Structurally diverse triterpenes obtained from the fruits of *Ziziphus jujuba* Mill. as inflammation inhibitors by NF-κB signaling pathway

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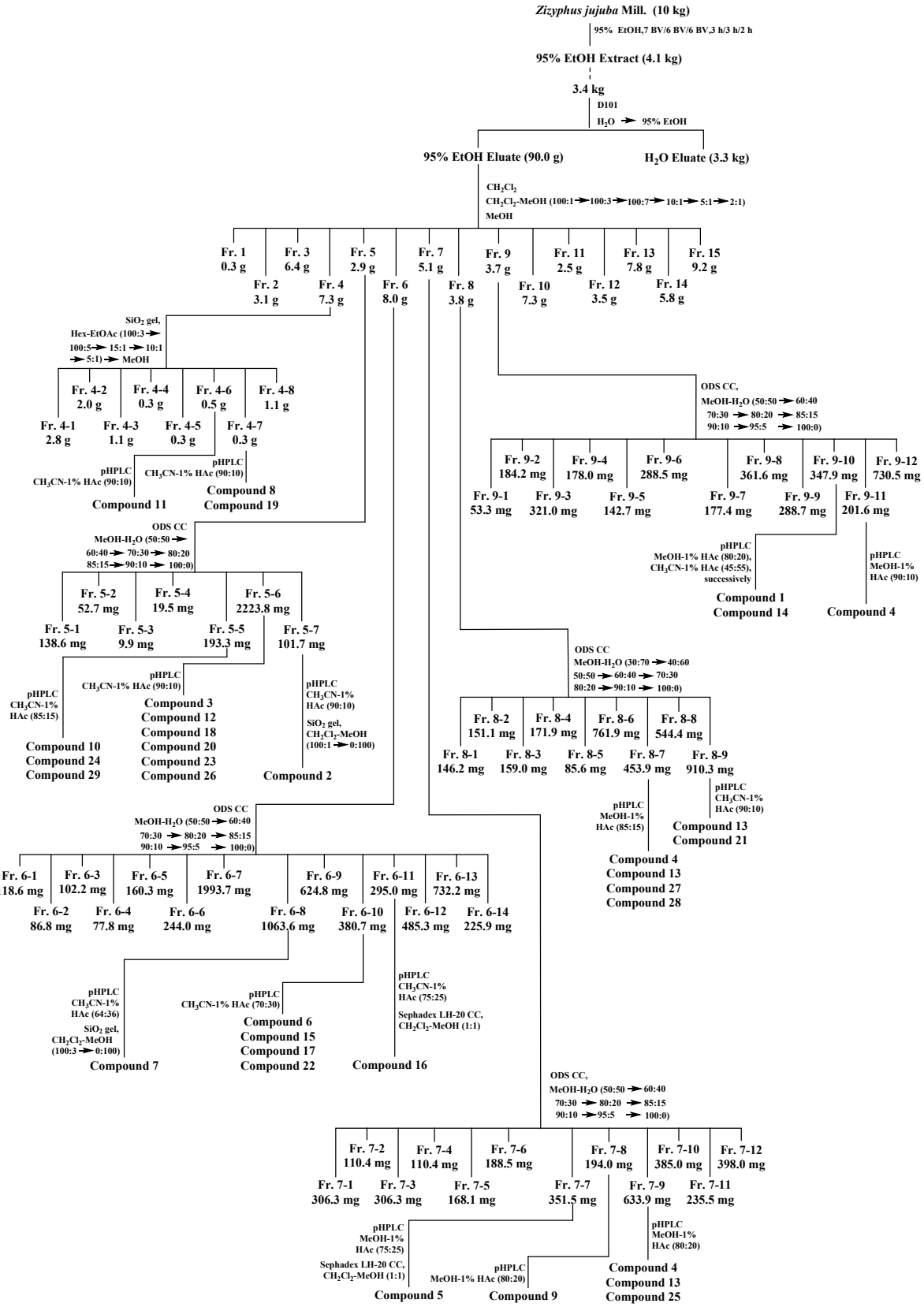


Chart S1. The extraction and isolation progress of triterpenes **1**–**29** from *Z. jujuba*

S1. The NMR data of compounds 2–29

*Lup-20 (29)-en-3-on-28-oic acid (**2**, purity percentage is 98.3%)*: White powder; ^{1}H NMR ($CDCl_3$, 500 MHz) spectroscopic data: δ 0.92, 0.99, 0.99, 1.02, 1.07, 1.70 (3H each, all s, H_3-26, 25, 27, 24, 23 and 29), 4.61, 4.75 (1H each, both br. s, H_2-30); ^{13}C NMR ($CDCl_3$, 125 MHz) spectroscopic data: see Tab. S1; ESI-Q-Orbitrap MS *m/z* 453.33734 $[M–H]^-$ (calcd for $C_{30}H_{47}O_3$, 453.33632).

*Betulinic acid (**3**, purity percentage is 99.5%)*: White powder; ^{1}H NMR (C_5D_5N, 600 MHz) spectroscopic data: δ 0.84, 1.02, 1.07, 1.08, 1.23, 1.80 (3H each, all s, H_3-24, 25, 26, 27, 23 and 29), 3.46 (1H, t like, *ca*. *J* = 8 Hz, H-3), 4.78, 4.95 (1H each, both br. s, H_2-30); ^{13}C NMR (C_5D_5N, 150 MHz) spectroscopic data: see Tab. S1; ESI-Q-Orbitrap MS *m/z* 455.35287 $[M–H]^-$ (calcd for $C_{30}H_{47}O_3$, 455.35197); and according to our identification, the chemical shift values of C-15 and C-21 in the literature were exchanged.

*2α-Hydroxybetulinic acid (**4**, purity percentage is 99.3%)*: White powder; ^{1}H NMR (C_5D_5N, 500 MHz) spectroscopic data: δ 0.91, 1.05, 1.05, 1.06, 1.25, 1.79 (3H each, all s, H_3-25, 24, 26, 27, 23 and 29), 3.38 (1H, d, *J* = 9.5 Hz, H-3), 4.08 (1H, dt, *J* = 4.5, 9.5 Hz, H-2), 4.77, 4.93 (1H each, both br. s, H_2-30); ^{13}C NMR (C_5D_5N, 125 MHz) spectroscopic data: see Tab. S1; ESI-Q-Orbitrap MS *m/z* 471.34763 $[M–H]^-$ (calcd for $C_{30}H_{47}O_4$, 471.34689); and according to our identification, the chemical shift values of C-23 and C-27, C-25 and C-26 in the literature were exchanged.

*3β,30-Dihydroxylup-20(29)-en-28-oic acid (**5**, purity percentage is 93.0%)*:

White powder; ^{1}H NMR (DMSO-d_6, 500 MHz) spectroscopic data: δ 0.65, 0.76, 0.87, 0.93, 1.24 (3H each, all s, H_3-24, 25, 26, 27 and 23), 2.97 (1H, t like, *ca*. J = 8 Hz, H-3), 3.89 (2H, s, H_2-29), 4.77, 4.86 (1H each, both br. s, H_2-30); ^{13}C NMR (DMSO-d_6, 125 MHz) spectroscopic data: see Tab. S1; ESI-Q-Orbitrap MS *m/z* 471.34747 [M–H]$^-$ (calcd for $C_{30}H_{47}O_4$, 471.34689).

*2-O-trans-p-Coumaroylalphitolic acid (**6**, purity percentage is 97.9%)*: White powder; ^{1}H NMR (C_5D_5N, 500 MHz) spectroscopic data: δ 1.01, 1.04, 1.09, 1.11, 1.30, 1.88 (3H each, all s, H_3-25, 26, 27, 24, 23 and 29), 3.66 (1H, d, J = 10.0 Hz, H-3), 4.81, 4.96 (1H each, both br. s, H_2-29), 5.65 (1H, dt, J = 4.5, 10.0 Hz, H-2), 6.63, 8.03 (1H each, both d, J = 16.5 Hz, H-8',7'), 7.17 (2H, d, J = 8.5 Hz, H-3',5'), 7.51 (2H, d, J = 8.5 Hz, H-2',6'); ^{13}C NMR (C_5D_5N, 125 MHz) spectroscopic data: see Tab. S1; ESI-Q-Orbitrap MS *m/z* 617.38452 [M–H]$^-$ (calcd for $C_{39}H_{53}O_6$, 617.38367).

*3-O-cis-p-Coumaroylalphitolic acid (**7**, purity percentage is 97.3%)*: White powder; ^{1}H NMR (C_5D_5N, 600 MHz) spectroscopic data: δ [1.32 (1H, t, J = 10.8 Hz), 2.37 (1H, dd, J = 4.2, 10.8 Hz), H_2-1], 4.26 (1H, dt, J = 4.2, 10.8 Hz, H-2), 5.20 (1H, d, J = 10.8 Hz, H-3), 1.03 (1H, m, overlapped, H-5), [1.35, 1.45 (1H, both m, overlapped), H_2-6], [1.32 (1H, m), 1.35 (1H, m, overlapped), H_2-7], 1.45 (1H, m, overlapped, H-9), 1.21, 1.50 (1H each, both m, H_2-11), 1.20, 1.92 (1H each, both m, H_2-12), 2.72 (1H, dt, J = 3.0, 11.4 Hz, H-13), 1.22, 1.85 (1H each, both m, H_2-15), [1.55 (1H, m), 2.63 (1H, dt, J = 3.0, 12.6 Hz), H_2-16], 1.74 (1H, t like, *ca*. J = 11 Hz, H-18), 3.53 (1H, dt, J = 4.2, 10.8 Hz, H-19), 1.53, 2.23 (2H, m, H_2-21), 1.60, 2.25 (1H each, both m, H_2-22), 1.03, 0.96, 0.89, 1.03, 1.04, 1.78 (3H each, all s, H_3-23, 24,

25, 26, 27 and 29), 4.71, 4.94 (1H each, both br. s, H_2-30), 8.15 (2H, d, J = 8.5 Hz, H-2',6'), 7.14 (2H, d, J = 8.5 Hz, H-3',5'), 6.93, 6.09 (1H each, both d, J = 12.6 Hz, H-7', 8'); ^{13}C NMR (C_5D_5N, 150 MHz) spectroscopic data: see Tab. S1; ESI-Q-Orbitrap MS *m/z* 617.38422 $[M–H]^-$ (calcd for $C_{39}H_{53}O_6$, 617.38367).

*(3α,4β,5β,8α,9β,10α,13α,14β,15β)-13-Carboxy-4,9-dimethyl-15-(1-methylethenyl)-3-(1-methylethyl)-18-norandrostane-4-propanoic acid (**8**, purity percentage is 96.5%):* White powder; ^{1}H NMR (C_5D_5N, 600 MHz) spectroscopic data: δ 1.97 (2H, m, overlapped, H_2-1), 2.51 (2H, t, J = 7.8 Hz, H_2-2), 1.94 (1H, m, H-4), 1.18 (1H, m, overlapped, H-5), 1.33 (2H, m, H_2-6), 1.36, 1.42 (1H each, both m, H_2-7), 1.72 (1H, br. d, *ca*. J = 12 Hz, H-9), 1.18, 1.54 (1H each, both m, overlapped, H_2-11), 1.24, 1.94 (1H each, both m, H_2-13), 2.79 (1H, t like, *ca*. J = 11 Hz, H-14), 1.27, 1.84 (1H each, both m, H_2-15), 1.55, 2.63 (1H each, both m, H_2-16), 1.79 (1H, m, overlapped, H-18), 3.55 (1H, t like, *ca*. J = 11 Hz, H-19), 1.53, 2.25 (2H, m, H_2-21), 1.57, 2.28 (1H each, both m, H_2-22), 0.94, 0.76, 0.79, 1.07, 1.12, 1.79 (3H each, all s, H_3-23, 24, 25, 26, 27 and 29), 4.78, 4.96 (1H each, both s, H_2-30); ^{13}C NMR (C_5D_5N, 150 MHz) spectroscopic data: see Tab. S1; ESI-Q-Orbitrap MS *m/z* 471.34756 $[M–H]^-$ (calcd for $C_{30}H_{47}O_4$, 471.34689).

*Ceanothic acid (**9**, purity percentage is 99.0%)*: White powder; ^{1}H NMR (C_5D_5N, 500 MHz) spectroscopic data: δ 1.08, 1.16, 1.27, 1.40, 1.43, 1.67 (3H each, all s, H_3-27, 26, 24, 25, 23 and 29), 4.67, 4.86 (1H each, both s, H_2-30); ^{13}C NMR (C_5D_5N, 125 MHz) spectroscopic data: see Tab. S1; ESI-Q-Orbitrap MS *m/z* 485.32706 $[M–H]^-$ (calcd for $C_{30}H_{45}O_5$, 485.32615). And according to our identification, the chemical

198 shift values of C-4 and C-8 in the literature were exchanged.

199 *Ceanothic acid 2-methyl ester (**10**, purity percentage is 98.2%)*: White powder;
200 ^{1}H NMR (C_5D_5N, 600 MHz) spectroscopic data: δ 1.11, 1.14, 1.22, 1.31, 1.33, 1.78
201 (3H each, all s, H_3-26, 27, 24, 25, 23 and 29), 3.01 (1H, br. s, H-1), 4.60 (1H, br. s, H-
202 3), 4.74, 4.95 (1H each, both s, H_2-30); ^{13}C NMR (C_5D_5N, 150 MHz) spectroscopic
203 data: see Tab. S1; ESI-Q-Orbitrap MS *m/z* 499.34256 $[M–H]^-$ (calcd for $C_{31}H_{47}O_5$,
204 499.3418).

205 *3-Oxo-oleana-12-en-28-oic acid (**11**, purity percentage is 96.3%)*: White powder;
206 ^{1}H NMR (C_5D_5N, 500 MHz) spectroscopic data: δ 0.90, 0.97, 1.01, 1.02, 1.02, 1.16,
207 1.26 (3H each, all s, H_3-25, 29, 26, 24, 30, 23 and 27), 5.50 (1H, br. s, H-12); ^{13}C
208 NMR (C_5D_5N, 125 MHz) spectroscopic data: see Tab. S1; ESI-Q-Orbitrap MS *m/z*
209 453.33710 $[M–H]^-$ (calcd for $C_{30}H_{45}O_3$, 453.33632). And according to our
210 identification, the chemical shift values of C-9 and C-17 in the literature were
211 exchanged.

212 *Oleanolic acid (**12**, purity percentage is 94.9%)*: White powder; ^{1}H NMR
213 (C_5D_5N, 600 MHz) spectroscopic data: δ 0.91, 0.97, 1.03, 1.04, 1.04, 1.26, 1.30 (3H
214 each, all s, H_3-25, 29, 30, 24, 26, 23 and 27), 3.46 (1H, dd, J = 4.8, 10.2 Hz, H-3),
215 5.52 (1H, t, J = 3.6 Hz, H-12); ^{13}C NMR (C_5D_5N, 150 MHz) spectroscopic data: see
216 Tab. S2; ESI-Q-Orbitrap MS *m/z* 455.35303 $[M–H]^-$ (calcd for $C_{30}H_{47}O_3$, 455.35197).

217 *Maslinic acid (**13**, purity percentage is 97.3%)*: White powder; ^{1}H NMR (C_5D_5N,
218 500 MHz) spectroscopic data: δ 0.95, 0.99, 1.01, 1.01, 1.07, 1.27, 1.27 (3H each, all s,
219 H_3-29, 25, 26, 30, 24, 23 and 27), 3.38 (1H, d, J = 9.5 Hz, H-3), 4.07 (1H, ddd, J = 4.5,

10.0, 14.0 Hz, H-2), 5.46 (1H, t, J = 4.0 Hz, H-12); ^{13}C NMR (C_5D_5N, 125 MHz) spectroscopic data: see Tab. S2; ESI-Q-Orbitrap MS *m/z* 471.34799 $[M–H]^-$ (calcd for $C_{30}H_{47}O_4$, 471.34689). And according to our identification, the chemical shift values of C-1 and C-17 in the literature were exchanged.

*11-Oxo-maslinic acid (2α,3β-dihydroxy-11-oxo-18β-olean-12-en-28-oic acid (**14**, purity percentage is 98.0%)*: White powder; ^{1}H NMR (CD_3OD, 600 MHz) spectroscopic data: δ 0.81, 0.94, 0.96, 0.98, 1.02, 1.17, 1.41 (3H each, all s, H_3-24, 29, 30, 26, 23, 25 and 27), 2.92 (1H, d, J = 9.6 Hz, H-3), 3.67 (1H, ddd, J = 4.2, 9.6, 14.4 Hz, H-2), 5.56 (1H, s, H-12); ^{13}C NMR (CD_3OD, 150 MHz) spectroscopic data: see Tab. S2; ESI-Q-Orbitrap MS *m/z* 485.32717 $[M–H]^-$ (calcd for $C_{30}H_{45}O_5$, 485.32615). And according to our identification, the chemical shift values of C-7 and C-22 in the literature were exchanged.

*2α-trans-p-Coumaroyloxy-2α,3β,23α-trihydroxy-olean-12-en-28-oic acid (**15**, purity percentage is 91.5%)*: White powder; ^{1}H NMR (DMSO-d_6, 600 MHz) spectroscopic data: δ 0.72, 0.77, 0.87, 0.87, 0.96, 0.99, 1.10 (3H each, all s, H_3-26, 24, 29, 30, 23, 25 and 27), 3.13 (1H, d, J = 10.8 Hz, H-3), 4.90 (1H, dt, *ca*. J = 4.8, 10.8 Hz, H-2), 5.17 (1H, br. s, H-12), 6.32, 7.54 (1H each, both d, J = 15.6 Hz, H-8',7'), 6.80 (2H, d, J = 8.4 Hz, H-3',5'), 7.52 (2H, d, J = 8.4 Hz, H-2',6'); ^{13}C NMR (DMSO-d_6, 150 MHz) spectroscopic data: see Tab. S2; ESI-Q-Orbitrap MS *m/z* 617.38428 $[M–H]^-$ (calcd for $C_{39}H_{53}O_6$, 617.38367).

*2α-cis-p-Coumaroyloxy-2α,3β,23α-trihydroxy-olean-12-en-28-oic acid (**16**, purity percentage is 98.0%)*: White powder; ^{1}H NMR (DMSO-d_6, 600 MHz)

242 spectroscopic data: δ 0.72, 0.77, 0.87, 0.87, 0.98, 0.99, 1.10 (3H each, all s, H_3-26, 24,
243 29, 30, 23, 25 and 27), 3.13 (1H, d, J = 10.8 Hz, H-3), 4.90 (1H, dt, *ca*. J = 4.8, 10.8
244 Hz, H-2), 5.14 (1H, br. s, H-12), 5.75, 6.81 (1H each, both d, J = 13.2 Hz, H-8',7'),
245 6.75 (2H, d, J = 8.4 Hz, H-3',5'), 7.69 (2H, d, J = 8.4 Hz, H-2',6'); ^{13}C NMR (DMSO-
246 d_6, 150 MHz) spectroscopic data: see Tab. S2; ESI-Q-Orbitrap MS *m/z* 617.38440
247 $[M–H]^-$ (calcd for $C_{39}H_{53}O_6$, 617.38367).

248 *3-O-trans-p-Coumaroyl maslinic acid (**17**, purity percentage is 98.0%)*: White
249 powder; ^{1}H NMR (C_5D_5N, 600 MHz) spectroscopic data: δ 0.97, 1.01, 1.01, 1.02,
250 1.04, 1.06, 1.28 (3H each, all s, H_3-29, 25, 26, 30, 24, 23 and 27), 4.29 (1H, ddd, J =
251 4.8, 10.2, 10.8 Hz, H-2), 5.24 (1H, d, J = 10.2 Hz, H-3), 5.47 (1H, br. s, H-12), 6.68,
252 8.00 (1H each, both d, J = 15.6 Hz, H-8',7'), 7.16 (2H, d, J = 8.4 Hz, H-3',5'), 7.56
253 (2H, d, J = 8.4 Hz, H-2',6'); ^{13}C NMR (C_5D_5N, 150 MHz) spectroscopic data: see Tab.
254 S2; ESI-Q-Orbitrap MS *m/z* 617.38403 $[M–H]^-$ (calcd for $C_{39}H_{53}O_6$, 617.38367).

255 *3,4-Seco-olean-12-ene-3,28-dioic acid (**18**, purity percentage is 98.3%)*: White
256 powder; ^{1}H NMR (C_5D_5N, 600 MHz) spectroscopic data: δ 0.77, 0.85, 0.95, 0.99,
257 1.02, 1.03, 1.26 (3H each, all s, H_3-24, 25, 23, 29, 30, 26 and 27), 5.49 (1H, br. s, H-
258 12); ^{13}C NMR (C_5D_5N, 150 MHz) spectroscopic data: see Tab. S2; ESI-Q-Orbitrap
259 MS *m/z* 471.34741 $[M–H]^-$ (calcd for $C_{30}H_{47}O_4$, 471.34689).

260 *3-Oxo-urs-12-en-28-oic acid (**19**, purity percentage is 96.5%)*: White powder;
261 ^{1}H NMR (C_5D_5N, 600 MHz) spectroscopic data: δ 0.89, 1.00, 1.02, 1.14, 1.20 (3H
262 each, all s, H_3-25, 24, 26, 23 and 27), 0.97 (3H, d, J = 6.0 Hz, H_3-30), 1.00 (1H, d, J =
263 6.0 Hz, H_3-29), 5.47 (1H, br. s, H-12); ^{13}C NMR (C_5D_5N, 150 MHz) spectroscopic

data: see Tab. S2; ESI-Q-Orbitrap MS *m/z* 453.33716 $[M–H]^-$ (calcd for $C_{30}H_{45}O_3$, 453.33632).

*Ursolic acid (**20**, purity percentage is 95.3%)*: White powder; ^1H NMR (C_5D_5N, 600 MHz) spectroscopic data: δ 0.91, 1.04, 1.07, 1.24, 1.26 (3H each, all s, H_3-25, 24, 26, 27 and 23), 0.97 (3H, d, J = 6.6 Hz, H_3-30), 1.02 (1H, d, J = 6.6 Hz, H_3-29), 3.47 (1H, dd, J = 5.4, 10.2 Hz, H-3), 5.51 (1H, t, J = 3.0 Hz, H-12); ^{13}C NMR (C_5D_5N, 150 MHz) spectroscopic data: see Tab. S3; ESI-Q-Orbitrap MS *m/z* 455.35297 $[M–H]^-$ (calcd for $C_{30}H_{47}O_3$, 455.35197).

*2α-Hydroxyursolic acid (**21**, purity percentage is 95.3%)*: White powder; ^1H NMR (C_5D_5N, 500 MHz) spectroscopic data: δ 0.97, 1.03, 1.06, 1.21, 1.26 (3H each, all s, H_3-25, 26, 24, 27 and 23), 0.96 (3H, d, J = 6.5 Hz, H_3-30), 0.99 (1H, d, J = 6.5 Hz, H_3-29), 3.38 (1H, d, J = 9.5 Hz, H-3), 4.07 (1H, ddd, J = 4.5, 9.5, 14.0 Hz, H-2), 5.47 (1H, t, J = 3.5 Hz, H-12); ^{13}C NMR (C_5D_5N, 125 MHz) spectroscopic data: see Tab. S3; ESI-Q-Orbitrap MS *m/z* 471.34784 $[M–H]^-$ (calcd for $C_{30}H_{47}O_4$, 471.34689).

*Jacoumaric acid (**22**, purity percentage is 93.0%)*: White powder; ^1H NMR (C_5D_5N, 500 MHz) spectroscopic data: δ 0.97 (3H, d, J = 6.0 Hz, H_3-30), 1.00 (3H, d, J = 5.0 Hz, H_3-29), 1.01, 1.05, 1.05, 1.09, 1.24 (3H each, all s, H_3-25, 24, 26, 23 and 27), 4.29 (1H, dt, J = 5.0, 9.5 Hz, H-2), 5.27 (1H, d, J = 9.5 Hz, H-3), 5.48 (1H, t, J = 4.0 Hz, H-12), 6.68, 8.00 (1H each, both d, J = 16.0 Hz, H-8',7'), 7.17 (2H, d, J = 8.5 Hz, H-3',5'), 7.51 (2H, d, J = 8.5 Hz, H-2',6'); ^{13}C NMR (C_5D_5N, 125 MHz) spectroscopic data: see Tab. S3; ESI-Q-Orbitrap MS *m/z* 617.38409 $[M–H]^-$ (calcd for $C_{39}H_{53}O_6$, 617.38367). And according to our identification, the chemical shift

values of C-26 and C-29, C-3',5' and C-8' in the literature were exchanged.

*(1S,2S,4aR,4bS,6aS,9R,10S,10aS,12aR)-6a-Carboxy-1,2,3,4,4a,4b,5,6,6a,7,8,9,10,10a,12,12a-hexadecahydro-1,4a,4b,9,10-pentamethyl-2-(1-methylethyl)-1-chrysenepropanoic acid (**23**, purity percentage is 92.8%)*: White powder; ^{1}H NMR (C_5D_5N, 600 MHz) spectroscopic data: δ 1.99 (2H, m, overlapped, H_2-1), 2.53 (2H, t, J = 7.2 Hz, H_2-2), 1.92 (1H, m, H-4), 1.22 (1H, m, overlapped, H-5), 1.35 (1H, m, H_2-6), 1.38, 1.46 (1H each, both m, H_2-7), 2.01 (1H, m, overlapped, H-9), 1.95, 2.09 (1H each, both m, H_2-11), 5.48 (1H, t like, *ca.* J = 4 Hz, H-12), [1.23 (1H, m, overlapped), 2.31 (1H, br. t, *ca*. J = 11 Hz), H_2-15], 2.07, 2.12 (1H each, both m, H_2-16), 2.64 (1H, d, J = 10.2 Hz, H-18), 1.45 (1H, m, H-19), 1.02 (1H, m, H-20), 2.00 (2H, m, overlapped, H_2-21), 1.37, 1.47 (1H each, both m, H_2-22), 0.93, 0.77, 0.85, 1.07, 1.24 (3H each, all s, H_3-23, 24, 25, 26 and 27), 0.94, 0.95 (3H each, both d, J = 6.0 Hz, H_3-29 and 30); ^{13}C NMR (C_5D_5N, 150 MHz) spectroscopic data:see Tab. S3; ESI-Q-Orbitrap MS *m/z* 471.34763 $[M–H]^-$ (calcd for $C_{30}H_{47}O_4$, 471.34689).

*Pomonic acid (**24**, purity percentage is 93.3%)*: White powder; ^{1}H NMR (C_5D_5N, 600 MHz) spectroscopic data: δ 0.93, 1.02, 1.10, 1.15, 1.71 (3H each, all s, H_3-25, 24, 26, 23 and 27), 1.14 (3H, d, J = 6.6 Hz, H_3-30), 5.61 (1H, br. s, H-12); ^{13}C NMR (C_5D_5N, 150 MHz) spectroscopic data: see Tab. S3; ESI-Q-Orbitrap MS *m/z* 469.33218 $[M–H]^-$ (calcd for $C_{30}H_{45}O_4$, 469.33124). And according to our identification, the chemical shift values of C-23 and C-29 in the literature were exchanged.

*Pomolic acid (**25**, purity percentage is 93.7%)*: White powder; ^{1}H NMR (C_5D_5N,

600 MHz) spectroscopic data: δ 0.94, 1.05, 1.13, 1.26, 1.75 (3H each, all s, H_3-25, 24, 26, 23 and 27), 1.14 (3H, d, J = 6.0 Hz, H_3-30), 3.46 (1H, br. d, *ca.* J = 9 Hz, H-3), 5.63 (1H, br. s, H-12); ^{13}C NMR (C_5D_5N, 150 MHz) spectroscopic data: see Tab. S3; ESI-Q-Orbitrap MS *m/z* 471.34744 $[M–H]^-$ (calcd for $C_{30}H_{47}O_4$, 471.34689).

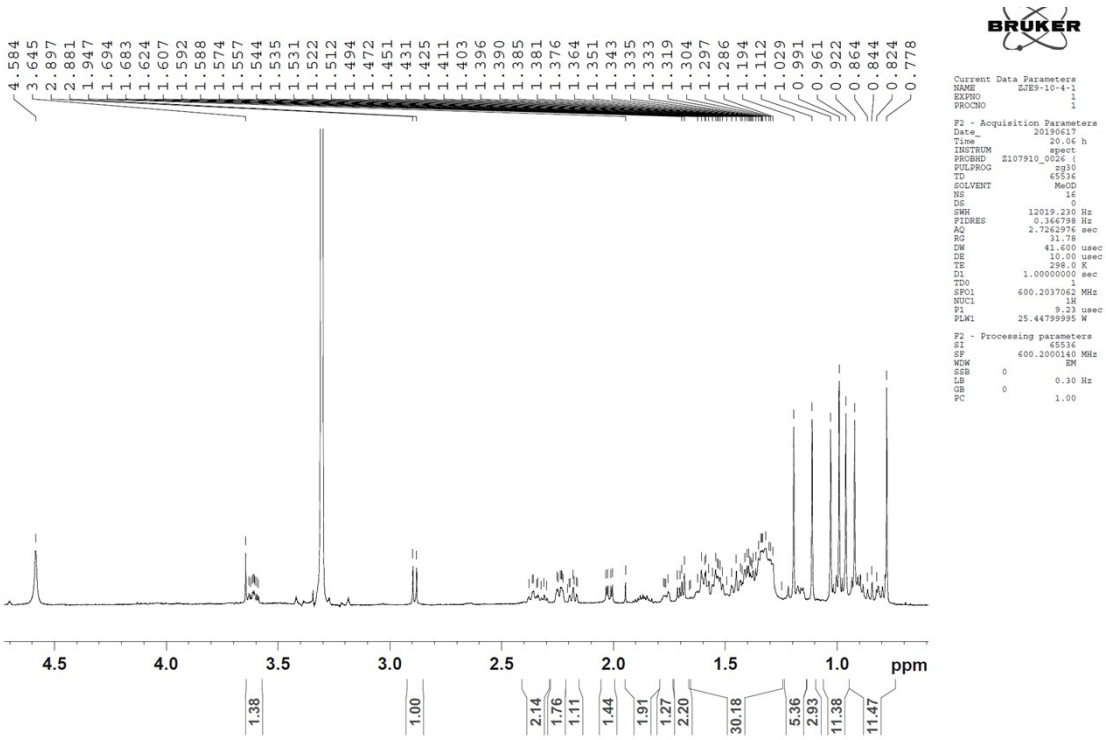
*2-Oxopomolic acid (**26**, purity percentage is 93.3%)*: White powder; ^{1}H NMR (C_5D_5N, 600 MHz) spectroscopic data: δ 0.88, 0.89, 1.06, 1.33, 1.76 (3H each, all s, H_3-24, 26, 25, 23 and 27), 1.14 (3H, d, J = 6.6 Hz, H_3-30), 1.44 (3H, s, H_3-29), 4.20 (1H, s, H-3), 5.58 (1H, t, J = 3.6 Hz, H-12); ^{13}C NMR (C_5D_5N, 150 MHz) spectroscopic data: see Tab. S3; ESI-Q-Orbitrap MS *m/z* 485.32736 $[M–H]^-$ (calcd for $C_{30}H_{45}O_5$, 485.32615). And the chemical shift value of C-11 in the literature was revised here.

*Euscaphic acid (**27**, purity percentage is 98.3%)*: White powder; ^{1}H NMR (C_5D_5N, 500 MHz) spectroscopic data: δ 0.92, 0.99, 1.12, 1.29, 1.66 (3H each, all s, H_3-24, 25, 26, 23 and 27), 1.13 (3H, d, J = 6.5 Hz, H_3-30), 3.79 (1H, d, J = 2.5 Hz, H-3), 4.33 (1H, dt, J = 2.5, 11.0 Hz, H-2), 5.60 (1H, br. s, H-12); ^{13}C NMR (C_5D_5N, 125 MHz) spectroscopic data: see Tab. S3; ESI-Q-Orbitrap MS *m/z* 487.34286 $[M–H]^-$ (calcd for $C_{30}H_{47}O_5$, 487.34180).

*2β,19α-Hydroxyursolic acid (**28**, purity percentage is 97.0%)*: White powder; ^{1}H NMR (C_5D_5N, 500 MHz) spectroscopic data: δ 1.15 (3H, d, J = 6.5 Hz, H_3-30), 1.19, 1.29, 1.41, 1.56, 1.79 (3H each, all s, H_3-26, 23, 24, 25 and 27), 1.49 (3H, s, H_3-29), 3.45 (1H, d, J = 3.0 Hz, H-3), 4.44 (1H, q, J = 3.0 Hz, H-2), 5.63 (1H, br. d, *ca.* J = 4 Hz, H-12); ^{13}C NMR (C_5D_5N, 125 MHz) spectroscopic data: see Tab. S3; ESI-Q-

330 Orbitrap MS *m/z* 487.34277 $[M–H]^-$ (calcd for $C_{30}H_{47}O_5$, 487.34180). And the
331 chemical shift value of C-2 in the literature was revised here.

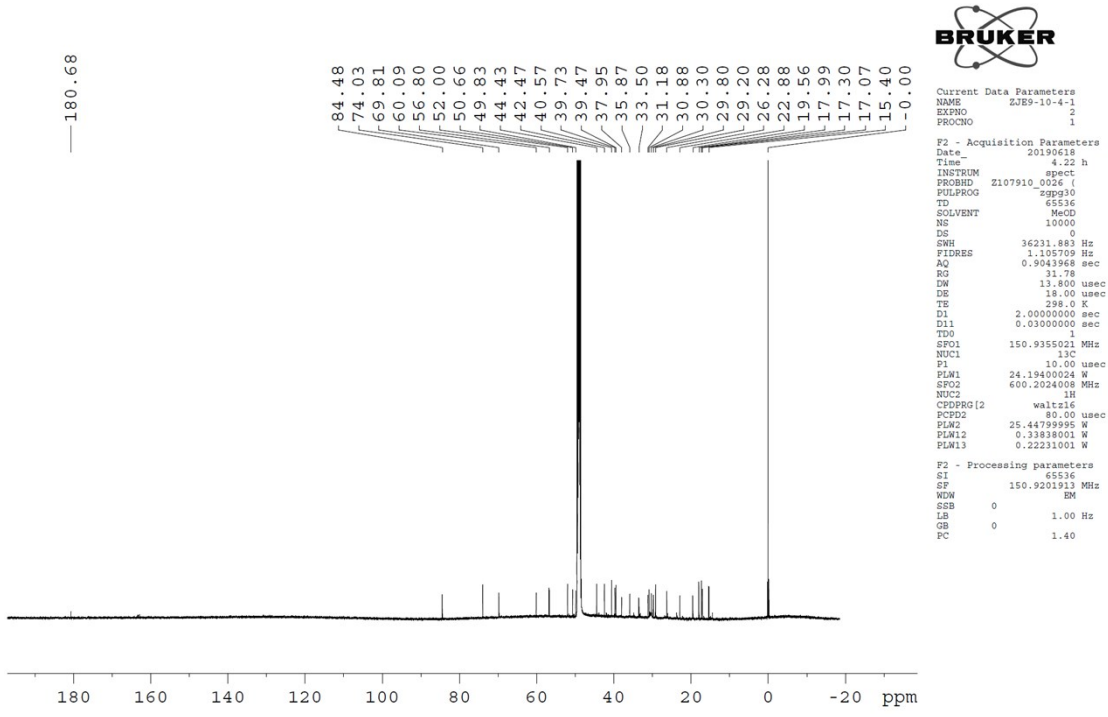
332 *Cecropiacic acid (**29**, purity percentage is 99.0%)*: White powder; ^1H NMR
333 (C_5D_5N, 600 MHz) spectroscopic data: δ 1.09 (3H, d, J = 6.6 Hz, H_3-30), 1.19, 1.20,
334 1.36, 1.56, 1.59, 1.88 (3H each, all s, H_3-26, 25, 29, 23, 24 and 27), 5.66 (1H, t like,
335 *ca.* J = 4 Hz, H-12); ^{13}C NMR (C_5D_5N, 150 MHz) spectroscopic data: see Tab. S3;
336 ESI-Q-Orbitrap MS *m/z* 517.31659 $[M–H]^-$ (calcd for $C_{30}H_{45}O_7$, 517.31598).
337 According to our identification, the chemical shift values of H_3-23 and H_3-24 in the
338 literature were exchanged.



