Electronic Supplementary Material (ESI) for Chemical Communications.

Supporting Information

Rhodium(II)-catalyzed annulation of *N*-sulfonyl-1,2,3-triazoles with 1,3,5-triazinanes to produce octahydro-1*H*-purine derivatives: a combined experimental and computational study

Jiemin Ge, Xueli Wu, Xiaoguang Bao*

College of Chemistry, Chemical Engineering and Materials Science, Soochow University, Suzhou 215123, China.

E-mail: xgbao@suda.edu.cn

Contents

1. General Information

All reagents were purchased from commercial suppliers and used without further purification. 1,3,5-Triazinanes[1] and *N*-sulfonyl-1,2,3-triazoles[2] could be prepared according to the methods reported in literature. All the reactions were performed under air atmosphere in dry tube. For column chromatography, 200-300 mesh silica gel was used. NMR spectra were recorded on Varian Inova–600 MHz, Inova–400 MHz, Bruker DRX–400 spectrometer in $CDCl_3$. Multiplicities were recorded as: s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, dt = doublet of triplets, m = multiplet. HRMS analyses were carried out using a Bruker micrOTOF–Q instrument or Agilent 1200/6220 instrument. IR spectra were recorded using a Bruker Vertex 70 instrument. X-ray crystal structure analyses were measured on a Bruker D8 Venture instrument. Melting points were determined with an INESA WRR melting point instrument.

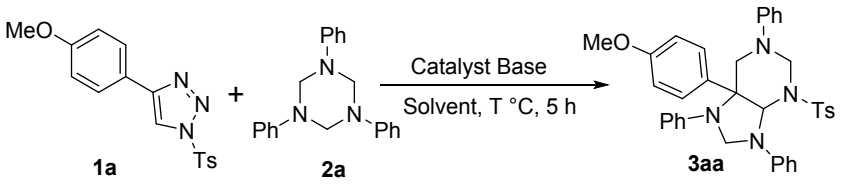
References

1 A. G. Giumanini and G. Verard, *J. Prakt. Chem.*, 1987, **329**, 417.

2 J. Raushel and V. V. Fokin, *Org. Lett.*, 2010, **12**, 4952.

2. Optimization of reaction conditions

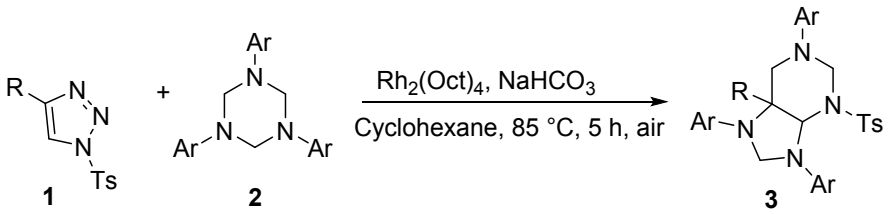
Table S1 Optimization of the reaction conditions[a]



Entry	Catalyst	Base	Solvent	*T* (℃)	**3aa**[b] [%]
1	$Rh_2(OAc)_4$	--	DCM	80	25
2	$Rh_2(TFA)_4$	--	DCM	80	-
3	$Rh_2(Oct)_4$	--	DCM	80	45
4	$Rh_2(Oct)_4$	Na_2CO_3	DCM	80	40
5	$Rh_2(Oct)_4$	$NaHCO_3$	DCM	80	71
6	$Rh_2(Oct)_4$	$KHCO_3$	DCM	80	44
7	$Rh_2(Oct)_4$	$NaHCO_3$	Neat	80	43
8	$Rh_2(Oct)_4$	$NaHCO_3$	DCE	80	-
9	$Rh_2(Oct)_4$	$NaHCO_3$	Toluene	80	-
10	$Rh_2(Oct)_4$	$NaHCO_3$	Cyclohexane	80	74
11	$Rh_2(Oct)_4$	$NaHCO_3$	Cyclohexane	75	61
12	**$Rh_2(Oct)_4$**	**$NaHCO_3$**	**Cyclohexane**	**85**	**82**
13	$Rh_2(Oct)_4$	$NaHCO_3$	Cyclohexane	90	79
14	$Rh_2(Oct)_4$	$NaHCO_3$	Cyclohexane	95	75
15[c]	$Rh_2(Oct)_4$	$NaHCO_3$	Cyclohexane	85	74
16[d]	$Rh_2(Oct)_4$	$NaHCO_3$	Cyclohexane	85	72
17[e]	$Rh_2(Oct)_4$	$NaHCO_3$	Cyclohexane	85	79

[a] Reaction conditions: **1a** (0.24 mmol), **2a** (0.2 mmol), catalyst (5 mol %), base (2 equiv), solvent (3 mL), under air. [b] Isolated yield. [c] Under an O_2 atmosphere. [d] Under an N_2 atmosphere. [e] Under an argon atmosphere.

