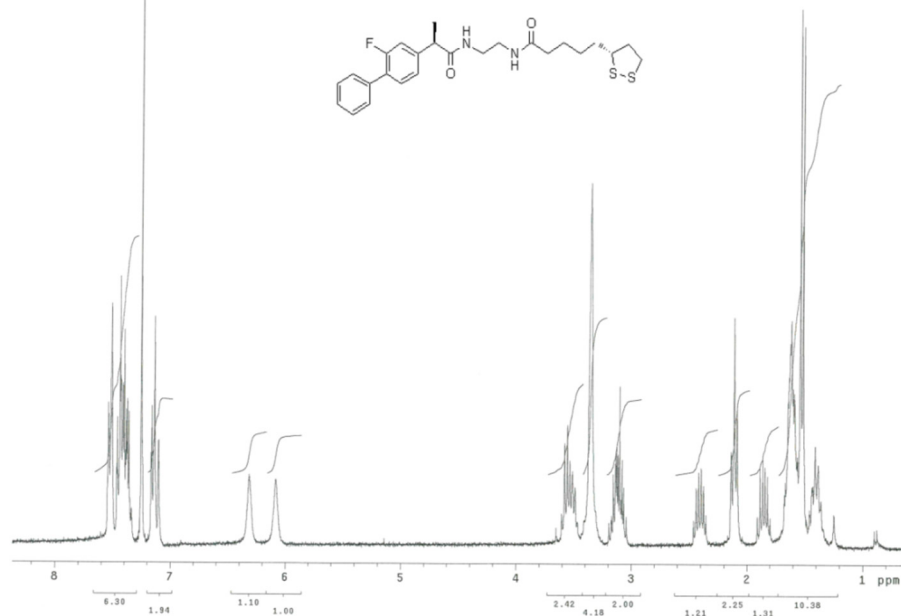
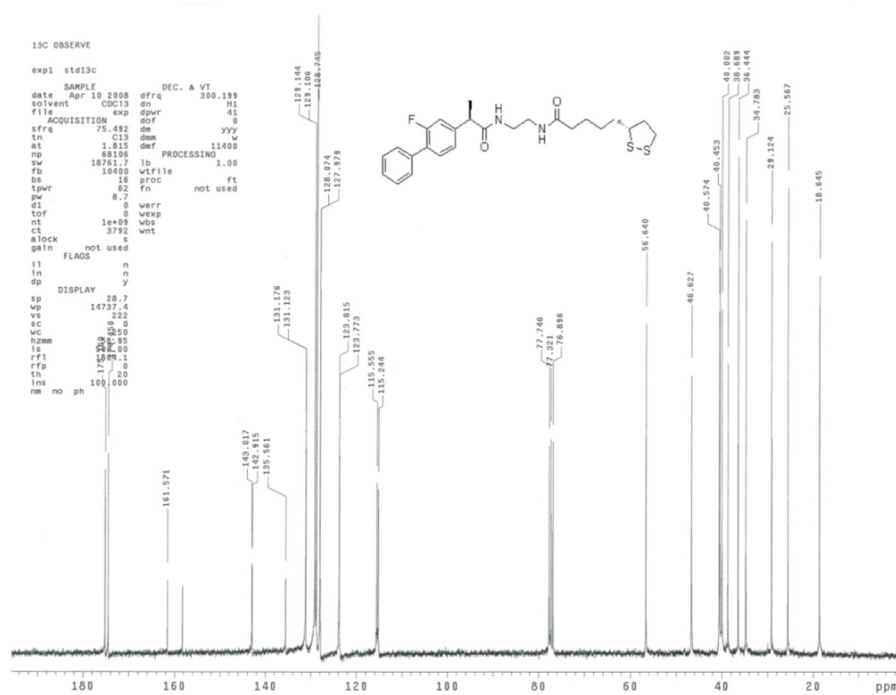
Figure S9. Expanded ^{13}C -NMR spectra of AL6.

Figure S10. HR-MS spectra of AL6.

(A)



(B)

Figure S11. (A) ¹H- and (B) ¹³C-NMR spectra of AL7.