341

342 **Fig. S1**. ^{1}H NMR (600MHz, CD_3OD) spectrum of compound **1**

343



344

345 **Fig. S2**. ^{13}C NMR (150MHz, CD_3OD) spectrum of compound **1**

346

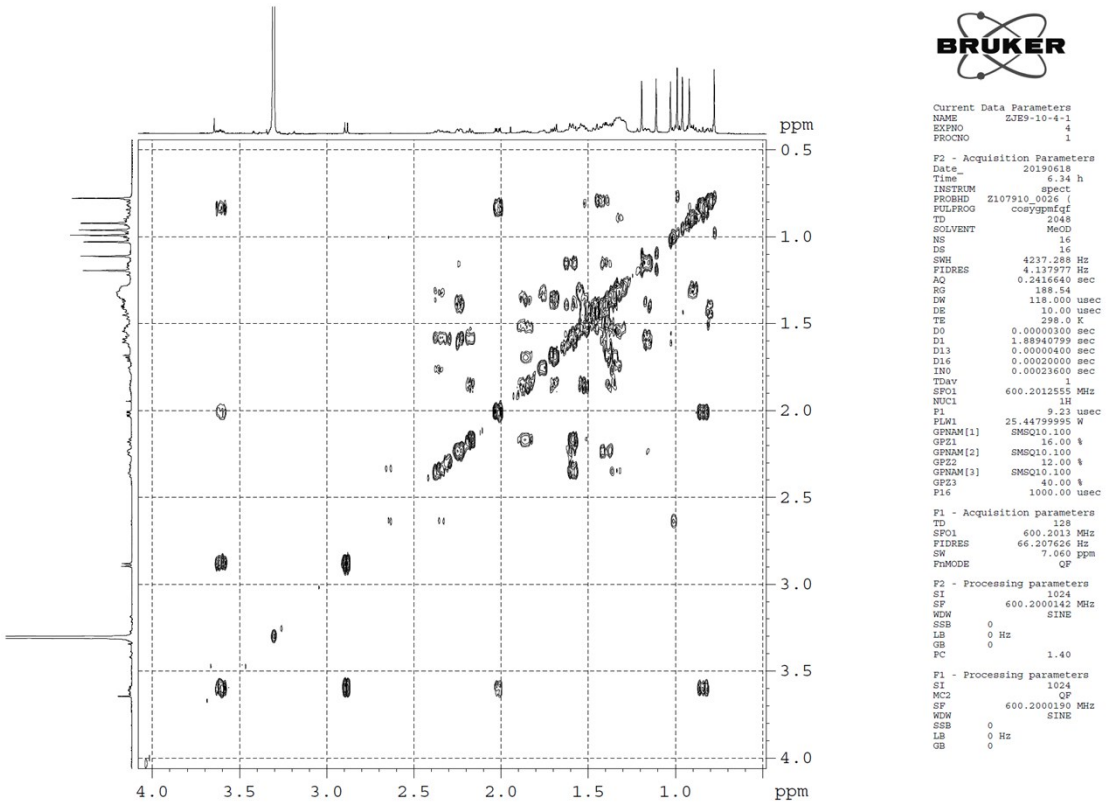


Fig. S3. The ^{1}H ^{1}H COSY (CD_3OD) spectrum of compound **1**

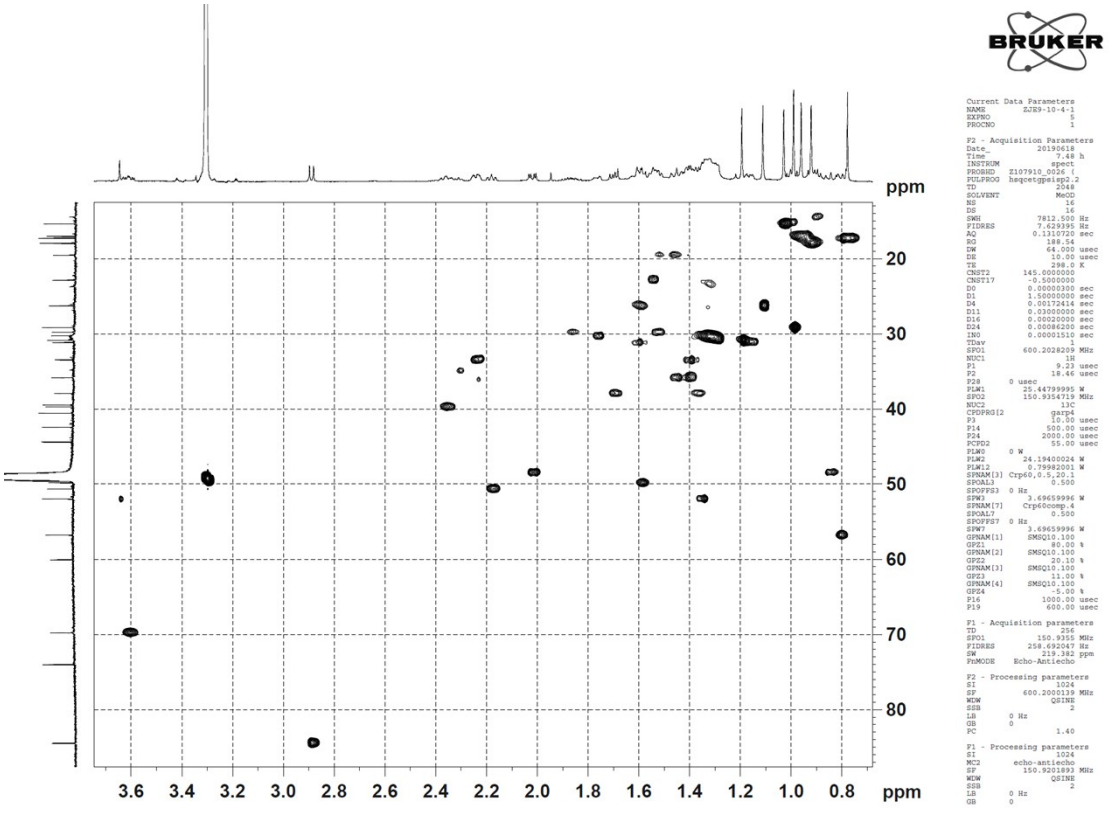
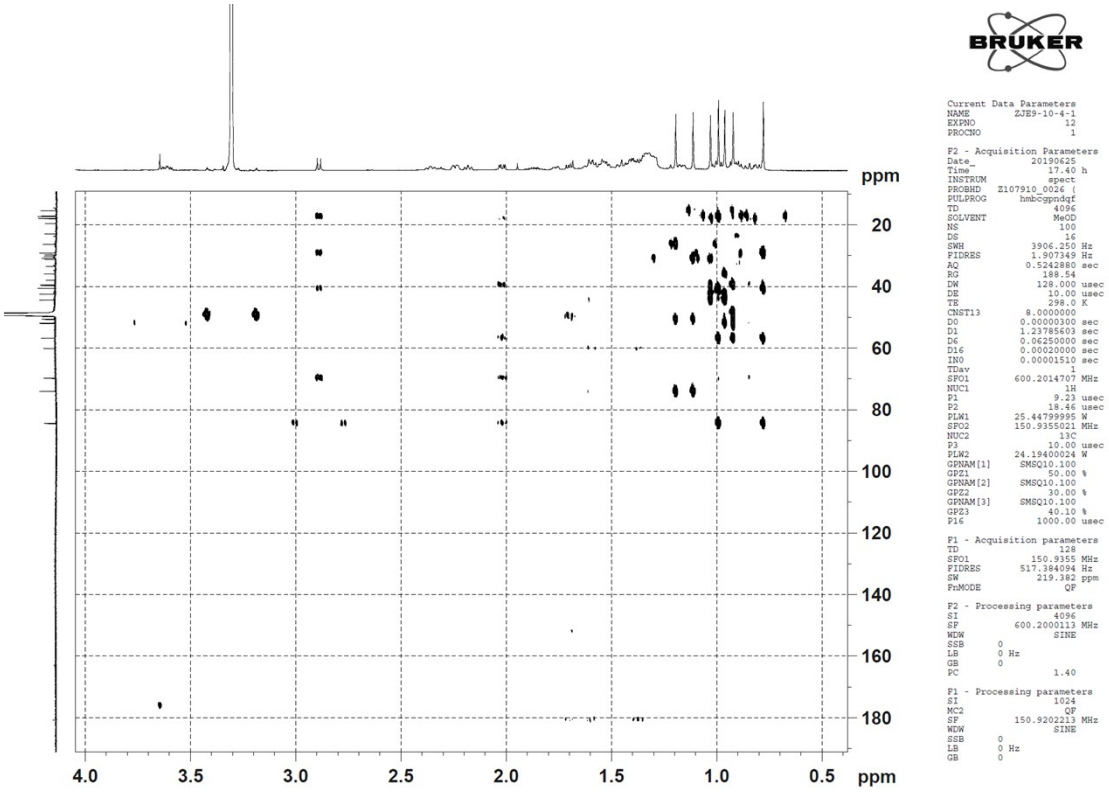


Fig. S4. The HSQC (CD_3OD) spectrum of compound **1**



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SOLVENT MeOD
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FIDRES 1.907349 Hz
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RG 188.54
DW 128.000 usec
DE 10.00 usec
TE 298.0 K
CNST13 8.0000000
D0 0.00000300 sec
D1 1.23785603 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001510 sec
TDav 1
SFO1 600.2014707 MHz
NUC1 1H
P1 9.23 usec
P2 18.46 usec
PLW1 25.44799995 W
SFO2 150.9355021 MHz
NUC2 13C
P3 10.00 usec
PLW2 24.19400024 W
GPNAM[1] SMSQ10.100
GPZ1 50.00 %
GPNAM[2] SMSQ10.100
GPZ2 30.00 %
GPNAM[3] SMSQ10.100
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
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FIDRES 517.384094 Hz
SW 219.382 ppm
FnMODE QF

F2 - Processing parameters
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WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
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MC2 QF
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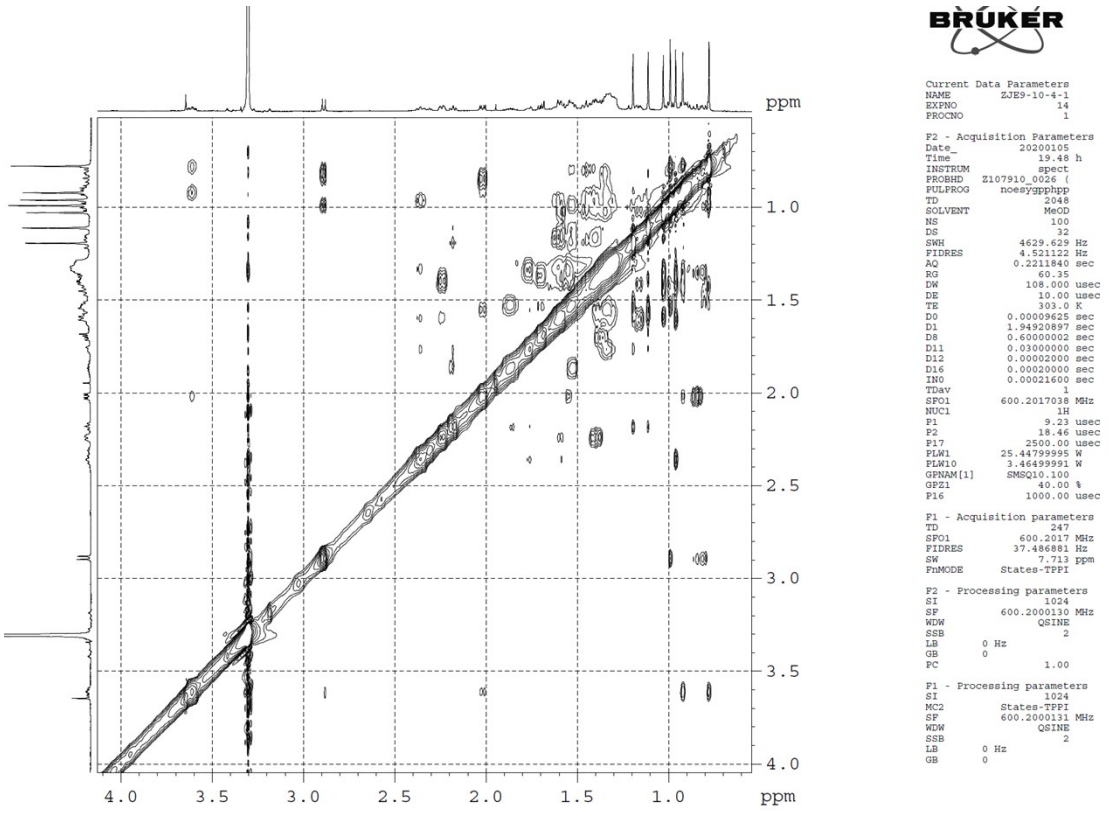
WDW SINE
SSB 0
LB 0 Hz
GB 0

Fig. S5. The HMBC (CD_3OD) spectrum of compound **1**



Current Data Parameters
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PROCNO 1

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FIDRES 4.521122 Hz
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D0 0.00009625 sec
D1 1.94920897 sec
D8 0.60000002 sec
D11 0.03000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.00021600 sec
TDav 1
SFO1 600.2017038 MHz
NUC1 1H
P1 9.23 usec
P2 18.46 usec
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PLW1 25.44799995 W
PLW10 3.46499991 W
GPNAM[1] SMSQ10.100
GPZ1 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
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SFO1 600.2017 MHz
FIDRES 37.486881 Hz
SW 7.713 ppm
FnMODE States-TPPI

F2 - Processing parameters
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SF 600.2000130 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 States-TPPI
SF 600.2000131 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

Fig. S6. The NOESY (CD_3OD) spectrum of compound **1**

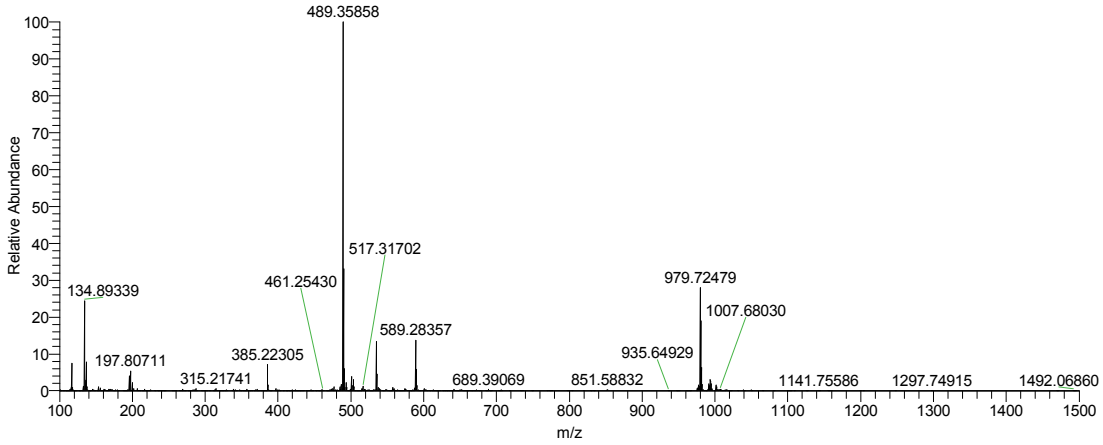


Fig. S7. The ESI-Q-Orbitrap MS spectrum of compound **1**

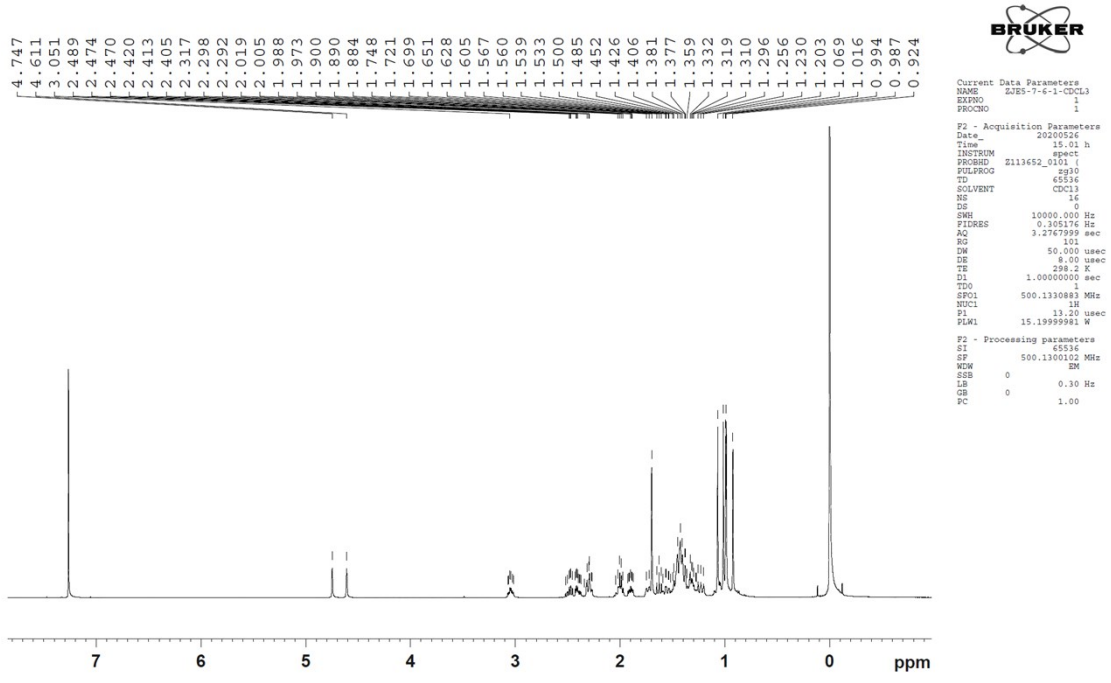


Fig. S8. ^{1}H NMR (500MHz, $CDCl_3$) spectrum of compound **2**

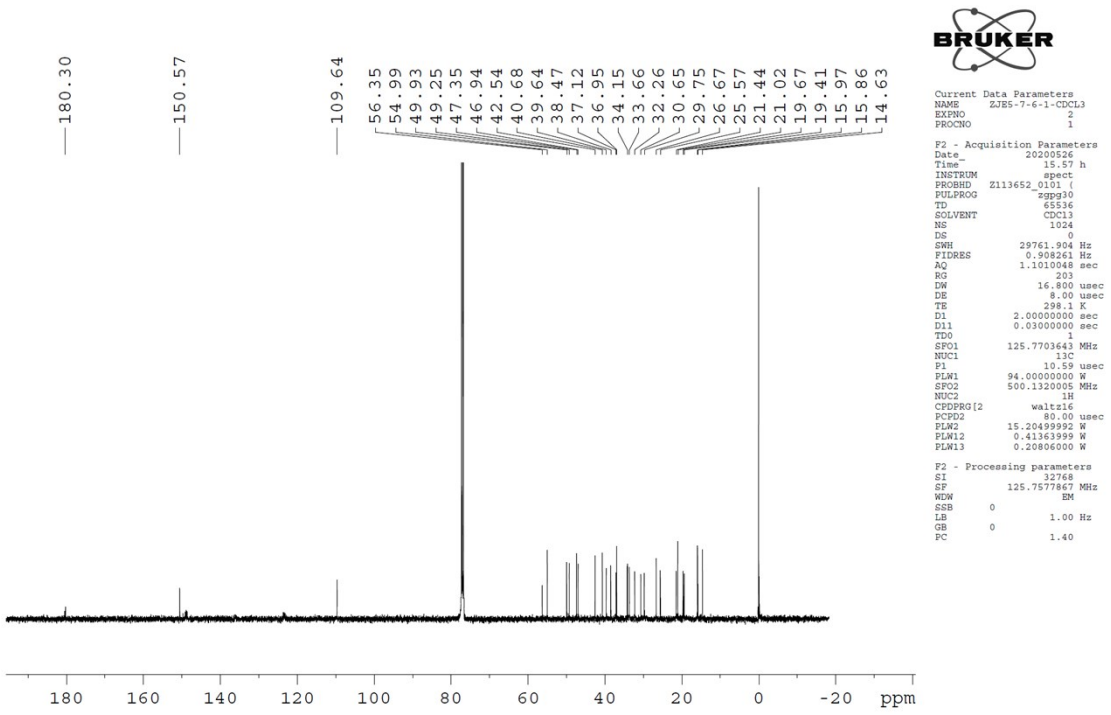


Fig. S9. ^{13}C NMR (125MHz, $CDCl_3$) spectrum of compound **2**

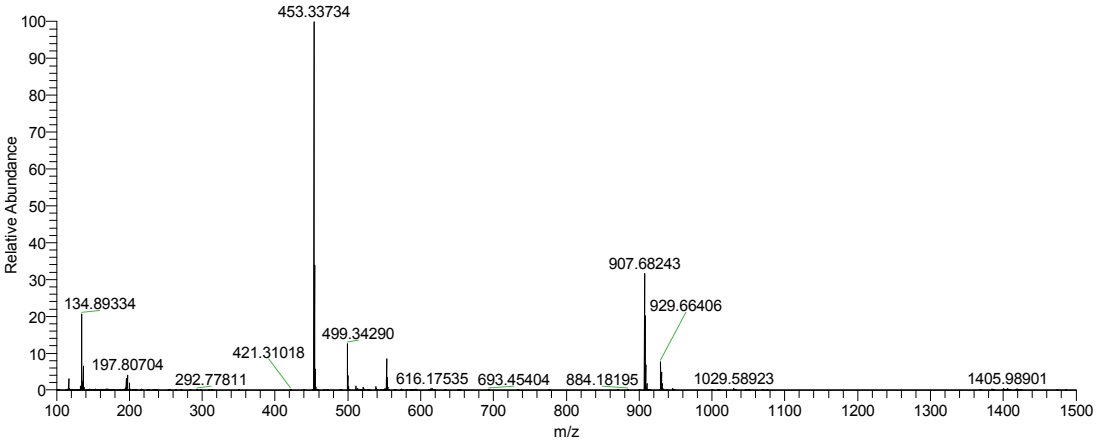


Fig. S10. The ESI-Q-Orbitrap MS spectrum of compound **2**

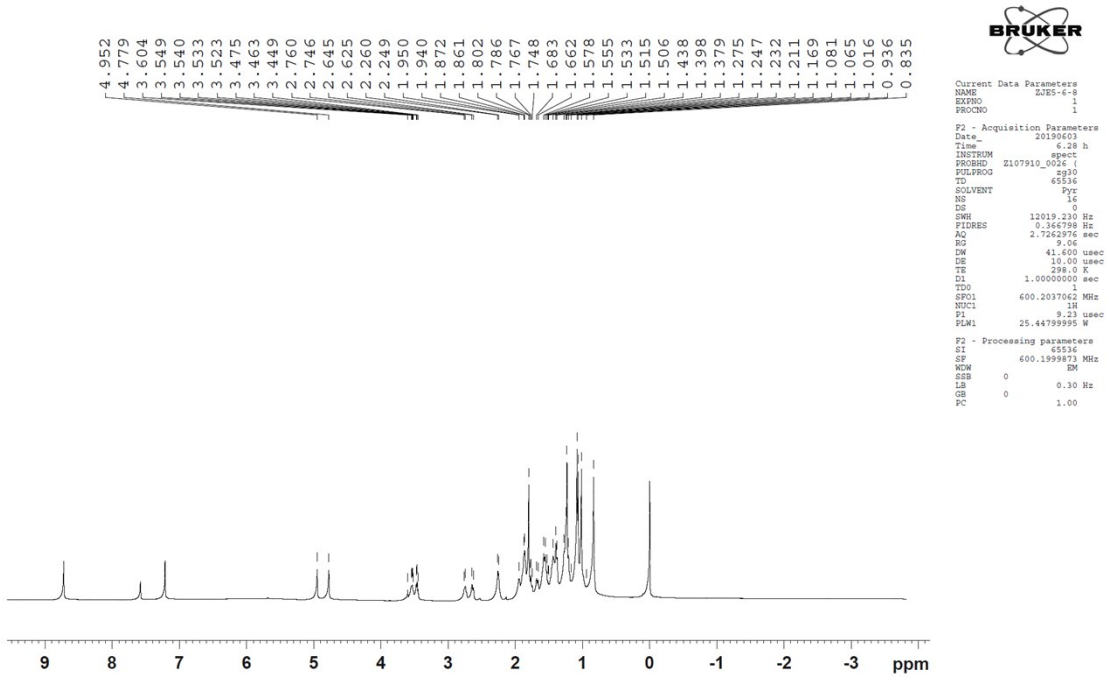


Fig. S11. ^{1}H NMR (600MHz, C_5D_5N) spectrum of compound **3**

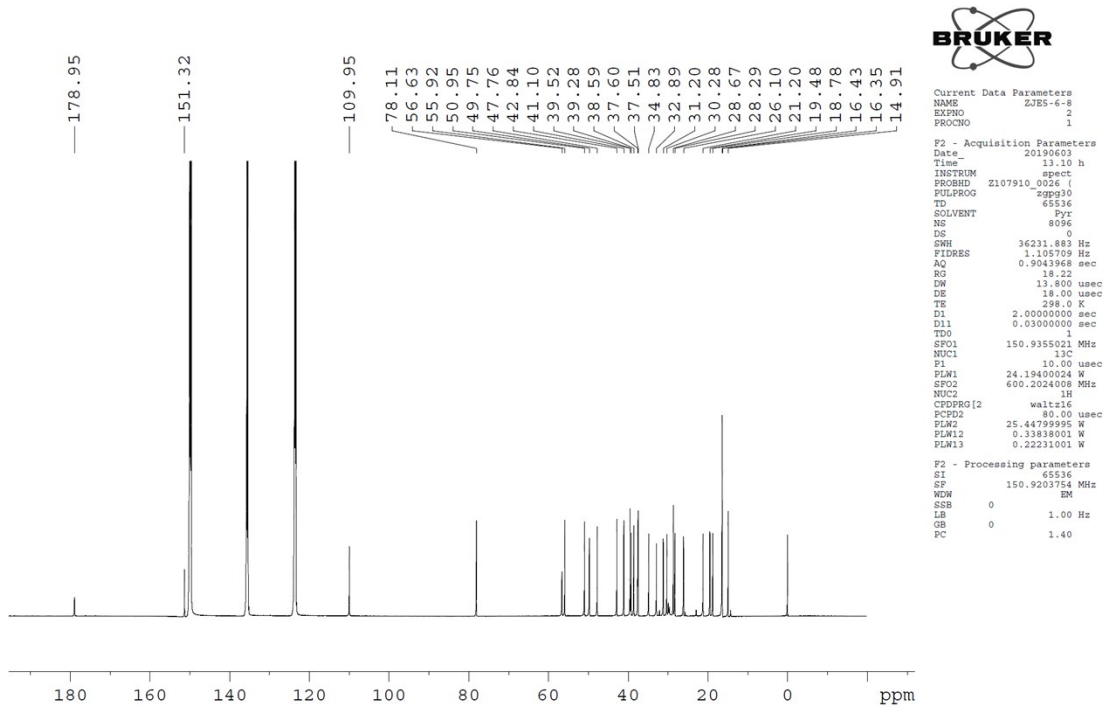


Fig. S12. ^{13}C NMR (150MHz, C_5D_5N) spectrum of compound **3**

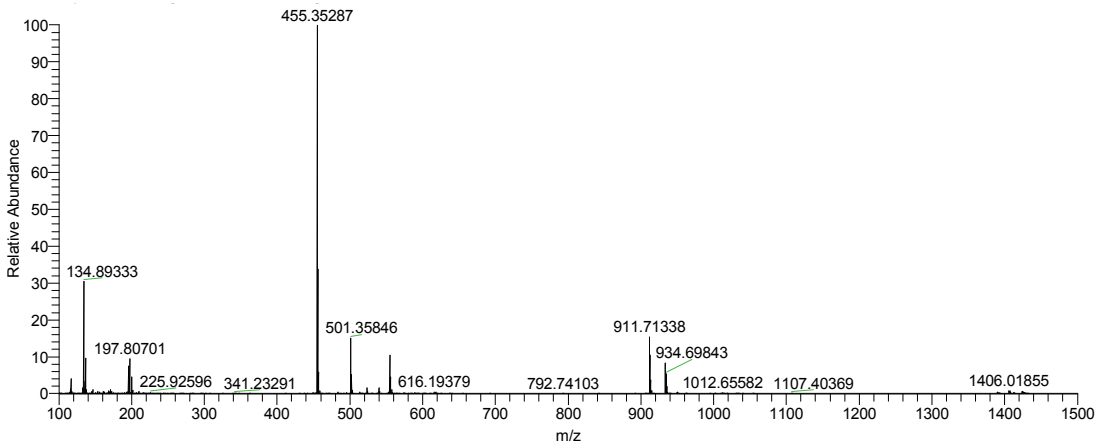


Fig. S13. The ESI-Q-Orbitrap MS spectrum of compound **3**

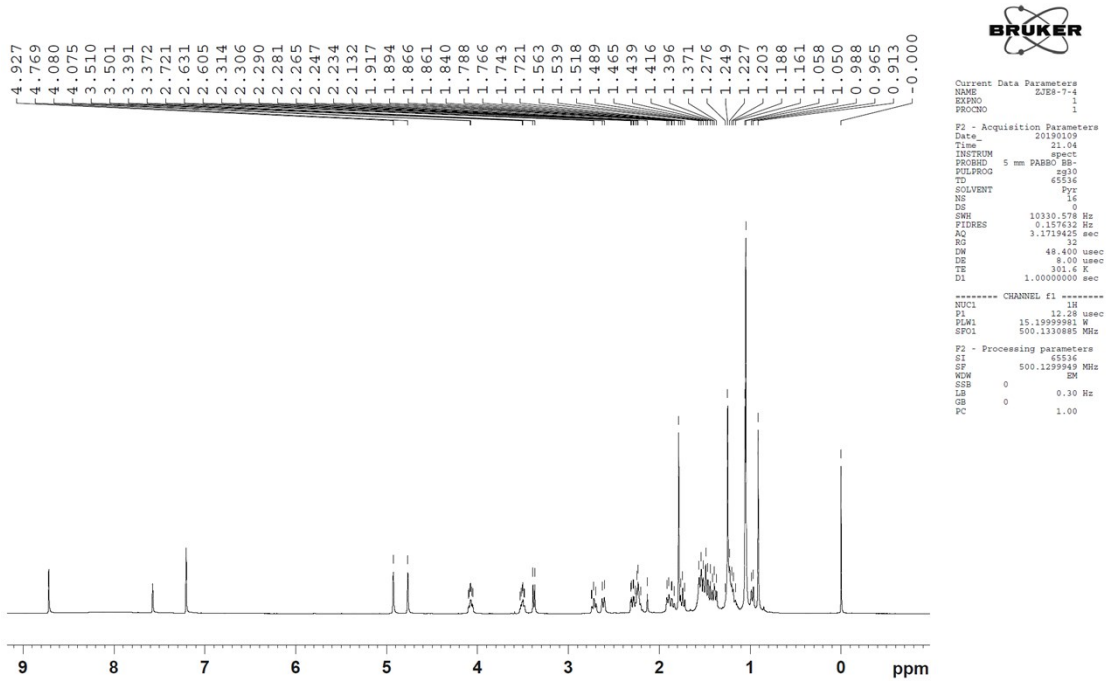


Fig. S14. ^{1}H NMR (500MHz, C_5D_5N) spectrum of compound **4**

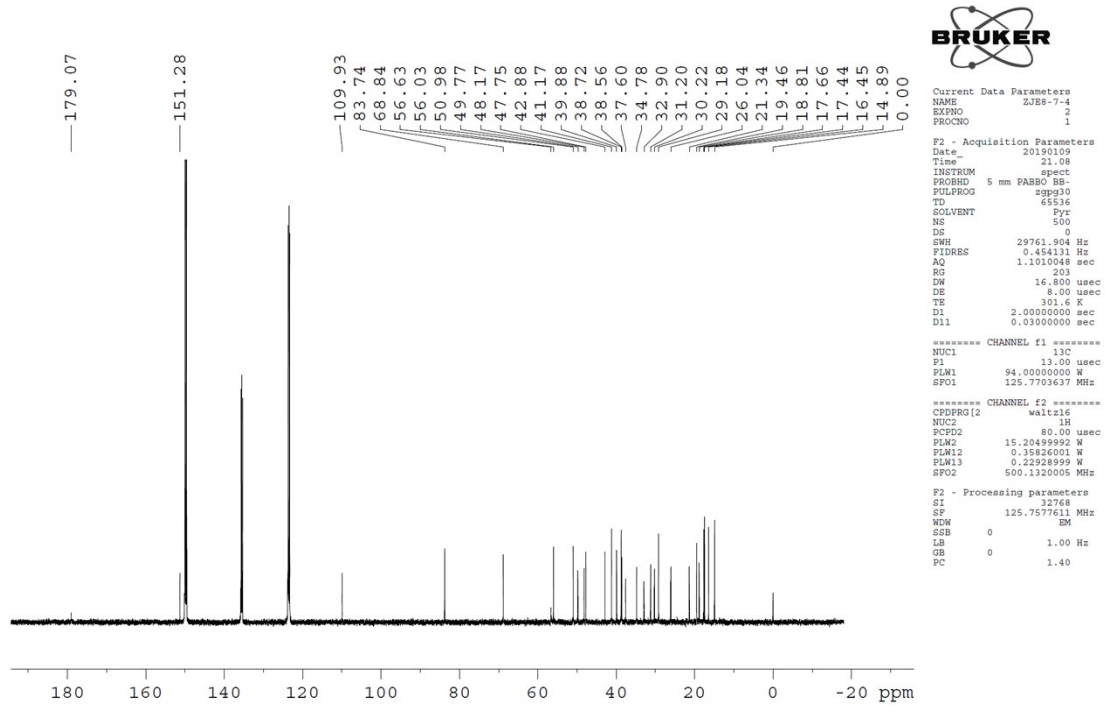


Fig. S15. ^{13}C NMR (125MHz, C_5D_5N) spectrum of compound **4**

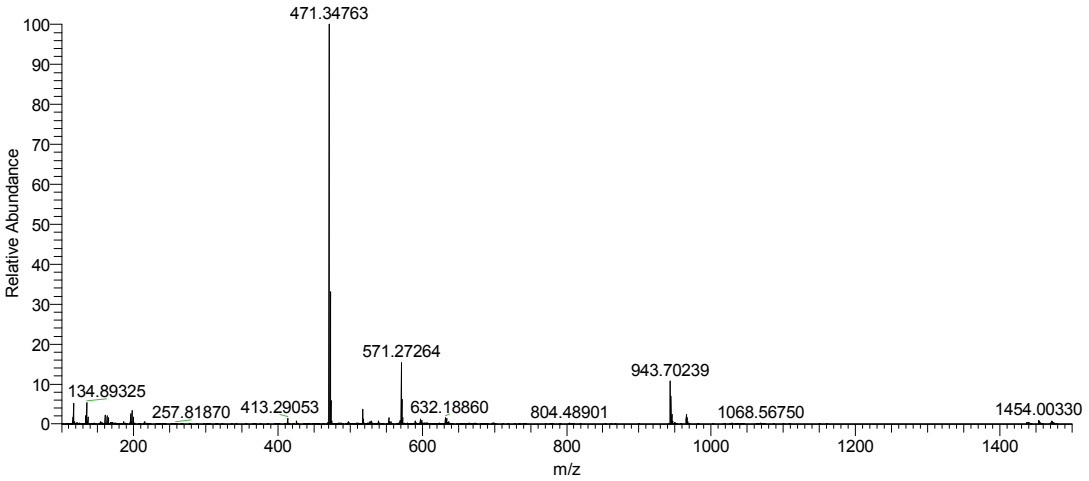
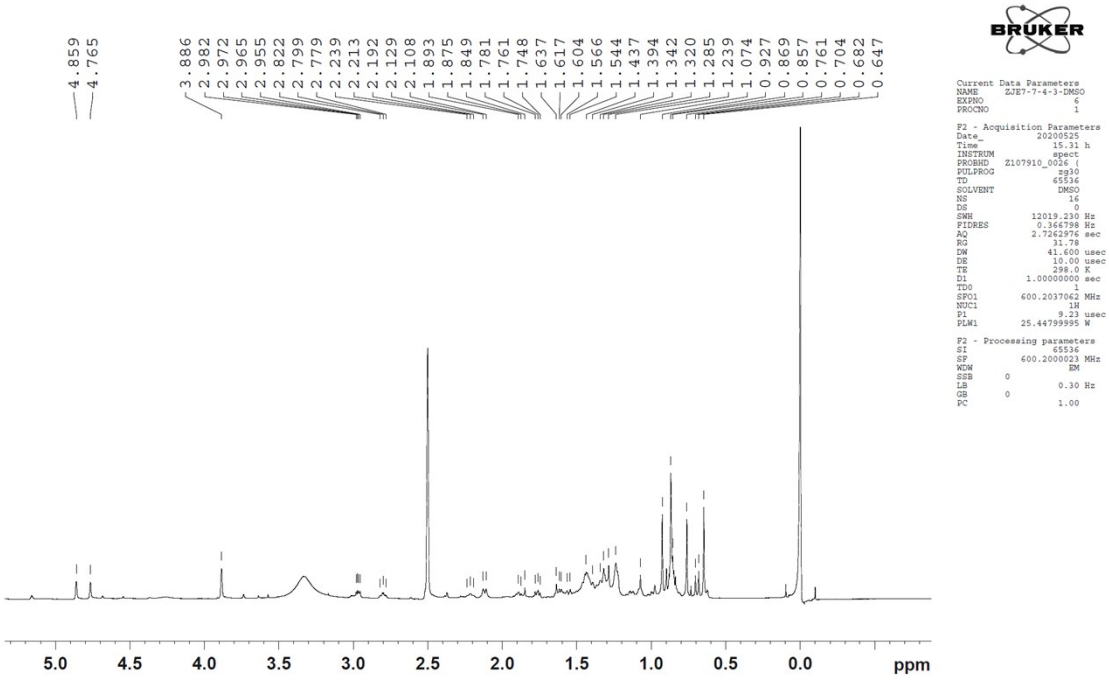