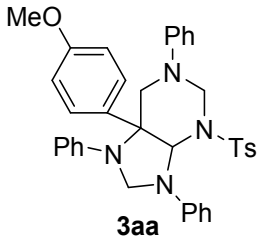
3. General Procedure and Characterization Data



A dry tube equipped with a magnetic stirrer bar was charged with *N*-sulfonyl-1,2,3-triazoles **1** (0.24 mmol, 1.1 equiv), 1,3,5-triazinanes **2** (0.2 mmol, 1 equiv), $Rh_2(OAc)_4$ [a], $NaHCO_3$ (2 equiv, 33.6 mg), and cyclohexane (3 mL). The mixture was stirred under air at 85 ℃ for 5 hours. After cooling to room temperature, the solvent was removed under vacuum. Then crude residue was purified by column chromatography (PE/EA =10:1) to afford the desired product **3.**

[a] $Rh_2(OAc)_4$ (5 mol %, 7.8 mg) for general products except **3ha**, **3ia**, **3la** and **3ma**, which used $Rh_2(OAc)_4$ (9 mol %, 14 mg).

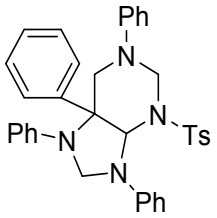
5-(4-methoxyphenyl)-1,7,9-triphenyl-3-tosyloctahydro-1H-purine (3aa):



3aa

White solid, 101mg, 82 %, m.p.: 158-160 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.3 Hz, 2H), 7.33 – 7.27 (m, 4H), 7.19 (d, *J* = 8.2 Hz, 2H), 7.08 – 7.00 (m, 6H), 6.92 (t, *J* = 7.3 Hz, 1H), 6.88 (d, *J* = 8.8 Hz, 2H), 6.72 (t, *J* = 7.3 Hz, 1H), 6.66 (t, *J* = 7.3 Hz, 1H), 6.44 (d, *J* = 8.0 Hz, 2H), 6.26 (d, *J* = 8.1 Hz, 2H), 6.16 (s, 1H), 5.11 (d, *J* = 2.9 Hz, 1H), 5.07 (d, *J* = 2.9 Hz, 1H), 4.85 (d, *J* = 11.3 Hz, 1H), 4.42 (d, *J* = 11.3 Hz, 1H), 4.26 (d, *J* = 13.5 Hz, 1H), 3.83 (s, 3H), 3.77 (d, *J* = 13.5 Hz, 1H), 2.42 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 159.14, 146.70, 143.95, 142.92, 142.70, 136.89, 133.50, 129.73, 129.29, 128.99, 127.73, 127.23, 119.55, 118.46, 117.97, 114.71, 114.49, 114.32, 112.80, 78.82, 69.49, 67.63, 57.35, 55.27, 44.03, 21.56. IR (neat): 3068, 2954, 2838, 1599, 1504, 1397, 1336, 1319, 1249, 1157, 932, 748, 691 cm^{-1}. HRMS (EI) calcd for $C_{37}H_{36}N_4O_3S$ $[M+Na]^+$: 639.2406; found: 639.2404.

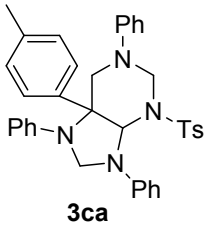
1,5,7,9-tetraphenyl-3-tosyloctahydro-1H-purine (3ba):



