Retusone A, A Guaiane-Type Sesquiterpene Dimer from *Wikstroemia retusa* and Its Inhibitory Effects on Histone Acetyltransferase HBO1 Expression

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Table S1**.** Crystallographic data for **1**.

Formula	$C_{31}H_{38}O_4$
$D_{calc.}$/ g cm^{-3}	1.215
μ/mm^{-1}	0.079
Formula Weight	474.61
Colour	colourless
Shape	plate
Size/mm^3	0.53×0.14×0.09
T/K	90
Crystal System	monoclinic
Flack Parameter	-1.0(6)
Hooft Parameter	-0.9(6)
Space Group	
a/Å	22.460(6)
b/Å	5.0621(13)
c/Å	24.319(6)
α/°	90
β/°	110.160(3)
γ/°	90
V/Å^3	2595.5(11)
Z	4
Z'	1
Wavelength/Å	0.71073
Radiation type	MoK_α
Θ_{min}/°	1.784
Θ_{max}/°	27.555
Measured Refl's.	36724
Indep't Refl's	5968
Refl's I≥2 σ(I)	4867
R_{int}	0.0777
Parameters	321
Restraints	1
Largest Peak	0.342
Deepest Hole	-0.236
GooF	1.036
wR_2 (all data)	0.1265
wR_2	0.1173
R_1 (all data)	0.0723
R_1	0.0530

Single colourless plate crystals of **1** slow crystallization from a methanol solution at room temperature. A suitable crystal with dimensions 0.53 × 0.14 × 0.09 mm^3 was selected and the crystal was mounted on a MicroMount using perfluoropolyether oil on a Bruker SMART APEX II ULTRA diffractometer. The crystal was kept at a steady T = 90 K during data collection. The structure was solved with the ShelXT 2014/5 solution program[1] using dual methods and by using Olex2 as the graphical interface. The model was refined with XL using full matrix least squares minimisation on $\boldsymbol{F^2}$.

Table S2. Calculated Relative Energies (kcal/mol) and Populations (%) of the Three Lowest Energy Conformers of **1**.

Conformer	ΔG	$P(\%)$[b]
a	0.00 [a]	48.8
b	0.49	21.2
c	0.79	12.9
d	0.88	11.0
e	1.23	6.1

[a] Calculated relative energies to **a** with $\Delta G = -944642.89839$ kcal/mol at the B3LYP/6–311+G (2df, 2p) level in MeOH.
[b] Boltzmann population at T = 298 K and 1 atm.

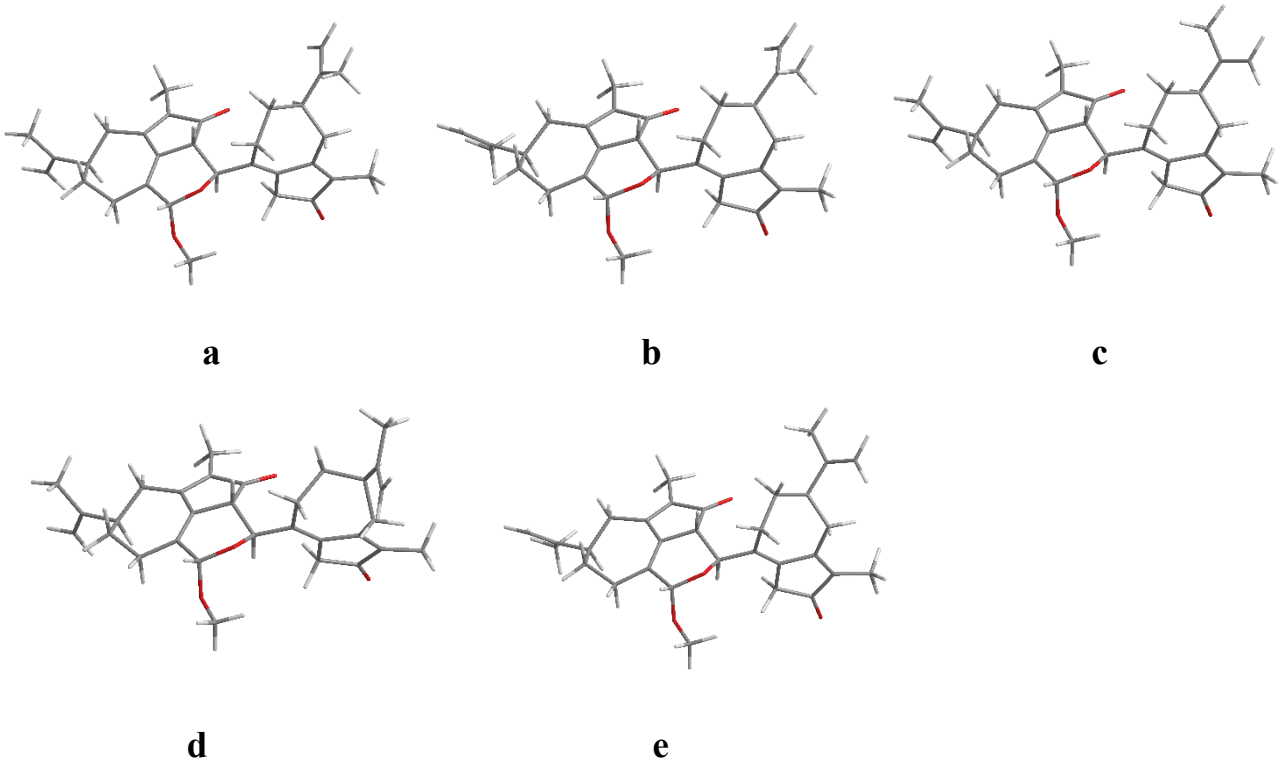


Figure S1. B3LYP/6–311+ G (2df,2p) optimized lowest energy conformers for **1**.

