Electronic Supplementary Material (ESI) for Food & Function.

Characterisation of pancreatic lipase inhibitors from *Brassica rapa* L. ssp. *Chinensis*

Joanne Yi Hui Toy [a], Yu yan Lim [a], Habiba Shalash [c], Dejian Huang [a, b, *]

[a] *Department of Food Science & Technology, National University of Singapore, Singapore 117542, Singapore*

[b] *National University of Singapore (Suzhou) Research Institute, 377 Lin Quan Street, Suzhou Industrial Park, Suzhou, Jiangsu 215123, PR China*

[c] *Wageningen University & Research, Droevendaalsesteeg 4, 6708 PB Wageningen, The Netherlands*

[*] *Corresponding author:* Email: dejian@nus.edu.sg

Supplementary figures

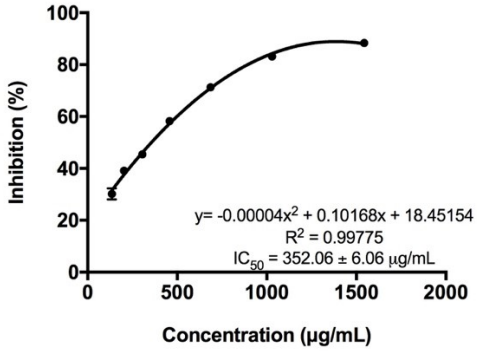


Figure S1: Dose-response curve of PL inhibition against concentration of naibai extract (a) DCM extract.

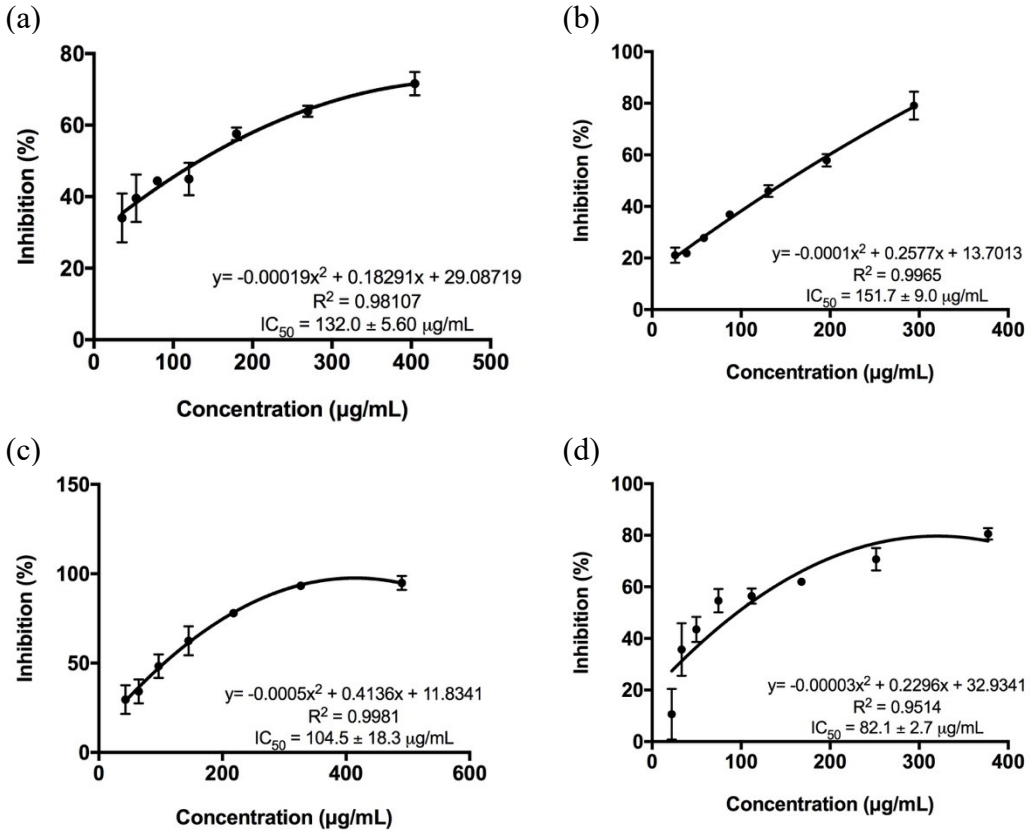


Figure S2: Dose-response curve of PL inhibition against different concentration of *Brassica rapa* ssp. *chinensis* extract (a) NB1, (b) NB2, (c) NB3 and (d) NB4.

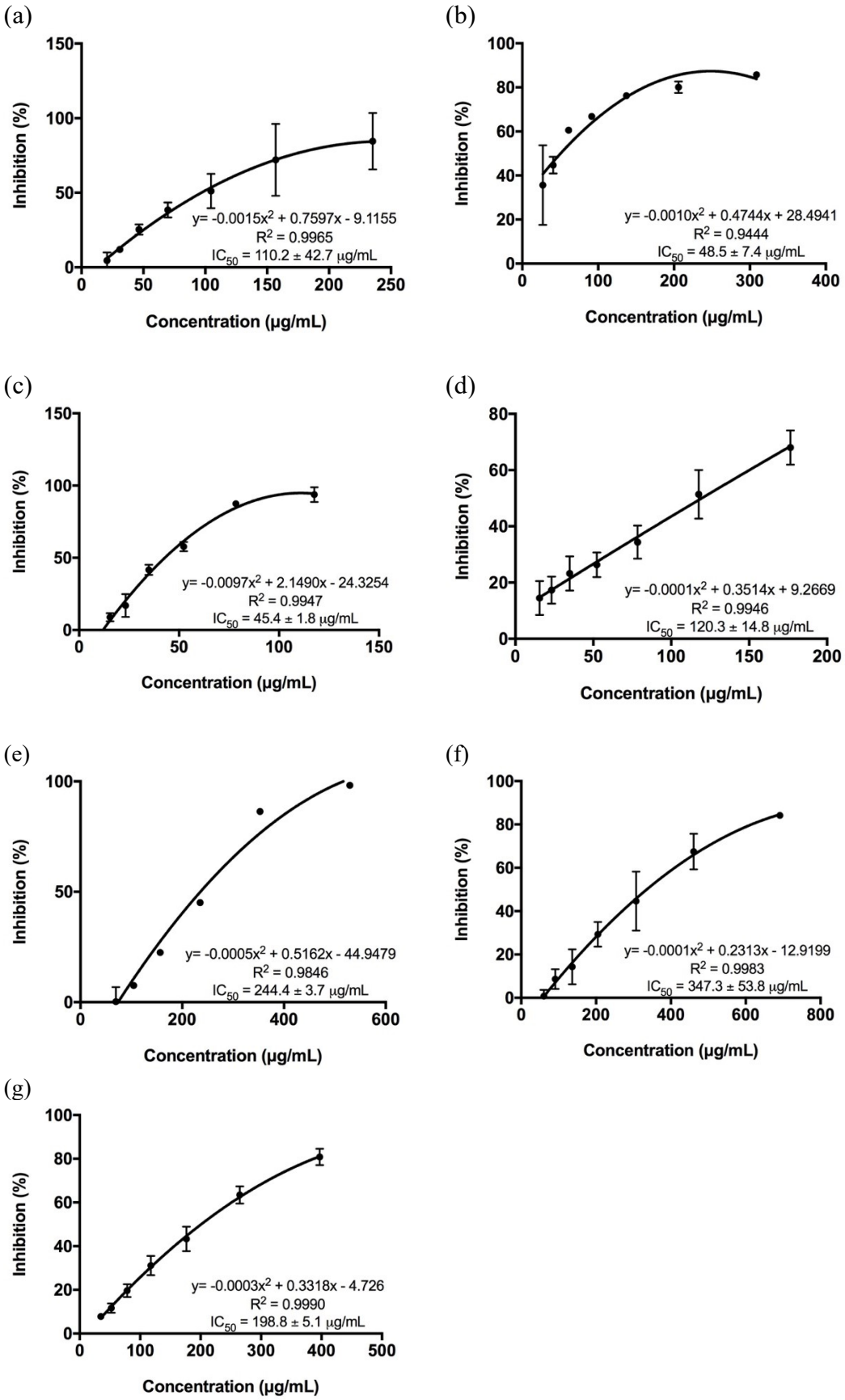
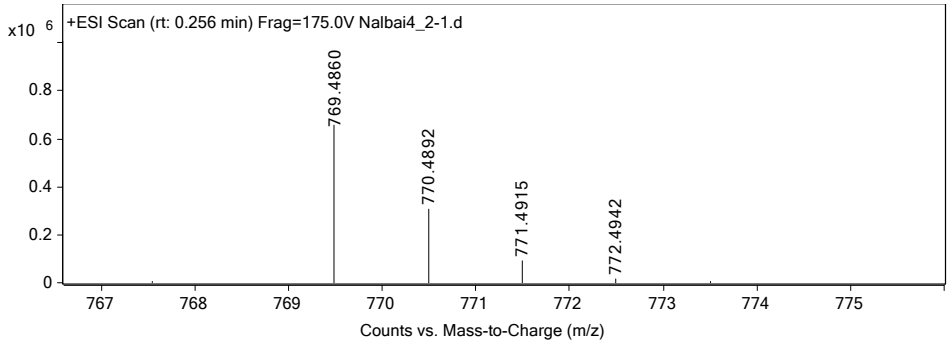


Figure S3: Dose-response curve of PL inhibition against different concentration of *Brassica rapa* ssp. *chinensis* extract after semi-preparative HPLC (a) NB4.1, (b) NB4.2, (c) NB4.3, (d) NB4.4, (e) NB4.5, (f) NB4.6, (g) NB4.7.

Mass Spectrum SmartFormula Report

Sample Name	Nalbai4.2	Data File	D:\MassHunter\Data\External\FST\20210817\Nalbai4_2-1.d
Instrument Name	Agilent 6546 LC-QTOF	IRM Calibration Status	Success
Acq Method	MS Scan_union-1.m	Acquired Time	17/8/2021 12:11:27 PM (UTC+08:00)
Comment	A/P Huang Dejian	Operator	

Meas. m/z	#	Formula	Calc. Mass	Err [ppm]
769.486	1	C43 H70 Na O10	769.4861	0.13



Page 1 of 1 Printed at 12:31 PM on 20-Aug-2021

Figure S4: HR-ESIMS of NB4.2 (Cationic mode).