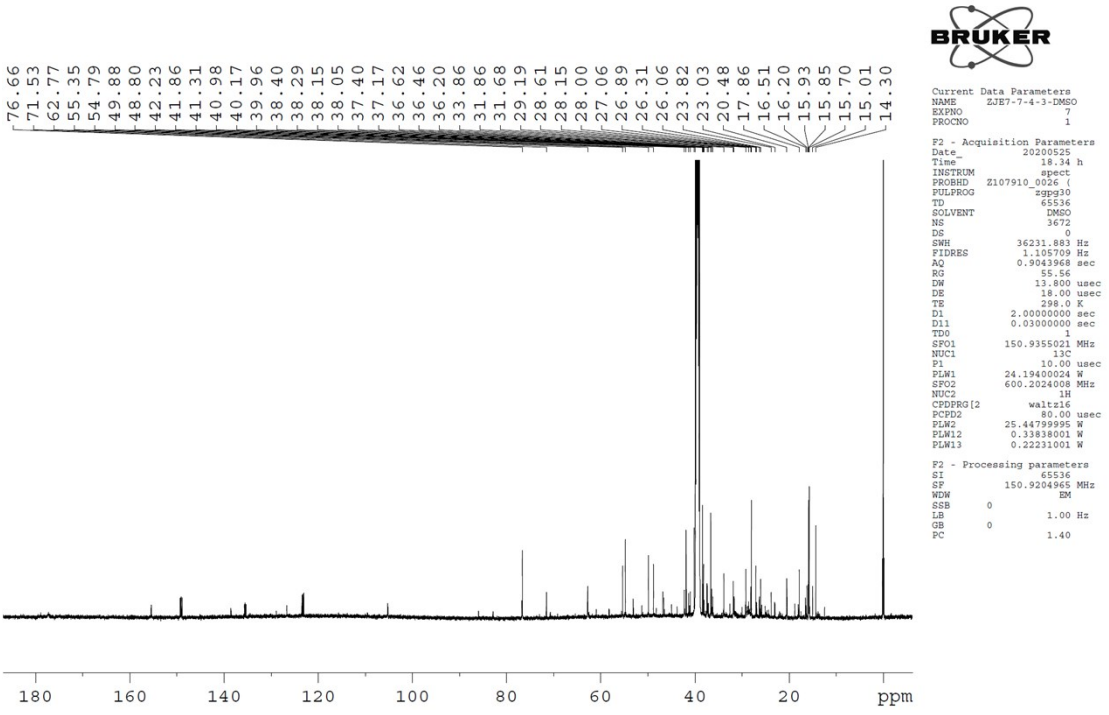
Fig. S16. The ESI-Q-Orbitrap MS spectrum of compound **4**



392

393 **Fig. S17**. ^{1}H NMR (500MHz, C_5D_5N) spectrum of compound **5**

394



395

396 **Fig. S18**. ^{13}C NMR (125MHz, C_5D_5N) spectrum of compound **5**

397

398

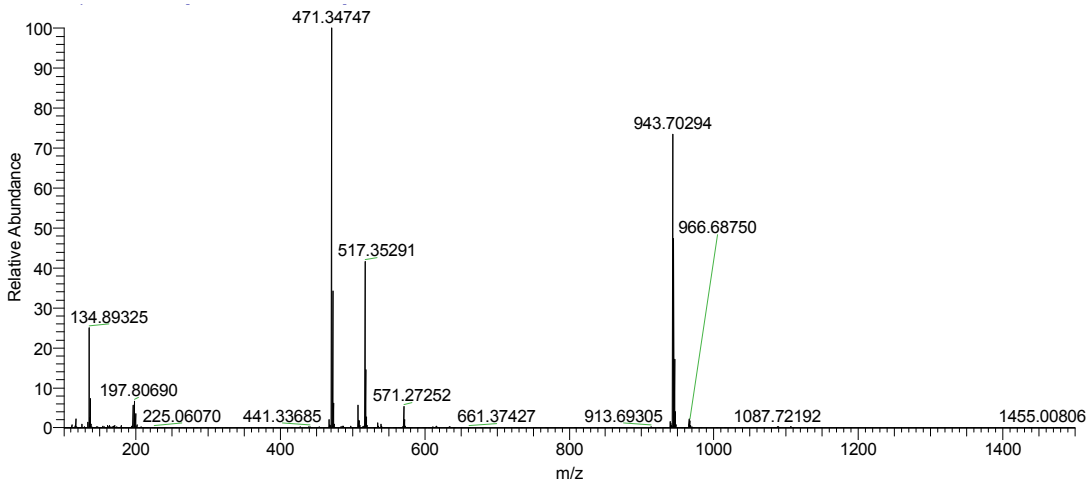


Fig. S19. The ESI-Q-Orbitrap MS spectrum of compound **5**

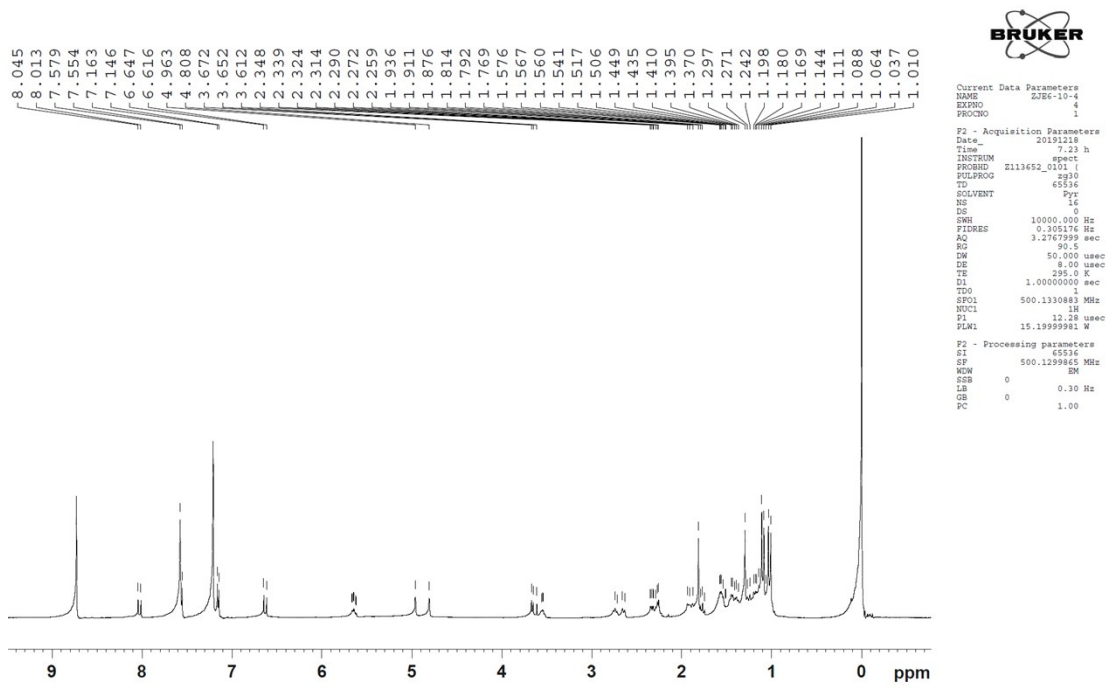


Fig. S20. ^{1}H NMR (500MHz, C_5D_5N) spectrum of compound **6**

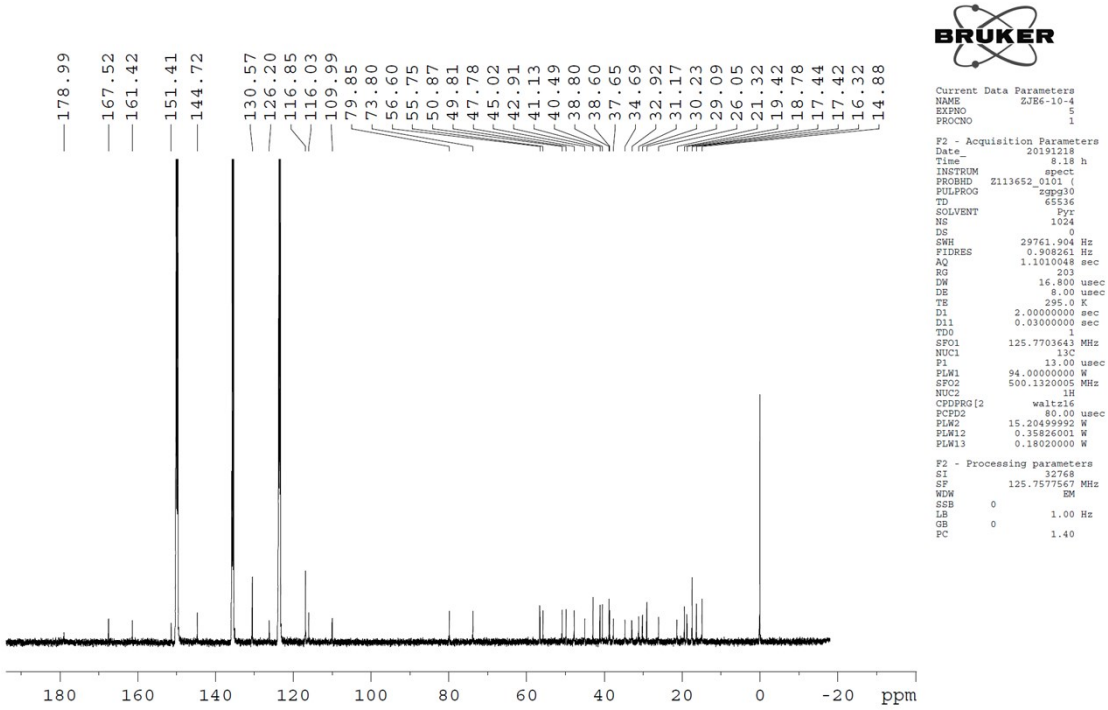


Fig. S21. ^{13}C NMR (125MHz, C_5D_5N) spectrum of compound **6**

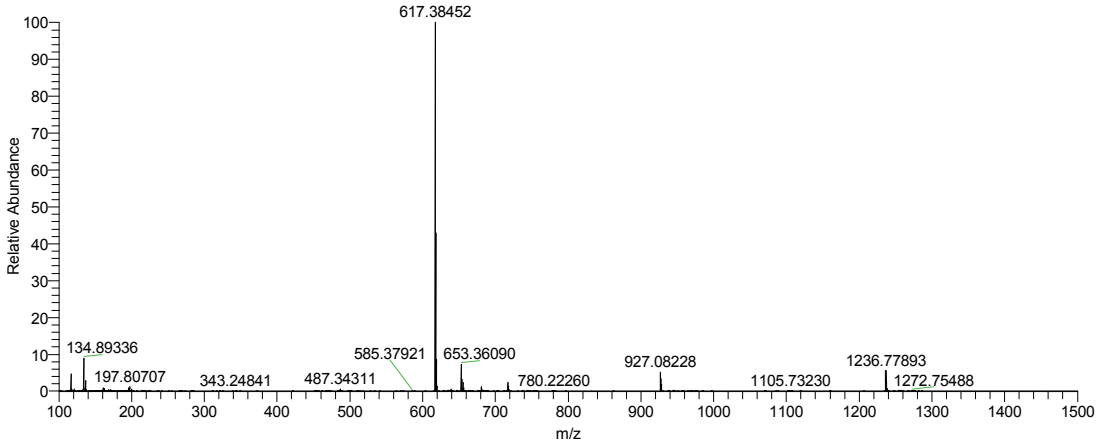
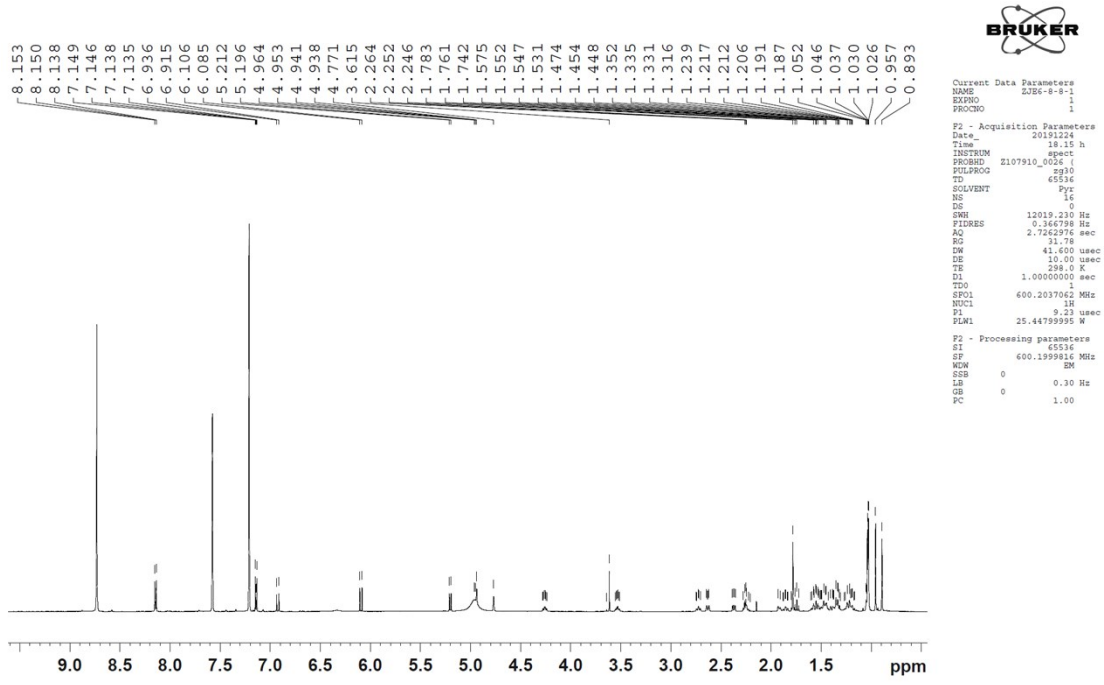


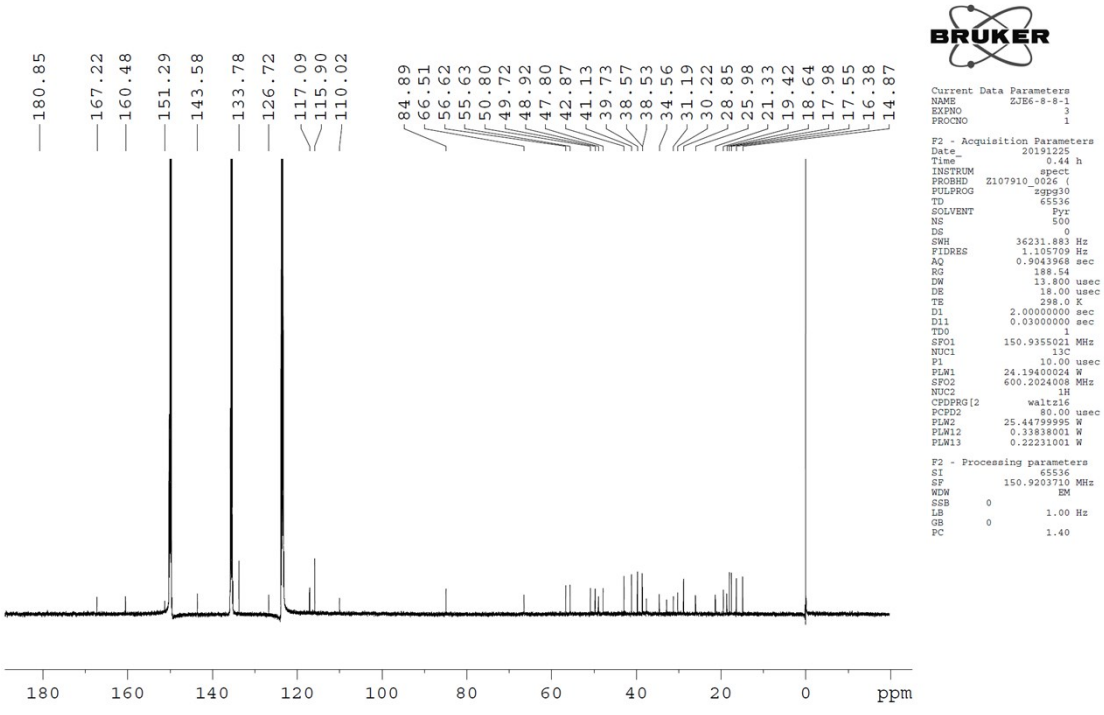
Fig. S22. The ESI-Q-Orbitrap MS spectrum of compound **6**



412

413 **Fig. S23**. ^{1}H NMR (600MHz, C_5D_5N) spectrum of compound **7**

414



415

416 **Fig. S24**. ^{13}C NMR (150MHz, C_5D_5N) spectrum of compound **7**

417

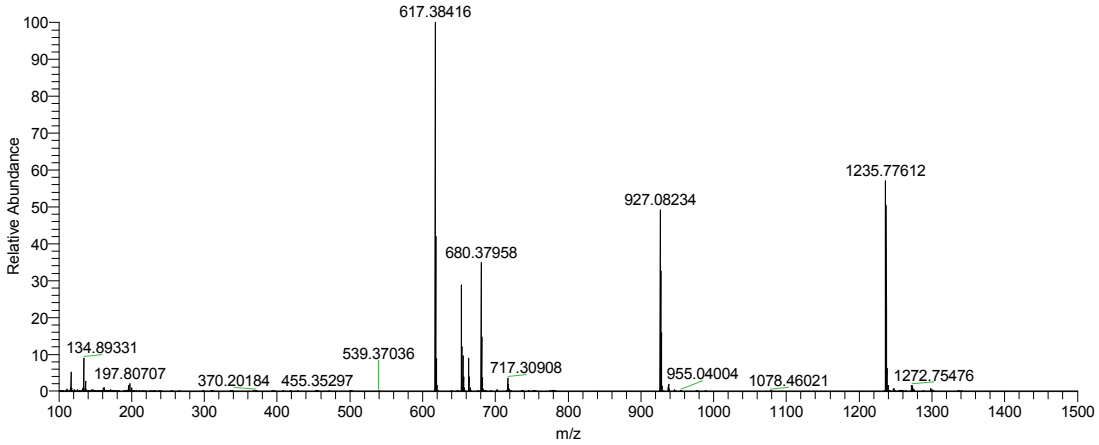


Fig. S25. The ESI-Q-Orbitrap MS spectrum of compound **7**

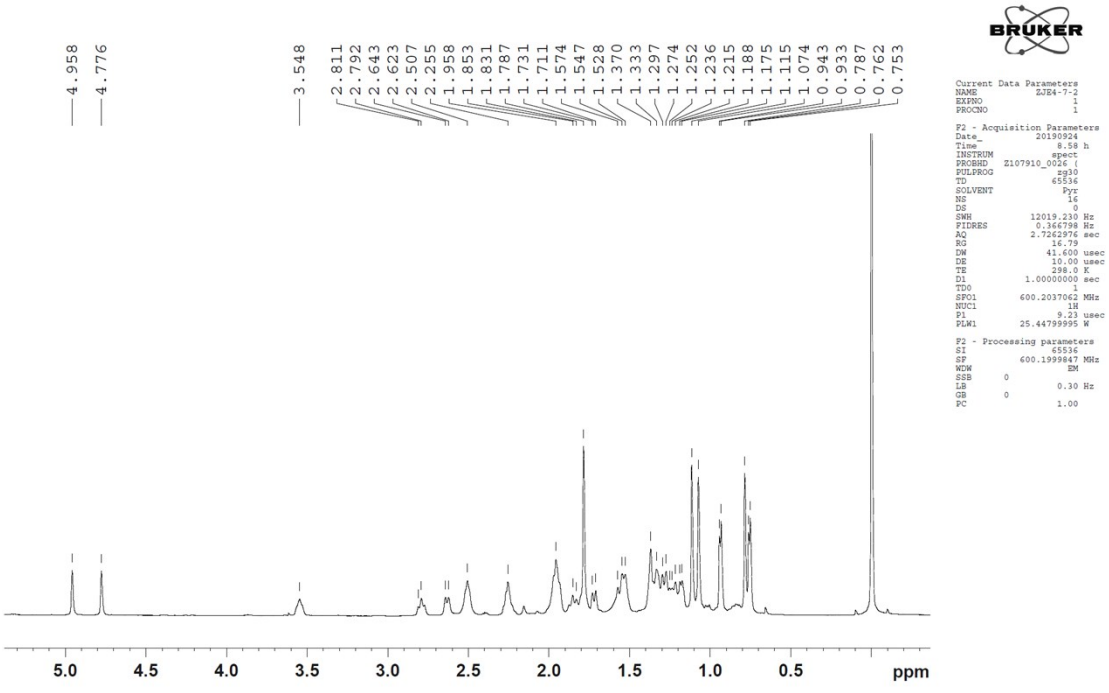


Fig. S26. ^{1}H NMR (600MHz, C_5D_5N) spectrum of compound **8**

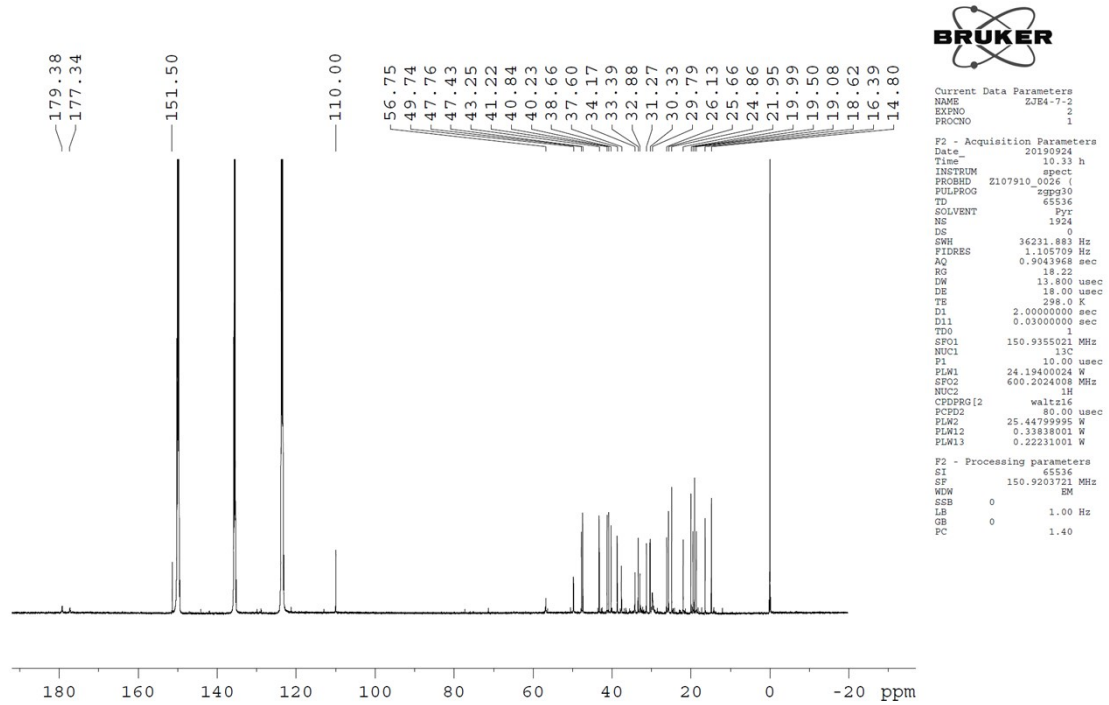


Fig. S27. ^{13}C NMR (150MHz, C_5D_5N) spectrum of compound **8**

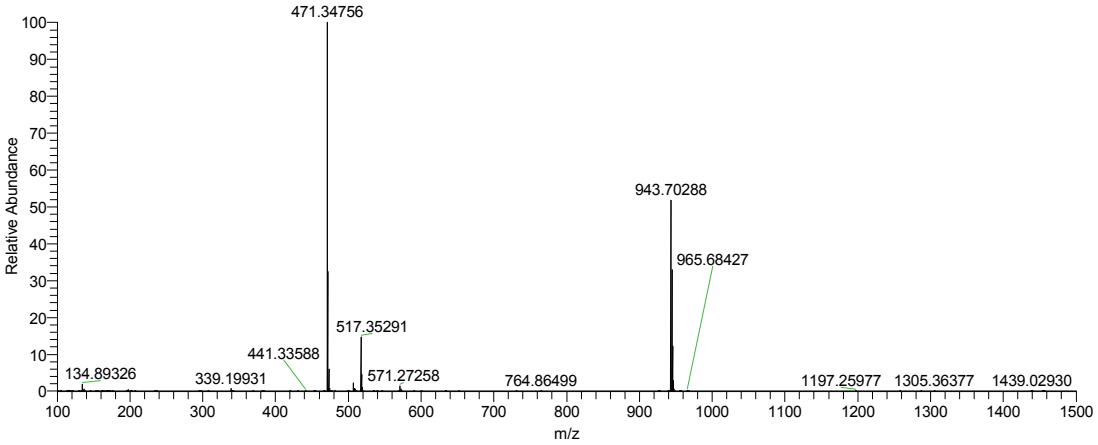
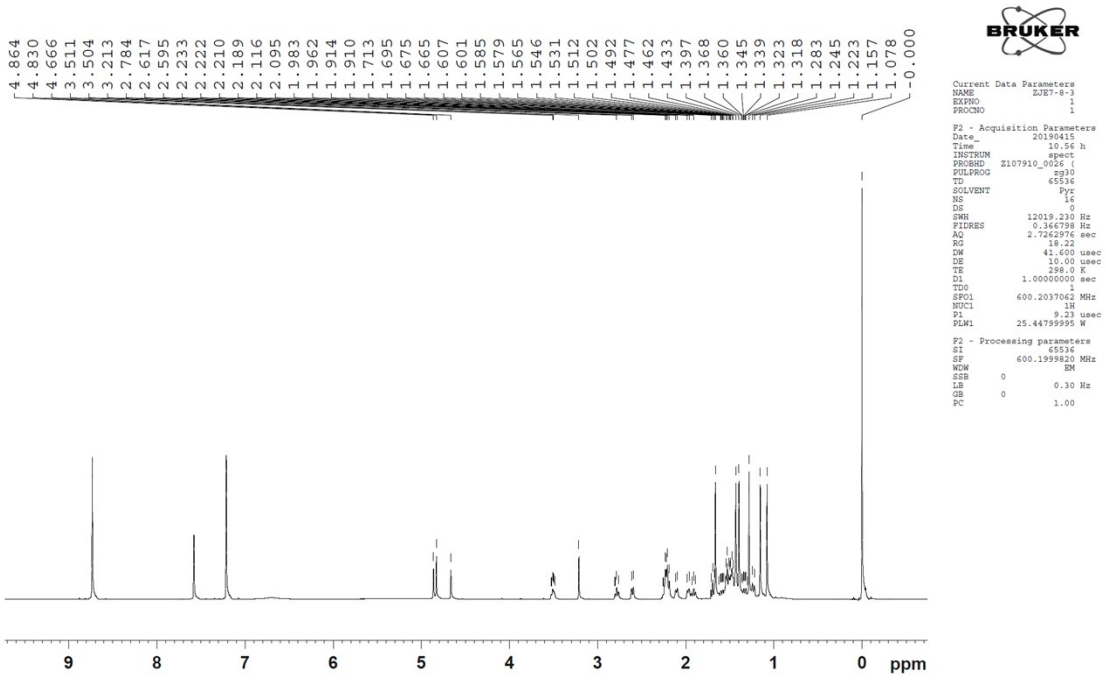


Fig. S28. The ESI-Q-Orbitrap MS spectrum of compound **8**



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FIDRES 0.366798 Hz
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RG 18.22
DW 41.600 usec
DE 10.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.2037062 MHz
NUC1 1H
P1 9.23 usec
PLW1 25.44799995 W

F2 - Processing parameters
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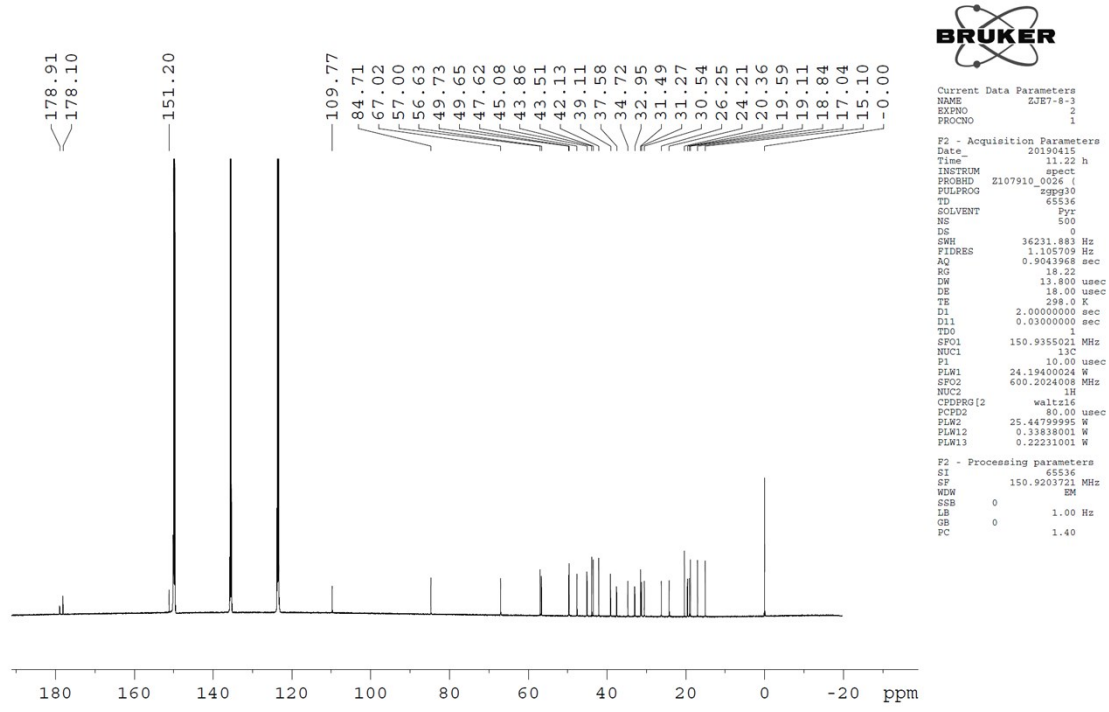
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