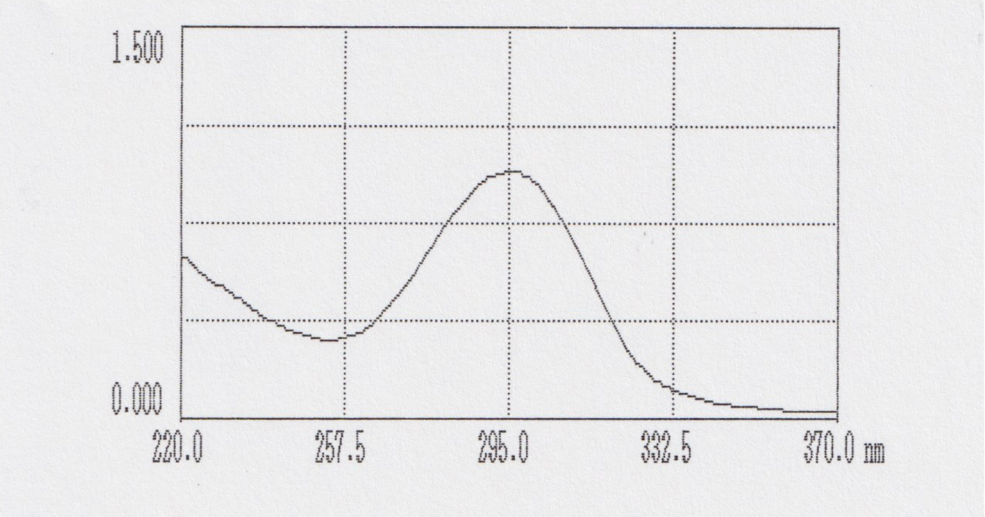


Figure S2. UV spectrum of **1**.

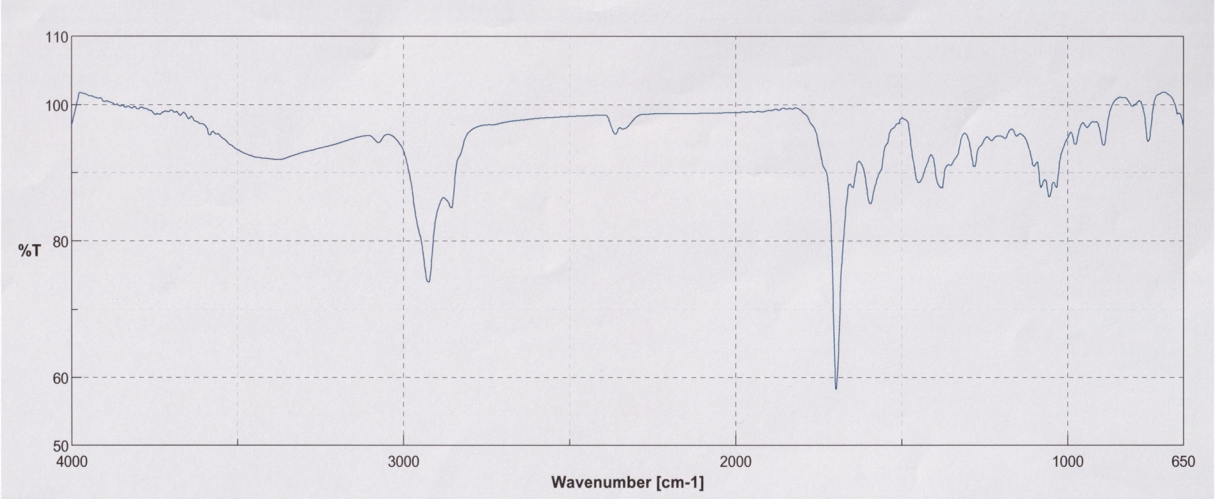
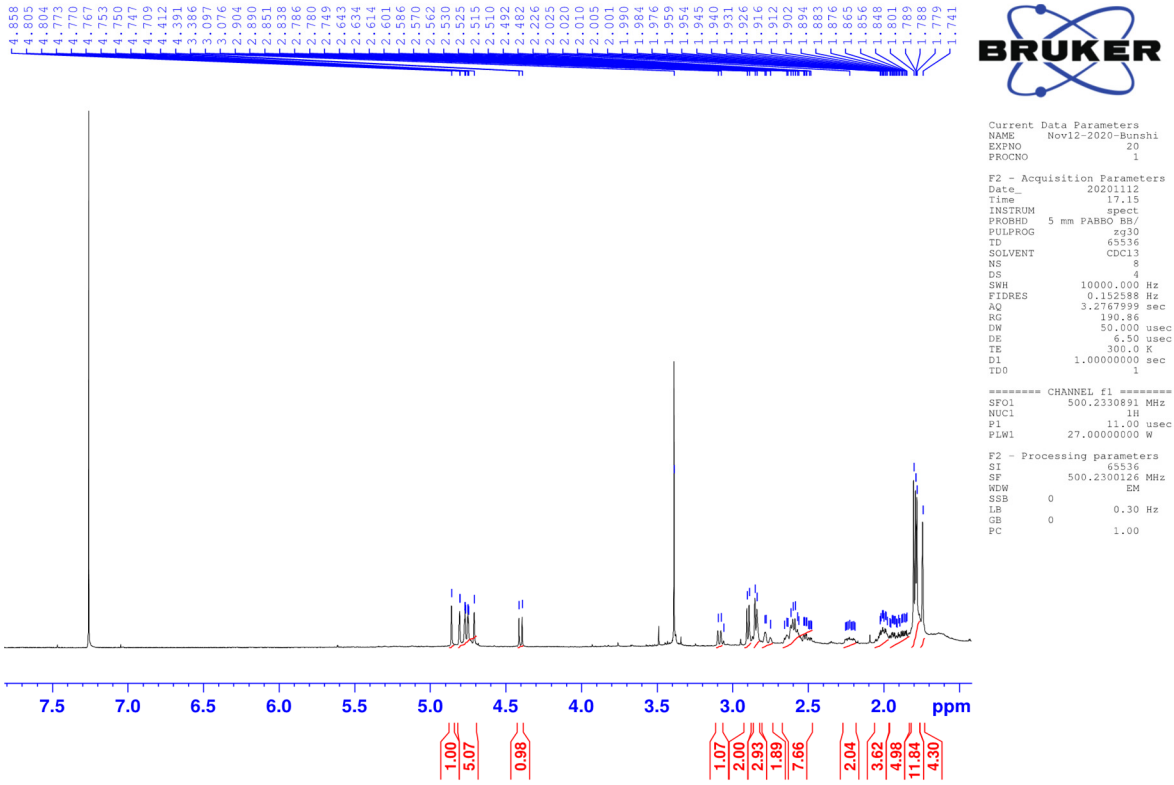