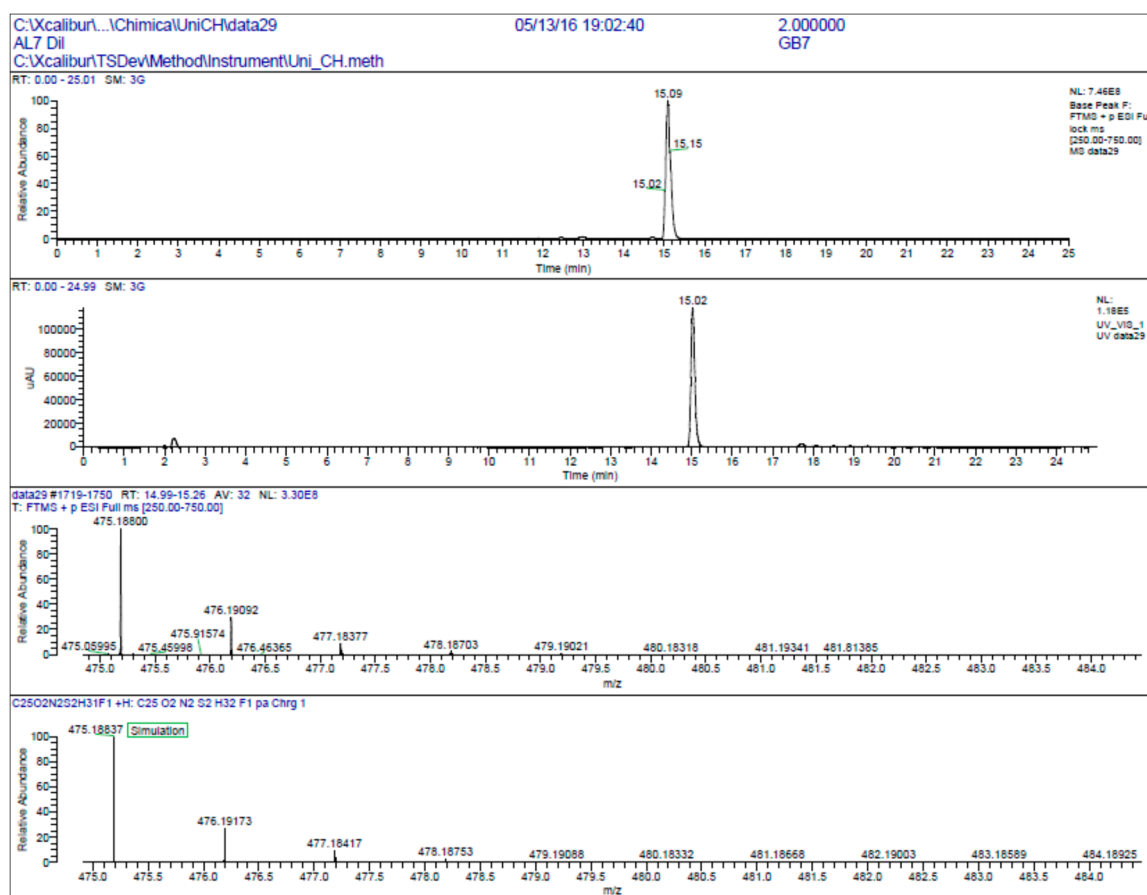


Figure S12. HR-MS spectra of AL7.

(A)