431

432 **Fig. S29**. ^{1}H NMR (600MHz, C_5D_5N) spectrum of compound **9**

433



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PROCNO 1

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SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 18.22
DW 13.800 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9355021 MHz
NUC1 13C
P1 10.00 usec
PLW1 24.19400024 W
SFO2 600.2024008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 25.44799995 W
PLW12 0.33838001 W
PLW13 0.22231001 W

F2 - Processing parameters
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SF 150.9203721 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

434

435 **Fig. S30**. ^{13}C NMR (150MHz, C_5D_5N) spectrum of compound **9**

436

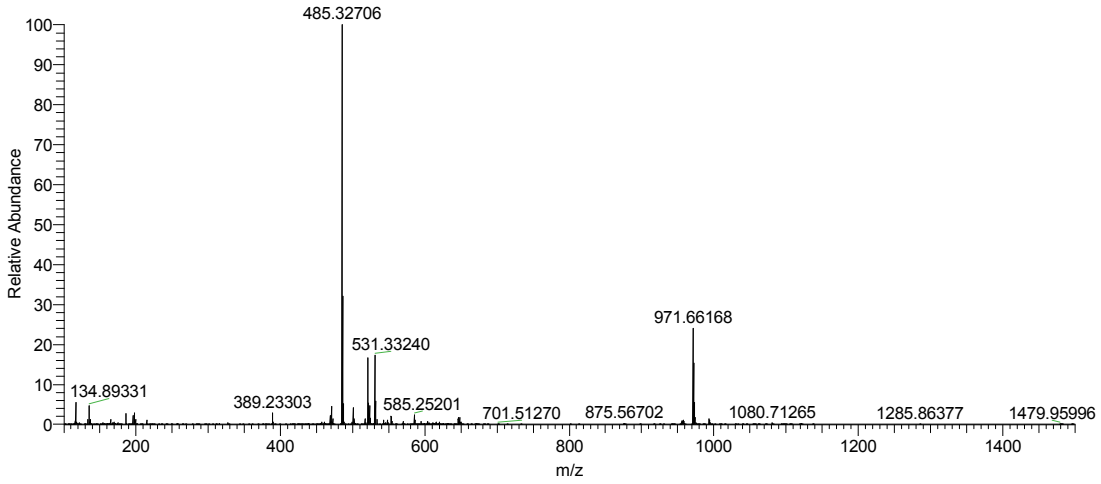
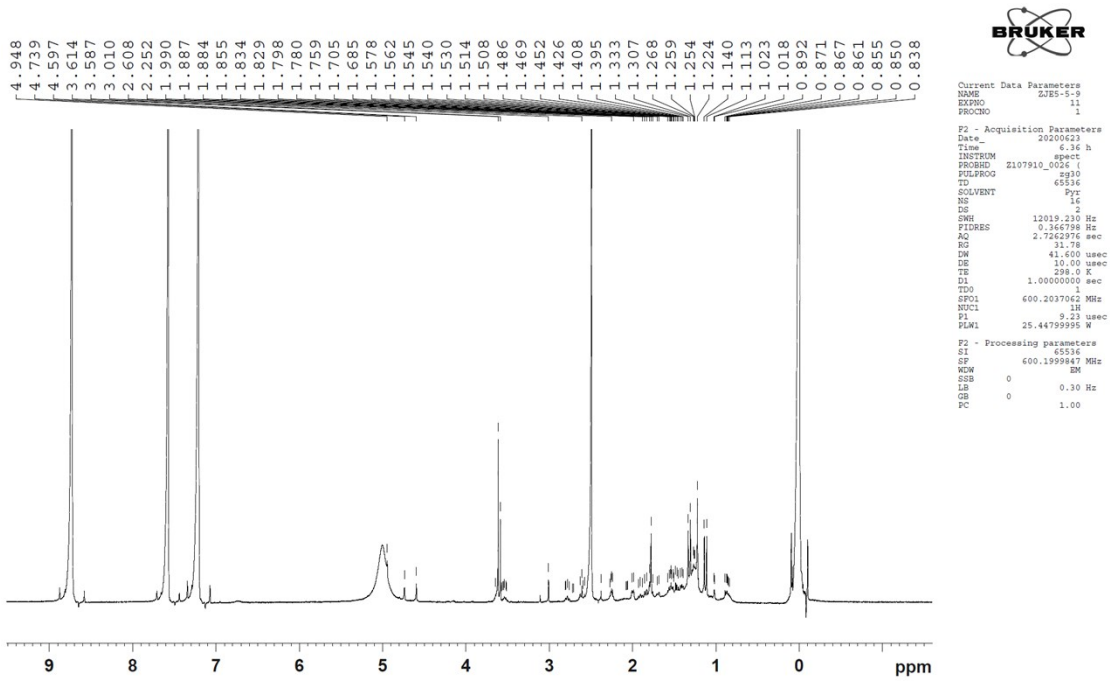


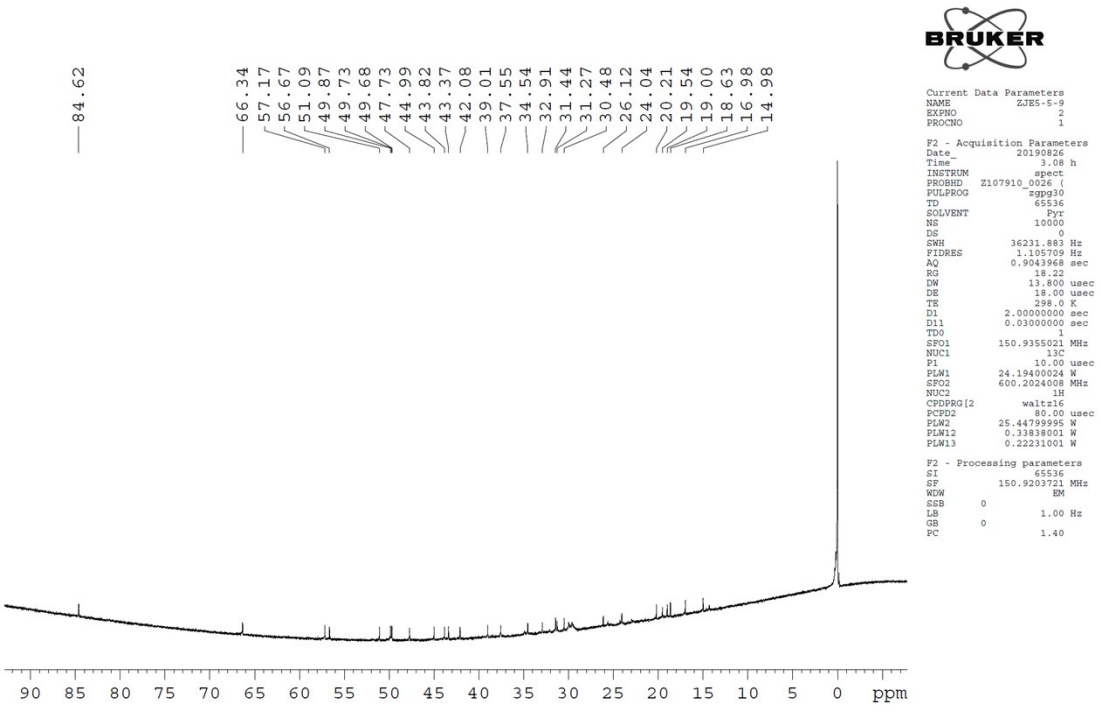
Fig. S31. The ESI-Q-Orbitrap MS spectrum of compound **9**



441

442 **Fig. S32**. ^{1}H NMR (600MHz, C_5D_5N) spectrum of compound **10**

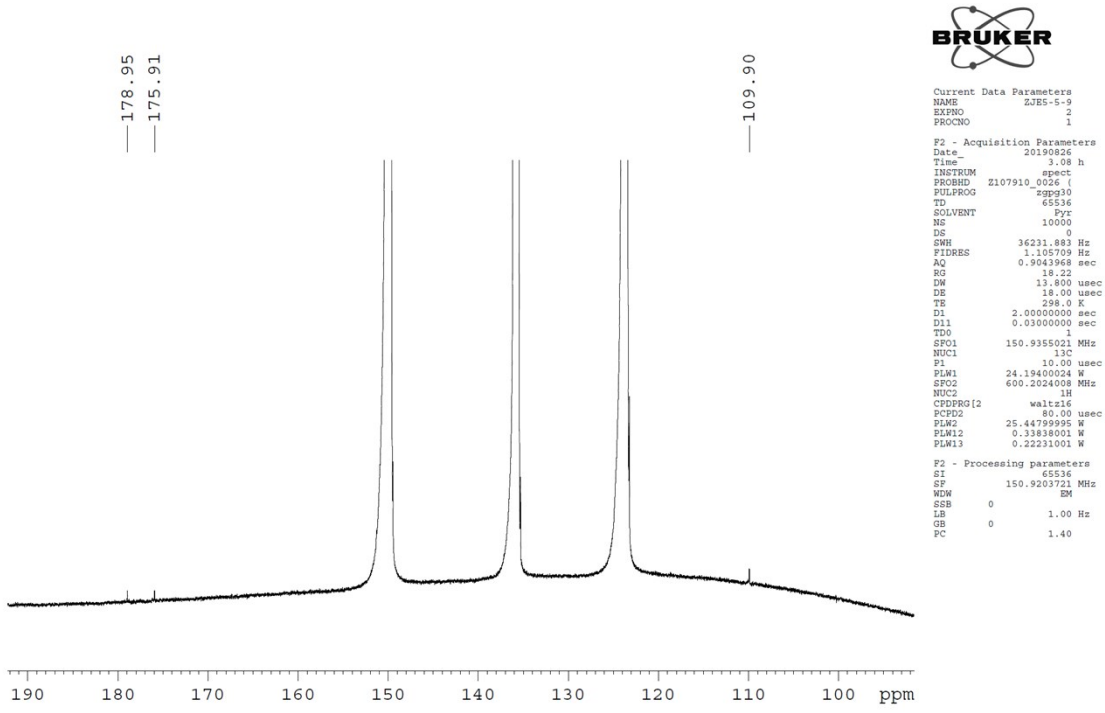
443



444

445 **Fig. S33**. ^{13}C NMR (150MHz, C_5D_5N) spectrum-1 of compound **10**

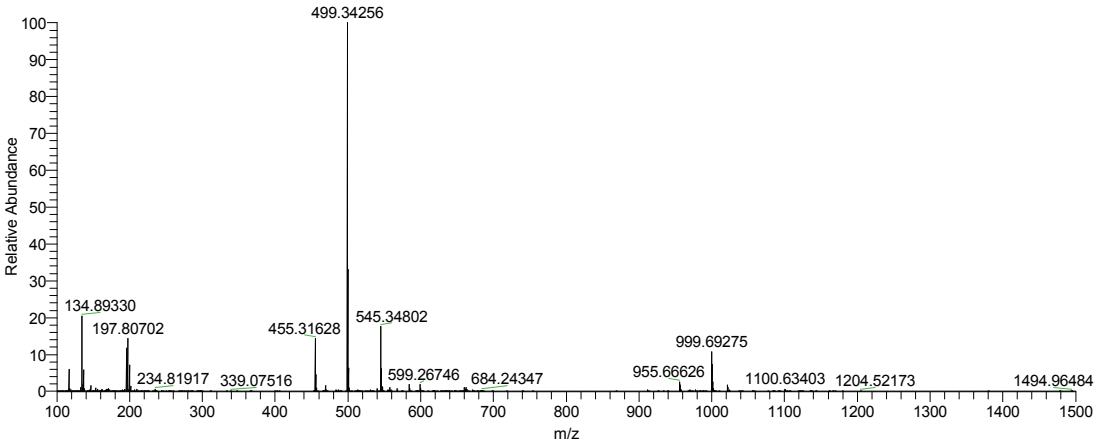
446



447

448 **Fig. S34**. ^{13}C NMR (150MHz, C_5D_5N) spectrum-2 of compound **10**

449



450

451 **Fig. S35**. The ESI-Q-Orbitrap MS spectrum of compound **10**

452

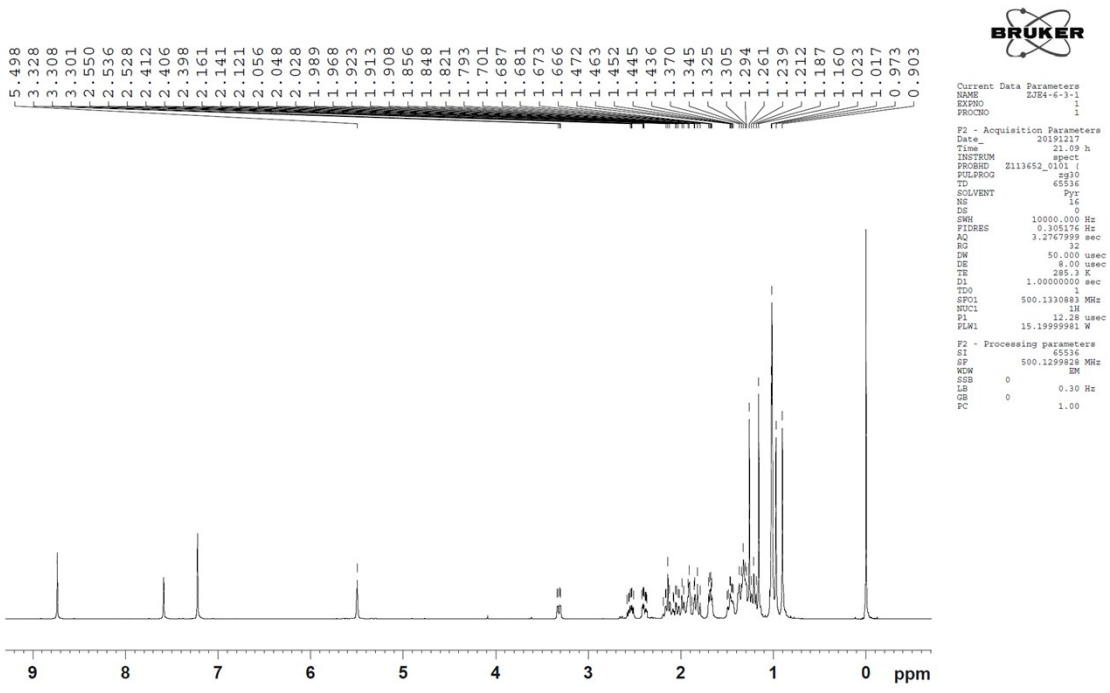


Fig. S36. ^{1}H NMR (500MHz, C_5D_5N) spectrum of compound **11**

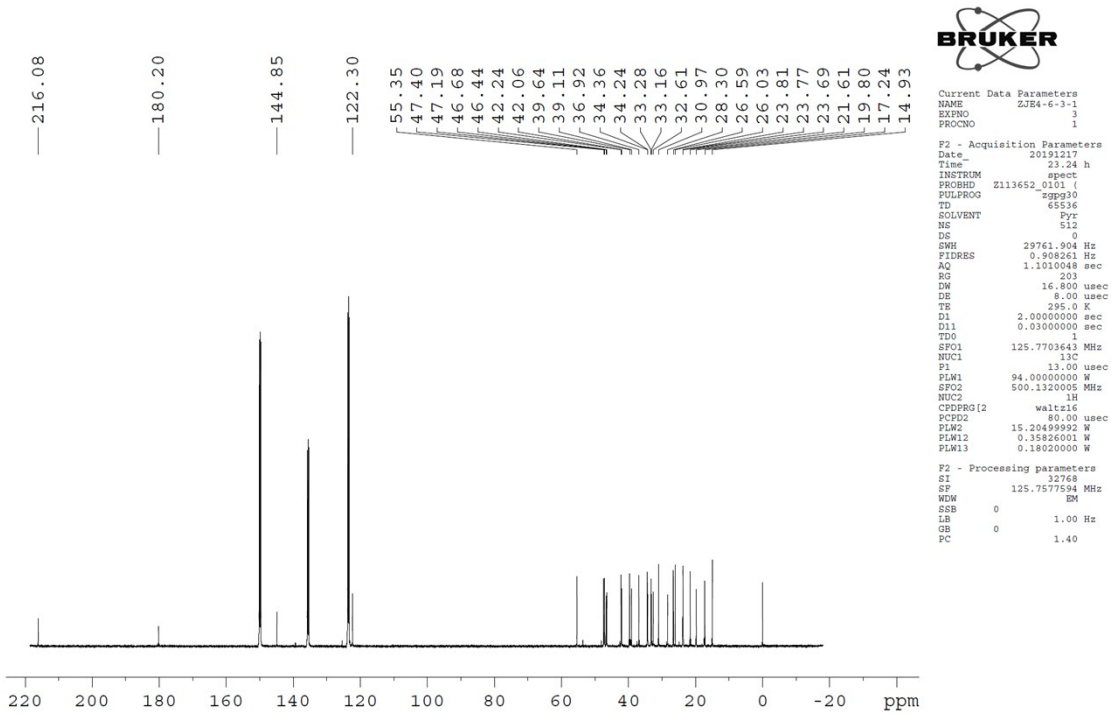


Fig. S37. ^{13}C NMR (125MHz, C_5D_5N) spectrum of compound **11**

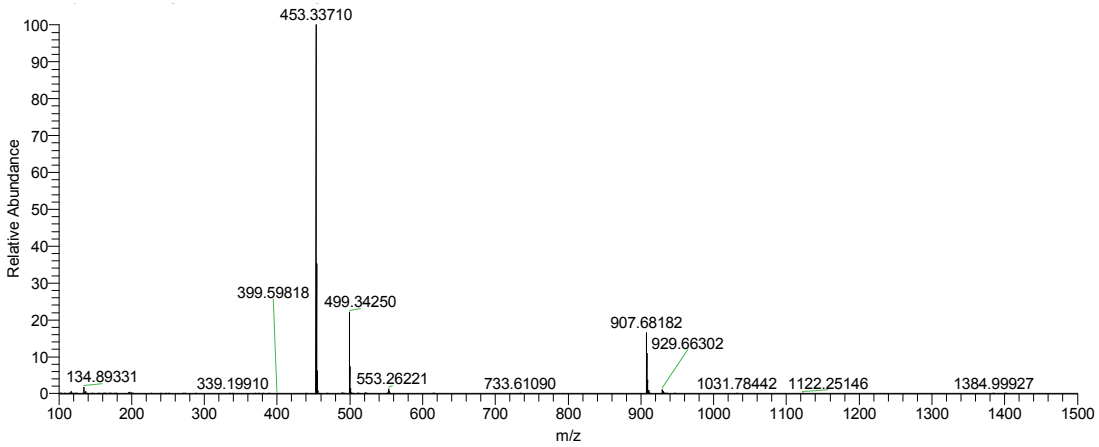
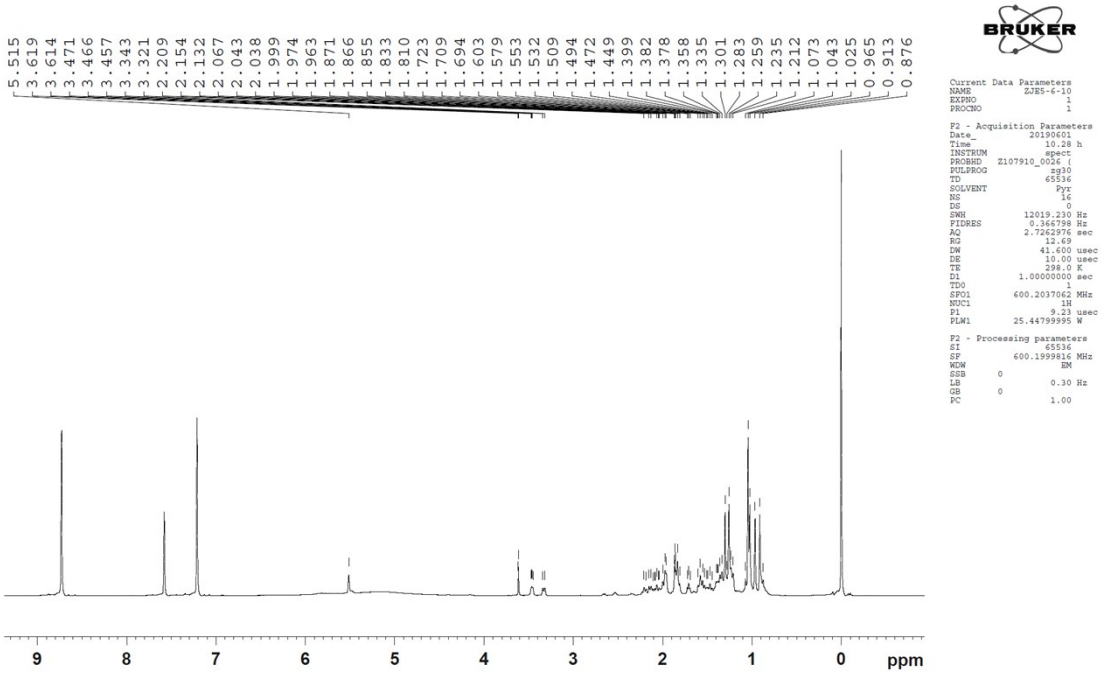


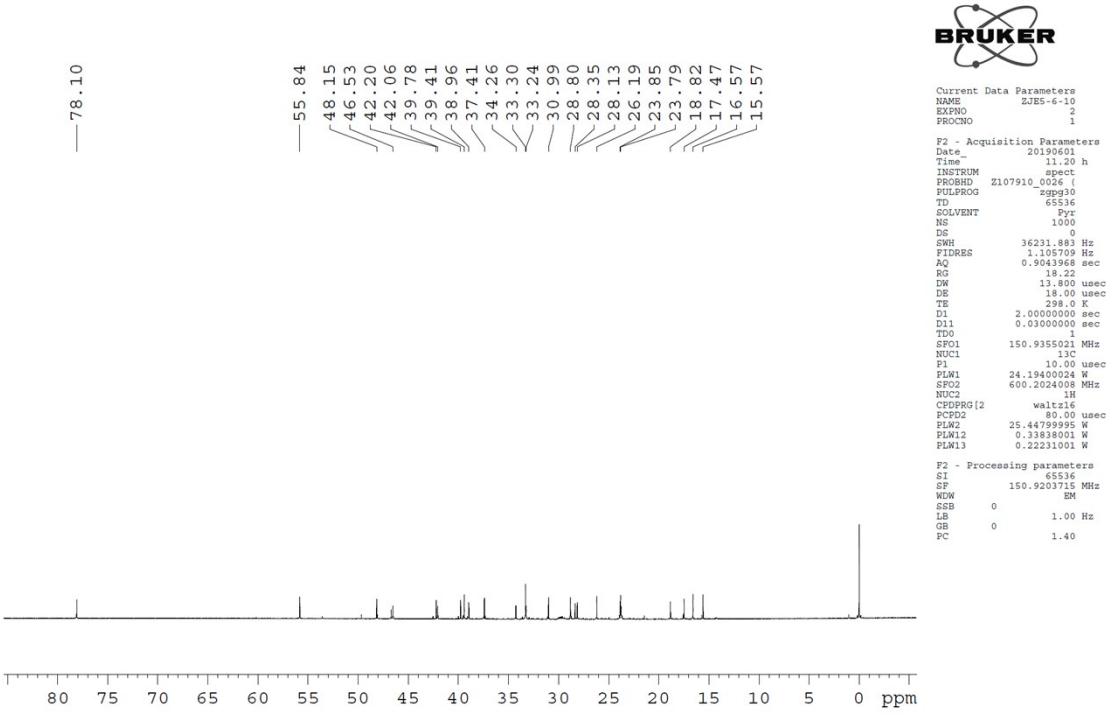
Fig. S38. The ESI-Q-Orbitrap MS spectrum of compound **11**



464

465 **Fig. S39**. ^{1}H NMR (600MHz, C_5D_5N) spectrum of compound **12**

466



467

468 **Fig. S40**. ^{13}C NMR (150MHz, C_5D_5N) spectrum-1 of compound **12**

469

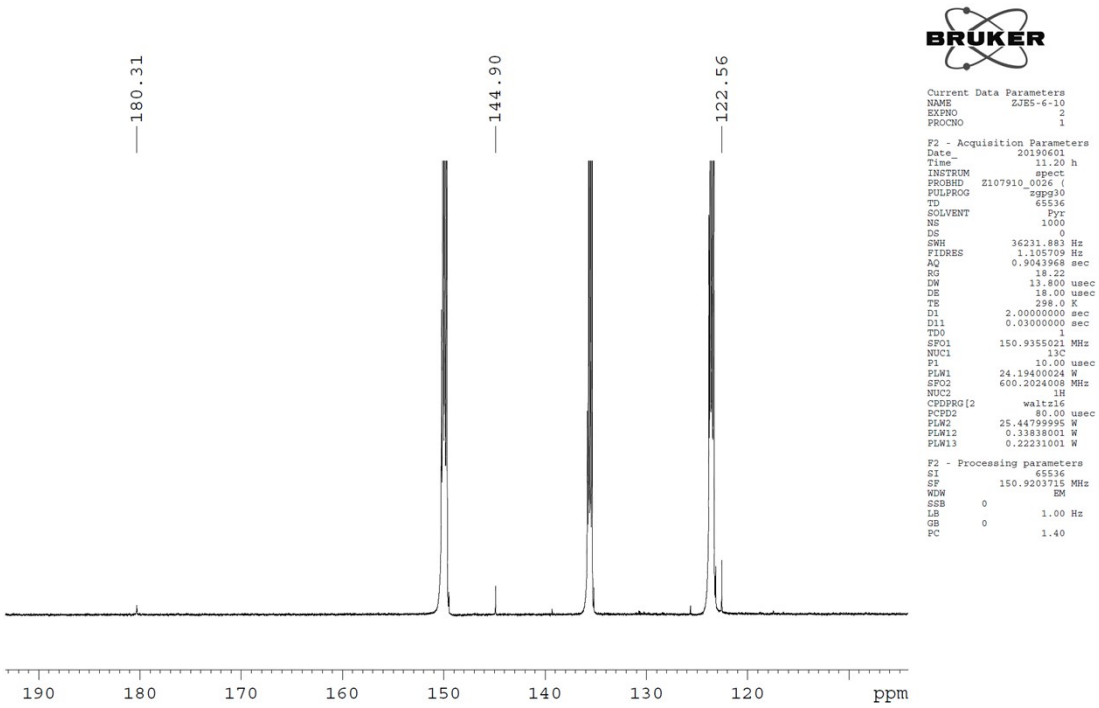


Fig. S41. ^{13}C NMR (150MHz, C_5D_5N) spectrum-2 of compound **12**

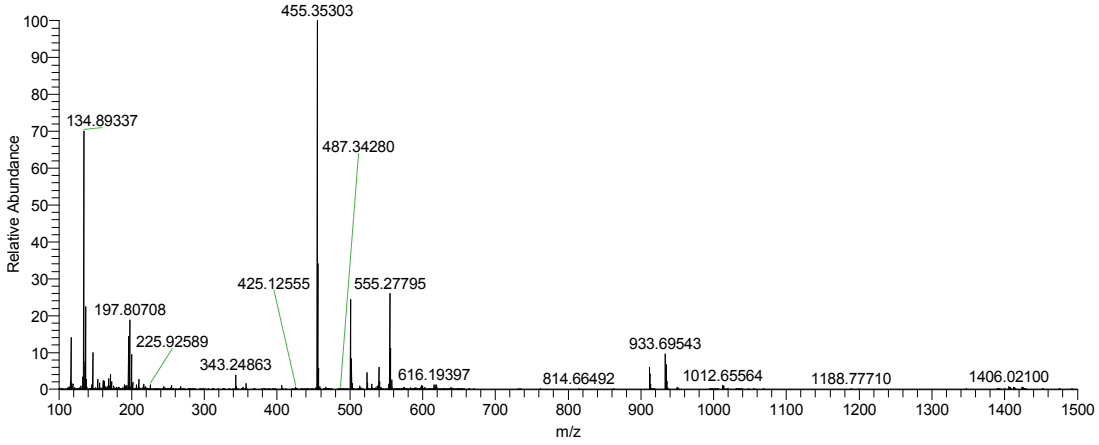


Fig. S42. The ESI-Q-Orbitrap MS spectrum of compound **12**

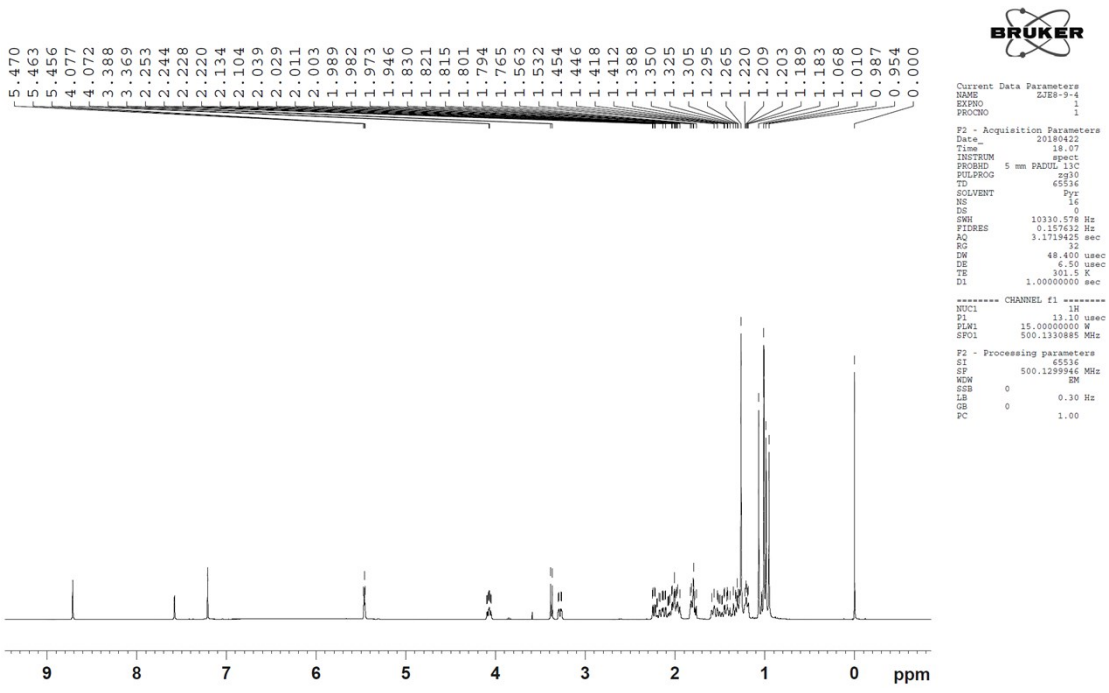


Fig. S43. ^{1}H NMR (500MHz, C_5D_5N) spectrum of compound **13**

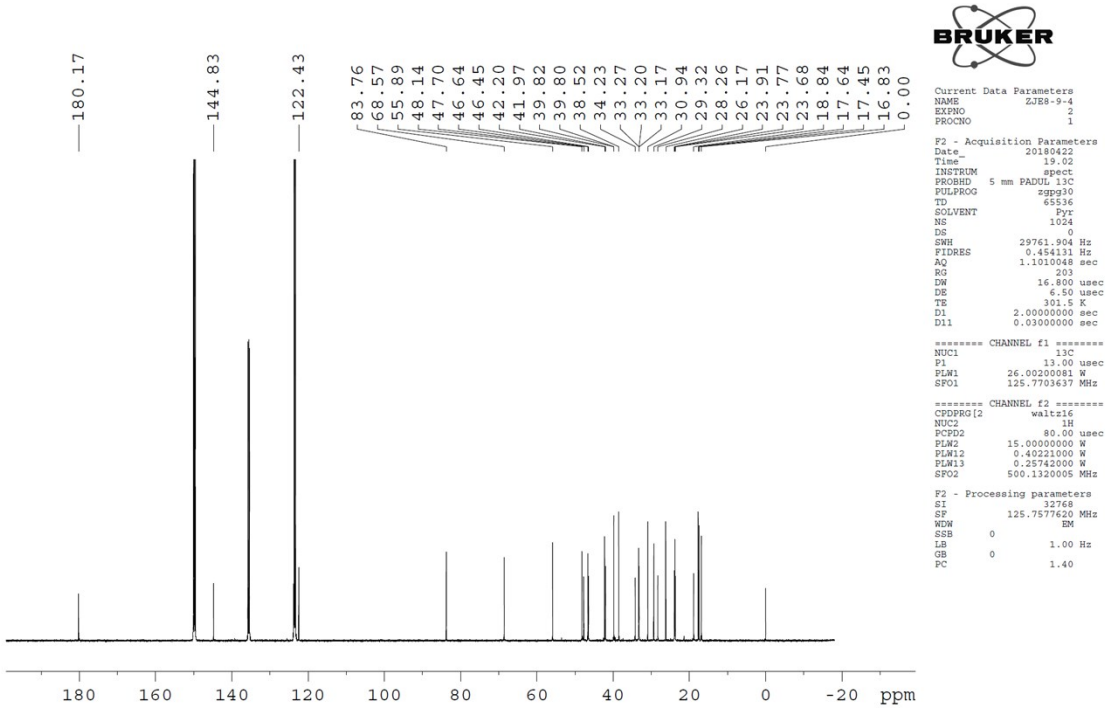


Fig. S44. ^{13}C NMR (125MHz, C_5D_5N) spectrum of compound **13**

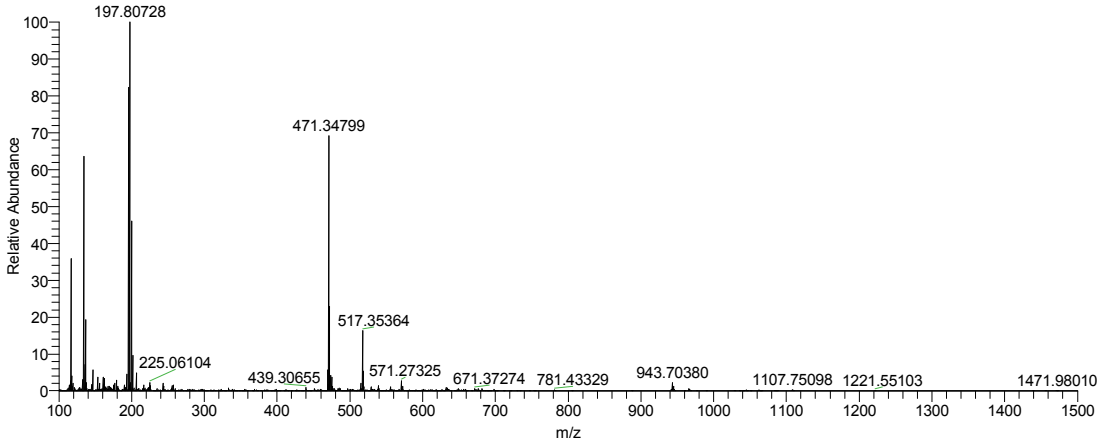
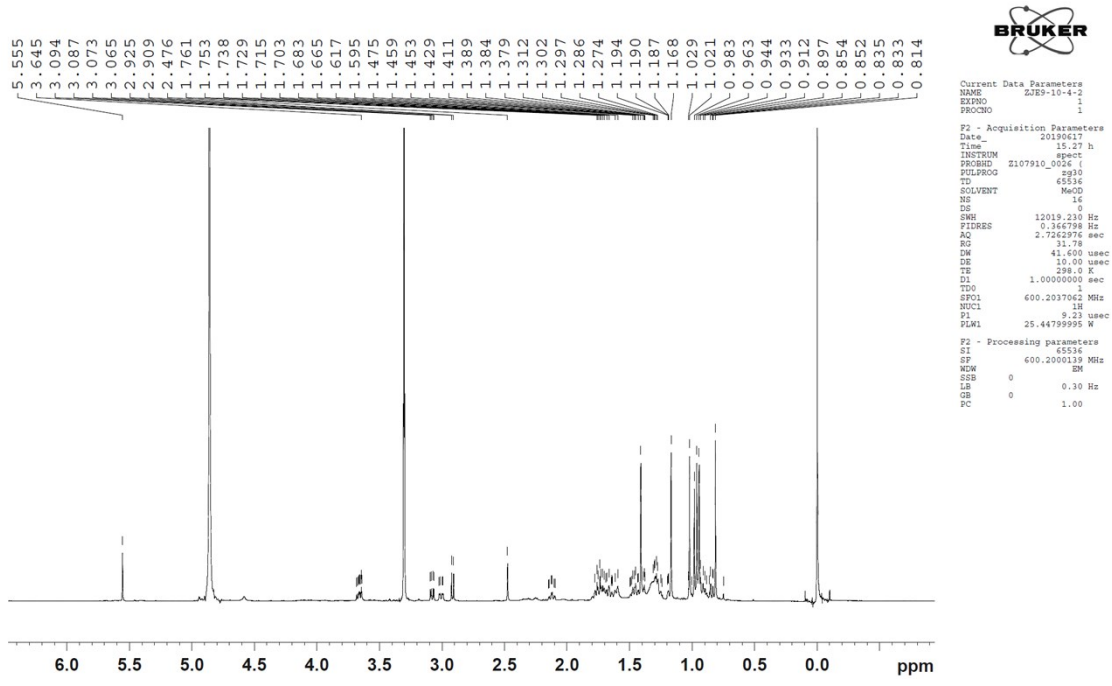