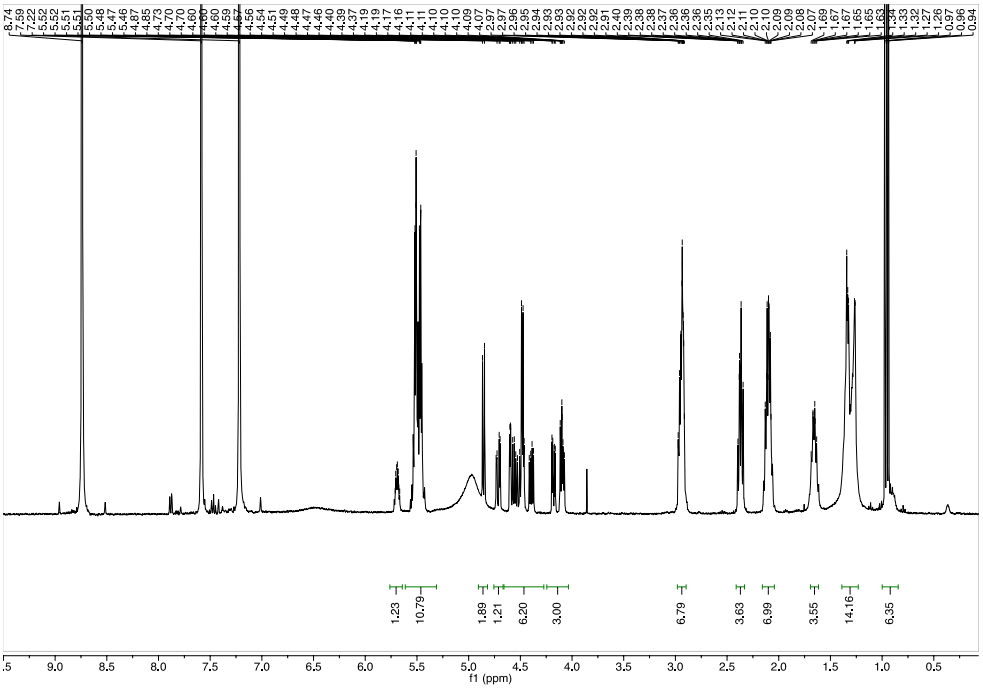


Figure S5: ^{1}H NMR spectrum of NB4.2 in pyridine-d_5

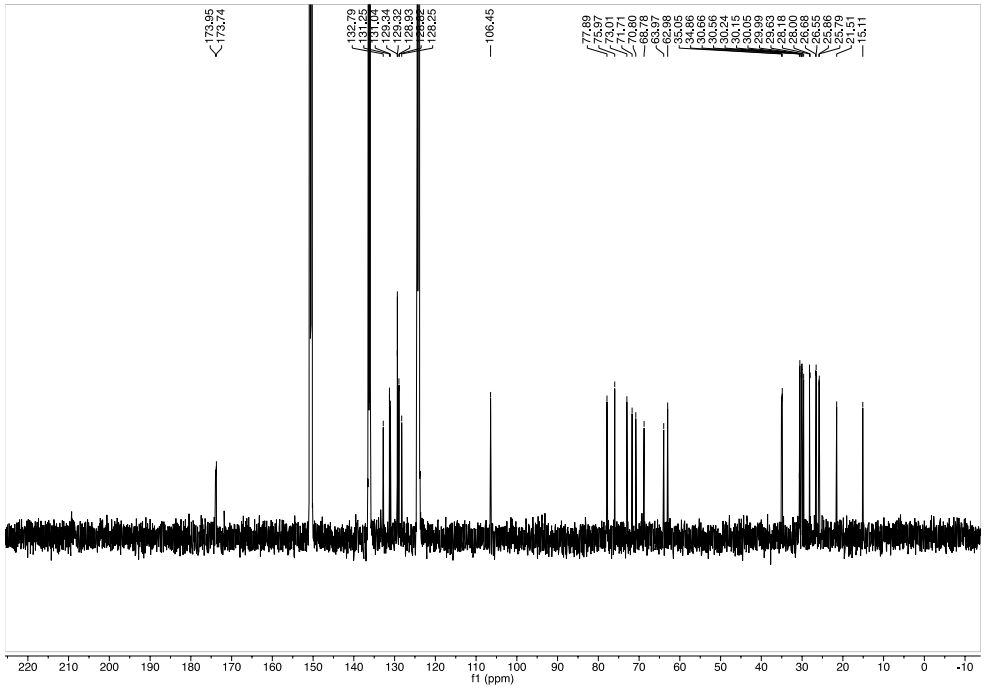


Figure S6: ^{13}C NMR spectrum of NB4.2 in pyridine-d_5

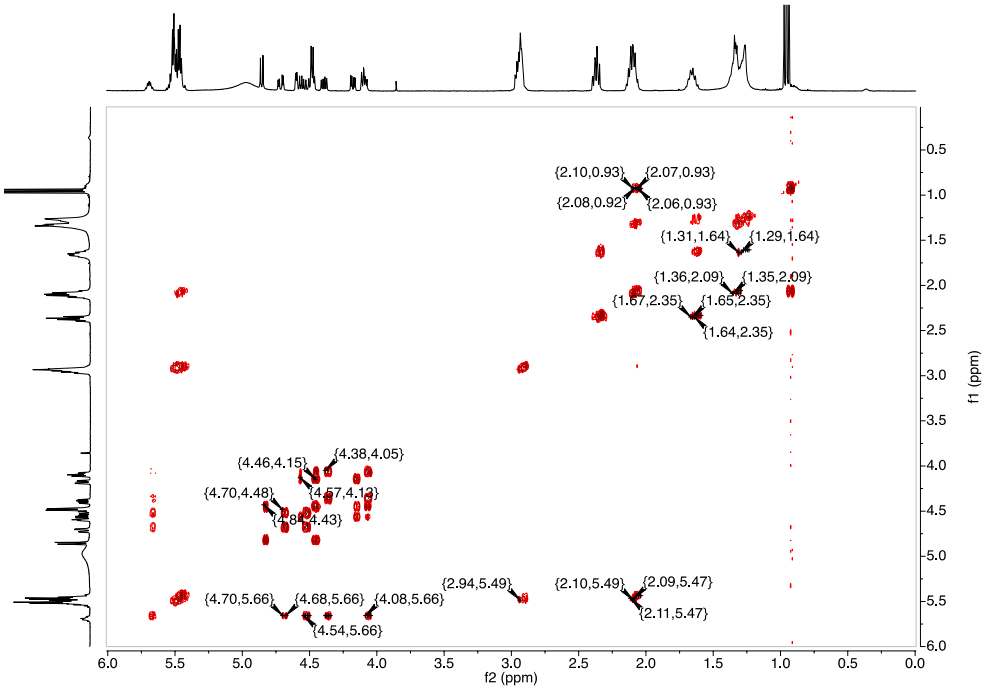


Figure S7: COSY NMR spectrum of NB4.2 in pyridine-d_5

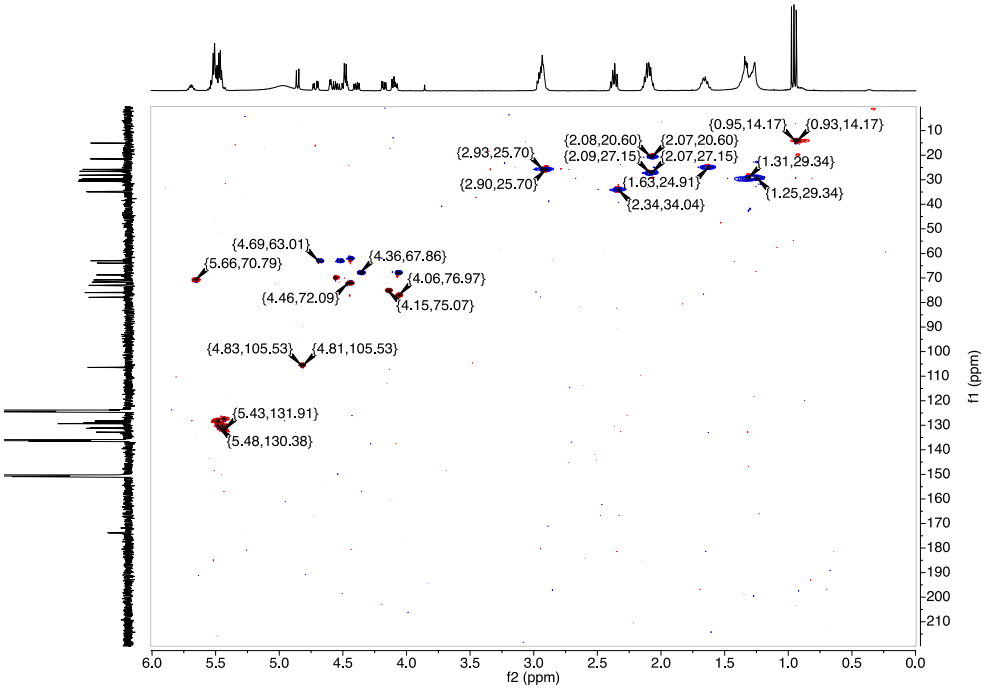


Figure S8: HSQC NMR spectrum of NB4.2 in pyridine-d_5

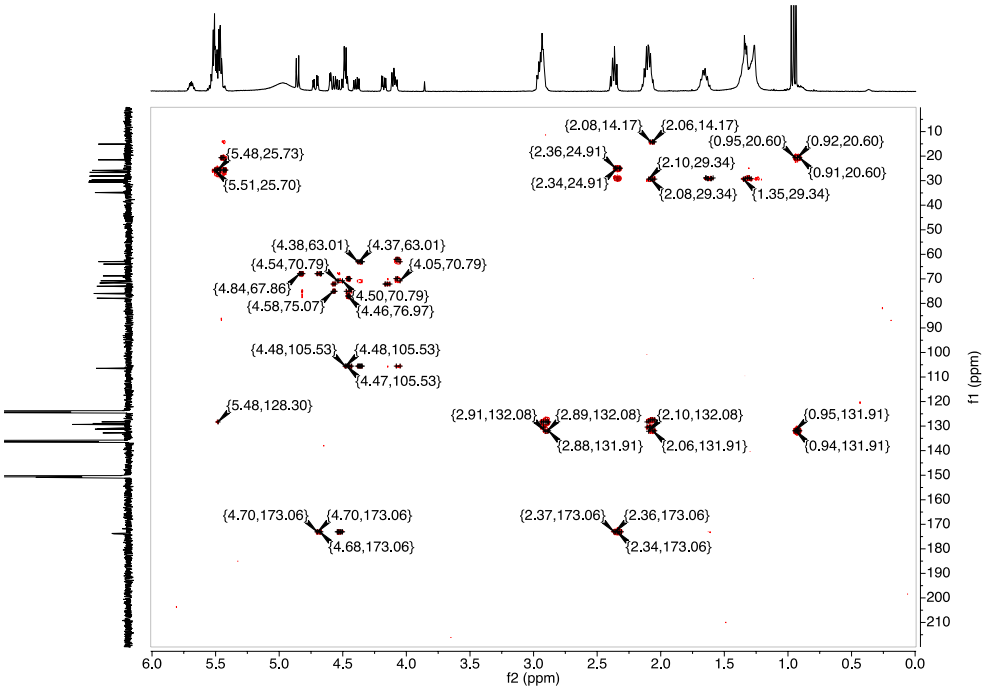


Figure S9: HMBC NMR spectrum of NB4.2 in pyridine-d_5

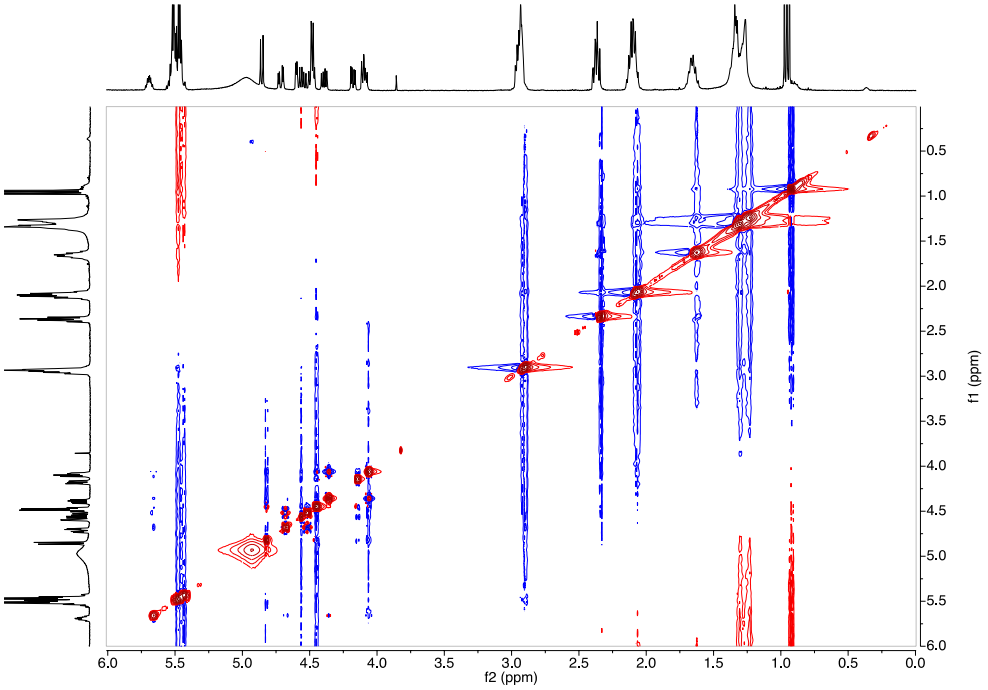
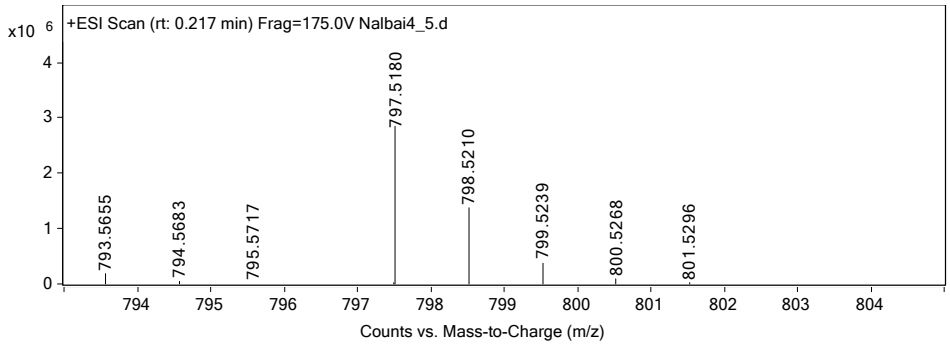


Figure S10: NOESY NMR spectrum of NB4.2 in pyridine-d_5

Mass Spectrum SmartFormula Report

Sample Name	Nalbai4.5	Data File	D:\MassHunter\Data\External\FST\20210817\Nalbai4_5.d
Instrument Name	Agilent 6546 LC-QTOF	IRM Calibration Status	Success
Acq Method	MS Scan_union-1.m	Acquired Time	17/8/2021 12:04:09 PM (UTC+08:00)
Comment	A/P Huang Dejian	Operator	

Meas. m/z	#	Formula	Calc. Mass	Err [ppm]
797.518	1	C47 H73 O10	797.5198	2.26
797.518	1	C54 H69 O5	797.514	5.02



Printed at 12:47 PM on 20-Aug-2021

Figure S11: HR-ESIMS of NB4.5 (Cationic mode)