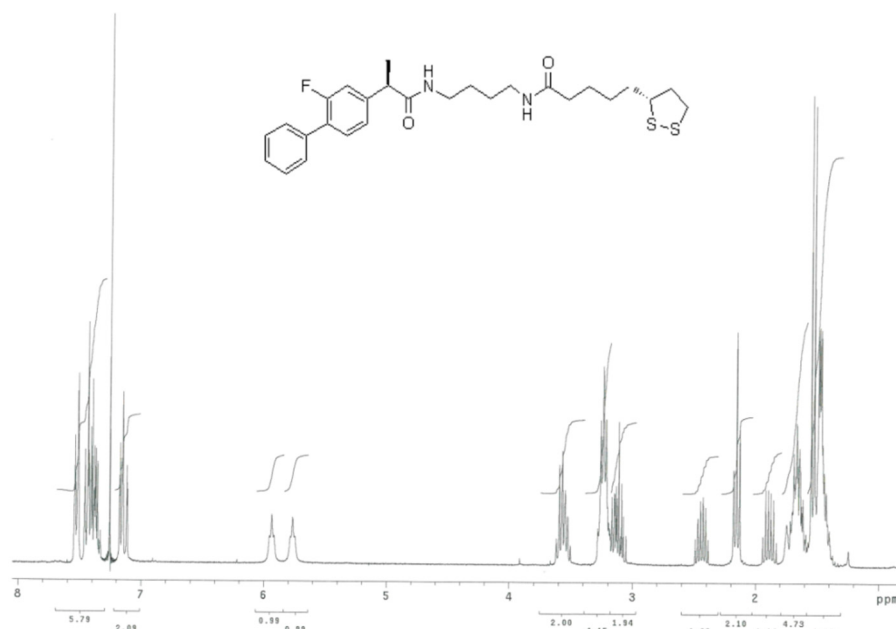
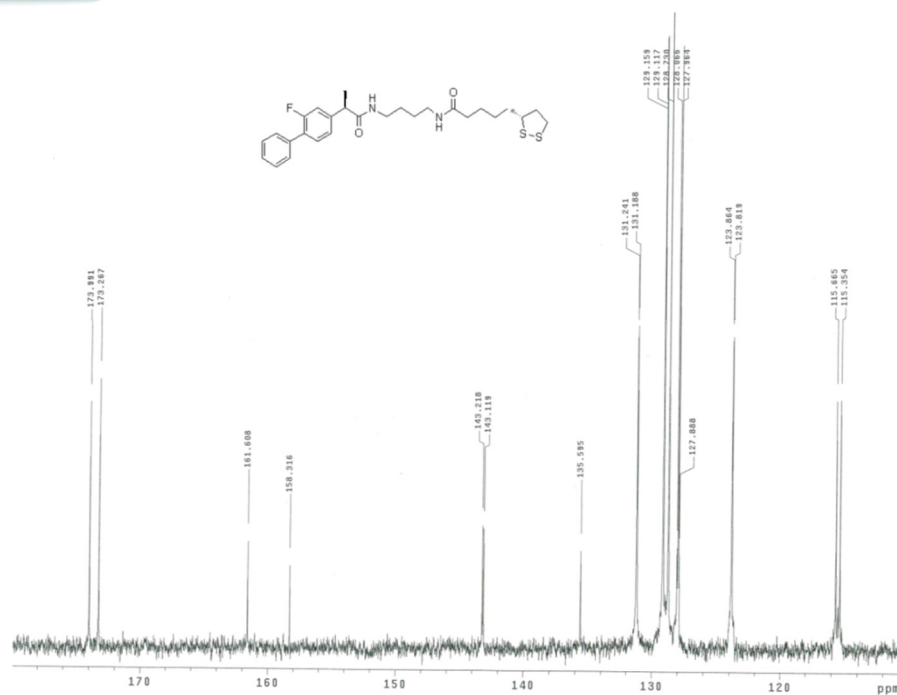
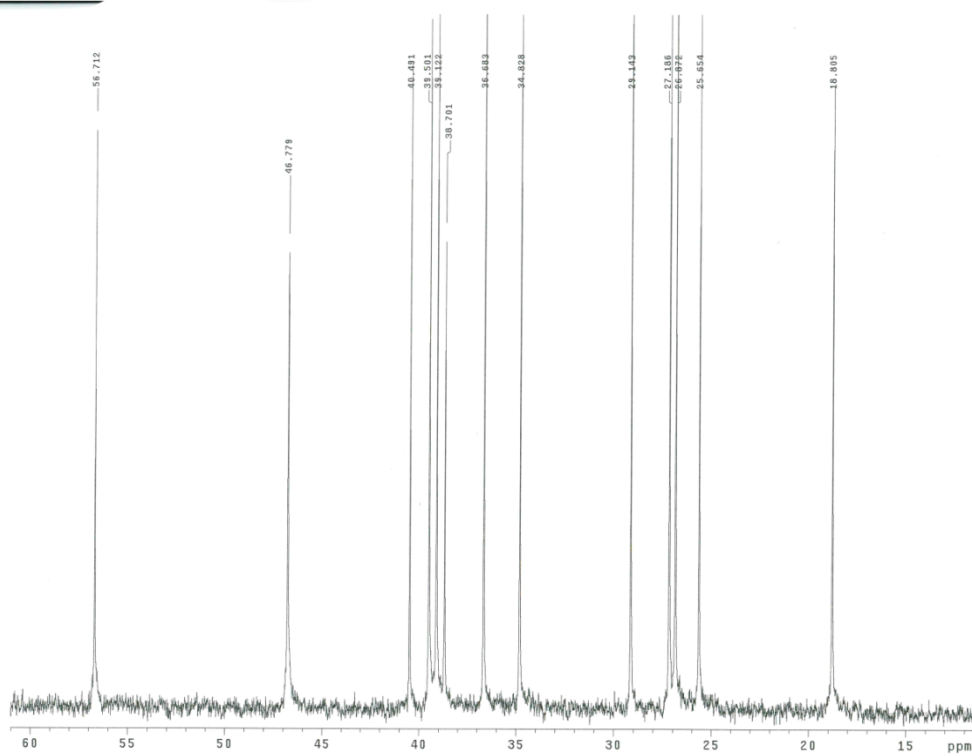