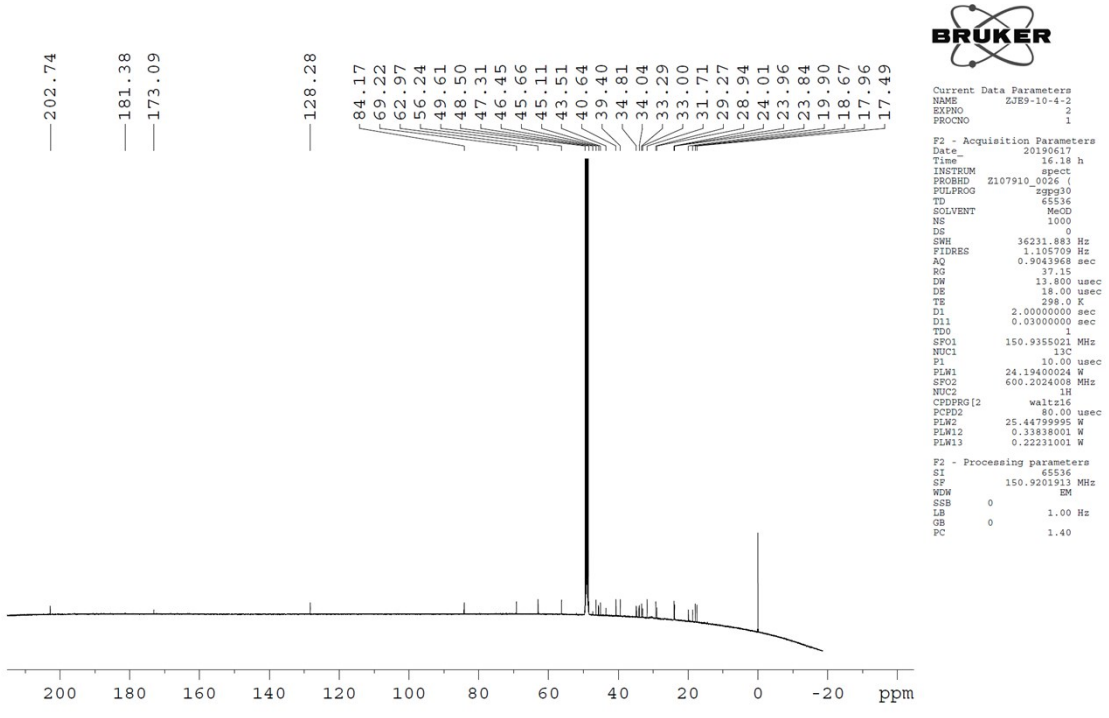
Fig. S45. The ESI-Q-Orbitrap MS spectrum of compound **13**



487

488 **Fig. S46**. ^{1}H NMR (600MHz, CD_3OD) spectrum of compound **14**

489



490

491 **Fig. S47**. ^{13}C NMR (150MHz, CD_3OD) spectrum of compound **14**

492

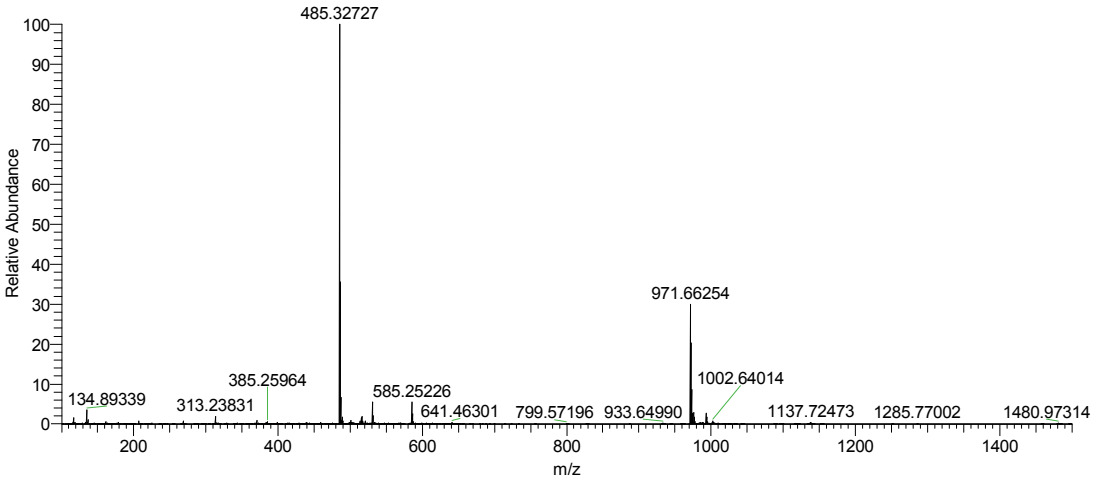
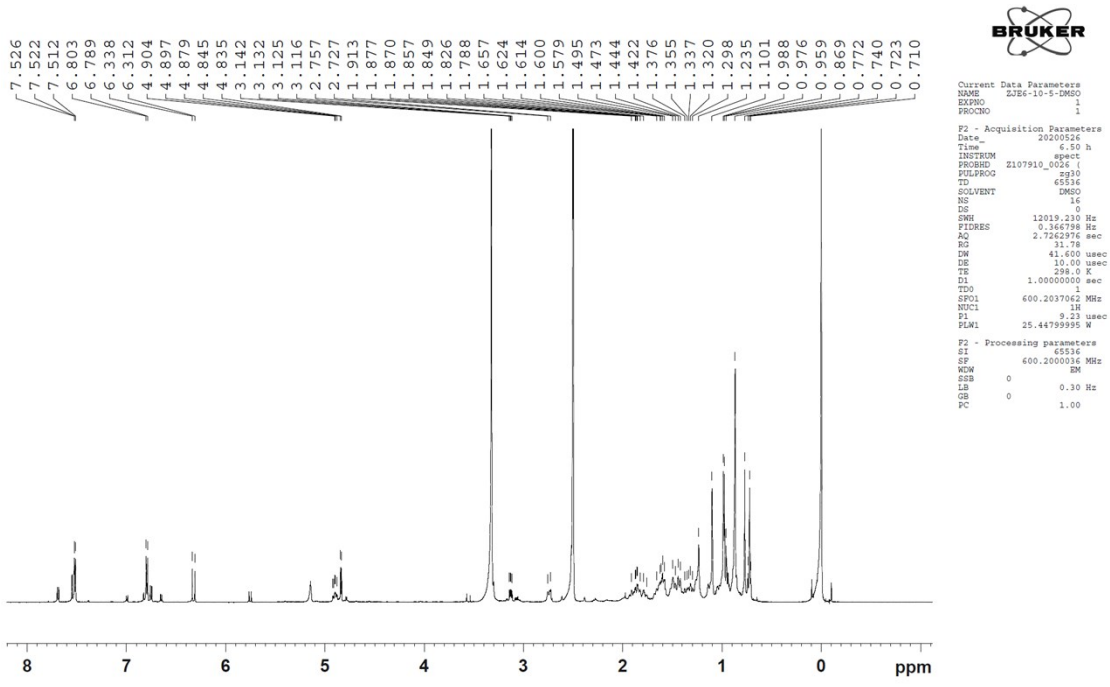


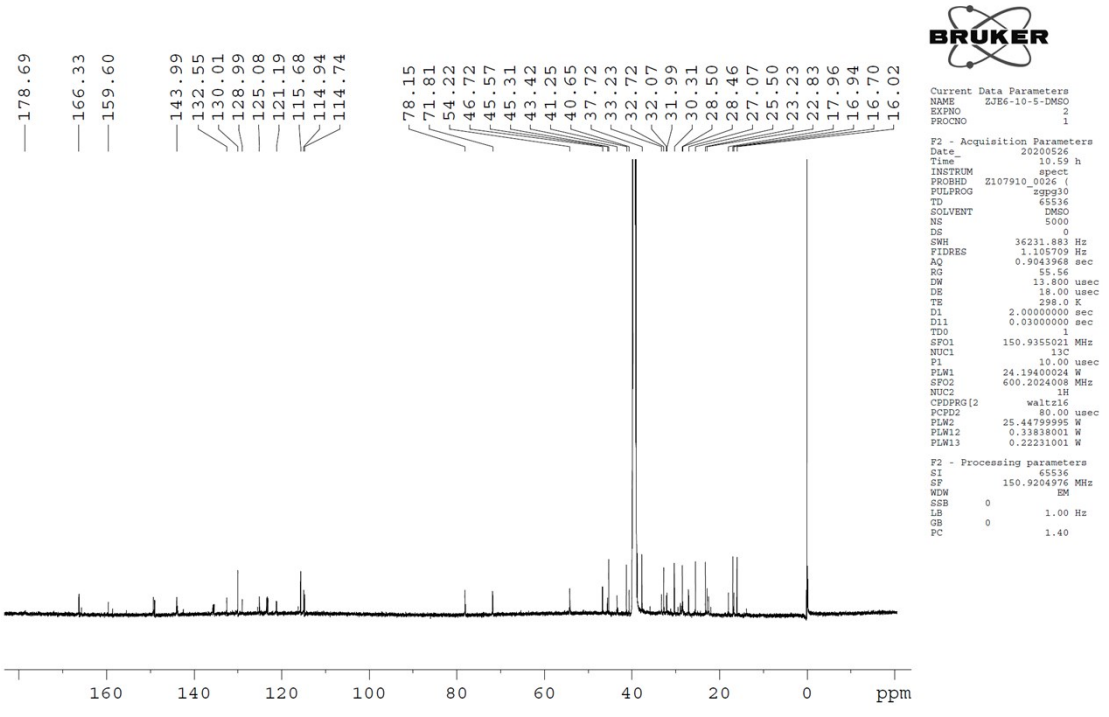
Fig. S48. The ESI-Q-Orbitrap MS spectrum of compound **14**



497

498 **Fig. S49**. ^{1}H NMR (600MHz, DMSO-d_6) spectrum of compound **15**

499



500

501 **Fig. S50**. ^{13}C NMR (150MHz, DMSO-d_6) spectrum of compound **15**

502

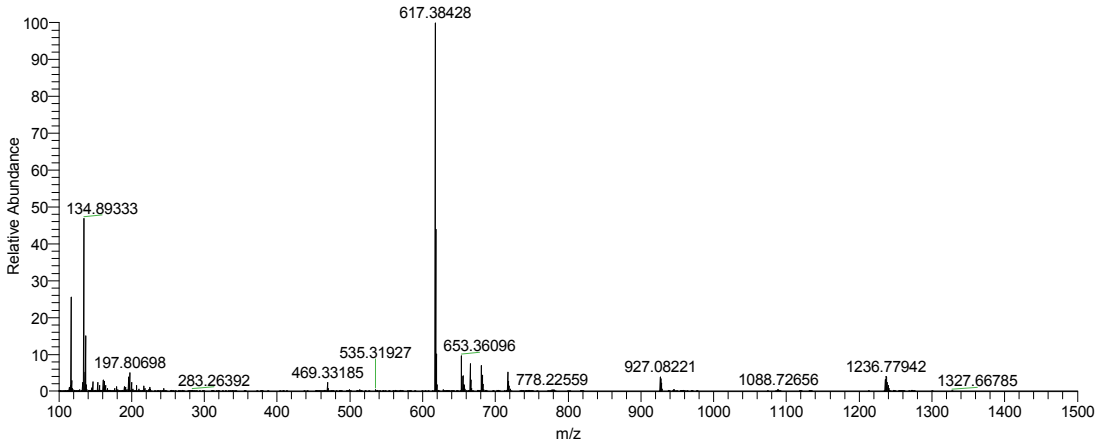


Fig. S51. The ESI-Q-Orbitrap MS spectrum of compound **15**

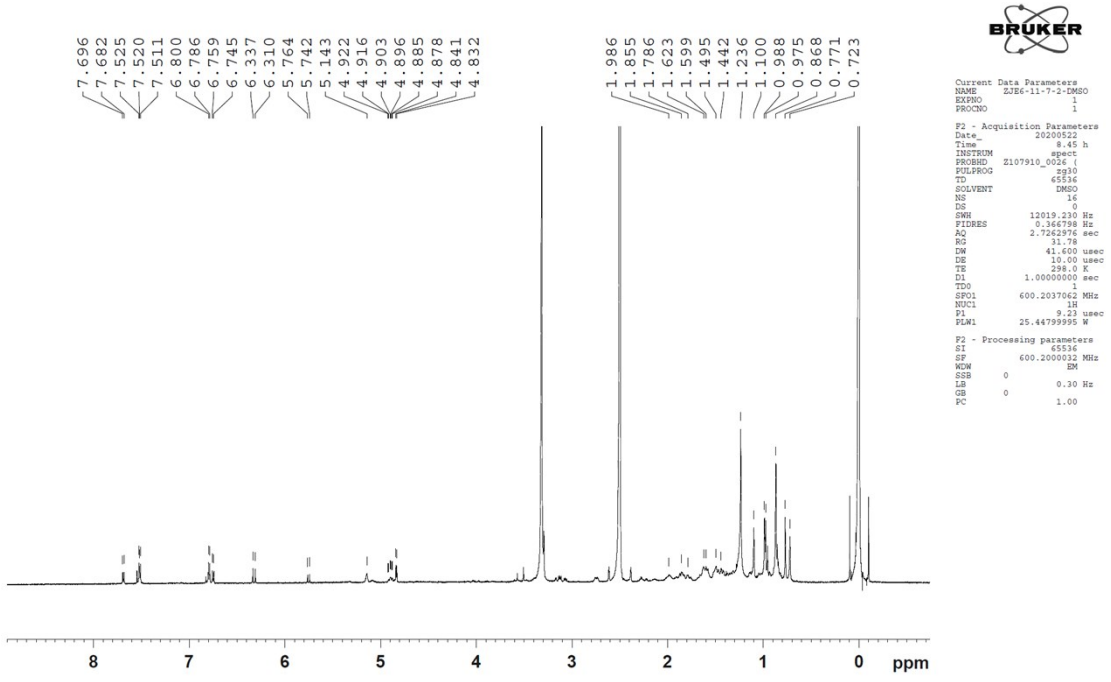


Fig. S52. ^{1}H NMR (600MHz, DMSO-d_6) spectrum of compound **16**

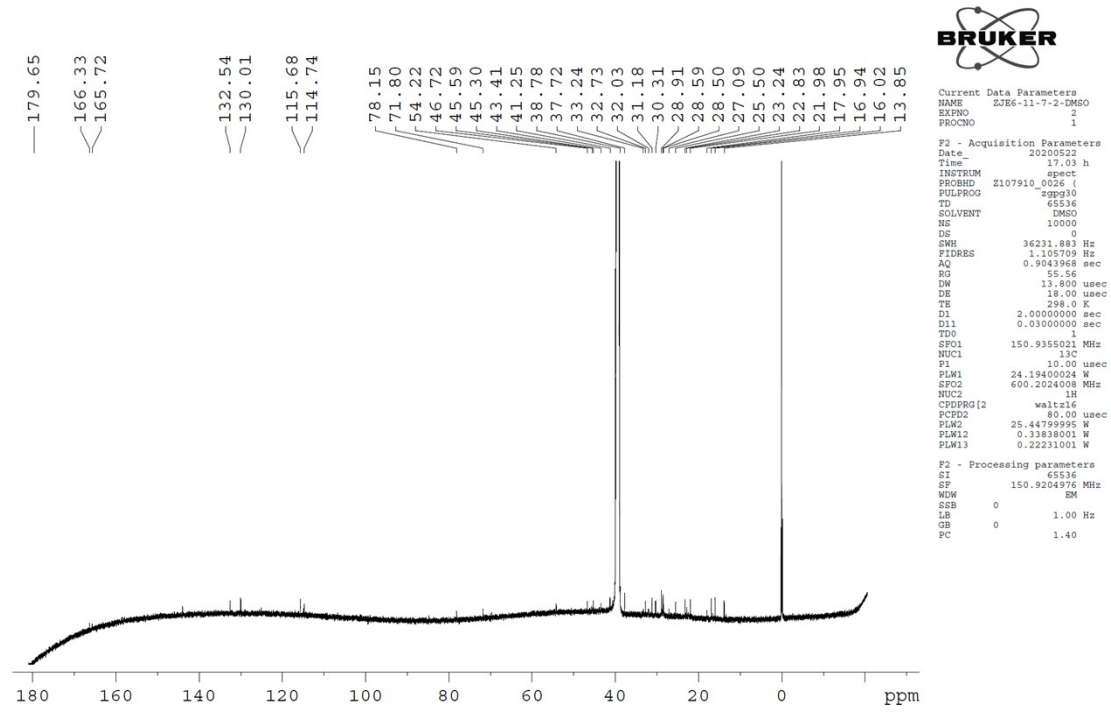


Fig. S53. ^{13}C NMR (150MHz, DMSO-d_6) spectrum of compound **16**

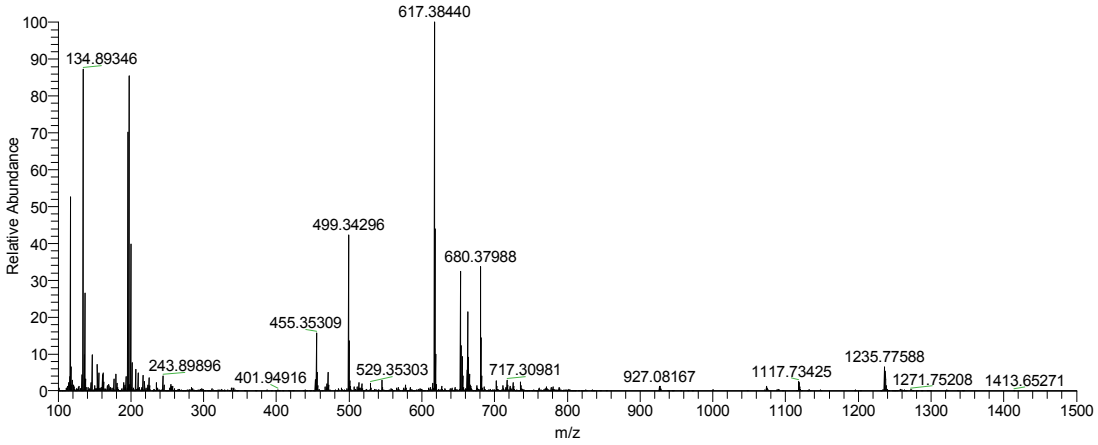


Fig. S54. The ESI-Q-Orbitrap MS spectrum of compound **16**

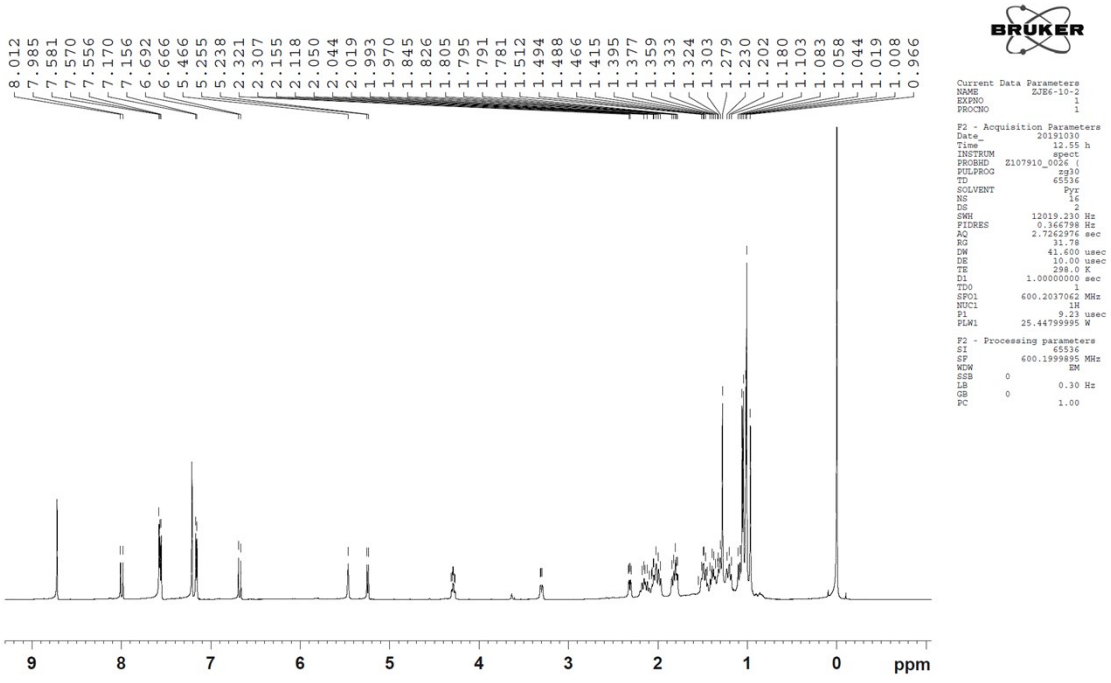


Fig. S55. ^{1}H NMR (600MHz, C_5D_5N) spectrum of compound **17**

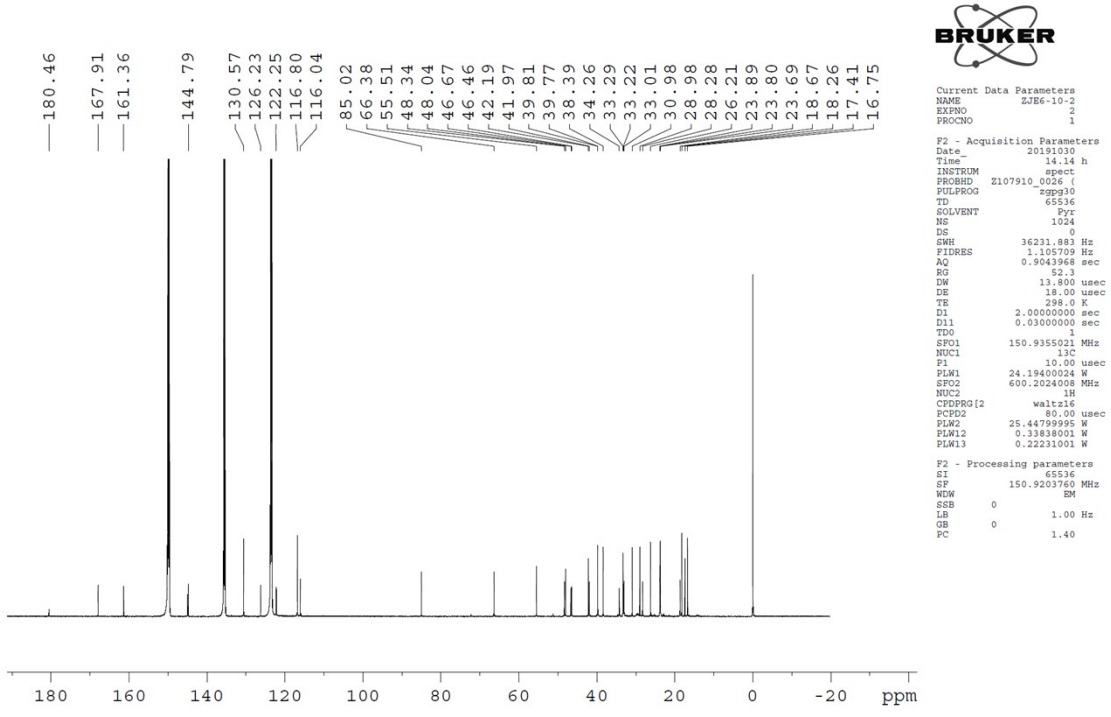


Fig. S56. ^{13}C NMR (150MHz, C_5D_5N) spectrum of compound **17**

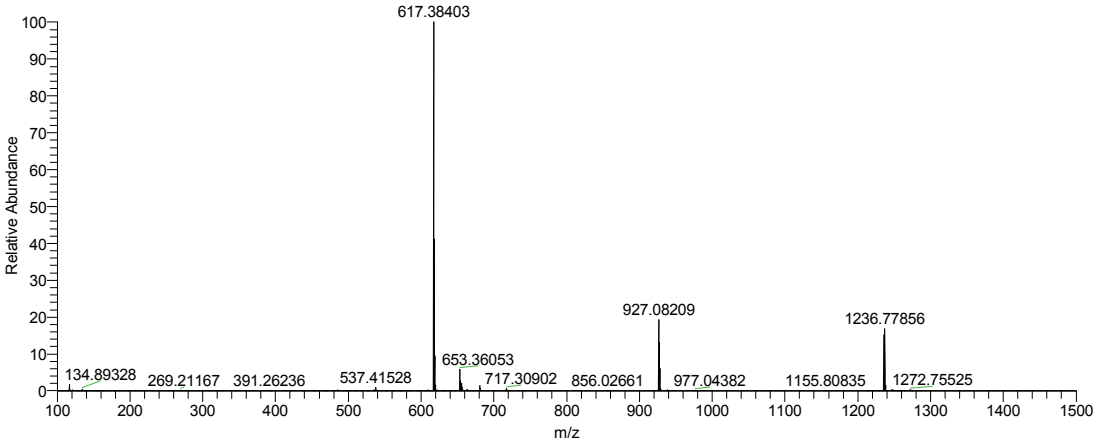
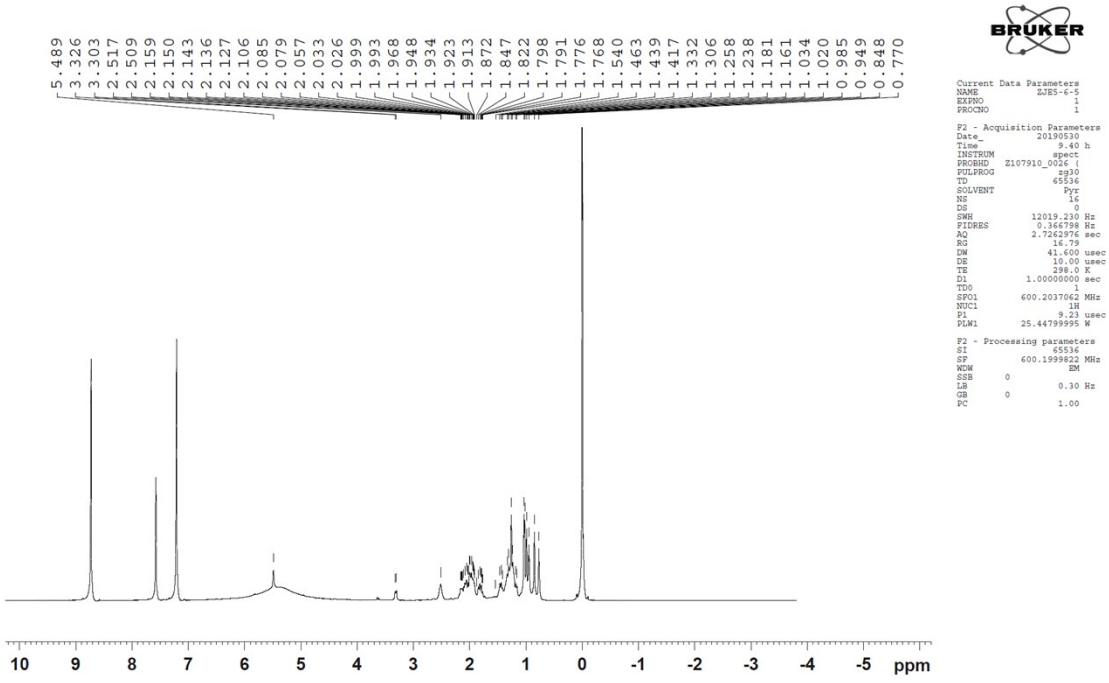


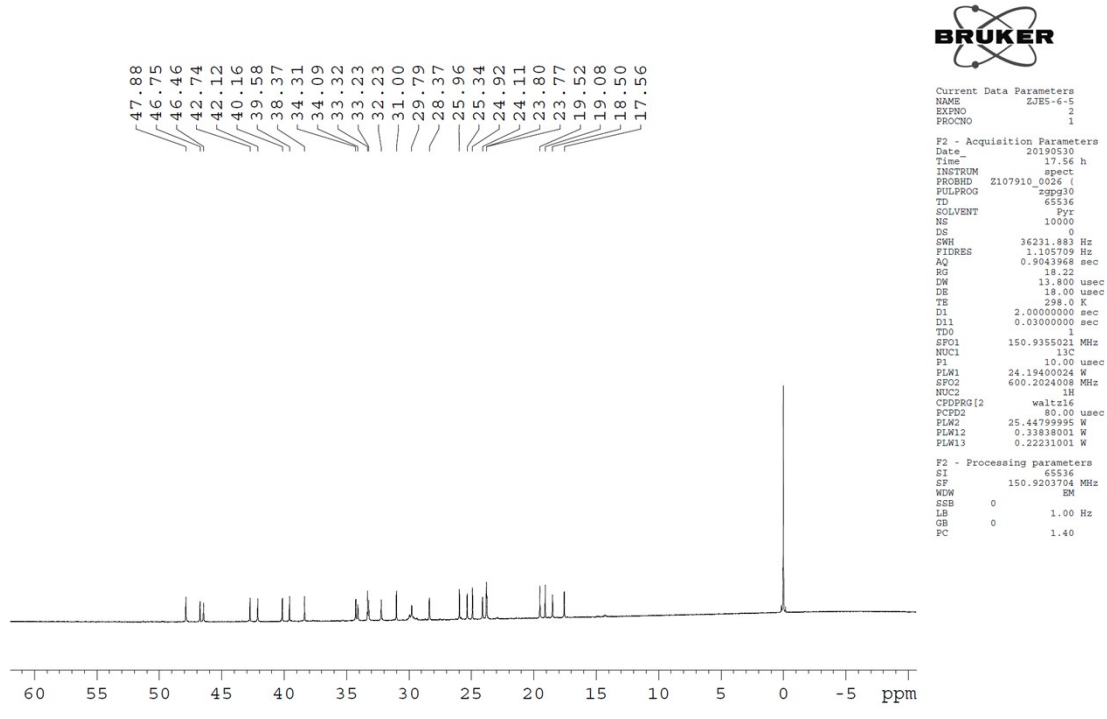
Fig. S57. The ESI-Q-Orbitrap MS spectrum of compound **17**