3ba

White solid, 83 mg, 70 %, m.p.: 144-146 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.3 Hz, 2H), 7.41 – 7.29 (m, 7H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.09 – 6.99 (m, 6H), 6.93 (t, *J* = 7.3 Hz, 1H), 6.72 (t, *J* = 7.3 Hz, 1H), 6.66 (t, *J* = 7.3 Hz, 1H), 6.43 (d, *J* = 8.0 Hz, 2H), 6.25 (d, *J* = 8.0 Hz, 2H), 6.21 (d, *J* = 0.6 Hz, 1H), 5.15 (d, *J* = 2.9 Hz, 1H), 5.10 (d, *J* = 2.9 Hz, 1H), 4.85 (dd, *J* = 11.3, 1.1 Hz, 1H), 4.44 (d, *J* = 11.3 Hz, 1H), 4.33 (d, *J* = 13.6 Hz, 1H), 3.80 (d, *J* = 13.6 Hz, 1H), 2.43 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 146.62, 143.95, 142.74, 142.50, 141.50, 136.74, 129.69, 129.19, 128.92, 127.98, 127.68, 125.90, 119.51, 118.42, 117.84, 114.60, 114.24, 112.62, 78.61, 69.93, 67.58, 57.27, 43.72, 21.49. IR (neat): 2880, 2838, 1599, 1495, 1396, 1329, 1192, 1159, 1117, 996, 750, 691 cm^{-1}. HRMS (EI) calcd for $C_{36}H_{34}N_4O_2S$ $[M+H]^+$: 587.2481; found: 587.2473.

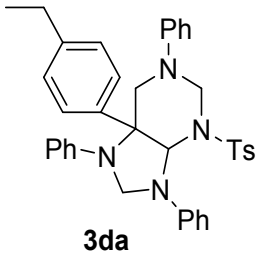
1,7,9-triphenyl-5-(p-tolyl)-3-tosyloctahydro-1H-purine (3ca):



3ca

White solid, 91 mg, 73 %, m.p.: 174-176 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.3 Hz, 2H), 7.31 (t, *J* = 8.0 Hz, 2H), 7.25 (d, *J* = 8.2 Hz, 2H), 7.18 (dd, *J* = 11.8, 8.2 Hz, 4H), 7.07 – 6.99 (m, 6H), 6.91 (t, *J* = 7.3 Hz, 1H), 6.71 (t, *J* = 7.3 Hz, 1H), 6.65 (t, *J* = 7.3 Hz, 1H), 6.44 (d, *J* = 8.1 Hz, 2H), 6.24 (d, *J* = 8.2 Hz, 2H), 6.17 (s, 1H), 5.13 (d, *J* = 2.8 Hz, 1H), 5.08 (d, *J* = 2.8 Hz, 1H), 4.85 (d, *J* = 10.9 Hz, 1H), 4.42 (d, *J* = 11.3 Hz, 1H), 4.29 (d, *J* = 13.6 Hz, 1H), 3.75 (d, *J* = 13.6 Hz, 1H), 2.42 (s, 3H), 2.37 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.76, 144.01, 142.95, 142.67, 138.59, 137.77, 136.91, 129.84, 129.33, 129.01, 127.79, 125.87, 119.54, 118.44, 117.90, 114.69, 114.31, 112.71, 78.84, 69.86, 67.66, 57.33, 43.83, 21.59, 21.14. IR (neat): 3030, 2880, 1600, 1497, 1396, 1326, 1158, 1116, 1098, 944, 749, 689 cm^{-1}. HRMS (EI) calcd for $C_{37}H_{36}N_4O_2S$ $[M+Na]^+$: 623.2457; found: 623.2448.

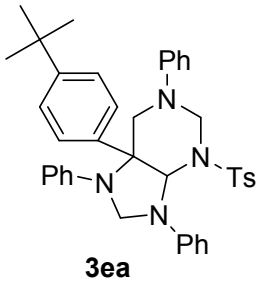
5-(4-ethylphenyl)-1,7,9-triphenyl-3-tosyloctahydro-1H-purine (3da):



3da

White solid, 88 mg, 72 %, m.p.: 192-194 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.3 Hz, 2H), 7.34 – 7.25 (m, 4H), 7.19 (d, *J* = 7.3 Hz, 4H), 7.08 – 6.99 (m, 6H), 6.92 (t, *J* = 7.4 Hz, 1H), 6.71 (t, *J* = 7.3 Hz, 1H), 6.64 (t, *J* = 7.3 Hz, 1H), 6.45 (d, *J* = 8.3 Hz, 2H), 6.24 (d, *J* = 8.3 Hz, 2H), 6.20 (s, 1H), 5.15 (d, *J* = 2.8 Hz, 1H), 5.08 (d, *J* = 2.8 Hz, 1H), 4.84 (d, *J* = 11.4 Hz, 1H), 4.43 (d, *J* = 11.4 Hz, 1H), 4.32 (d, *J* = 13.6 Hz, 1H), 3.74 (d, *J* = 13.6 Hz, 1H), 2.68 (q, *J* = 7.6 Hz, 2H), 2.43 (s, 3H), 1.27 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.75, 143.99, 142.92, 142.59, 138.73, 136.84 (s), 129.74 (s), 129.30 (s), 128.97 (d, *J* = 3.1 Hz), 128.66 (s), 127.79 (s), 125.87 (s), 119.47 (s), 118.40 (s), 117.78 (s), 114.69 (s), 114.22 (s), 112.58 (s), 78.77 (s), 77.28 (d, *J* = 11.5 Hz), 77.02 (s), 76.70 (s), 69.99 (s), 67.59 (s), 57.25 (s), 43.75 (s), 28.41 (s), 21.57 (s), 15.29 (s). IR (neat): 3029, 2970, 2928, 2878, 2814, 1600, 1496, 1395, 1325, 1158, 1117, 1096, 942, 747, 689 cm^{-1}. HRMS (EI) calcd for $C_{38}H_{38}N_4O_2S$ $[M+H]^+$: 615.2794, found: 615.2797.