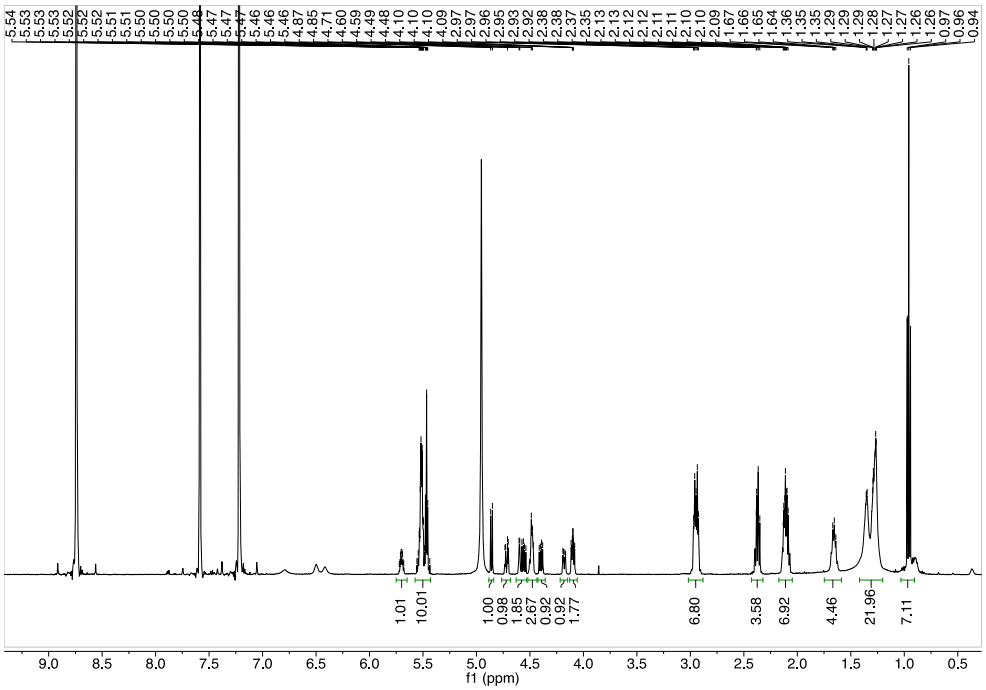


Figure S12: ^{1}H NMR spectrum of NB4.5 in pyridine-d_5

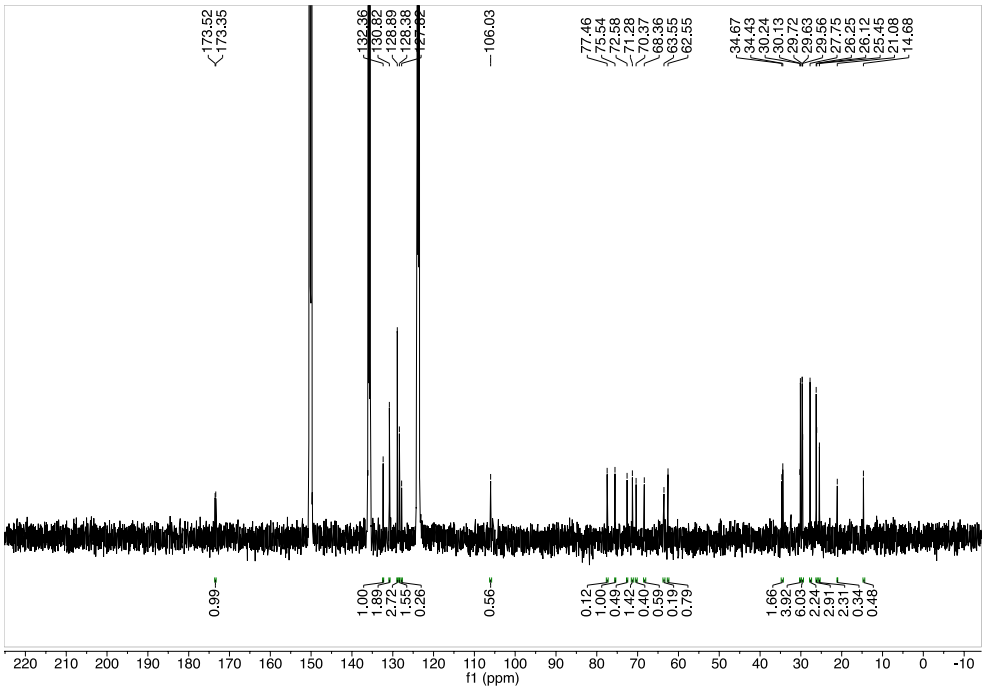


Figure S13: ^{13}C NMR spectrum of NB4.5 in pyridine-d_5

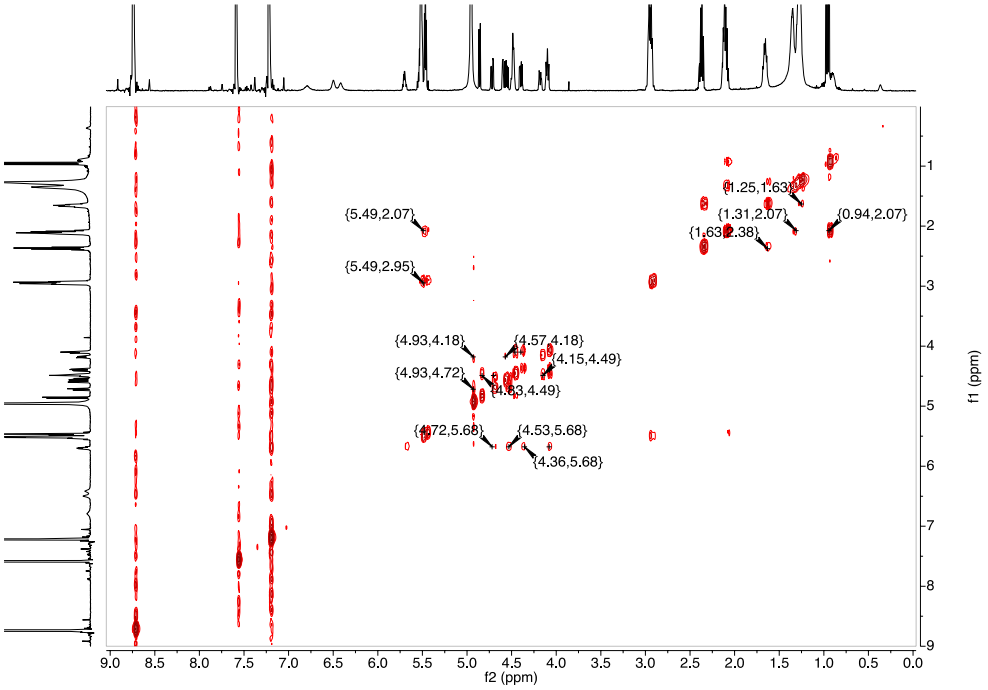


Figure S14: COSY NMR spectrum of NB4.5 in pyridine-d_5

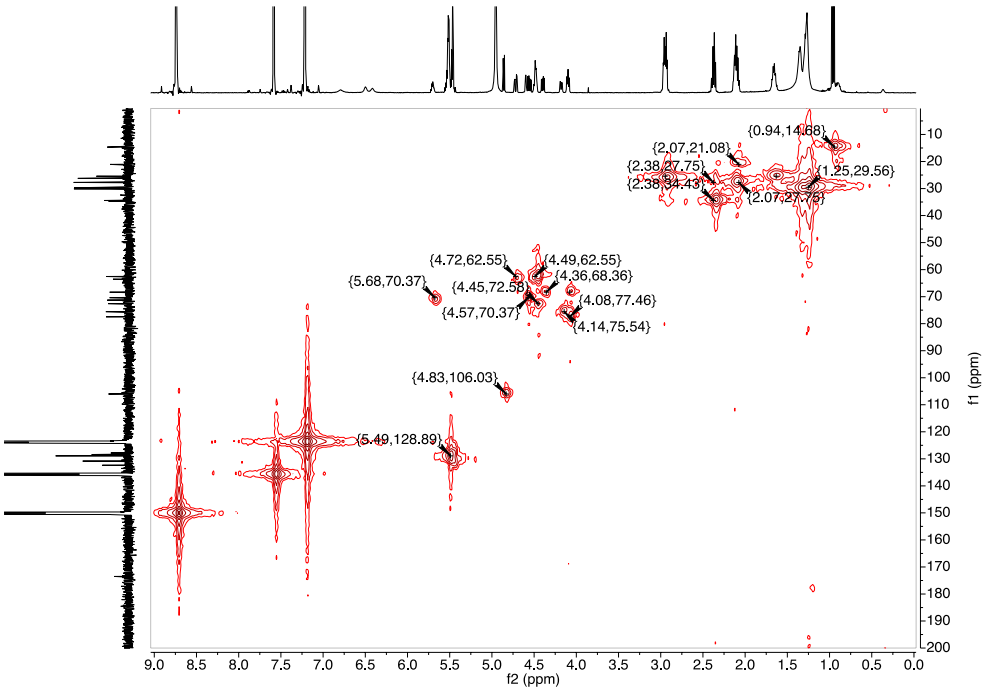


Figure S15: HSQC NMR spectrum of NB4.5 in pyridine-d_5

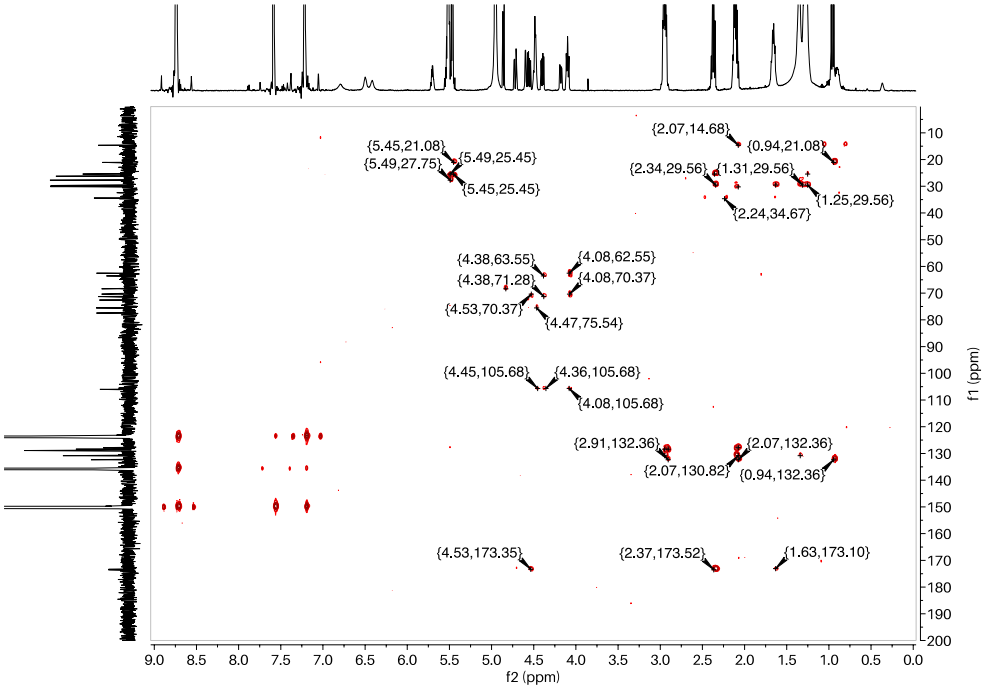


Figure S16: HMBC NMR spectrum of NB4.5 in pyridine-d_5

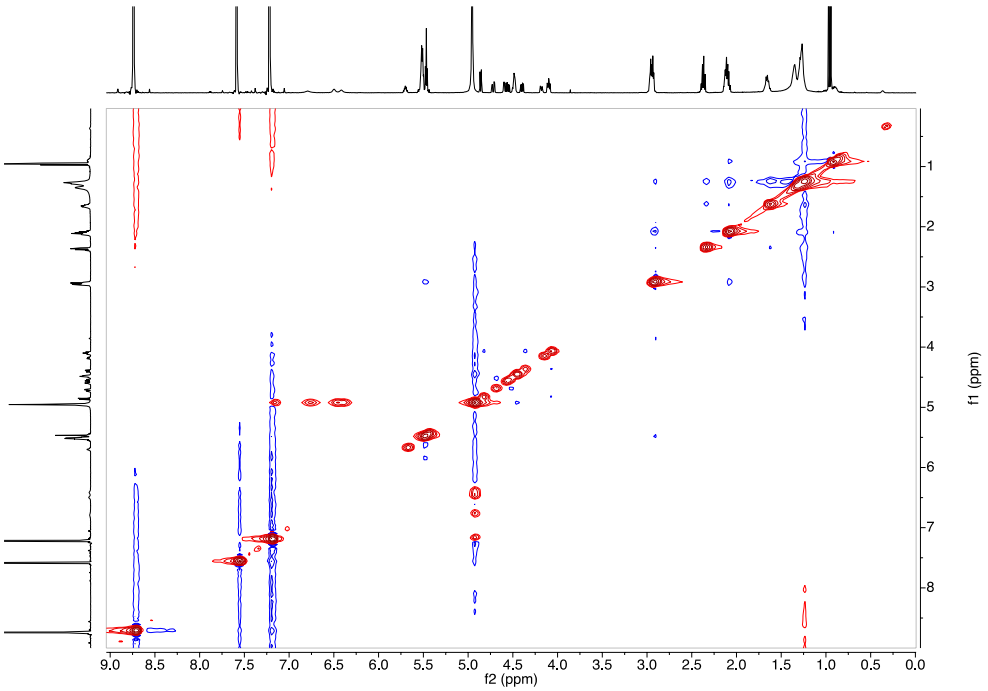


Figure S17: NOESY NMR spectrum of NB4.5 in pyridine-d_5

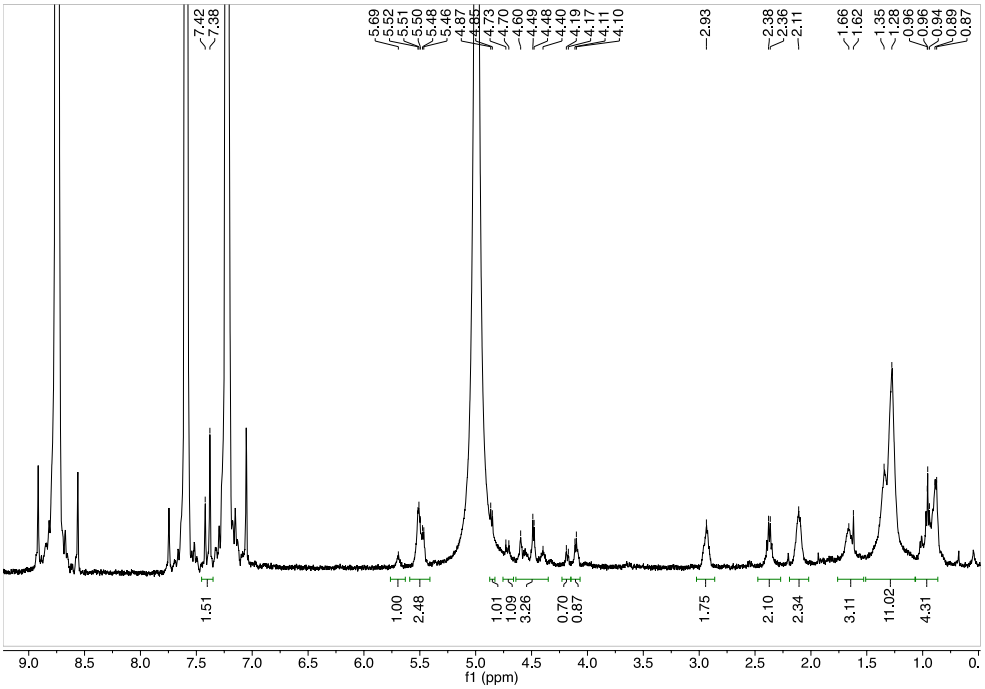


Figure S18: ^{1}H NMR spectrum of NB4.4 in pyridine-d_5

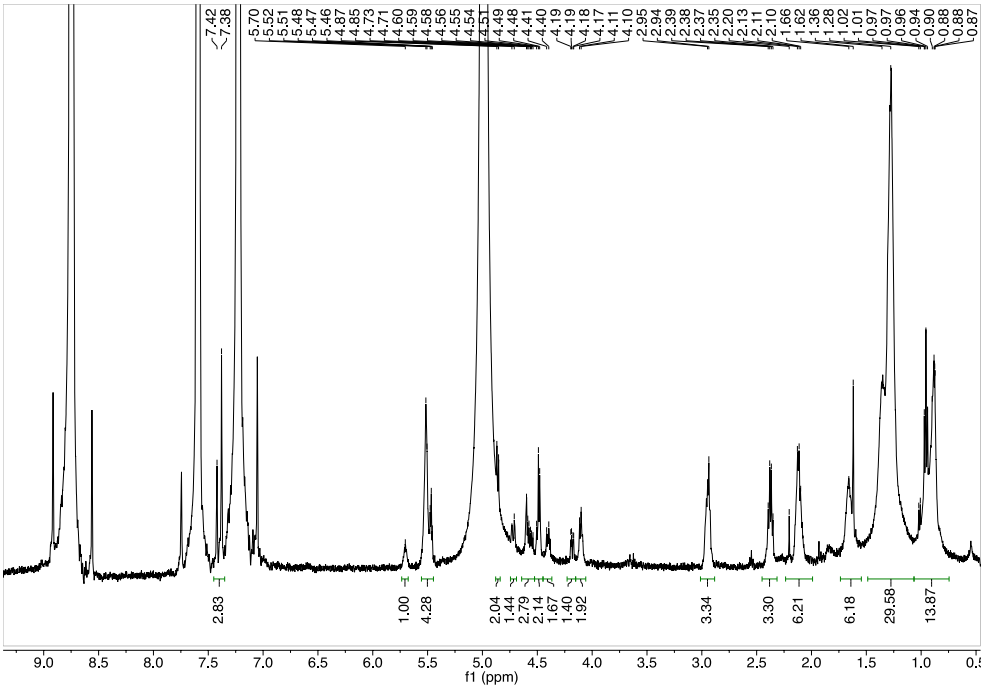