Figure S3. IR spectrum of **1**.


4.858 4.805 4.804 4.773 4.770 4.767 4.753 4.750 4.747 4.709 4.412 4.391 3.386 3.097 3.076 2.904 2.890 2.851 2.838 2.786 2.780 2.749 2.643 2.634 2.614 2.601 2.586 2.570 2.562 2.530 2.525 2.515 2.510 2.492 2.482 2.226 2.025 2.020 2.010 2.005 2.001 1.990 1.984 1.976 1.959 1.954 1.945 1.940 1.931 1.926 1.916 1.912 1.902 1.894 1.883 1.876 1.865 1.856 1.848 1.801 1.789 1.788 1.779 1.741
BRUKER
Current Data Parameters
NAME Nov12-2020-Bunshi
EXPNO 20
PROCNO 1
F2 - Acquisition Parameters
Date_ 20201112
Time 17.15
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 4
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 190.86
DW 50.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
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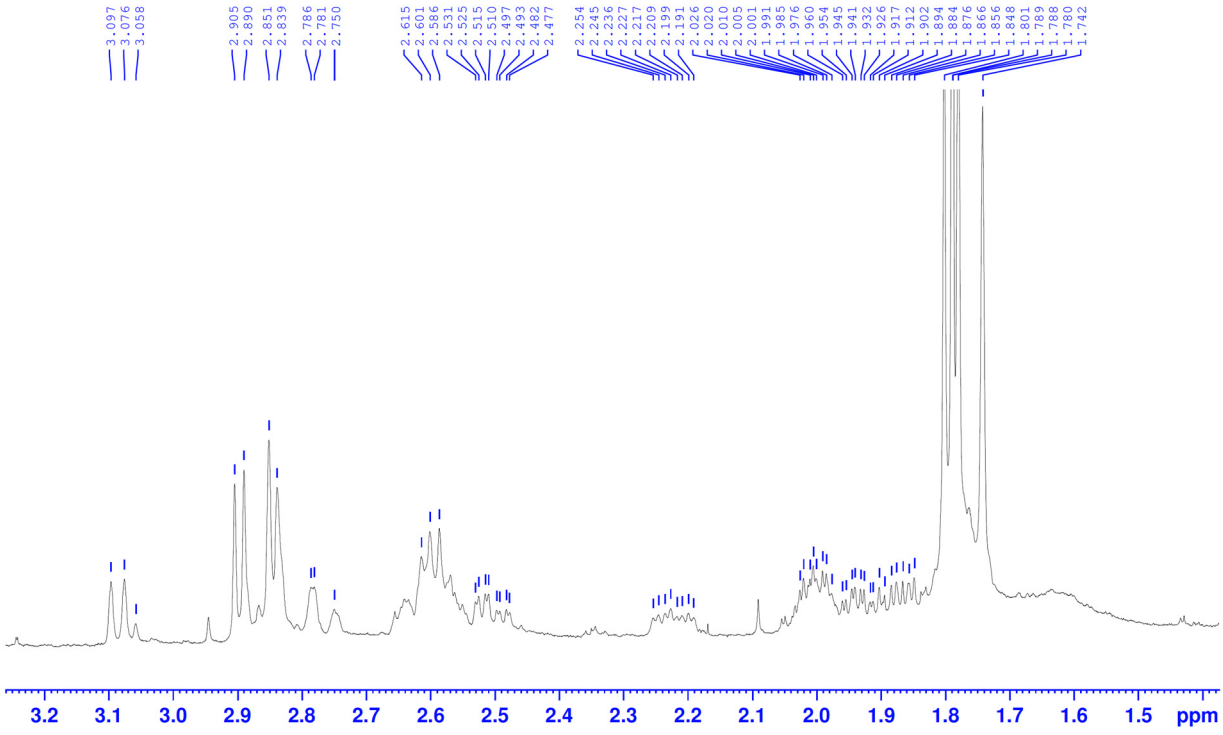
SFO1 500.2330891 MHz
NUC1 1H
P1 11.00 usec
PLW1 27.00000000 W
F2 - Processing parameters
SI 65536
SF 500.2300126 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 ppm
1.00 5.07 0.98 1.07 2.00 2.93 1.89 7.66 2.04 3.62 4.98 11.84 4.30