528

529 **Fig. S58**. ^{1}H NMR (600MHz, C_5D_5N) spectrum of compound **18**

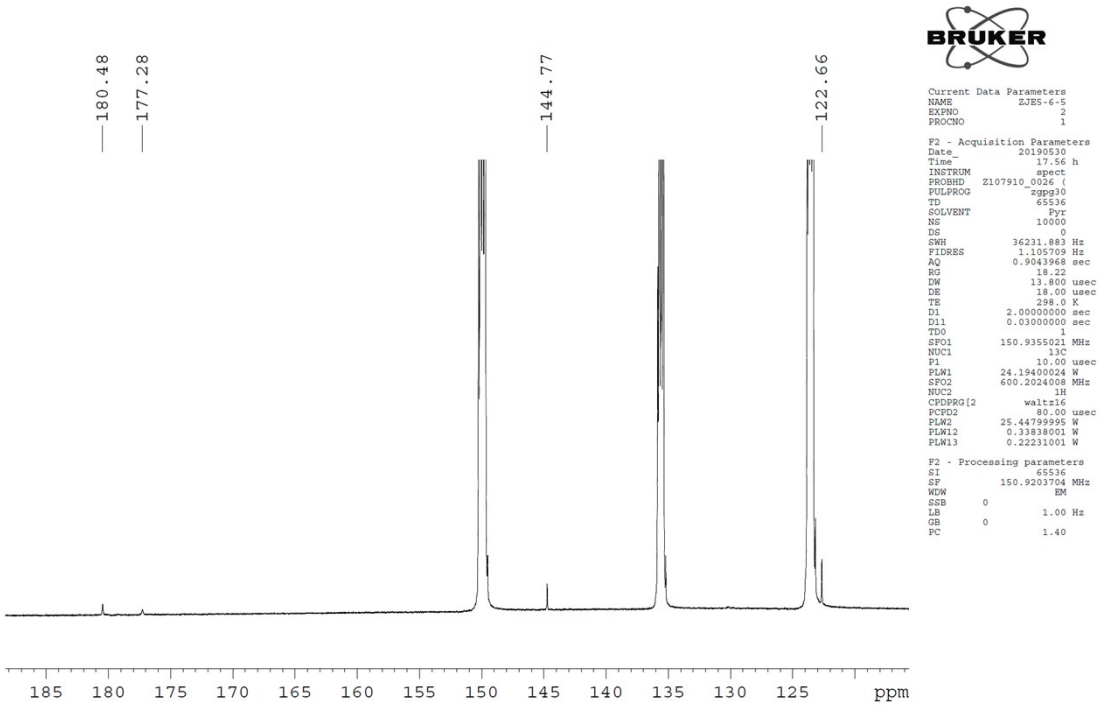
530



531

532 **Fig. S59**. ^{13}C NMR (150MHz, C_5D_5N) spectrum-1 of compound **18**

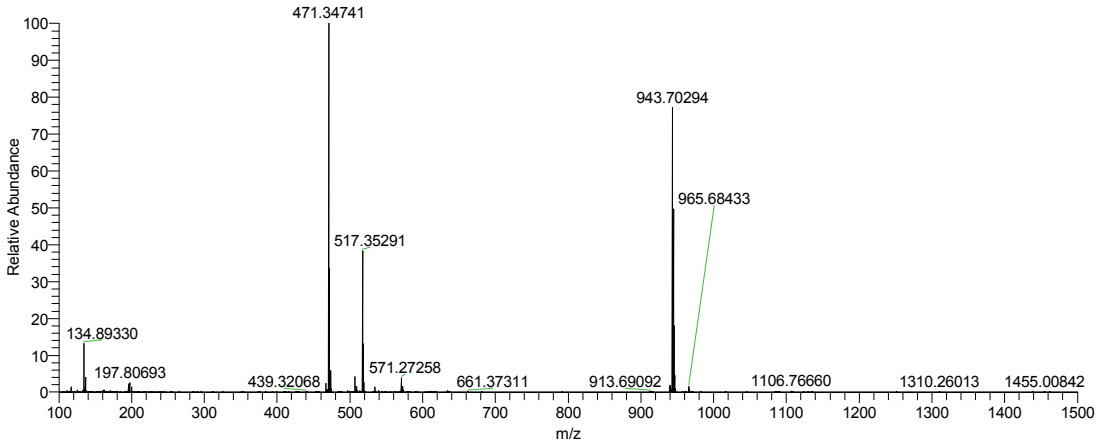
533



534

535 **Fig. S60**. ^{13}C NMR (150MHz, C_5D_5N) spectrum-2 of compound **18**

536



537

538 **Fig. S61**. The ESI-Q-Orbitrap MS spectrum of compound **18**

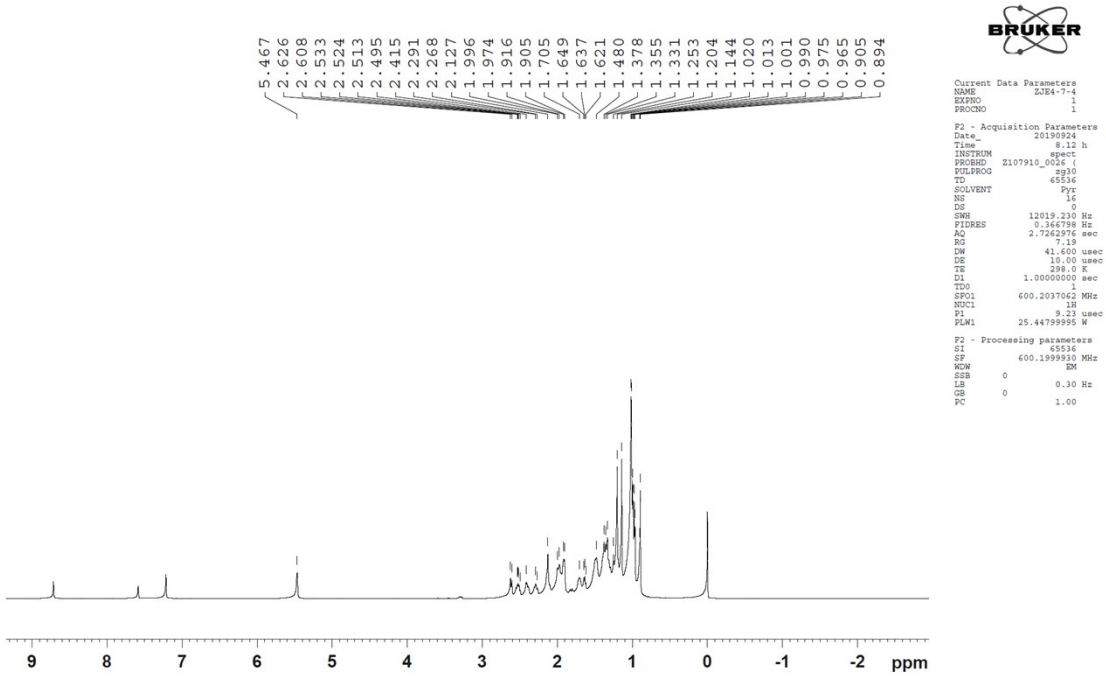


Fig. S62. ^{1}H NMR (600MHz, C_5D_5N) spectrum of compound **19**

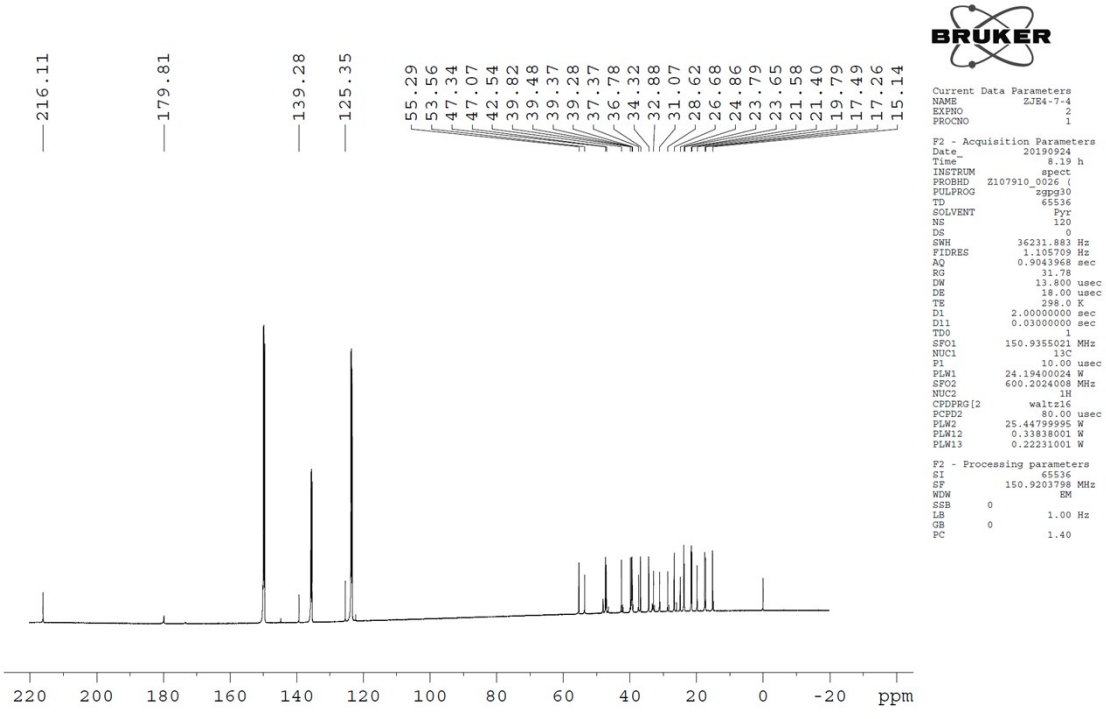
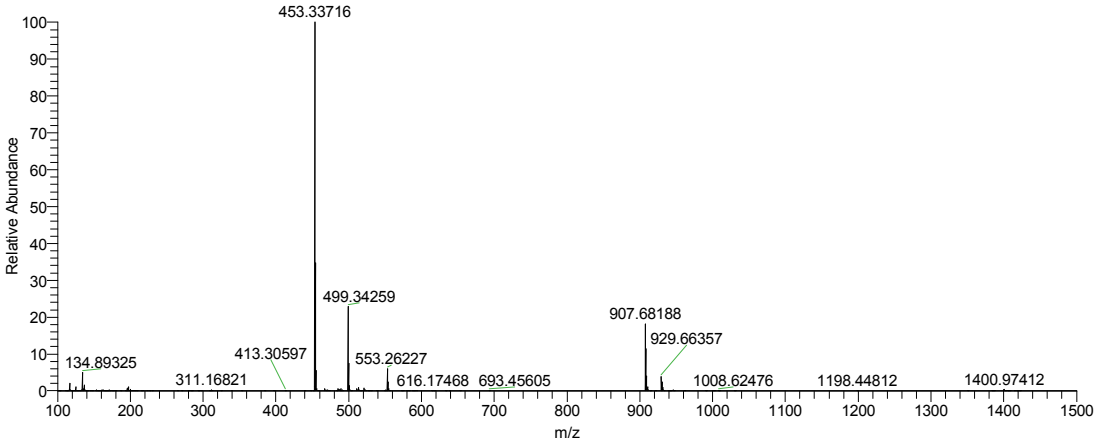