Figure S19: ^{1}H NMR spectrum of NB4.6 in pyridine-d_5

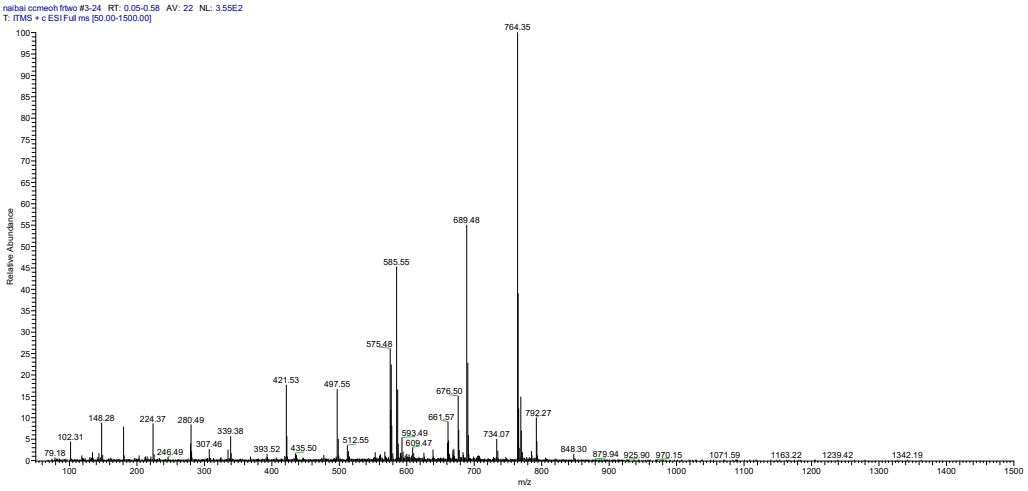


Figure S20: ESI-MS spectrum of NB4.2 (Cationic mode)

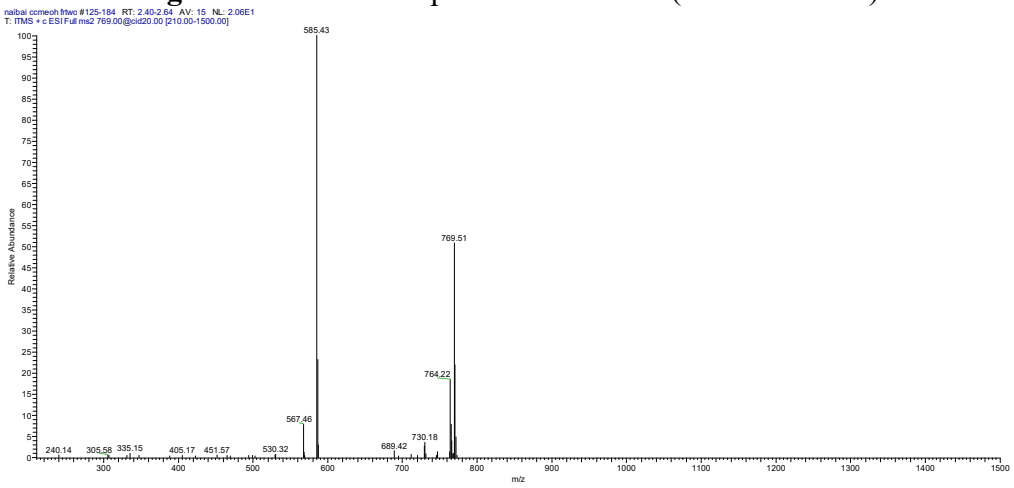


Figure S21: ESI-MS/MS spectrum of *m/z* 769 from NB4.2 (Cationic mode)

Sample Name	NB4.4	**Instrument Name**	Instrument 1	**Operator**	WLK
Inj Vol	5	**IRM Calibration Status**	Success	**Data Filename**	NB4.4_msms.d
ACQ Method	MS Scan_union_APCI-1.m	**Comment**	FST, Prof Huang Dejian	**Acquired Time**	28/7/2022 4:47:17 PM (UTC+08:00)

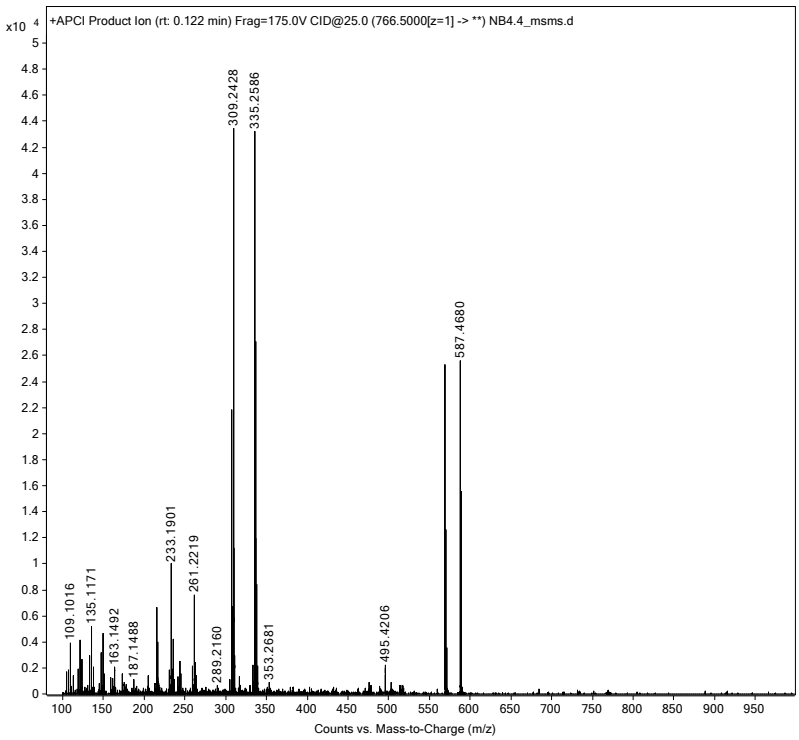


Figure S22: APCI-MS/MS spectrum of *m/z* 766 from NB4.4 (Cationic mode)

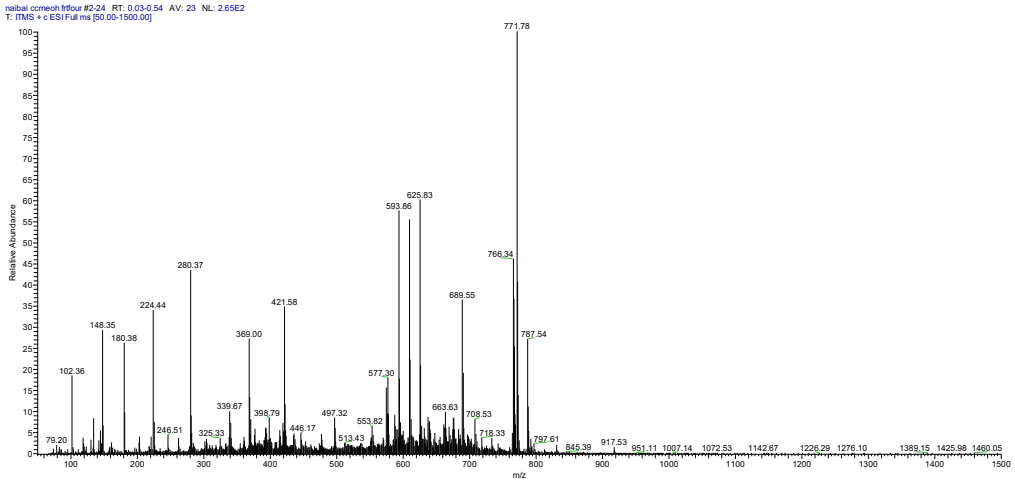


Figure S23: ESI-MS spectrum of NB4.4 (Cationic mode)