3.097 3.076 3.058 2.905 2.890 2.851 2.839 2.786 2.781 2.750 2.615 2.601 2.586 2.531 2.525 2.515 2.510 2.497 2.493 2.482 2.477 2.254 2.245 2.236 2.227 2.217 2.209 2.199 2.191 2.026 2.020 2.010 2.005 2.001 1.991 1.985 1.976 1.960 1.954 1.945 1.941 1.932 1.926 1.917 1.912 1.902 1.894 1.884 1.876 1.866 1.856 1.848 1.801 1.789 1.788 1.780 1.742
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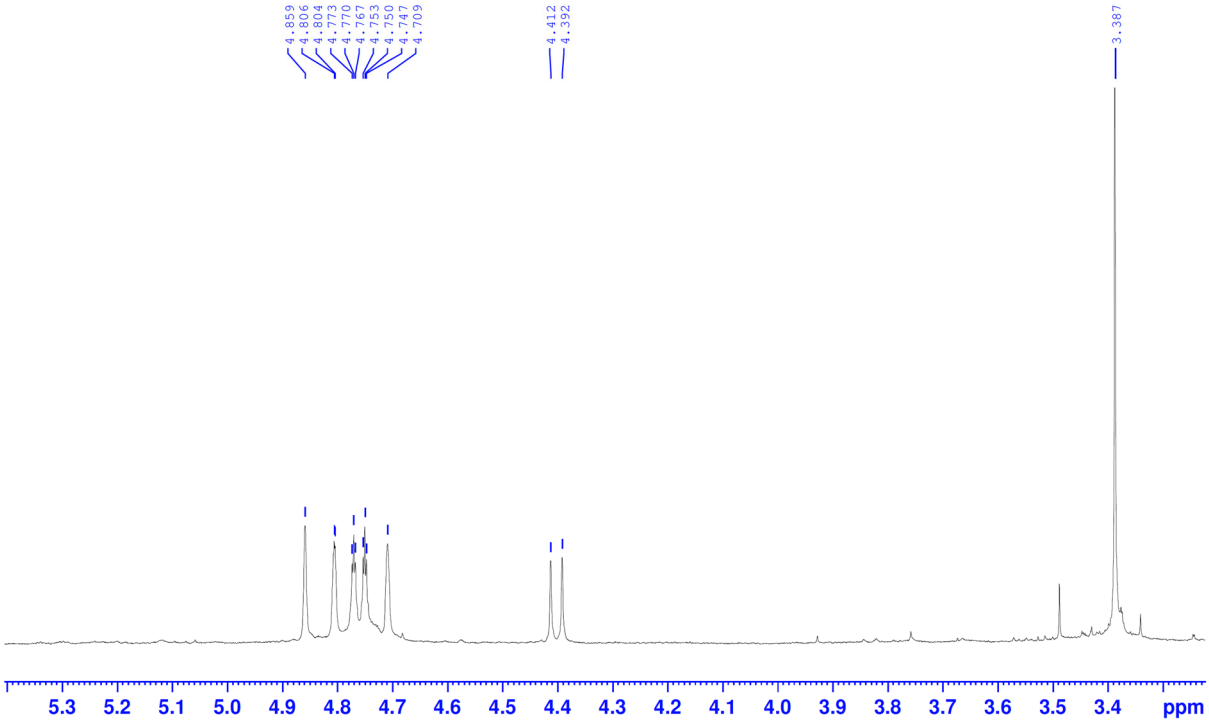


Figure S4. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **1**.