Fig. S63. ^{13}C NMR (150MHz, C_5D_5N) spectrum of compound **19**



546

547 **Fig. S64**. The ESI-Q-Orbitrap MS spectrum of compound **19**

548

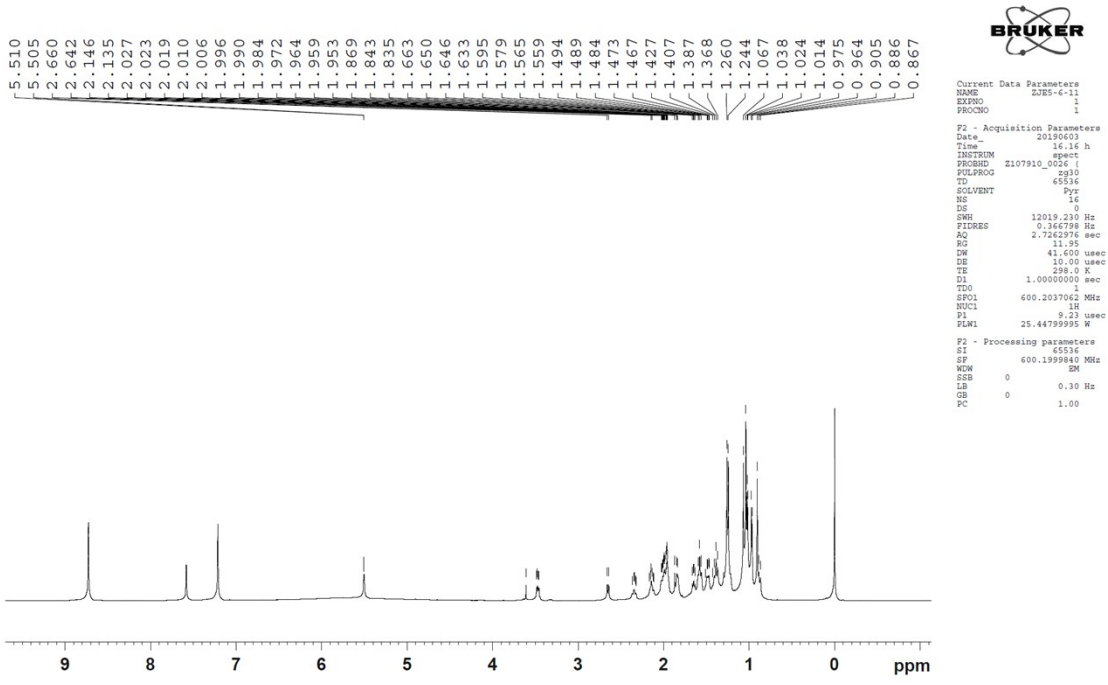


Fig. S65. ^{1}H NMR (600MHz, C_5D_5N) spectrum of compound **20**

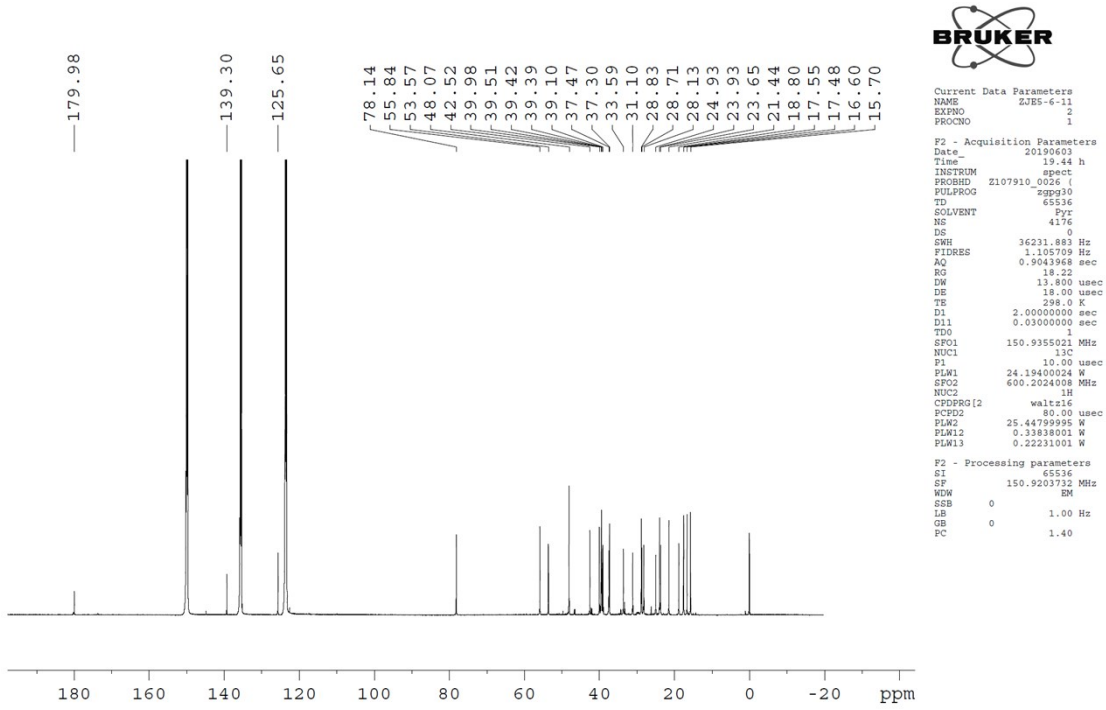


Fig. S66. ^{13}C NMR (150MHz, C_5D_5N) spectrum of compound **20**

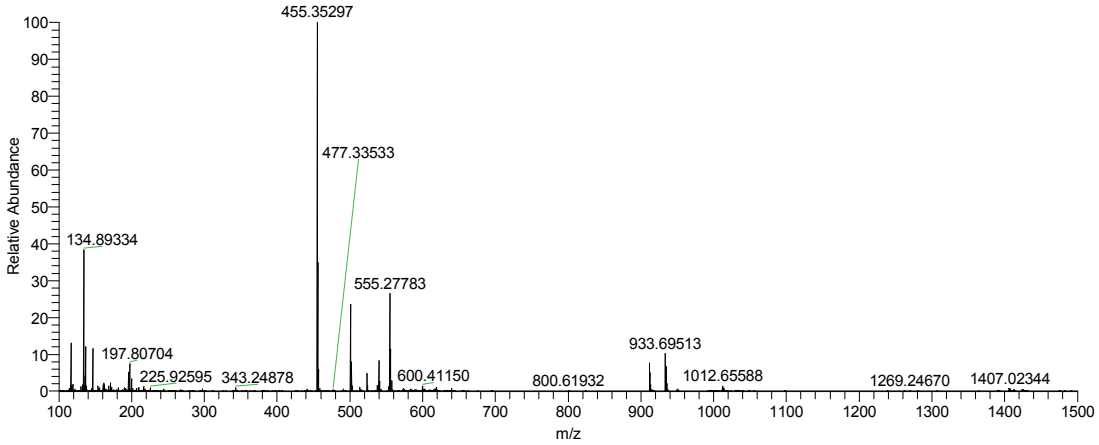


Fig. S67. The ESI-Q-Orbitrap MS spectrum of compound **20**

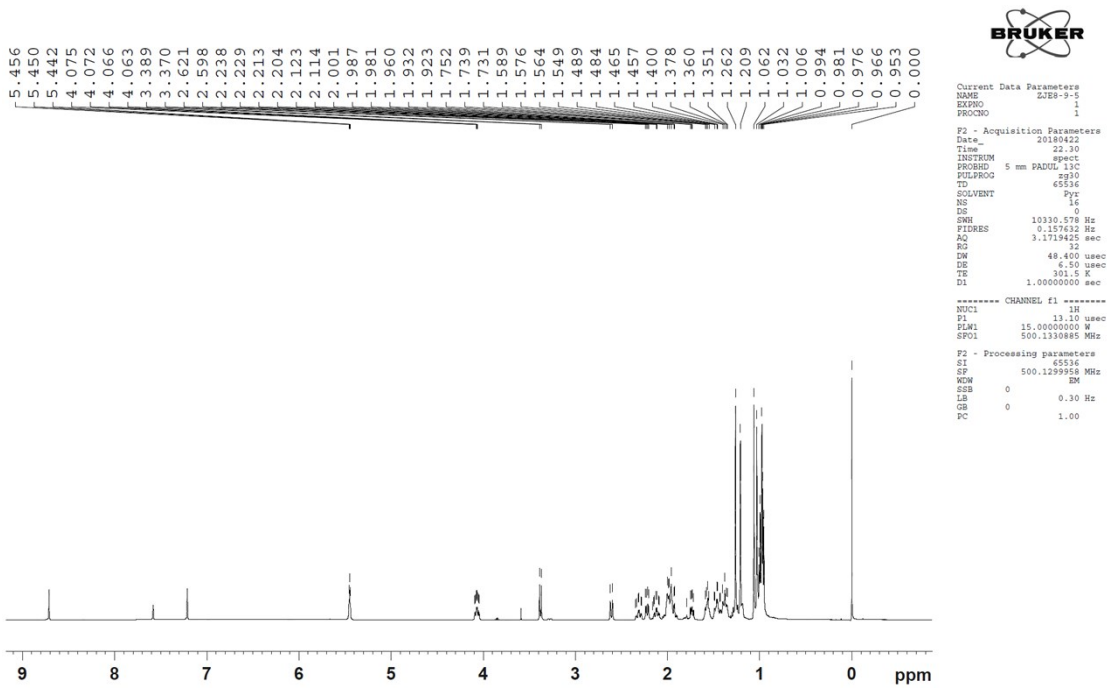


Fig. S68. ^{1}H NMR (500MHz, C_5D_5N) spectrum of compound **21**

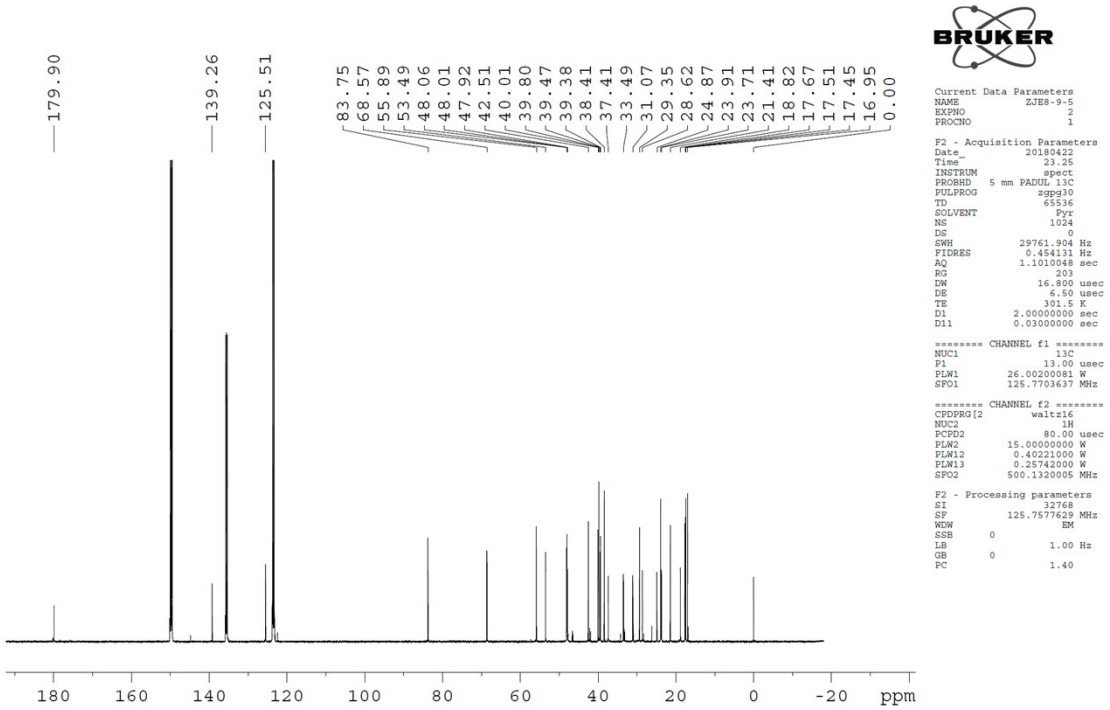


Fig. S69. ^{13}C NMR (125MHz, C_5D_5N) spectrum of compound **21**

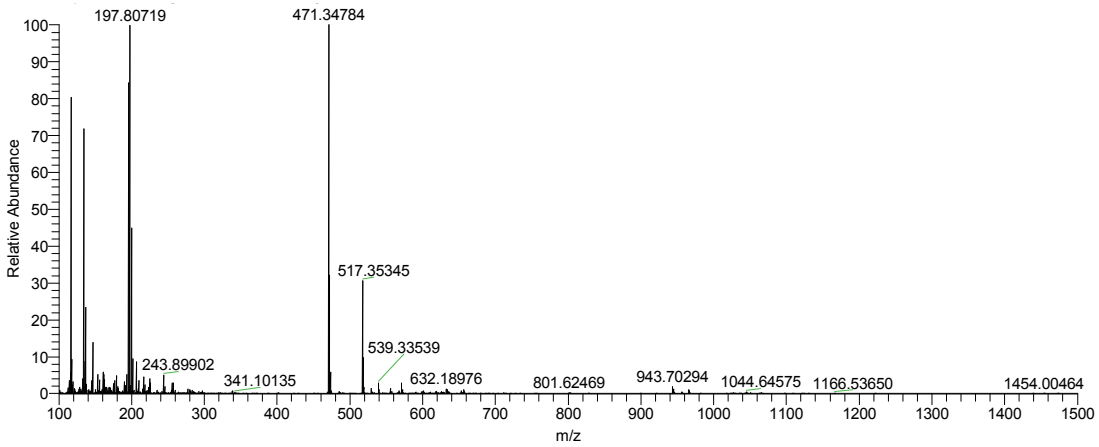


Fig. S70. The ESI-Q-Orbitrap MS spectrum of compound **21**

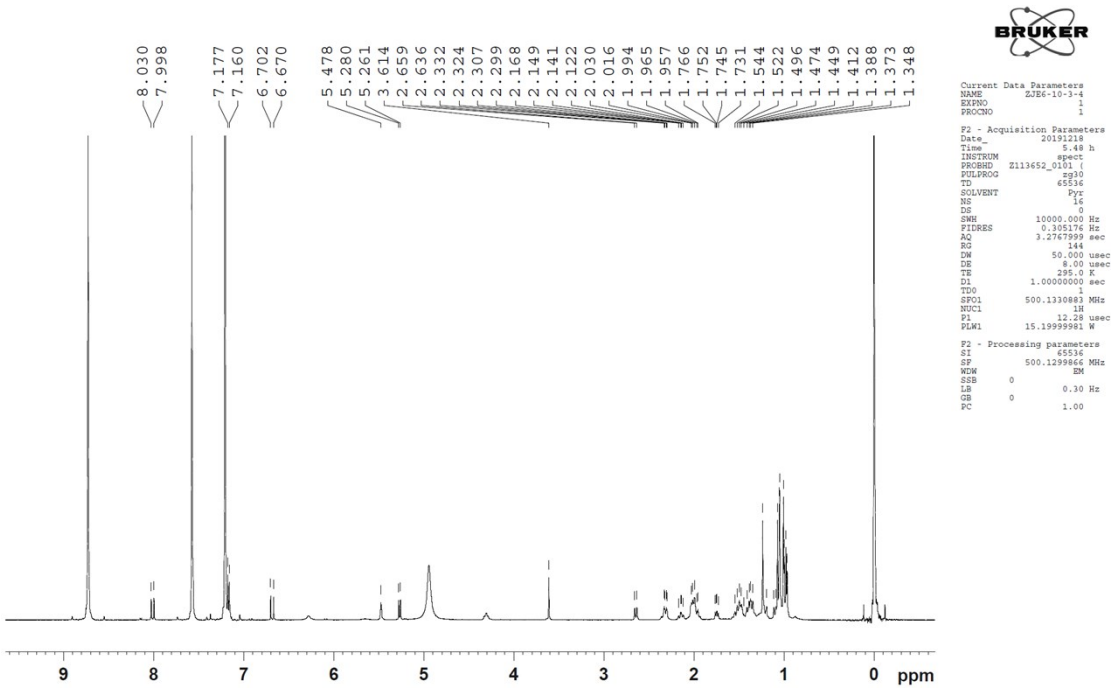


Fig. S71. ^{1}H NMR (500MHz, C_5D_5N) spectrum of compound **22**

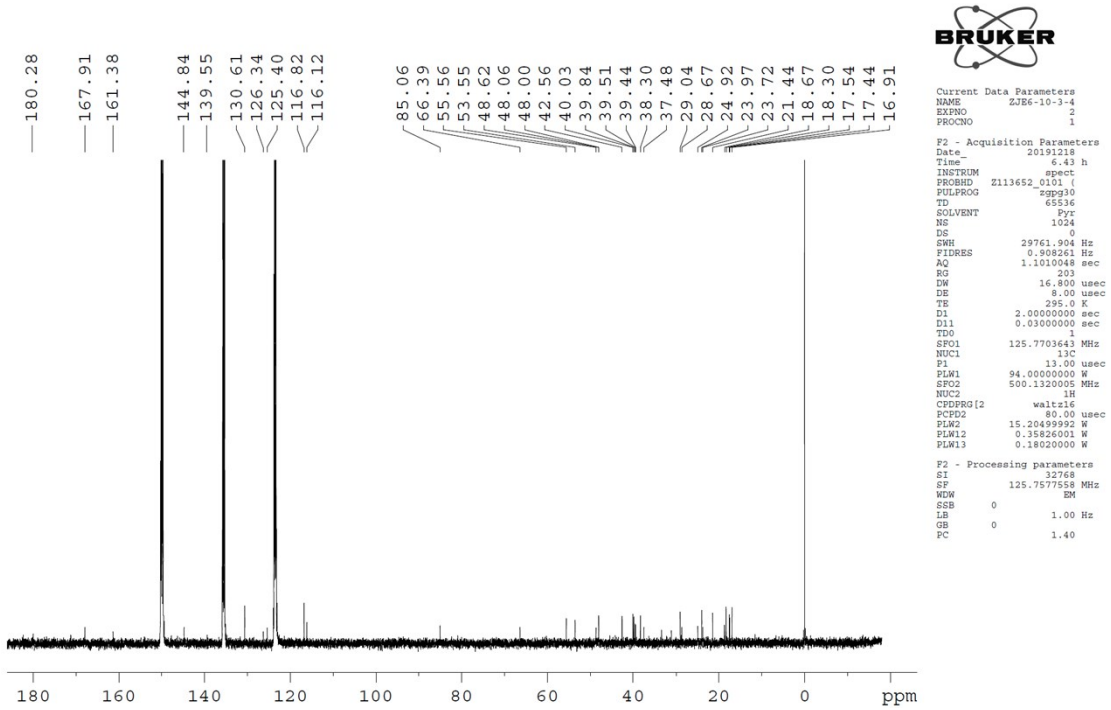


Fig. S72. ^{13}C NMR (125MHz, C_5D_5N) spectrum of compound **22**

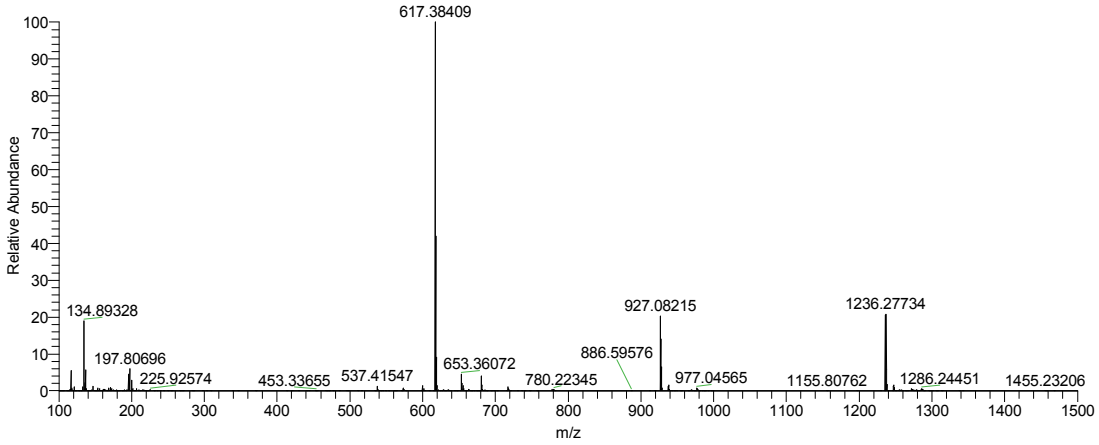


Fig. S73. The ESI-Q-Orbitrap MS spectrum of compound **22**

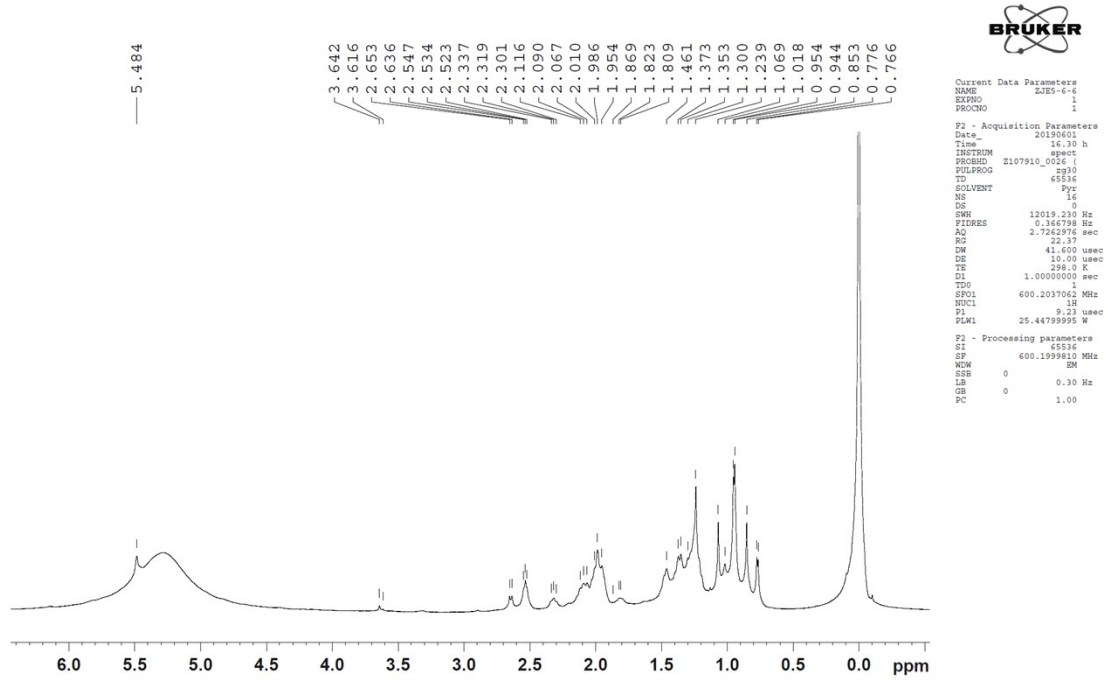


Fig. S74. ^{1}H NMR (600MHz, C_5D_5N) spectrum of compound **23**

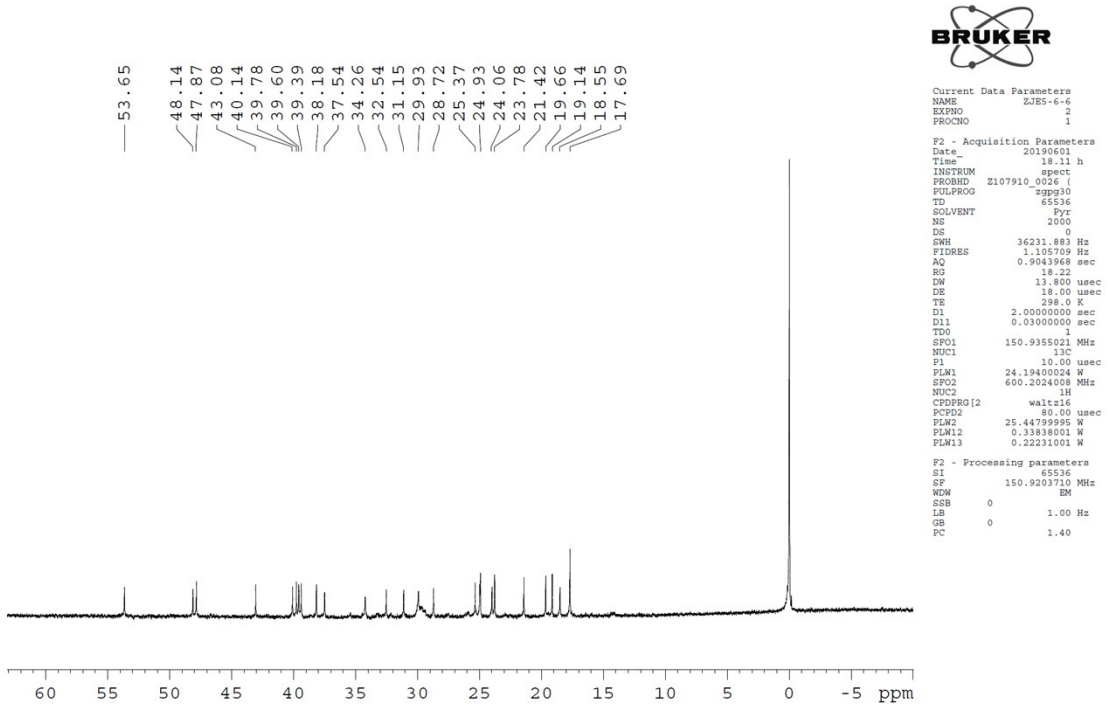


Fig. S75. ^{13}C NMR (150MHz, C_5D_5N) spectrum-1 of compound **23**

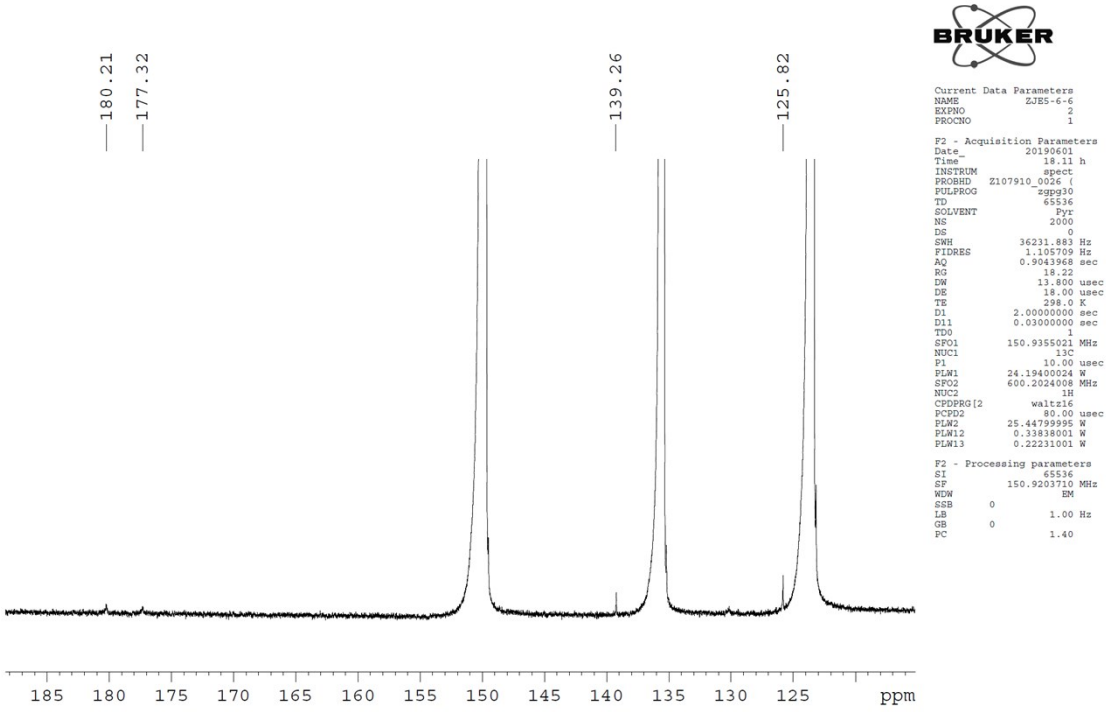


Fig. S76. ^{13}C NMR (150MHz, C_5D_5N) spectrum-2 of compound **23**

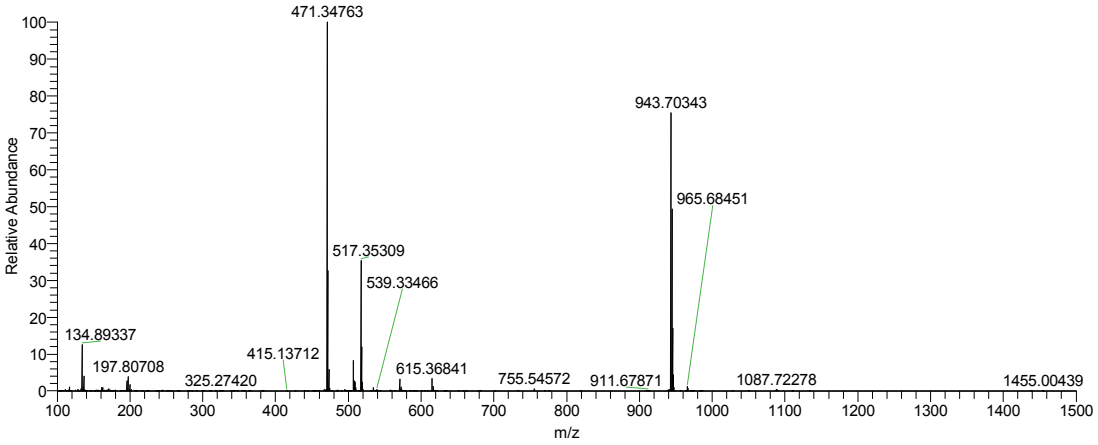


Fig. S77. The ESI-Q-Orbitrap MS spectrum of compound **23**

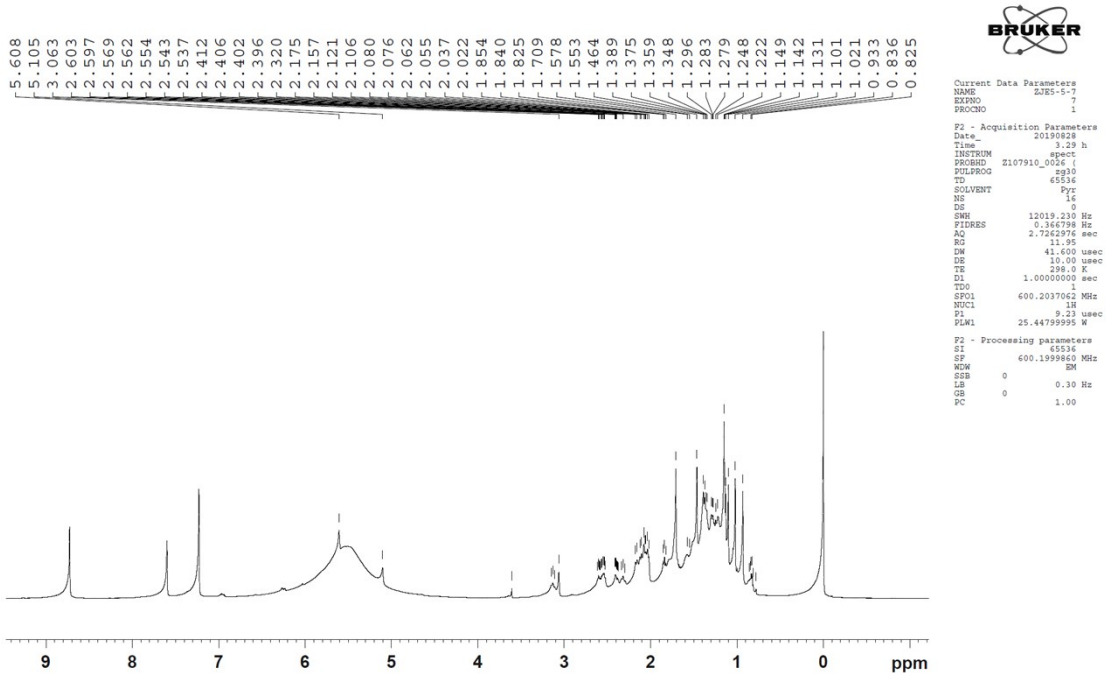


Fig. S78. ^{1}H NMR (600MHz, C_5D_5N) spectrum of compound **24**

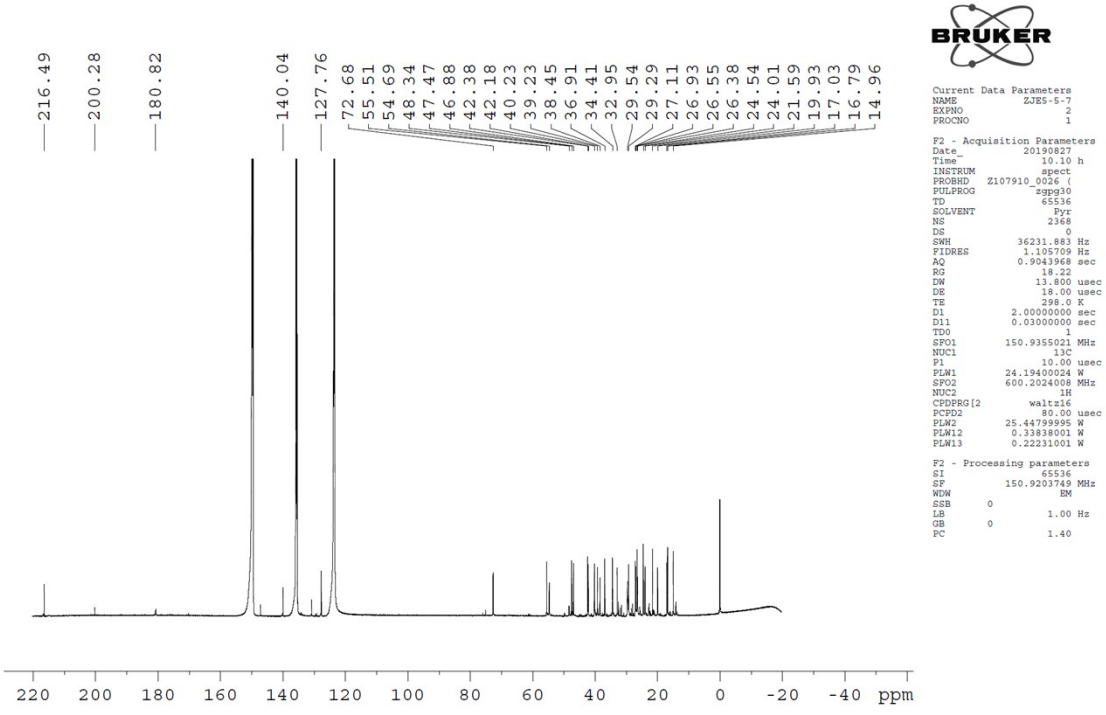


Fig. S79. ^{13}C NMR (150MHz, C_5D_5N) spectrum of compound **24**

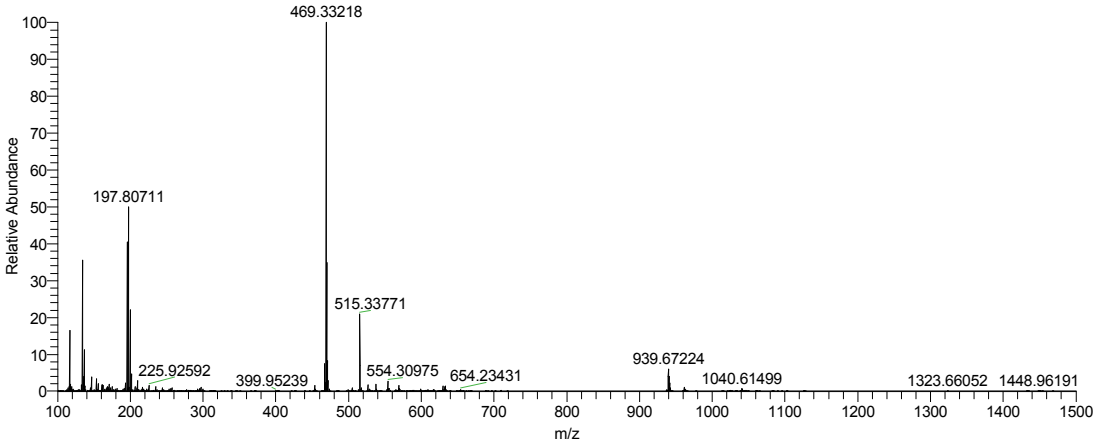
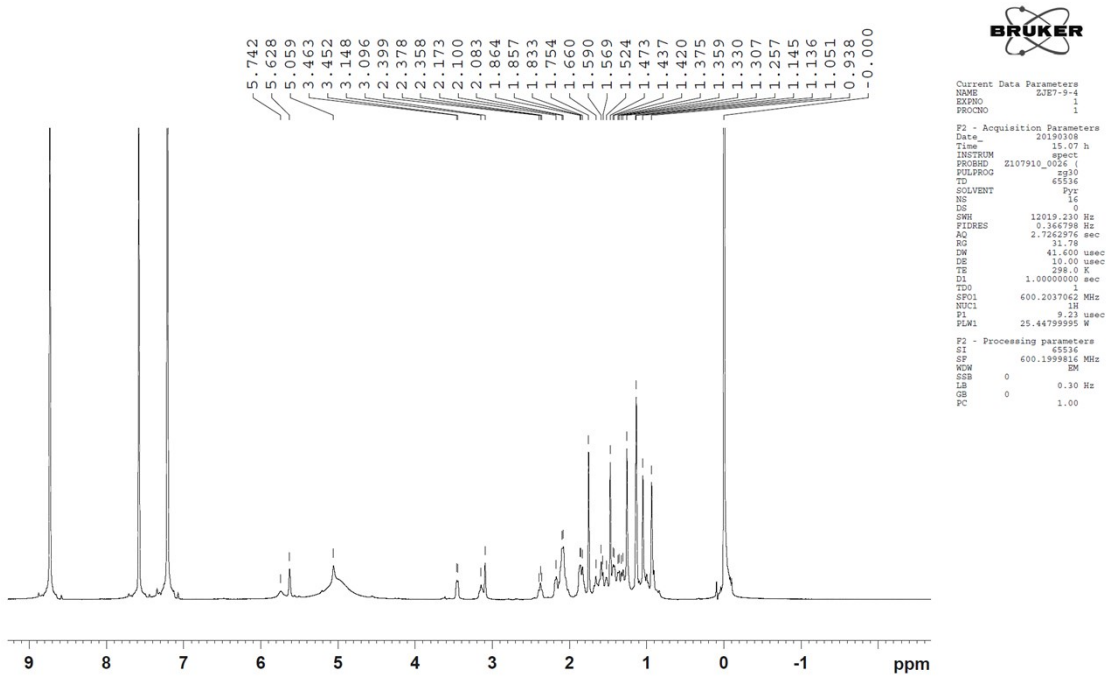


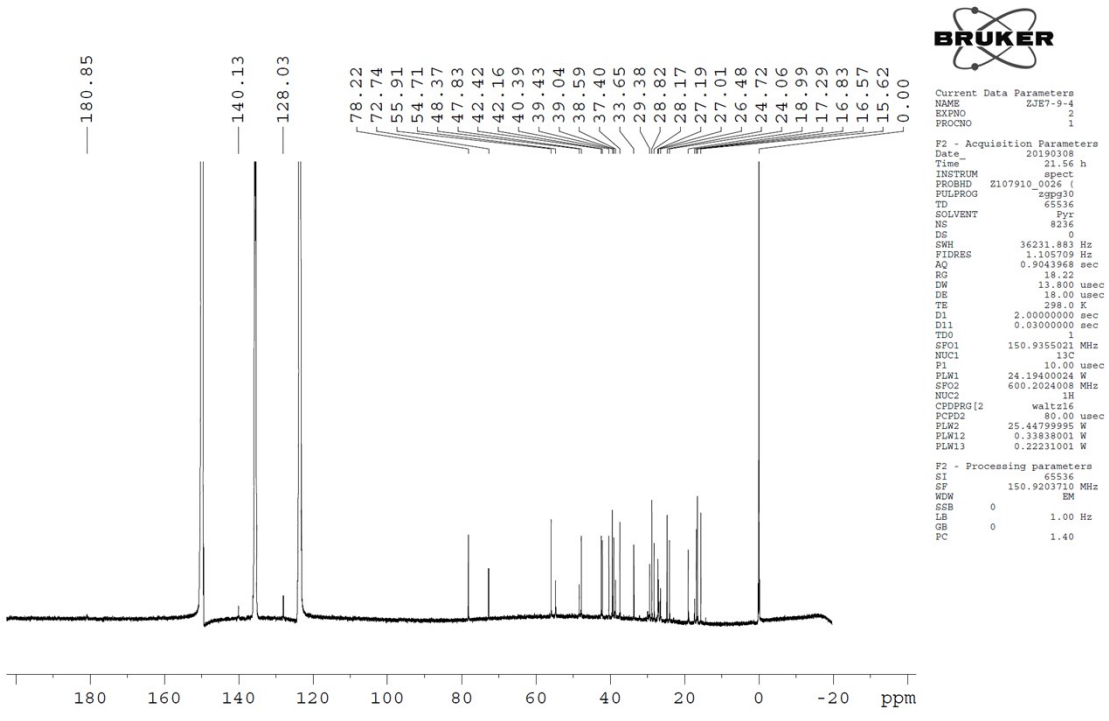
Fig. S80. The ESI-Q-Orbitrap MS spectrum of compound **24**



601

602 **Fig. S81**. ^{1}H NMR (600MHz, C_5D_5N) spectrum of compound **25**

603



604

605 **Fig. S82**. ^{13}C NMR (150MHz, C_5D_5N) spectrum of compound **25**

606

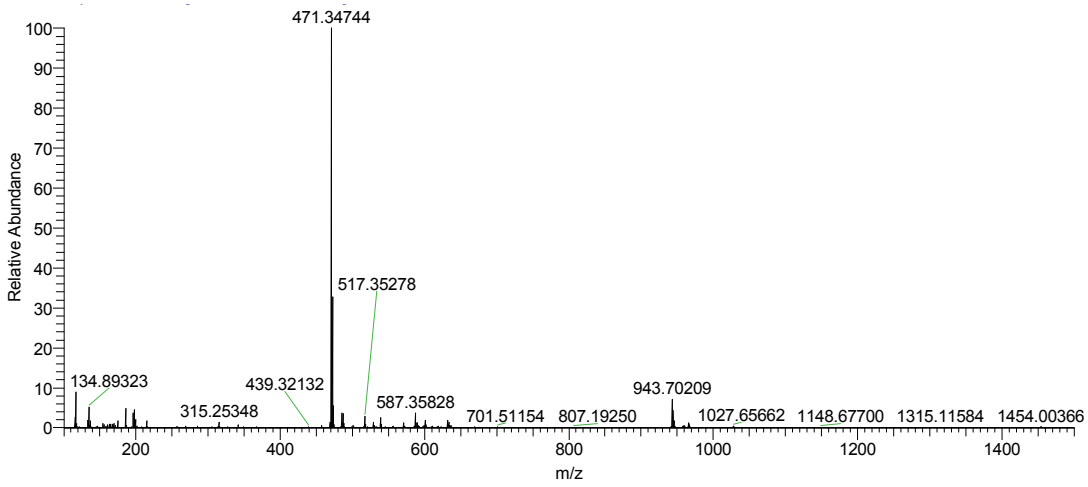
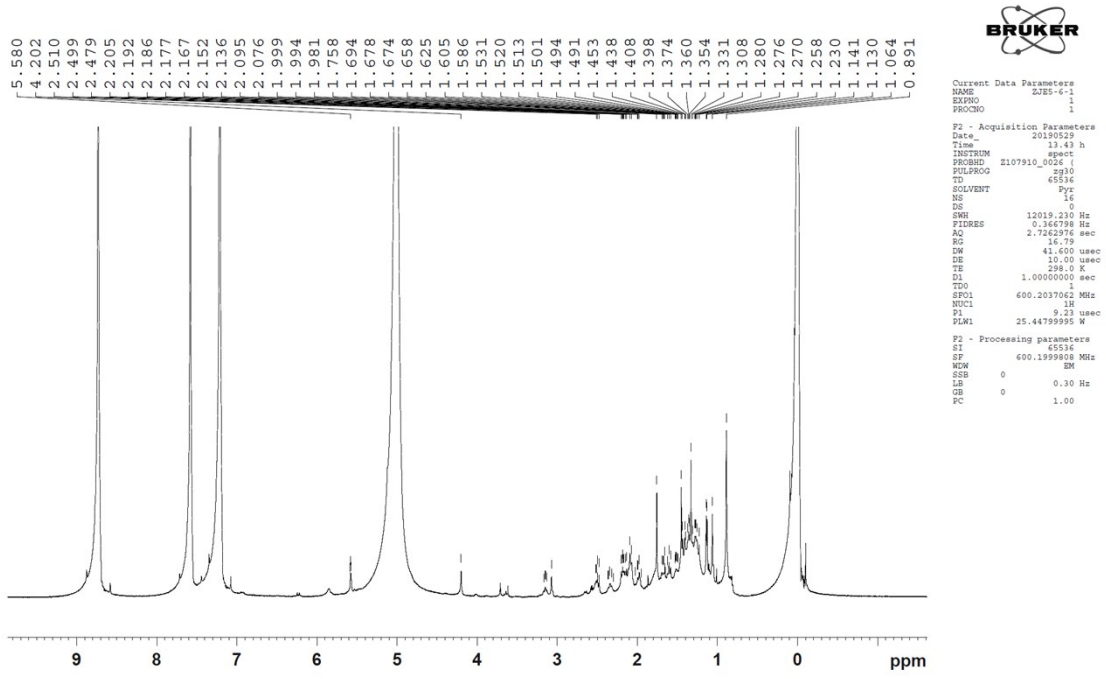


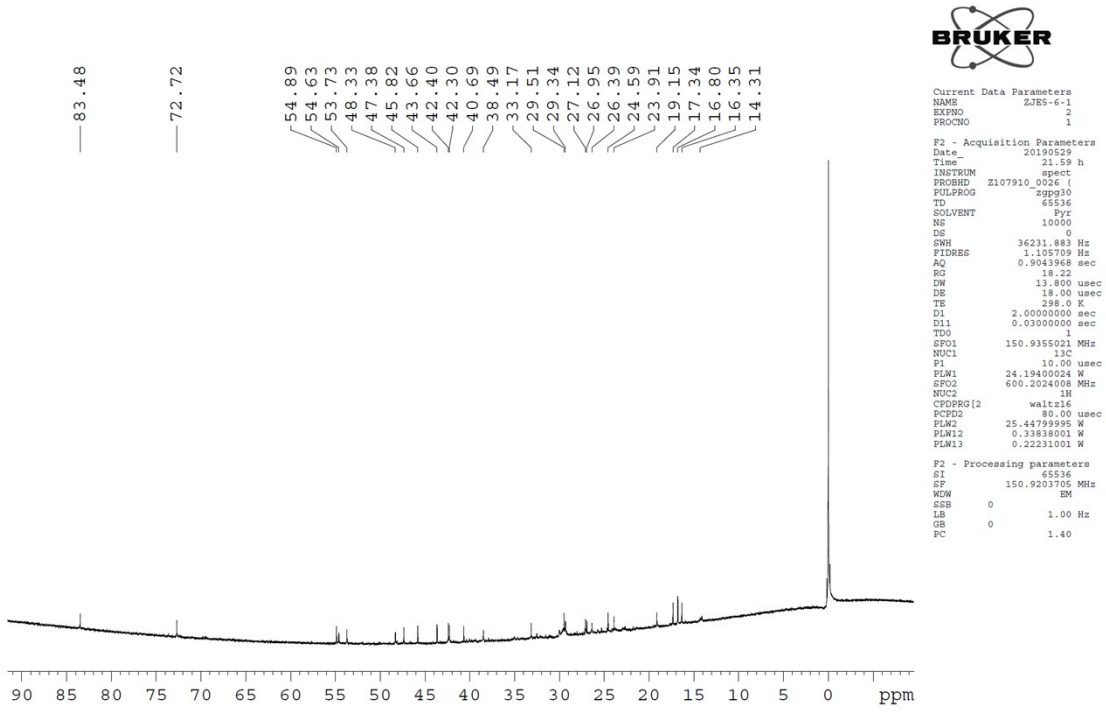
Fig. S83. The ESI-Q-Orbitrap MS spectrum of compound **25**



610

611 **Fig. S84**. ^{1}H NMR (600MHz, C_5D_5N) spectrum of compound **26**

612



613

614 **Fig. S85**. ^{13}C NMR (150MHz, C_5D_5N) spectrum-1 of compound **26**

615

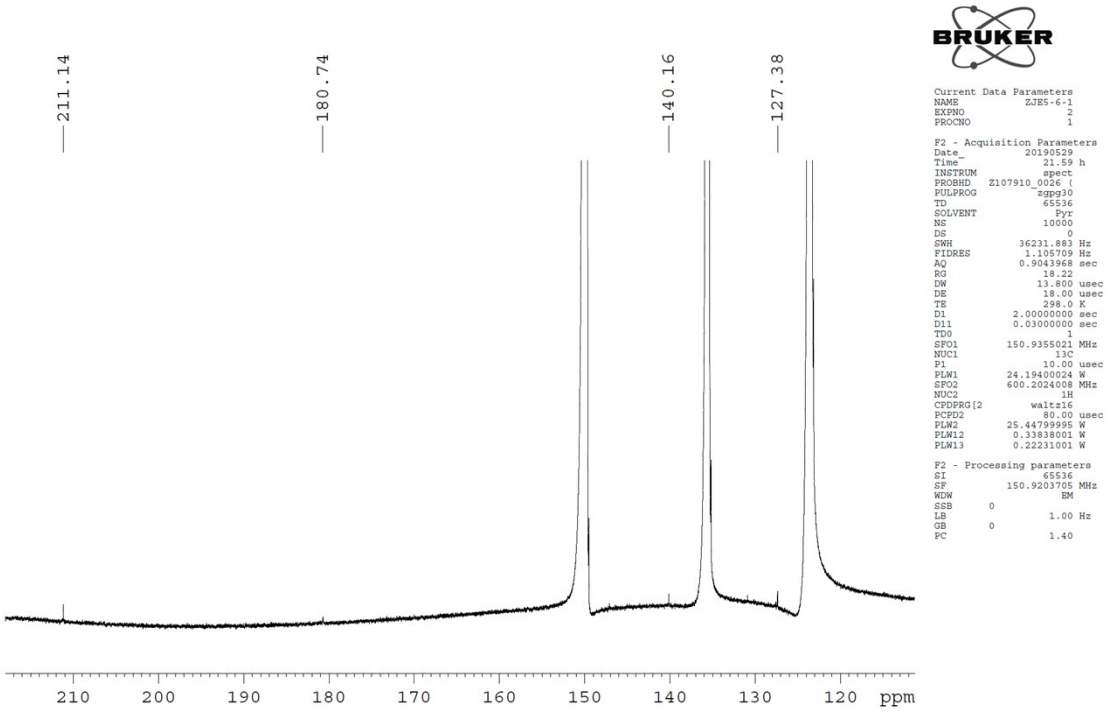


Fig. S86. ^{13}C NMR (150MHz, C_5D_5N) spectrum-2 of compound **26**

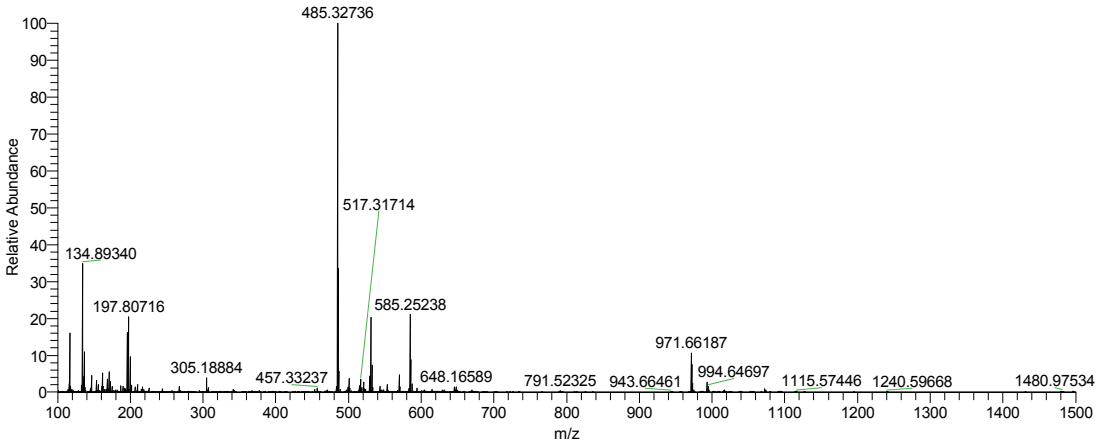


Fig. S87. The ESI-Q-Orbitrap MS spectrum of compound **26**

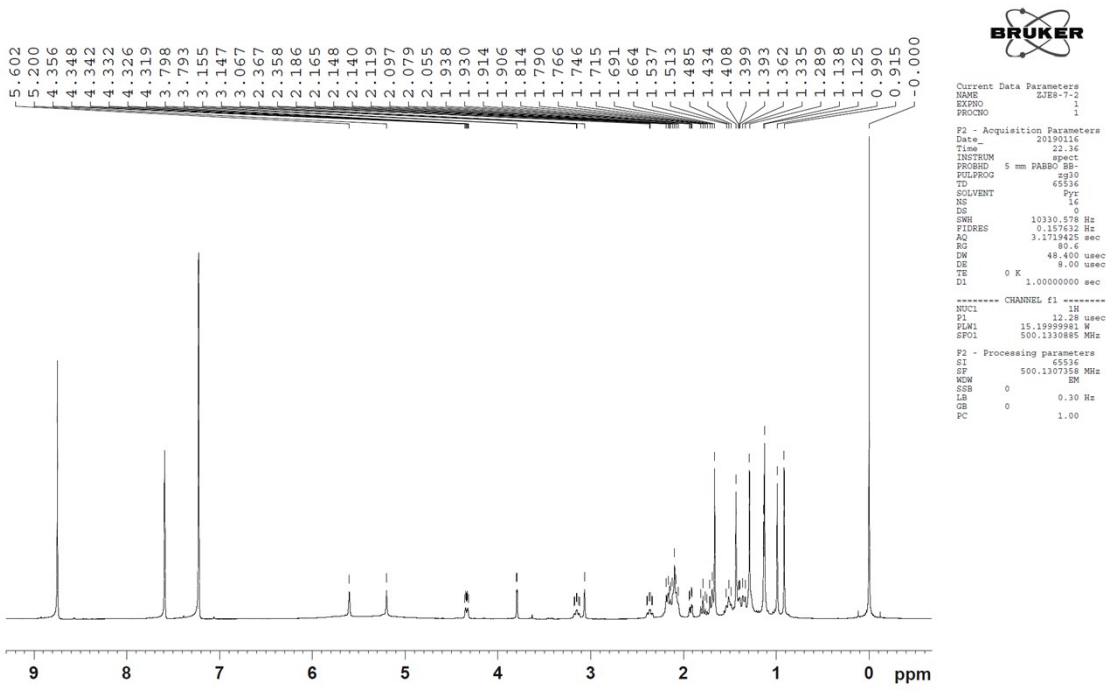


Fig. S88. ^{1}H NMR (500MHz, C_5D_5N) spectrum of compound **27**

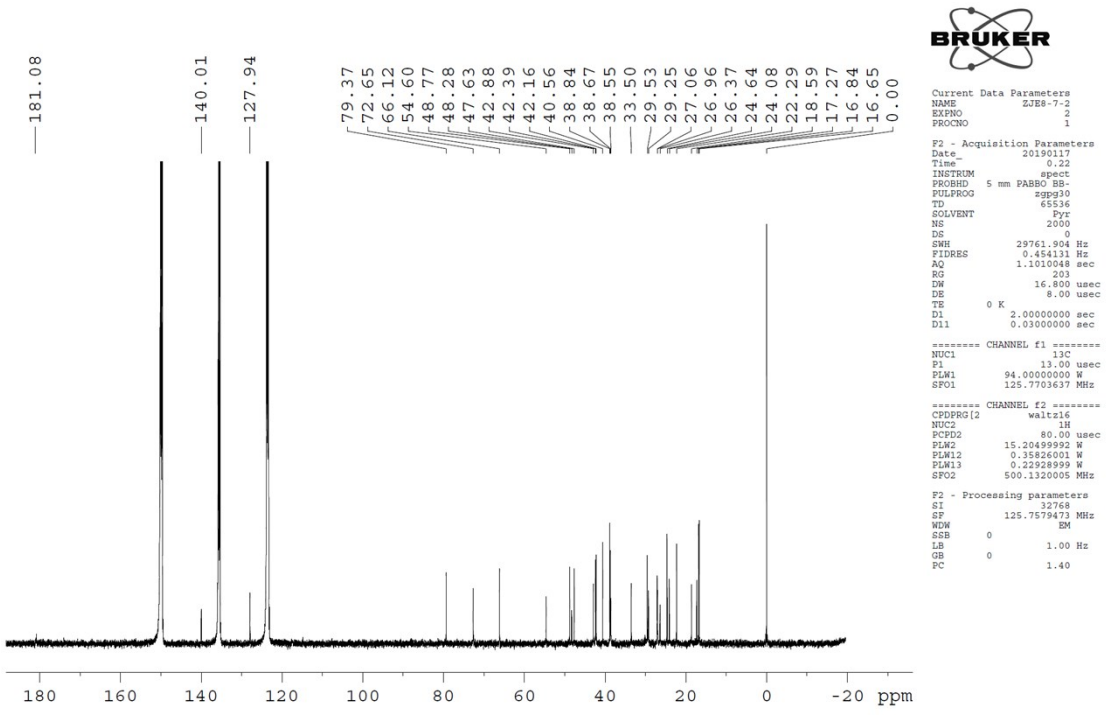


Fig. S89. ^{13}C NMR (125MHz, C_5D_5N) spectrum of compound **27**

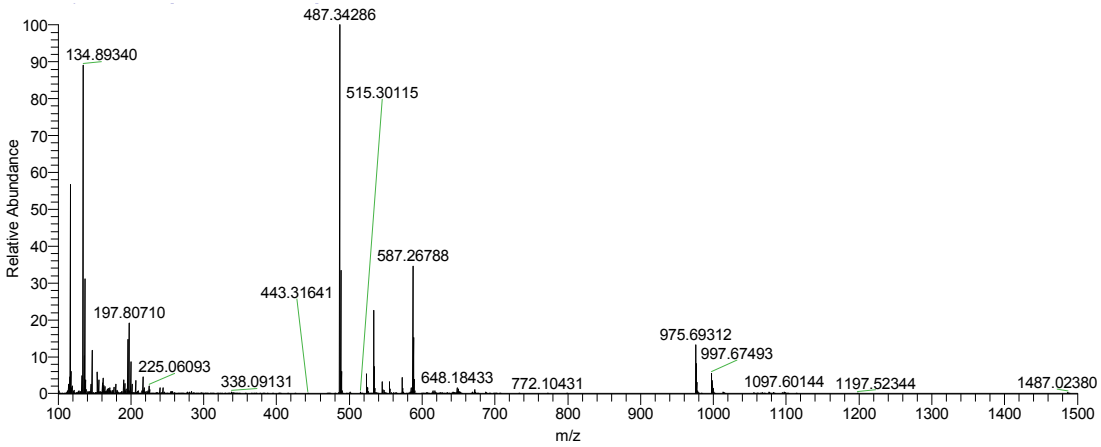
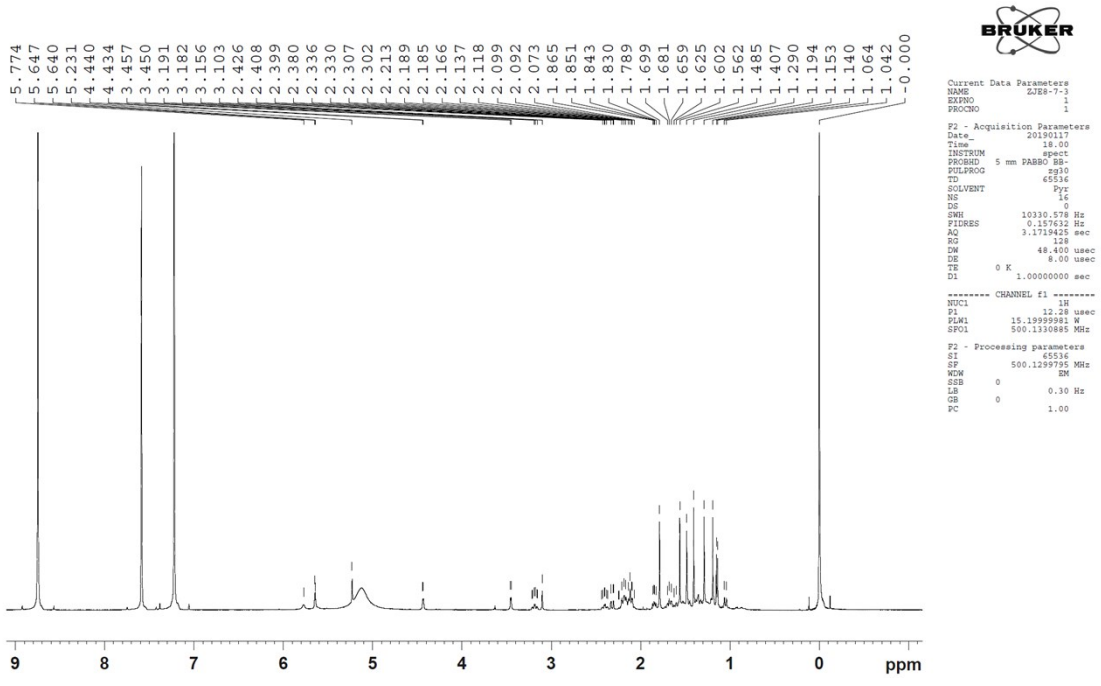