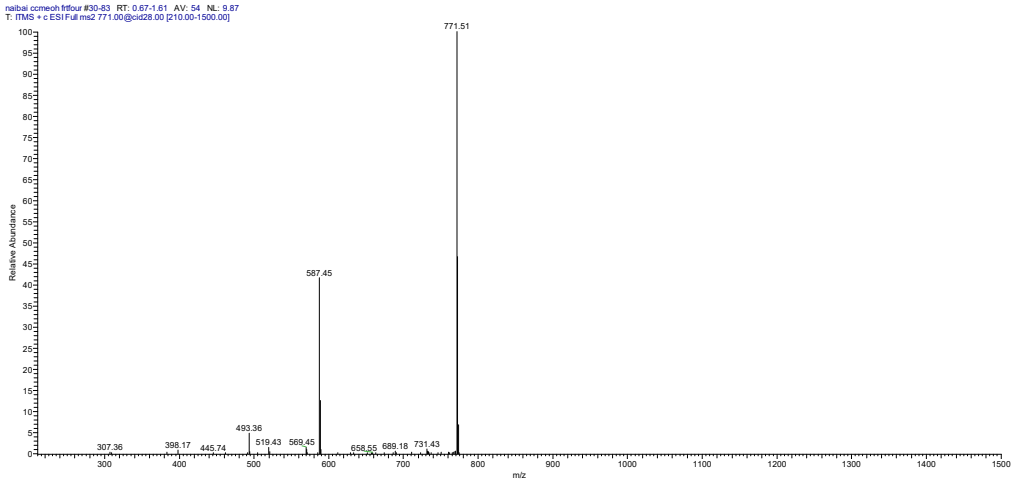


Figure S24: ESI-MS/MS spectrum of *m/z* 771 from NB4.4 (Cationic mode)

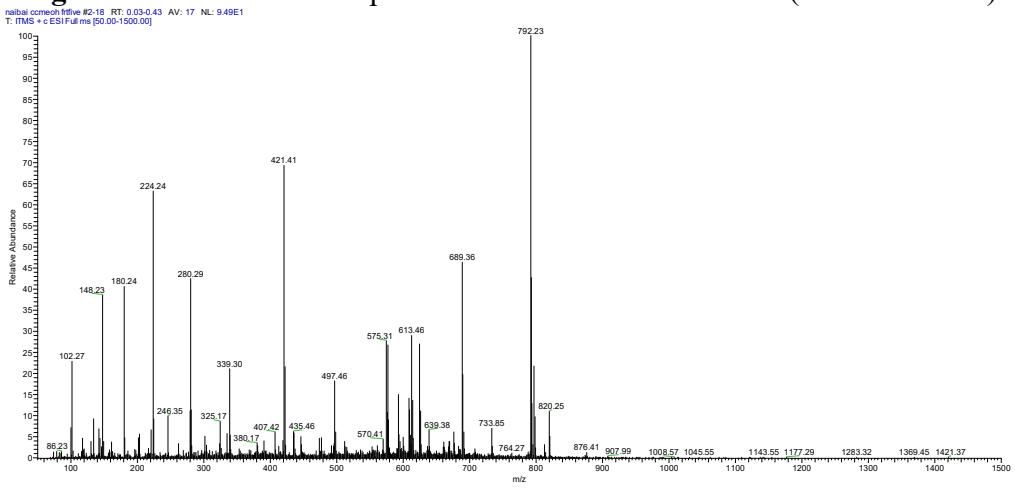


Figure S25: ESI-MS spectrum of NB4.5 (Cationic mode)

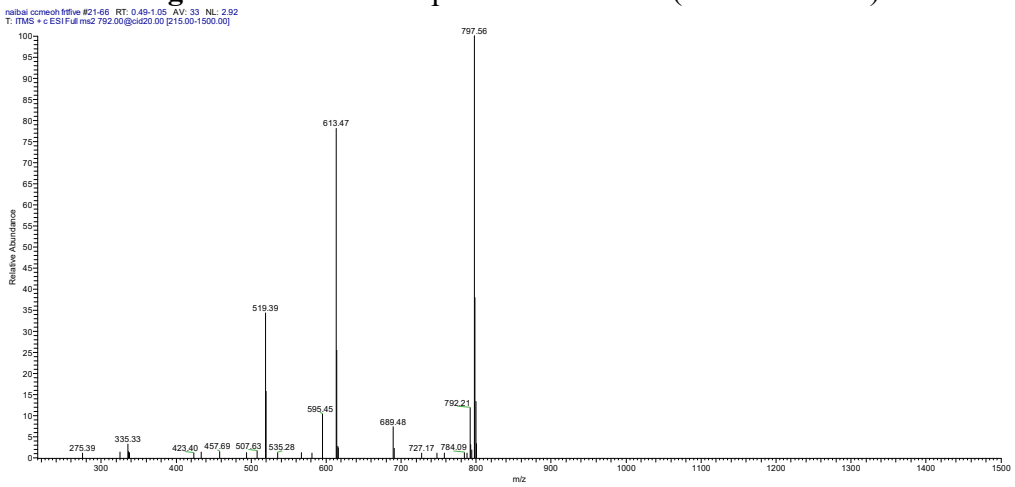


Figure S26: ESI-MS/MS spectrum of *m/z* 792 from NB4.5 (Cationic mode)

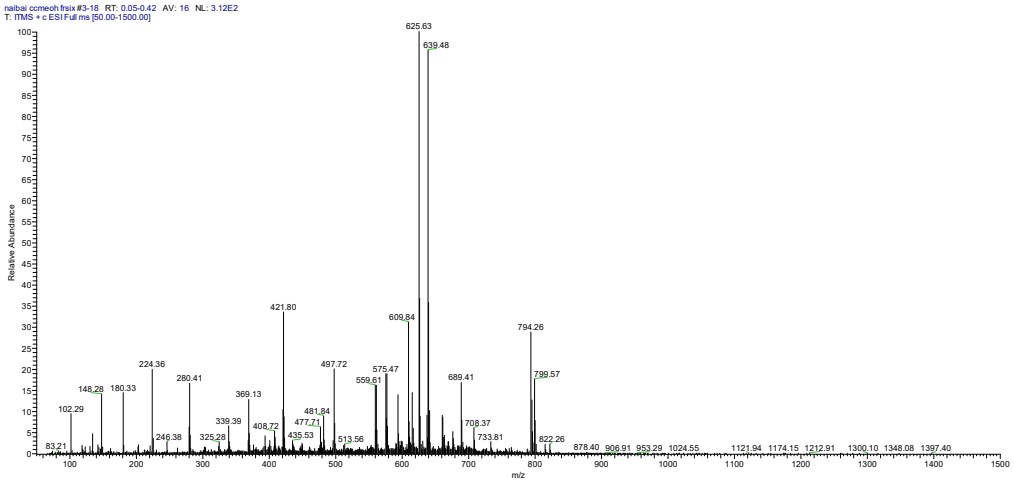


Figure S27: ESI-MS spectrum of NB4.6 (Cationic mode)

Sample Name	NB4.6	Instrument Name	Instrument 1	Operator	WLK
Inj Vol	10	IRM Calibration Status	Success	Data Filename	NB4.6_msms1.d
ACQ Method	MS Scan_union_APCI-1.m	Comment	FST, Prof Huang Dejian	Acquired Time	28/7/2022 5:09:07 PM (UTC+ 08:00)

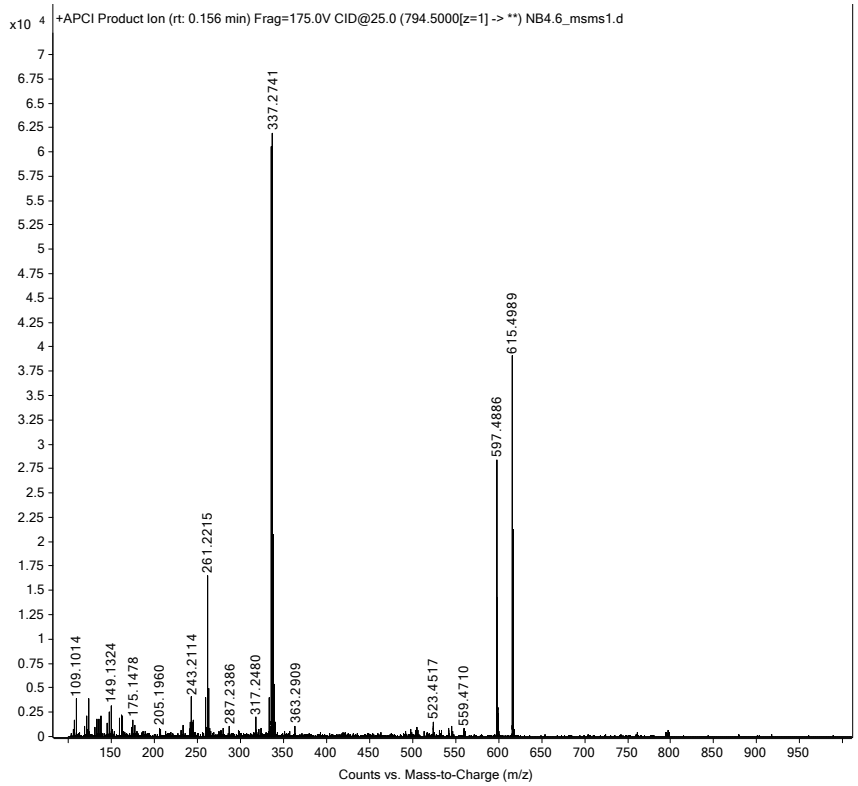


Figure S28: APCI-MS/MS spectrum of *m/z* 794 from NB4.6 (Cationic mode)

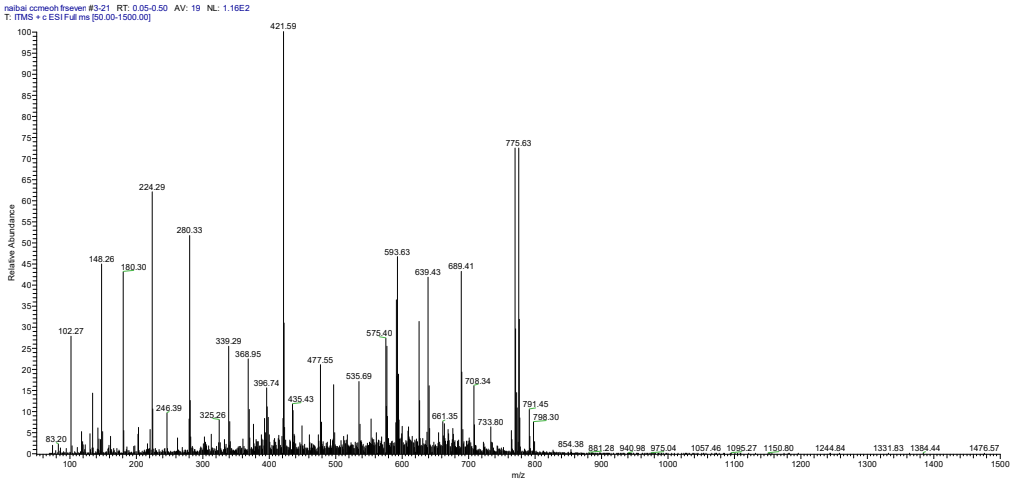


Figure S29: ESI-MS spectrum of NB4.7 (Cationic mode)