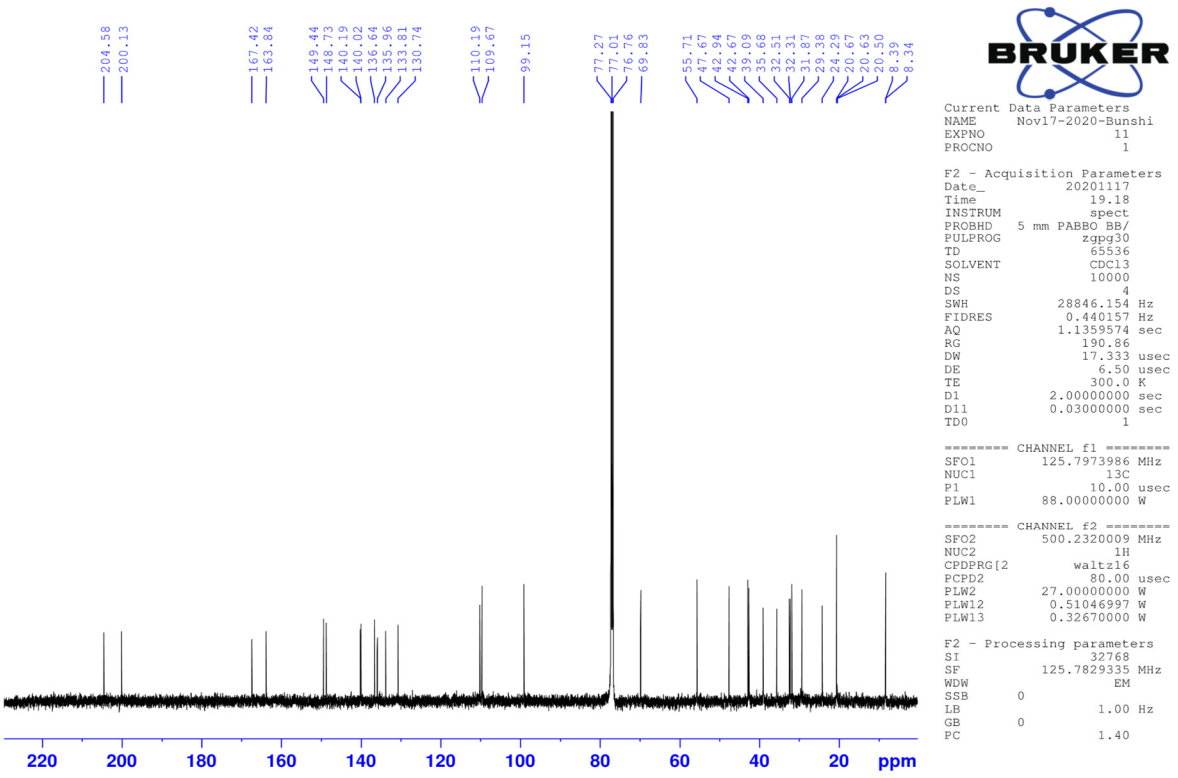


Figure S5. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of **1**.

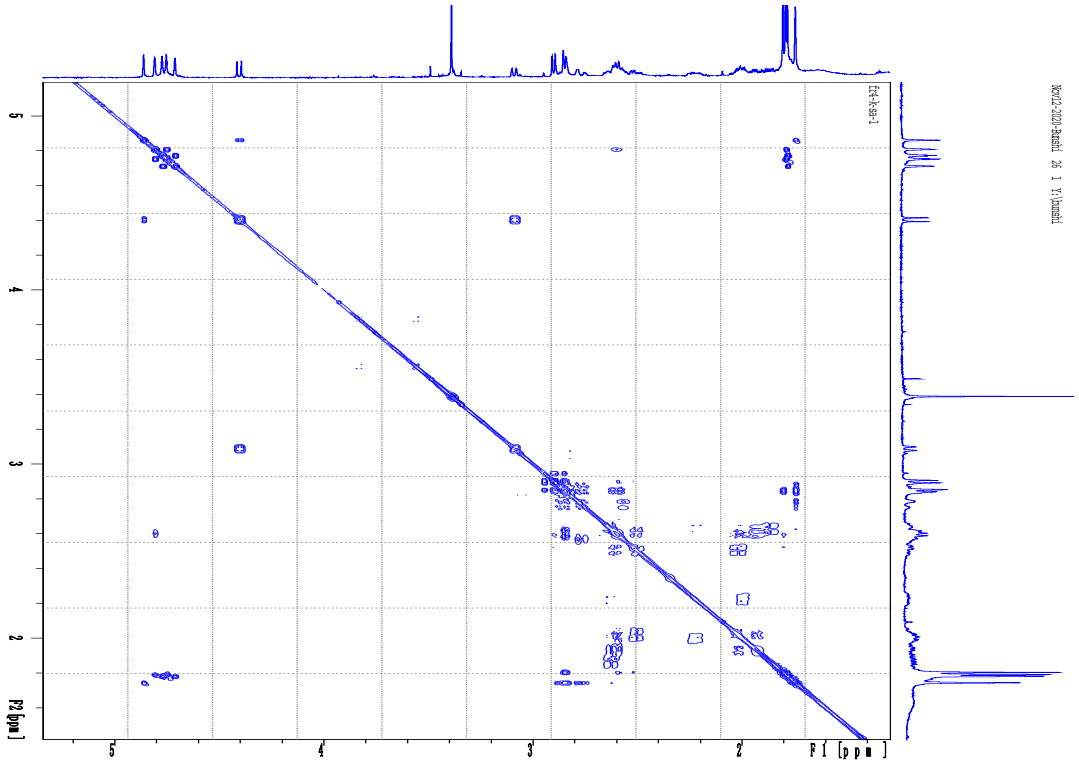


Figure S6. ^{1}H-^{1}H COSY spectrum of **1**.