Figure S13. Cont.

(B)

Figure S13. (A) ¹H- and (B) ¹³C-NMR spectra of AL8.Figure S14. Expanded ¹³C-NMR spectra of AL8.

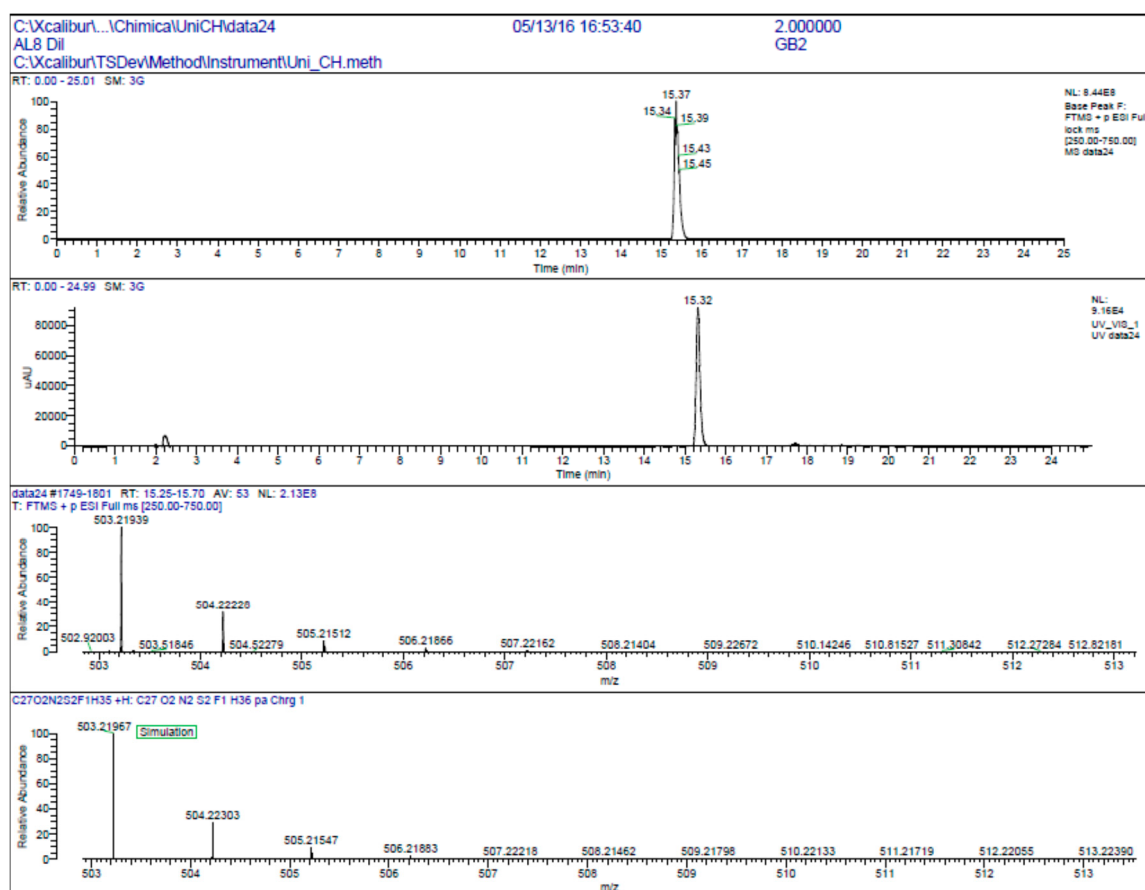


Figure S15. HR-MS spectra of AL8.