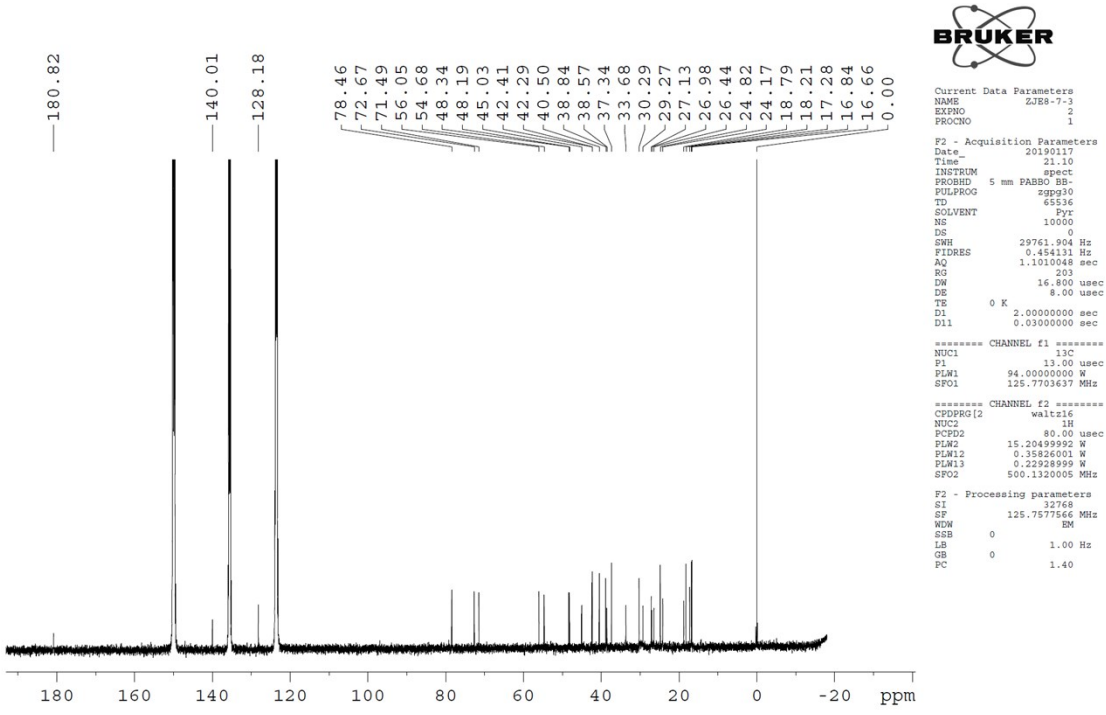
Fig. S90. The ESI-Q-Orbitrap MS spectrum of compound **27**



633

634 **Fig. S91**. ^{1}H NMR (500MHz, C_5D_5N) spectrum of compound **28**

635



636

637 **Fig. S92**. ^{13}C NMR (125MHz, C_5D_5N) spectrum of compound **28**

638

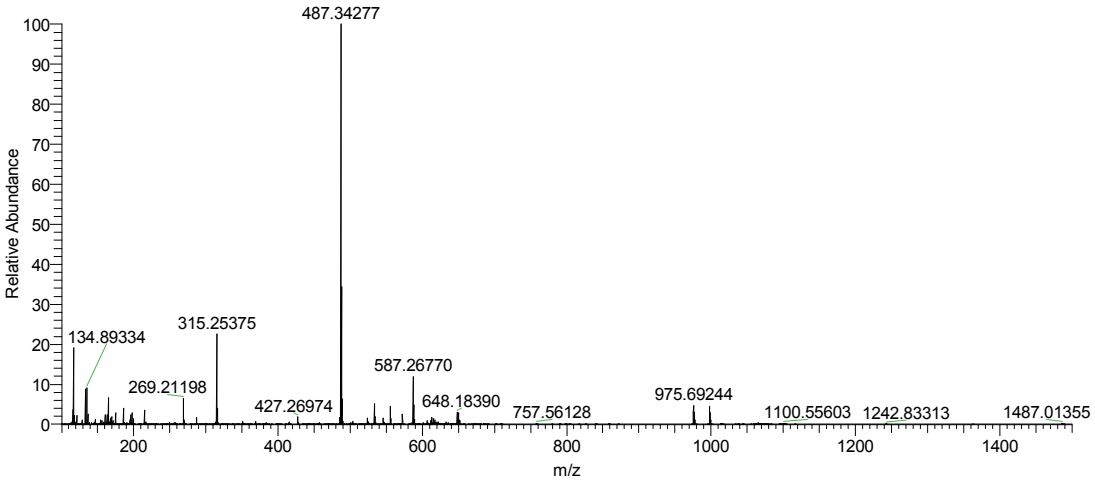
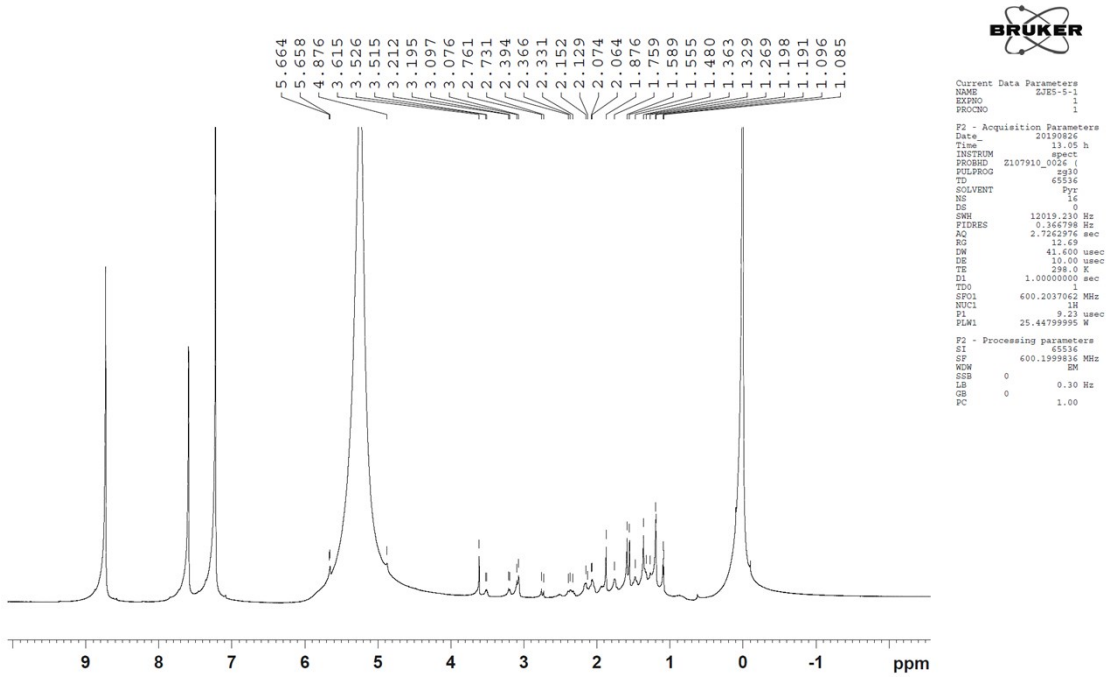


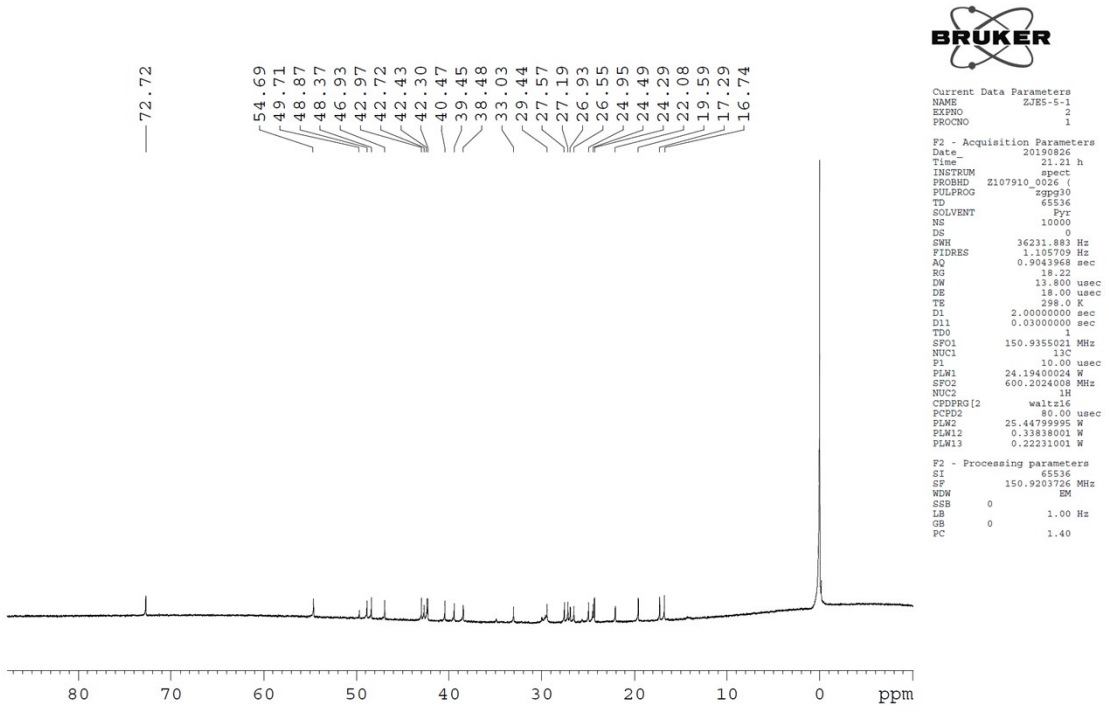
Fig. S93. The ESI-Q-Orbitrap MS spectrum of compound **28**



643

644 **Fig. S94**. ^{1}H NMR (600MHz, C_5D_5N) spectrum of compound **29**

645



646

647 **Fig. S95**. ^{13}C NMR (150MHz, C_5D_5N) spectrum-1 of compound **29**

648

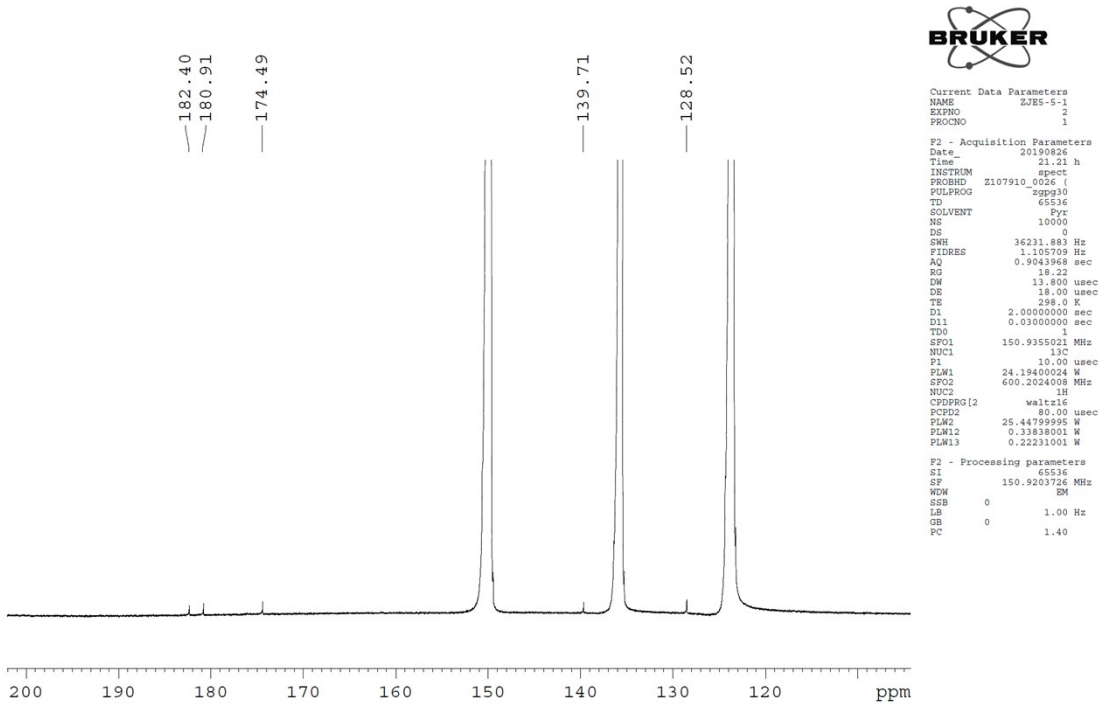


Fig. S96. ^{13}C NMR (150MHz, C_5D_5N) spectrum-2 of compound **29**

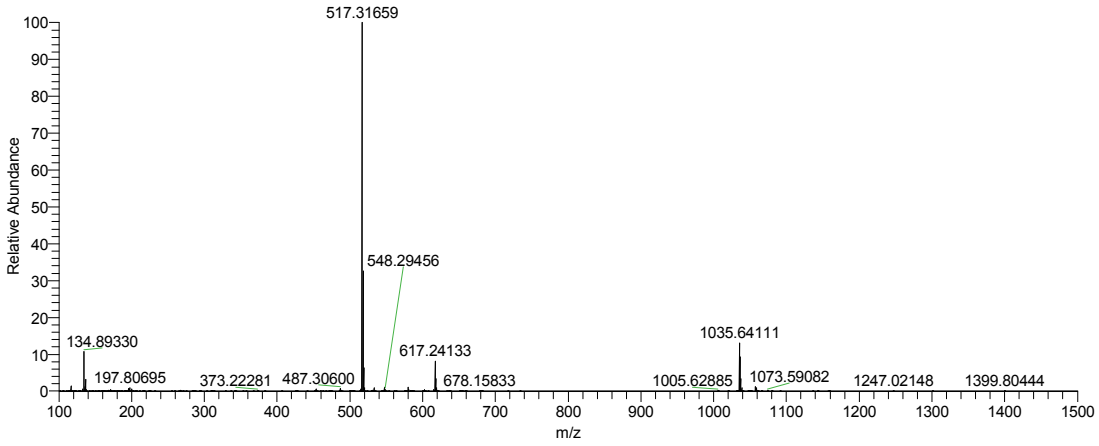


Fig. S97. The ESI-Q-Orbitrap MS spectrum of compound **29**

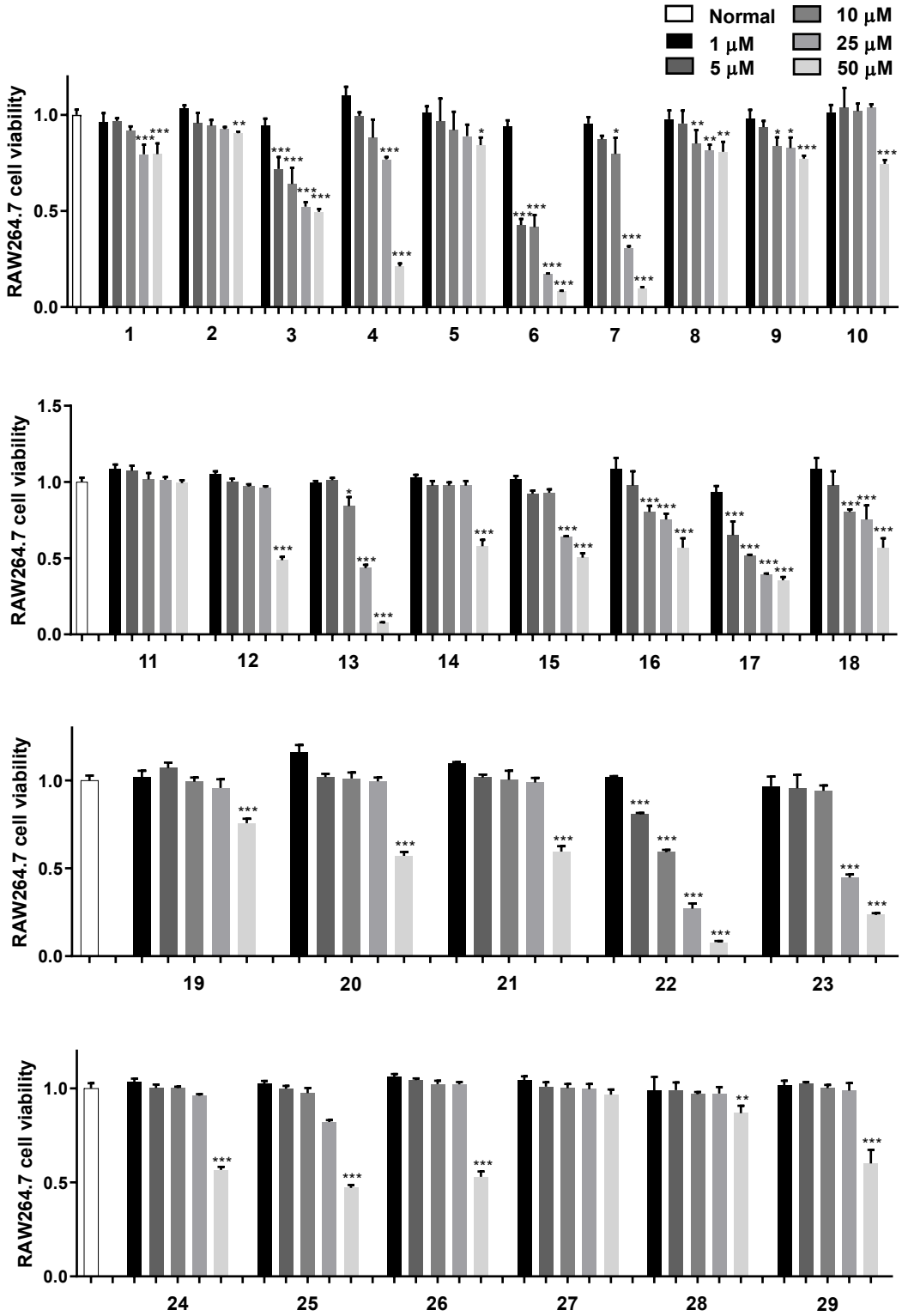


Fig. S98. The MTT assay compounds **1–29** at 1, 5, 10, 25 and 50 μM

N: normal group without tested samples. Values represent the mean ± SD of six determinations. $^{**}P < 0.01$, $^{***}P < 0.001$ (Differences between compound-treated group and normal group). n = 6.

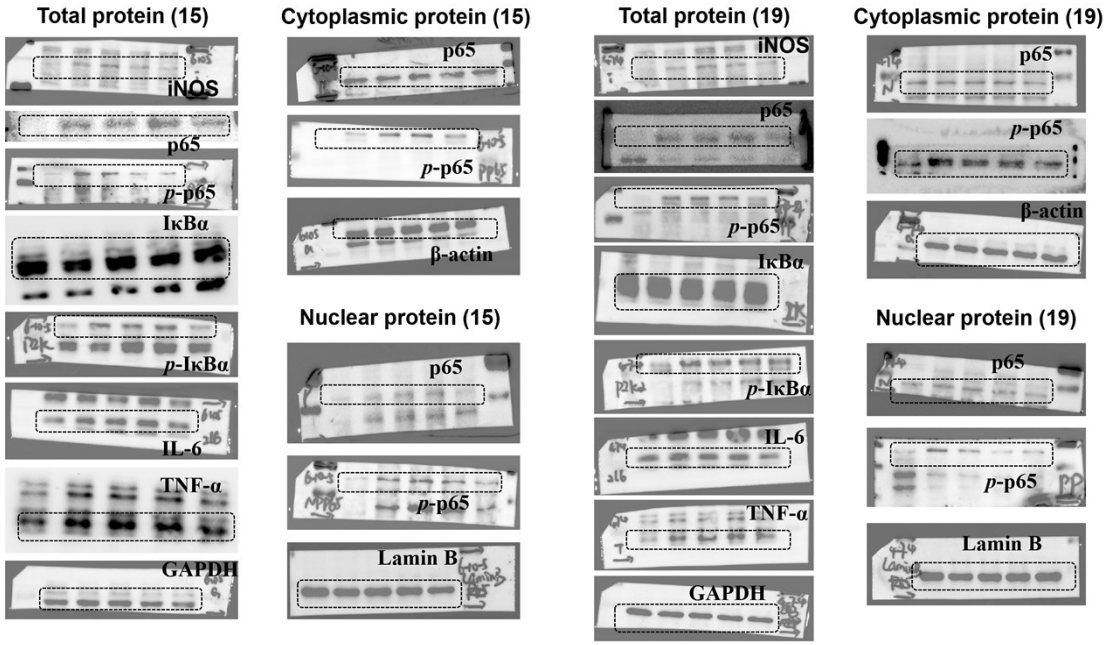


Fig. S99. The raw data of Fig. 3

Tab. S1. ^{13}C-NMR data for **2**–**11**

No.	2[a]	3[b]	4[b]	5[c]	6[b]	7[b]	8[b]	9[b]	10[b]	11[b]
1	39.6	39.5	48.2	38.2	45.0	48.9	34.2	67.0	66.3	39.1
2	34.2	28.3	68.8	27.1	73.8	66.5	29.8	178.1	175.9	34.4
3	218.1	78.1	83.7	76.7	79.9	84.9	177.3	84.7	84.6	216.0
4	47.4	39.4	39.9	38.4	40.5	39.7	25.7	43.5	43.4	47.4
5	55.0	55.9	56.0	54.8	55.8	55.6	47.4	57.0	57.2	55.4
6	19.7	18.8	18.8	17.9	18.8	18.6	18.6	19.1	19.0	19.8
7	33.7	34.8	34.8	33.9	32.9	34.6	33.4	34.7	34.5	32.6
8	40.7	41.1	41.2	42.2	41.1	41.1	40.8	43.9	43.8	39.6
9	49.9	51.0	51.0	49.9	50.9	50.8	41.2	45.1	45.0	47.2
10	37.1	37.5	38.7	38.4	38.8	38.6	40.2	49.7	49.7	36.9
11	21.4	21.2	21.3	20.5	21.3	21.3	22.0	24.2	24.0	23.8
12	25.6	26.1	26.0	26.1	26.1	26.0	26.1	26.3	26.1	122.3
13	38.5	38.6	38.6	37.4	38.6	38.5	38.7	39.1	39.0	144.9
14	42.5	42.8	42.9	40.2	42.9	42.9	43.3	42.1	42.1	42.2
15	29.8	30.3	30.2	29.2	30.2	30.2	30.3	30.5	30.5	28.3
16	32.3	32.9	32.9	31.7	32.9	32.8	32.9	33.0	32.9	23.7
17	56.4	56.6	56.6	55.4	56.6	56.6	56.8	56.6	56.7	46.7
18	49.3	49.8	49.8	48.8	49.8	49.7	49.7	49.7	49.7	42.1
19	46.9	47.8	47.8	41.9	47.8	47.8	47.8	47.6	47.7	46.4
20	150.6	151.3	151.3	155.5	151.4	151.3	151.5	151.2	151.2	31.0
21	30.7	31.2	31.2	28.6	31.2	31.2	31.3	31.3	31.3	34.2
22	37.0	37.6	37.6	36.2	37.7	37.6	37.6	37.6	37.6	33.2
23	26.7	28.7	29.2	28.0	29.1	28.9	24.9	31.5	31.5	26.6
24	21.0	16.4	17.4	15.7	16.3	18.0	19.1	20.4	20.2	21.6
25	15.9	16.4	17.7	15.9	17.4	17.6	20.0	18.8	18.6	14.9
26	16.0	16.4	16.5	15.9	17.4	16.4	16.4	17.0	17.0	17.2
27	14.6	14.9	14.9	14.3	14.9	14.9	14.8	15.1	15.0	26.0
28	180.3	179.0	179.1	177.2	179.0	179.0	179.4	178.9	179.0	180.2
29	19.4	19.5	19.5	62.8	19.4	19.4	19.5	19.6	19.5	33.3
30	109.6	110.0	109.9	105.3	110.0	110.0	110.0	109.8	109.9	23.7
2-OCH_3									51.1	
1'					126.2	126.7				
2'					130.6	133.8				
3'					116.9	115.9				
4'					161.4	160.5				
5'					116.9	115.9				
6'					130.6	133.8				
7'					144.7	143.6				
8'					116.0	117.1				
9'					167.5	167.2				

[a] $CDCl_3$; [b] C_5D_5N; [c] DMSO-d_6; [d] CD_3OD

669

670 **Tab. S2.** ^{13}C-NMR data for **12**–**20**

No.	12[b]	13[b]	14[d]	15[c]	16[c]	17[b]	18[b]	19[b]	20[b]
1	39.0	47.7	48.5	43.4	43.4	48.3	34.1	39.3	39.1
2	28.1	68.6	69.2	71.8	71.8	66.4	29.8	34.3	28.1
3	78.1	83.8	84.2	78.2	78.2	85.0	177.3	216.1	78.1
4	39.4	39.8	40.6	40.7	40.9	39.8	25.3	47.1	39.4
5	55.8	55.9	56.2	54.2	54.2	55.5	47.9	55.3	55.8
6	18.8	18.8	18.7	18.0	18.0	18.7	18.5	19.8	18.8
7	33.2	33.2	34.0	32.1	32.1	33.0	32.2	32.9	33.6
8	39.8	39.8	45.1	39.2	38.8	39.8	39.6	39.8	40.0
9	48.2	48.1	63.0	46.7	46.7	48.0	38.4	47.3	48.1
10	37.4	38.5	39.4	37.7	37.7	38.4	40.2	36.8	37.5
11	23.9	23.9	202.7	23.2	23.2	23.9	24.1	23.7	23.7
12	122.6	122.4	128.3	121.2	121.2	122.3	122.7	125.4	125.7
13	144.9	144.8	173.1	143.9	143.9	145.0	144.8	139.3	140.1
14	42.2	42.2	46.5	41.3	41.3	42.2	42.7	42.5	42.5
15	28.4	28.3	28.9	27.1	27.1	28.3	28.4	28.6	28.7
16	23.7	23.7	24.0	22.8	22.8	23.7	23.8	24.9	24.9
17	46.7	46.6	47.3	45.6	45.6	46.7	46.8	48.1	48.1
18	42.1	42.0	43.5	41.3	40.9	42.0	42.1	53.6	53.6
19	46.5	46.5	45.7	45.3	45.3	46.5	46.5	39.5	39.5
20	31.0	30.9	31.7	30.3	30.0	31.0	31.0	39.4	39.4
21	34.3	34.2	34.8	33.2	33.2	34.3	34.3	31.1	31.1
22	33.2	33.2	33.0	32.0	32.1	33.2	33.2	37.4	37.3
23	28.8	29.3	29.3	28.5	28.4	29.0	24.9	26.7	28.8
24	16.6	17.6	17.5	16.9	16.7	18.3	19.1	21.6	16.6
25	15.6	16.8	18.0	16.0	16.0	16.8	19.5	15.1	15.7
26	17.5	17.5	19.9	16.7	16.9	17.4	17.6	17.3	17.5
27	26.2	26.2	24.0	25.5	25.5	26.2	26.0	23.7	23.9
28	180.3	180.2	181.4	178.7	179.7	180.5	180.5	179.8	180.0
29	33.3	33.3	33.3	32.7	32.7	33.3	33.3	17.5	17.6
30	23.8	23.8	23.8	23.3	23.3	23.8	23.8	21.4	21.4
1'				125.1	125.8	126.2			
2'				130.0	132.5	130.6			
3'				115.7	114.7	116.8			
4'				159.6	159.2	161.4			
5'				115.7	114.7	116.8			
6'				130.0	132.5	130.6			
7'				144.0	142.3	144.8			
8'				114.9	116.2	116.0			
9'				166.3	166.3	167.9			

671 [a] $CDCl_3$; [b] C_5D_5N; [c] DMSO-d_6; [d] CD_3OD

673

674 **Tab. S3.** ^{13}C-NMR data for **21**–**29**

No.	21[b]	22[b]	23[b]	24[b]	25[b]	26[b]	27[b]	28[b]	29[b]
1	47.9	48.6	34.3	39.2	39.0	53.7	42.9	45.0	42.4
2	68.6	66.4	29.9	34.4	28.2	211.2	66.1	71.5	174.5
3	83.8	85.1	177.3	216.5	78.2	83.5	79.4	78.5	182.4
4	39.8	39.8	25.4	47.5	39.4	45.8	38.8	38.8	46.9
5	55.9	55.6	47.9	55.5	55.9	54.9	48.8	56.1	48.9
6	18.8	18.7	18.6	19.9	19.0	19.2	18.6	18.8	22.1
7	33.5	33.4	31.2	33.0	33.7	33.2	33.5	33.7	33.0
8	40.0	40.0	39.8	40.2	40.4	42.3	40.6	40.5	40.5
9	48.1	48.0	38.2	46.9	47.8	47.4	47.6	48.2	39.5
10	38.4	38.3	40.1	36.9	37.4	40.7	38.7	37.3	48.4
11	23.9	23.7	24.1	24.0	24.1	23.9	24.1	24.2	24.5
12	125.5	125.4	125.8	127.8	128.0	127.4	127.9	128.2	128.5
13	139.3	139.6	139.3	140.0	140.1	140.2	140.0	140.0	139.7
14	42.5	42.6	43.1	42.2	42.2	43.7	42.2	42.3	42.7
15	28.6	28.7	28.7	29.3	29.4	29.5	29.3	29.3	29.4
16	24.9	24.9	25.0	26.4	26.5	26.4	26.4	26.4	26.6
17	48.0	48.1	48.1	48.3	48.4	48.3	48.3	48.3	48.4
18	53.5	53.6	53.7	54.7	54.7	54.6	54.6	54.7	54.7
19	39.5	39.5	39.6	72.7	72.7	72.7	72.7	72.7	72.7
20	39.4	39.4	39.4	42.4	42.4	42.4	42.4	42.4	42.3
21	31.1	31.1	32.5	26.9	27.0	27.0	27.0	27.0	26.9
22	37.4	37.5	37.5	38.5	38.6	38.5	38.6	38.6	38.5
23	29.4	29.0	24.9	26.6	28.8	29.3	29.5	30.3	27.6
24	17.7	18.3	19.7	21.6	16.6	16.8	22.3	18.2	25.0
25	17.0	16.8	19.7	15.0	15.6	16.4	16.7	16.7	19.6
26	17.5	17.4	17.7	17.0	17.3	17.3	17.3	17.3	17.3
27	23.7	24.0	23.8	24.5	24.7	24.6	24.6	24.8	24.3
28	179.9	180.3	180.2	180.8	180.9	180.7	181.1	180.8	180.9
29	17.5	17.5	17.7	27.1	27.2	27.1	27.1	27.1	27.2
30	21.4	21.4	21.4	16.8	16.8	16.8	16.8	16.8	16.7
1'		126.3							
2'		130.6							
3'		116.8							
4'		161.4							
5'		116.8							
6'		130.6							
7'		144.8							
8'		116.1							
9'		167.9							

675 [a] $CDCl_3$; [b] C_5D_5N; [c] DMSO-d_6; [d] CD_3OD

677

678 **Tab. S4.** Comparison ^{1}H and ^{13}C NMR chemical shifts of maslinic acid, augustic acid,
679 bredemolic acid and 3-*epi*-maslinic acid

	Maslinic acid (2*α*3*β*)	**3-*epi*-Maslinic acid (2*α*3*α*)**	**Bredemolic acid (2*β*3*α*)**	**Augustic acid (2*β*3*β*)**
$\delta_{H\text{-}2}$	4.11	4.21	4.36	4.41
$\delta_{H\text{-}3}$	3.41	3.77	4.00	3.44
$\Delta\delta_{H2\text{-}H3}$	0.7	0.56	0.36	0.97
$J_{H2,3}$	9.4	2.6	7.5	4.0
$\delta_{C\text{-}2}$	69.0	66.5	71.1	71.8
$\delta_{C\text{-}3}$	84.3	79.7	78.7	78.7
$\Delta\delta_{C3\text{-}C2}$	15.3	13.2	7.6	6.9

680