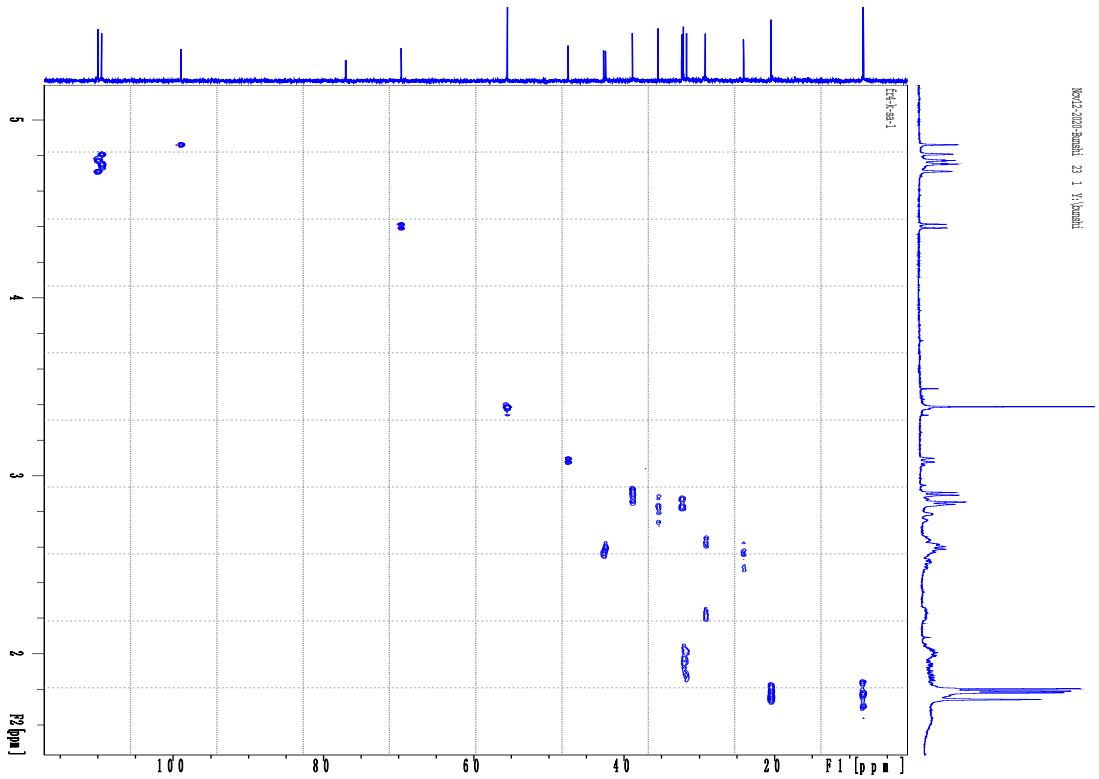


Figure S7. HMQC spectrum of **1**.

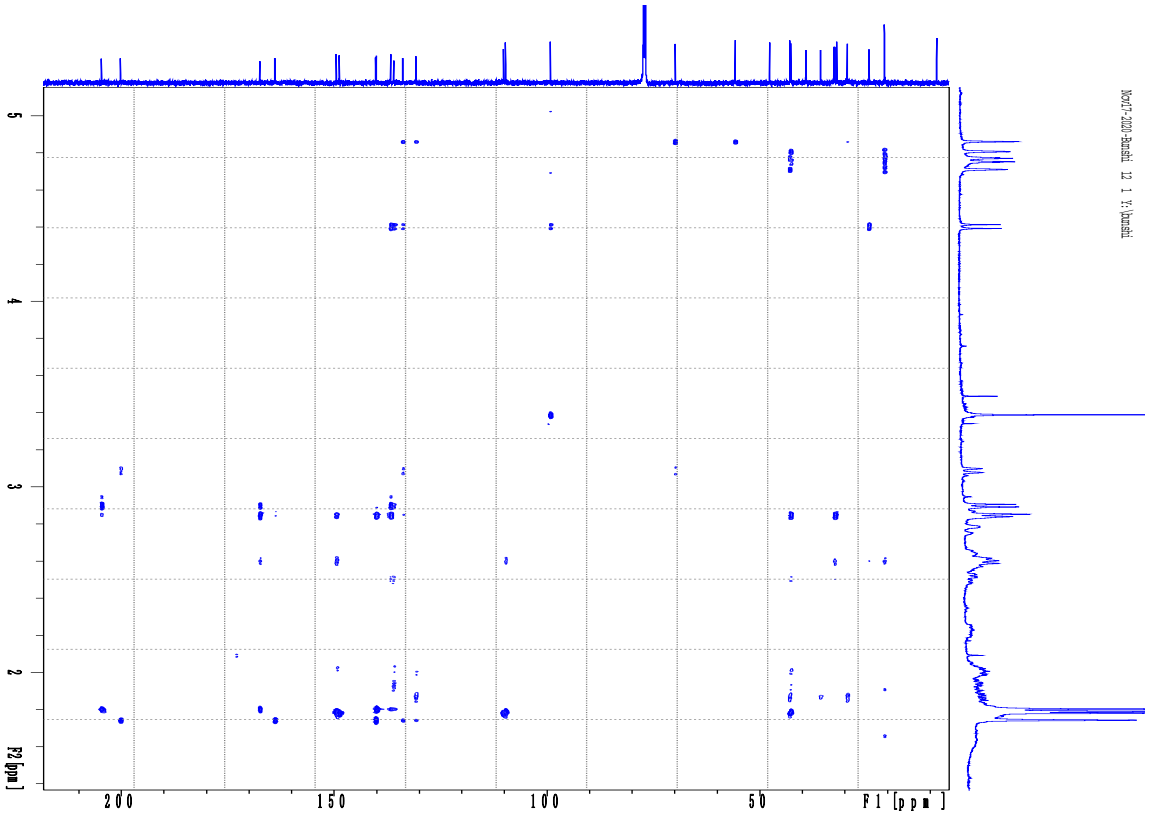


Figure S8. HMBC spectrum of **1**.