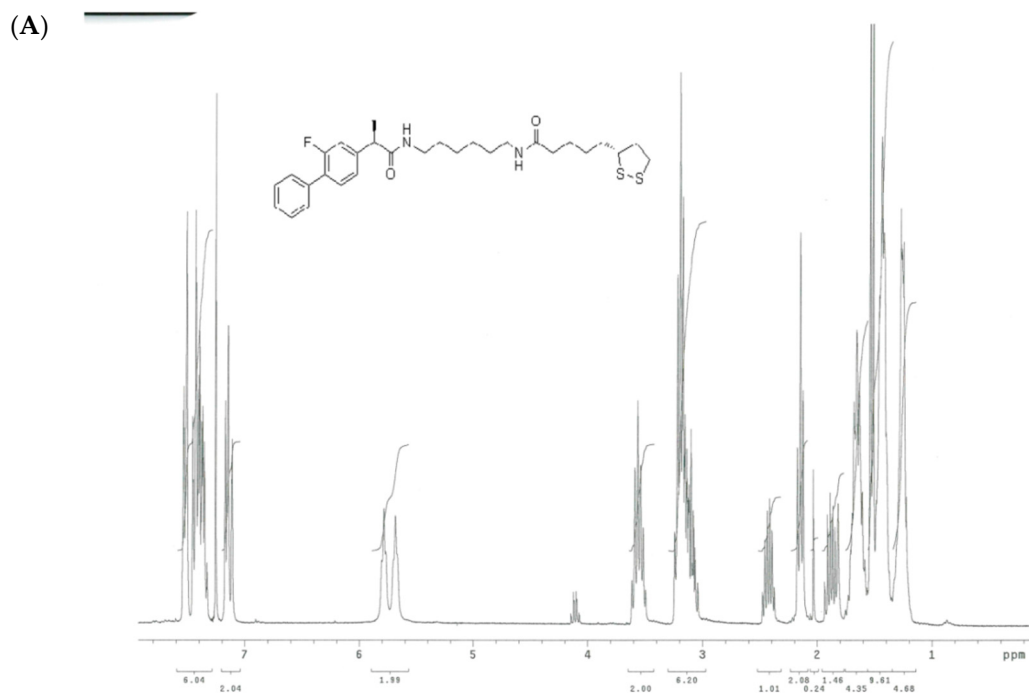


Figure S16. Cont.

(B)