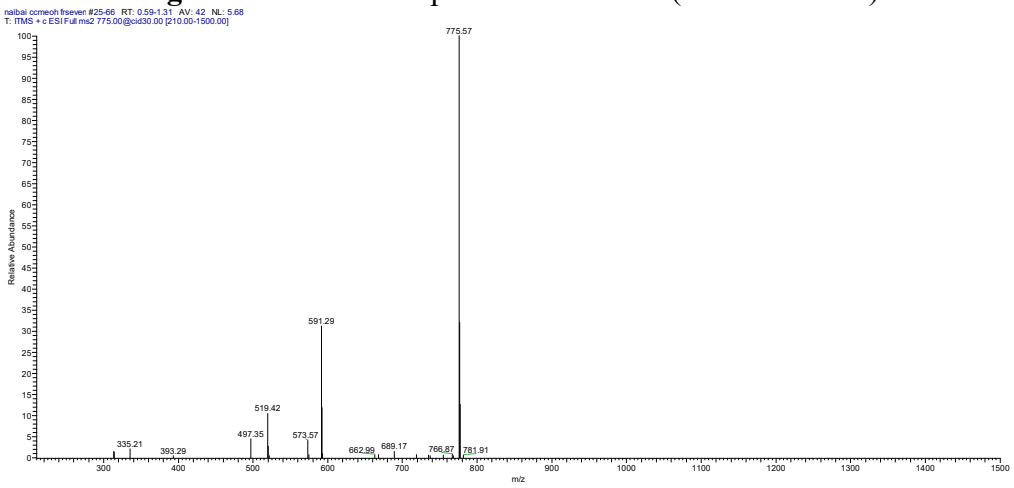


Figure S30: ESI-MS/MS spectrum of *m/z* 775 from NB4.7 (Cationic mode)

Sample Name	NB4.7	Instrument Name	Instrument 1	Operator	WLK
Inj Vol	5	IRM Calibration Status	Success	Data Filename	NB4.7_msms.d
ACQ Method	MS Scan_union_APCI-1.m	Comment	FST, Prof Huang Dejian	Acquired Time	28/7/2022 5:14:31 PM (UTC+08:00)

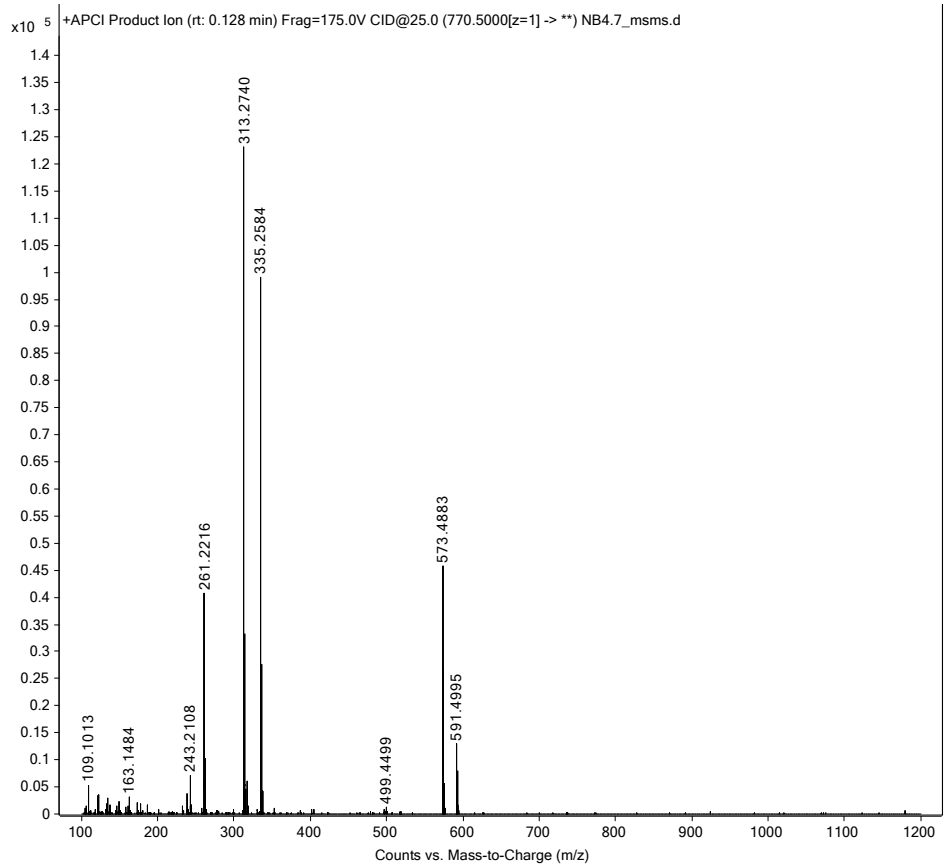


Figure S31: APCI-MS/MS spectrum of *m/z* 775 from NB4.7 (Cationic mode)

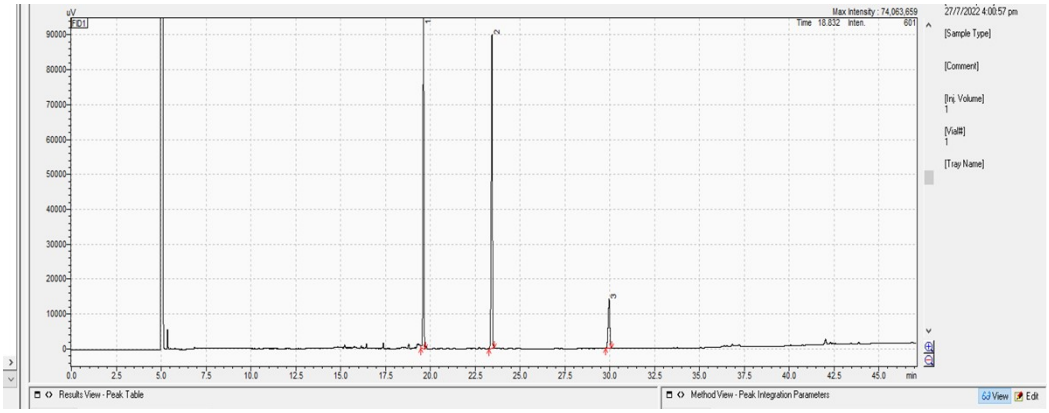


Figure S32: GC-MS/FID of NB4.2 after alkaline hydrolysis (Tricosanoic acid is internal standard)

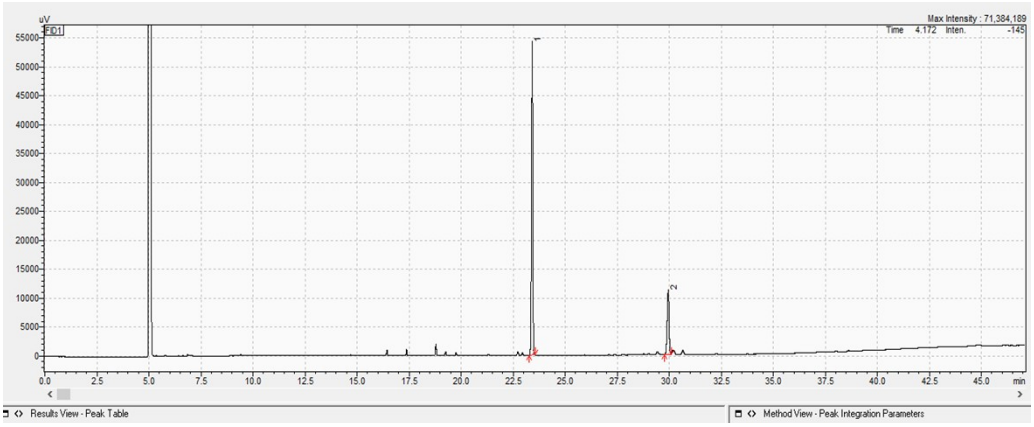


Figure S33: GC-MS/FID of NB4.5 after alkaline hydrolysis (Tricosanoic acid is internal standard)