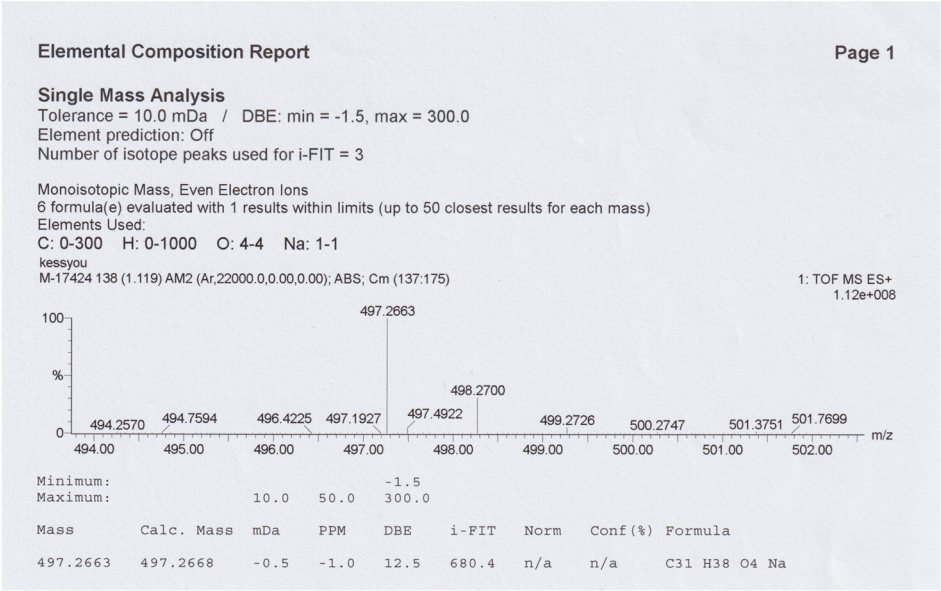


Figure S9. HR-ESI-MS chart of **1**.

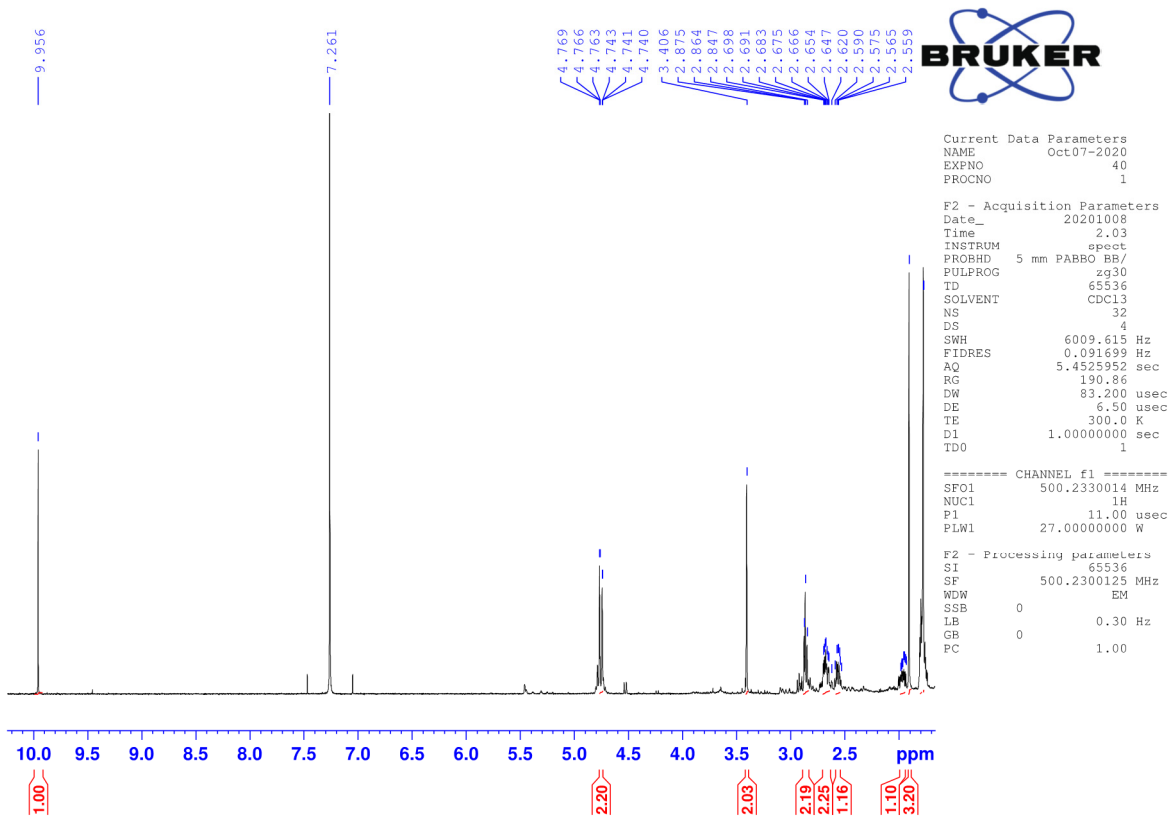


Figure S10. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **2**.