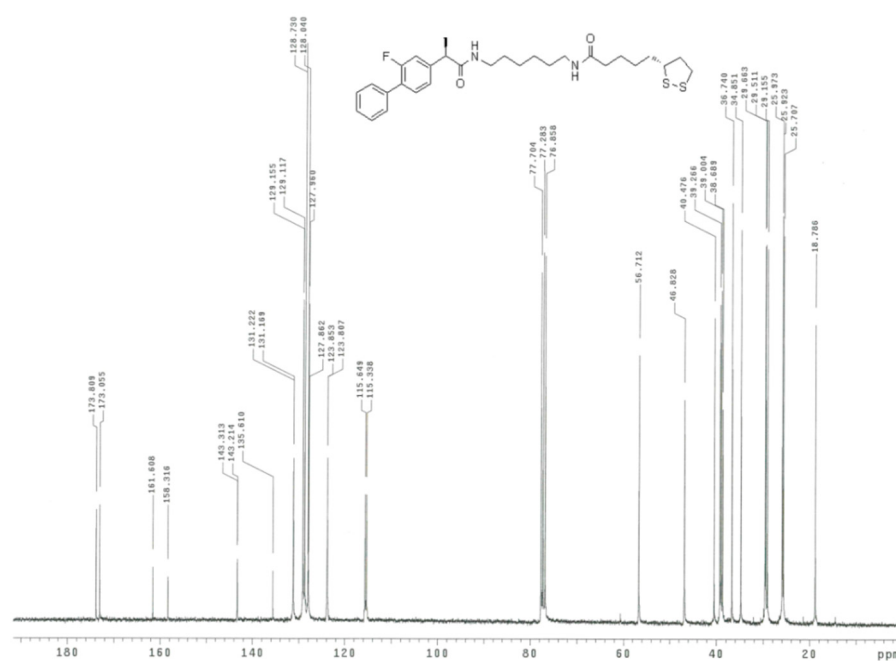
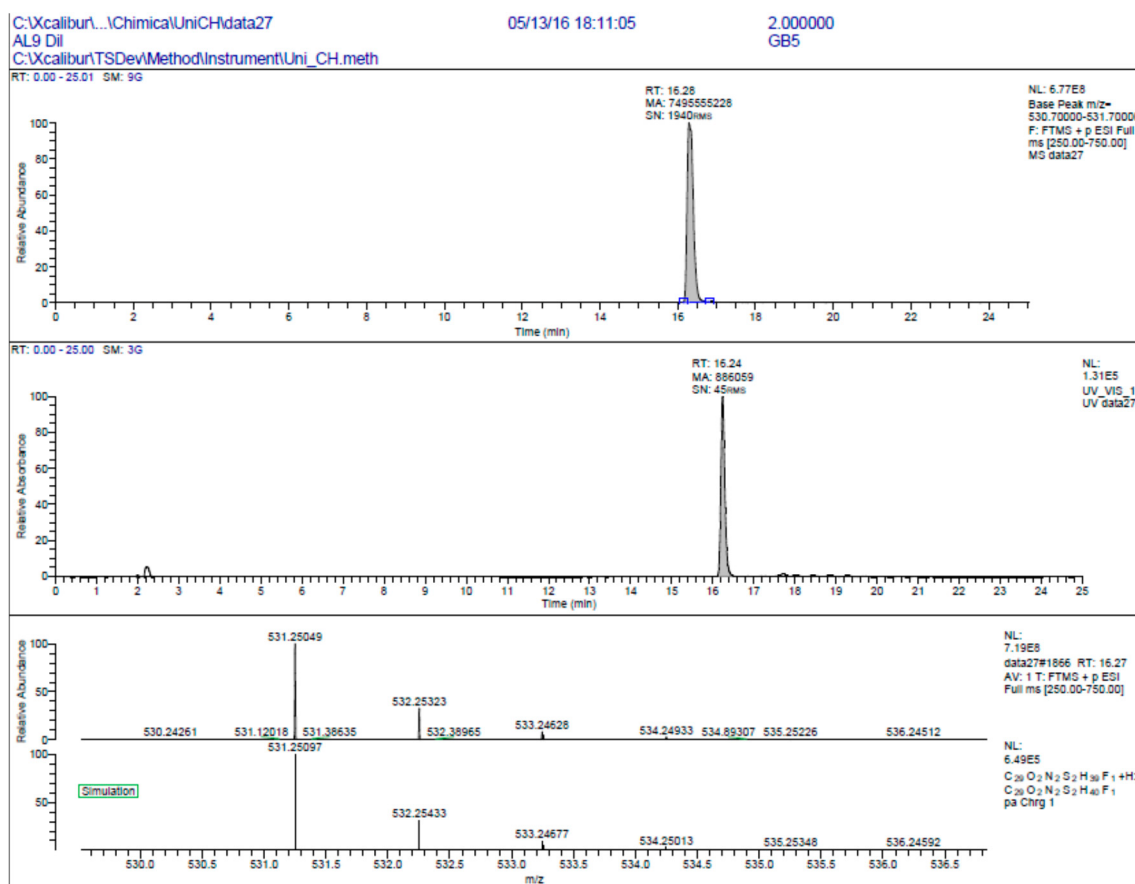
Figure S16. (A) ¹H- and (B) ¹³C-NMR spectra of AL9.

Figure S17. HR-MS spectra of AL9.

Table S1. Experimental conditions HR-MS.