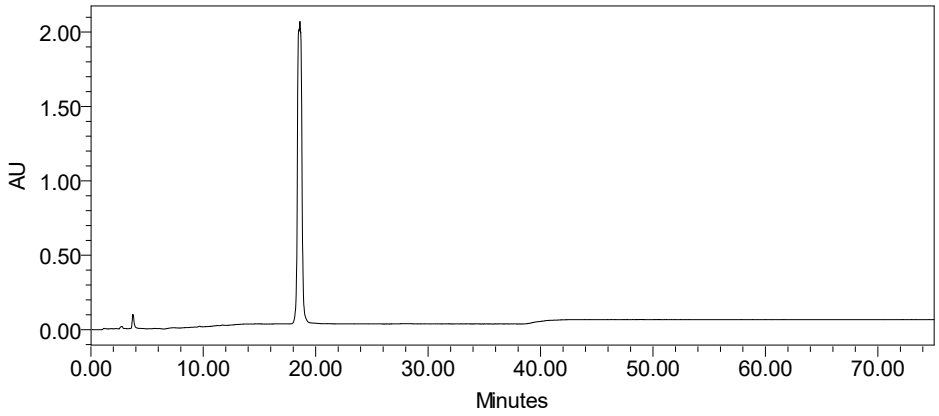


Figure S34: HPLC chromatogram of NB4.2 at 210 nm

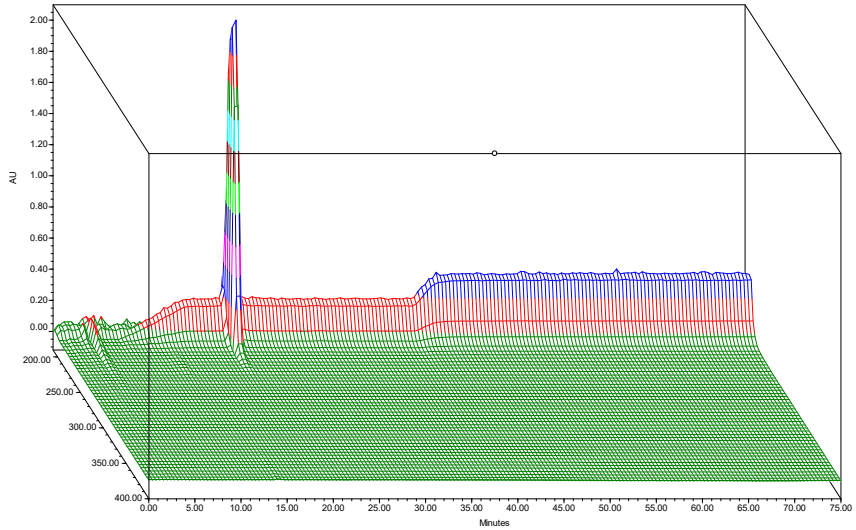


Figure S35: 3D HPLC chromatogram of NB4.2

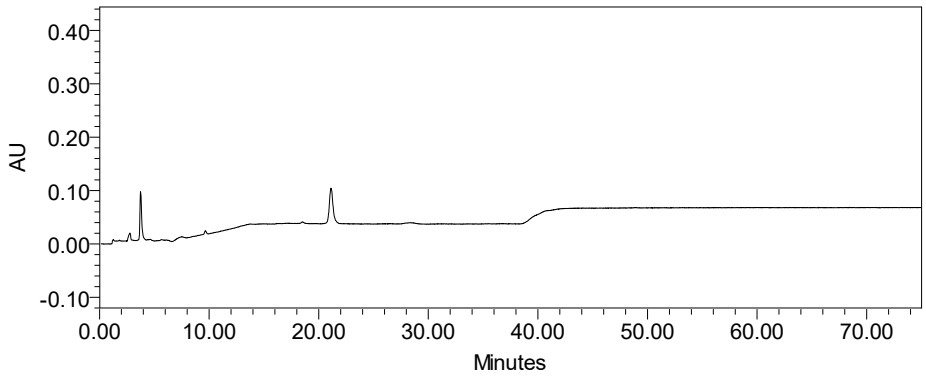


Figure S36: HPLC chromatogram of NB4.4 at 210 nm

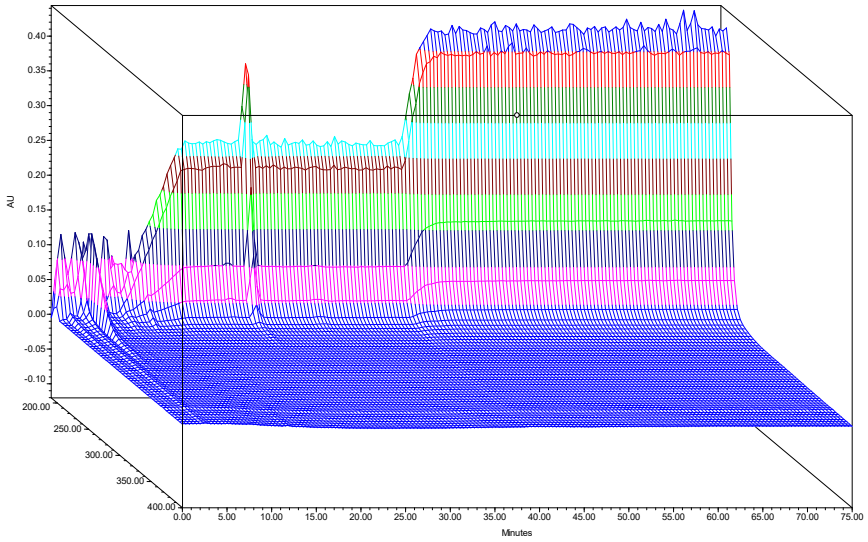


Figure S37: 3D HPLC chromatogram of NB4.4

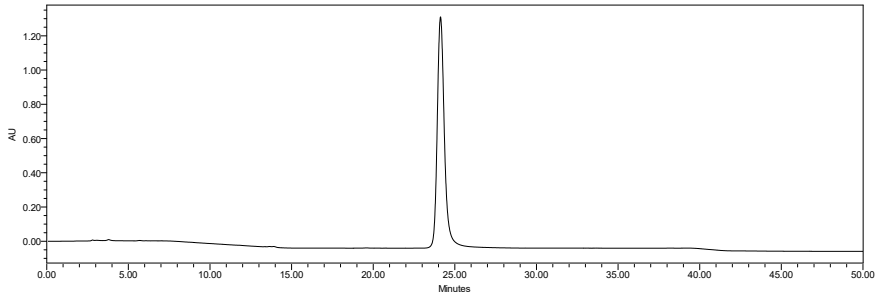


Figure S38: HPLC chromatogram of NB4.5 at 210 nm

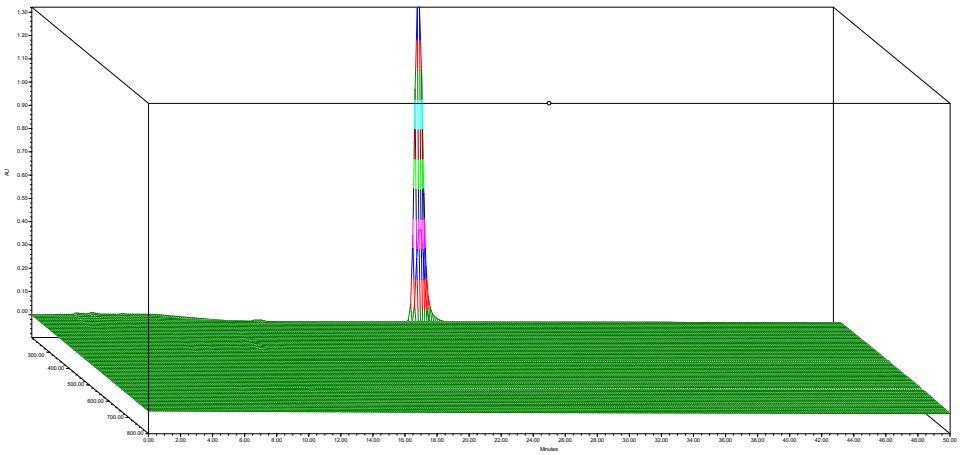


Figure S39: 3D HPLC chromatogram of NB4.5

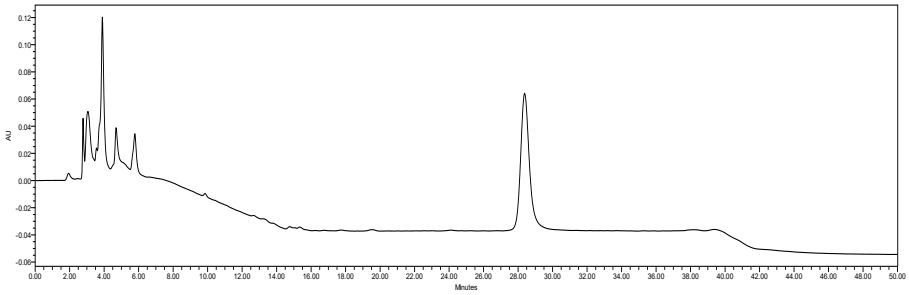


Figure S40: HPLC chromatogram of NB4.6 at 210 nm

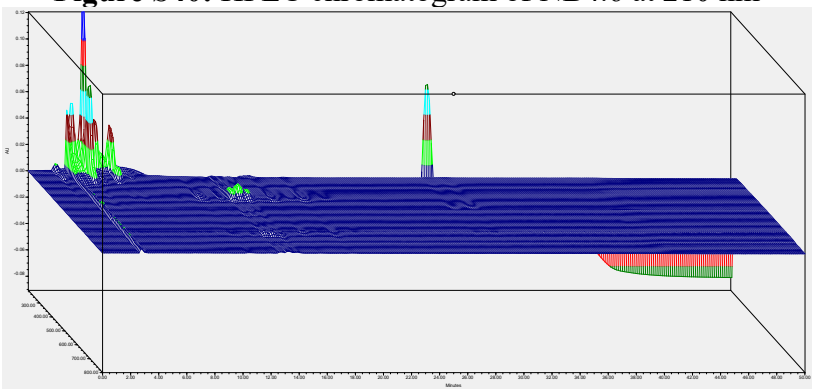


Figure S41: 3D HPLC chromatogram of NB4.6

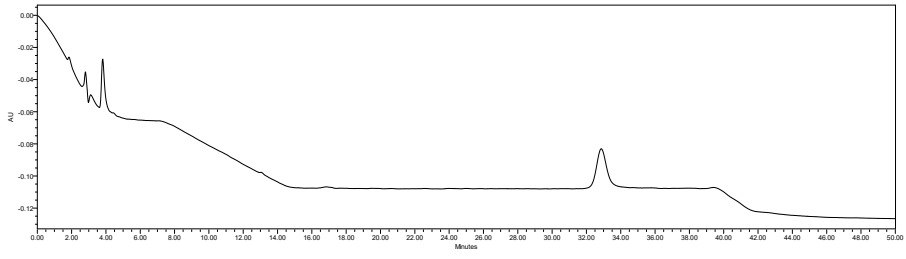


Figure S42: HPLC chromatogram of NB4.7 at 210 nm

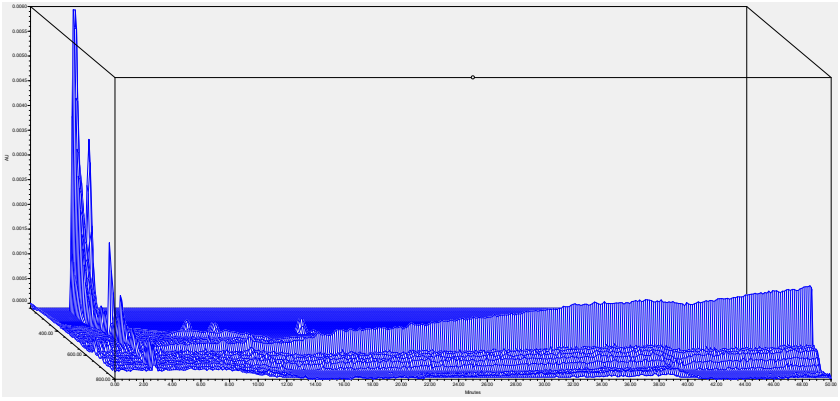


Figure S43: 3D HPLC chromatogram of NB4.7