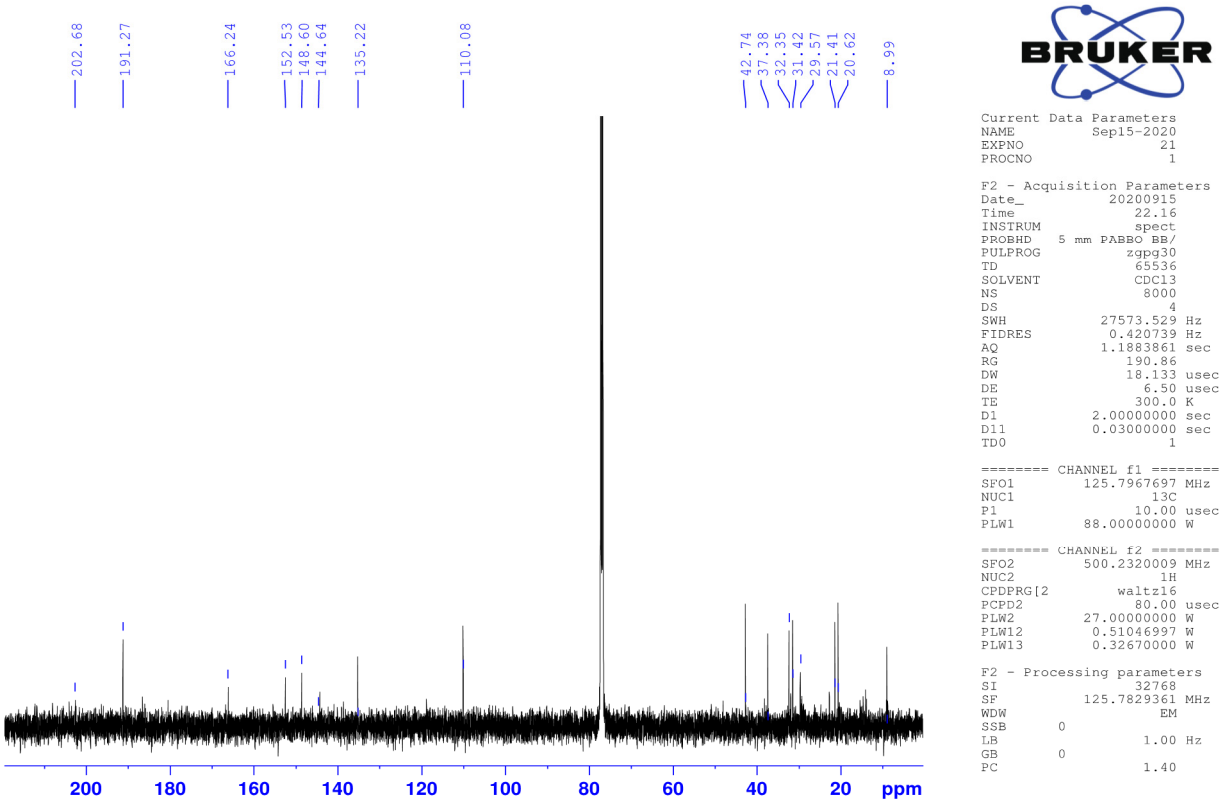


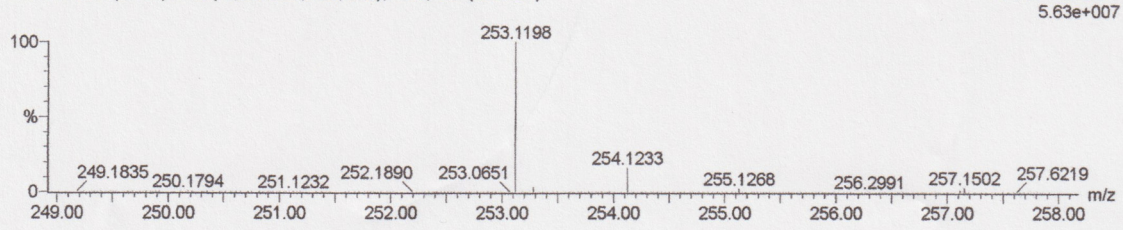
Figure S11. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of **2**.

Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 10.0 mDa / DBE: min = -1.5, max = 300.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
3 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 1-300 H: 1-1000 O: 2-2 Na: 1-1
fr3-3-2-1
M-17259 265 (2.133) AM2 (Ar,22000.0,0.00,0.00); ABS; Cm (230:267)

1: TOF MS ES+
5.63e+007



	Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
Minimum:					-1.5				
Maximum:			10.0	50.0	300.0				
	253.1198	253.1204	-0.6	-2.4	6.5	1001.6	n/a	n/a	C15 H18 O2 Na

Figure S12. HR-ESI-MS chart of **2**.