Instrument Method: Uni_CH
Wednesday, 18 May 2016, 09:30:36; Page 1 of 4
Program for Dionex Chromatography MS Link
Column Oven. Temp Ctrl = On
Column Oven. Temperature. Nominal = 40.0 °C
Column Oven. Temperature. Lower Limit = 5.0 °C
Column Oven. Temperature. Upper Limit = 80.0 °C
Equilibration Time = None
Column Oven. Ready Temp Delta = 3.0 °C
Sampler. Temp Ctrl = Off
Pressure. Lower Limit = 10 bar
Pressure. Upper Limit = 468 bar
Maximum Flow Ramp Down = 0.250 mL/min ²
Maximum Flow Ramp Up = 0.250 mL/min ²
%A. Equate = "%A"
%B. Equate = "%B"
%C. Equate = "%C"
%D. Equate = "%D"
Draw Speed = 5.000 µL/s
Draw Delay = 3000 ms
Disp Speed = 20.000 µL/s
Dispense Delay = 0 ms
Waste Speed = 32.000 µL/s
Sample Height = 2.000 mm
Inject Wash = No Wash
Loop Wash Factor = 2.000
Puncture Offset = 0.0 mm
Pump Device = "Pump"
Inject Mode = Normal
Response Time = 2.000 s
UV_VIS_1.Wavelength = 280.0 nm
UV_VIS_1.Band width = 1 nm
UV_VIS_1.Ref Wavelength = Off
UV_VIS_1.Ref Band width = 1 nm
0.000 Wait UV. Ready and Pump. Ready and Column Oven. Ready and
Sampler. Ready and Pump Module. Ready
Chromeleon sets this property to signal to Xcalibur that it is ready to start a run.
Ready To Run = 1
Xcalibur sets this property to start the run or injection.
Wait StartRun
Autozero
Flow = 0.200 mL/min
%B = 0.0%
%C = 20.0%
%D = 80.0%
Curve = 5
Wait UV. Ready and Pump. Ready and Column Oven. Ready and
Sampler. Ready and Pump Module. Ready
Inject
Inject Response = 1
Chromeleon sets this property to signal the injection to Xcalibur.

Depending on your system configuration it might be necessary to manually insert a “Relay” command below in order to send the start signal to the MS.

Instrument Method: Uni_CH

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Typical syntaxes:

Pump_Relay_1. Closed Duration = 2.00

UM3PUMP_Relay1. On Duration = 2.00

UV_VIS_1.AcqOn

Flow = 0.200 mL/min

%B = 0.0%

%C = 20.0%

%D = 80.0%

Curve = 5

15.000 Flow = 0.200 mL/min

%B = 0.0%

%C = 95.0%

%D = 5.0%

Curve = 5

20.000 Flow = 0.200 mL/min

%B = 0.0%

%C = 95.0%

%D = 5.0%

Curve = 5

Flow = 0.200 mL/min

%B = 0.0%

%C = 20.0%

%D = 80.0%

Curve = 5

24.000 Flow = 0.200 mL/min

%B = 0.0%

%C = 20.0%

%D = 80.0%

Curve = 5

25.000 UV_VIS_1. AcqOff

Inject Response = 0

End

Instrument Method: Uni_CH

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Method of Q Exactive

Overall method settings

Global Settings

use lock masses best

Lock mass injection—

Chrom. peak width (FWHM) 30 s

Time

Method duration 25.00 min

Customized Tolerances (+/-)

Inclusion

Exclusion

Neutral Loss

Mass Tags

Dynamic Exclusion

Experiment
Full MS—SIM
General
Runtime 0 to 25 min
Polarity Positive
In-source CID 0.0 eV
Full MS—SIM
Microscans 1
Resolution 140,000
AGC target 5 e 5
Maximum IT 200 ms
Number of scan ranges 1
Scan range 250 to 750 m/z
Spectrum data type Profile
Setup
Tunefiles
General
Switch Count 0
Base Tune C:\Xcalibur\TSDiv\Method\cal mix.mstune
Contact Closure
General
Used False
Start in Closed True
Switch Count 0
Syringe
General
Instrument Method: Uni_CH
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Used False
Start in OFF True
Stop at end of run False
Switch Count 0
Pump setup
Syringe type Hamilton
Flow rate 3.000 µL/min
Inner diameter 2.303 mm
Volume 250 µL
Divert Valve A
General
Used False
Start in 1-2 True
Switch Count 0
Divert Valve B
General
Used False
Start in 1-2 True
Switch Count 0
Lock Masses
1 entry
Mass Polarity Start End Comment