5-(4-(tert-butyl)phenyl)-1,7,9-triphenyl-3-tosyloctahydro-1H-purine (3ea):

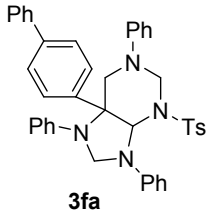


3ea

White solid, 110 mg, 86 %, m.p.: 156-158 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 8.3 Hz, 2H), 7.37 (d, *J* = 8.5 Hz, 2H), 7.34 – 7.24 (m, 4H), 7.19 (d, *J* = 8.2 Hz, 2H), 7.03 (dt, *J* = 16.0, 7.3 Hz, 6H), 6.91 (t, *J* = 7.3 Hz, 1H), 6.70 (t, *J* = 7.3 Hz, 1H), 6.63 (t, *J* = 7.3 Hz, 1H), 6.46 (d, *J* = 8.1 Hz, 2H), 6.22 (d, *J* = 8.0 Hz, 3H), 5.18 (d, *J* = 2.8 Hz, 1H), 5.08 (d, *J* = 2.8 Hz, 1H), 4.83 (d, *J* = 10.7 Hz, 1H), 4.44 (d, *J* = 11.4 Hz, 1H), 4.34 (d, *J* = 13.6 Hz, 1H), 3.72 (d, *J* = 13.6 Hz, 1H), 2.42 (s, 3H), 1.34 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.88, 146.84, 144.04, 142.96, 142.55, 138.37, 136.78, 129.76, 129.32, 128.97, 127.84, 126.11, 125.59, 119.44, 118.42, 117.70, 114.80, 114.17, 112.47, 77.36 , 67.54, 57.18, 43.73, 34.55, 31.33, 21.59. IR (neat): 3035, 2961, 2875,

1599, 1502, 1401, 1324, 1162, 1147, 941, 743, 688 cm^{-1}. HRMS (EI) calcd for $C_{40}H_{42}N_4O_2S$ $[M+Na]^+$: 665.2926; found: 665.2925.

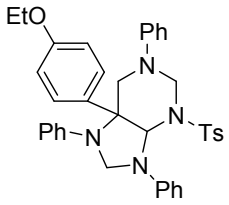
5-([1,1'-biphenyl]-4-yl)-1,7,9-triphenyl-3-tosyloctahydro-1H-purine (3fa):



3fa

White solid, 65 mg, 49 %, m.p.: 174-176 ℃. ^1H NMR (400 MHz, $CDCl_3$) δ 7.65 – 7.57 (m, 6H), 7.49 – 7.43 (m, 4H), 7.39 – 7.30 (m, 3H), 7.19 (d, *J* = 8.1 Hz, 2H), 7.10 – 7.00 (m, 6H), 6.93 (t, *J* = 7.3 Hz, 1H), 6.72 (t, *J* = 7.3 Hz, 1H), 6.66 (t, *J* = 7.3 Hz, 1H), 6.47 (d, *J* = 8.1 Hz, 2H), 6.28 (d, *J* = 8.1 Hz, 2H), 6.24 (s, 1H), 5.14 (dd, *J* = 16.5, 2.9 Hz, 2H), 4.87 (d, *J* = 10.9 Hz, 1H), 4.44 (d, *J* = 11.4 Hz, 1H), 4.34 (d, *J* = 13.6 Hz, 1H), 3.85 (d, *J* = 13.6 Hz, 1H), 2.40 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.70, 144.05, 142.84, 142.62, 140.72, 140.51, 140.29, 136.86, 129.77, 129.33, 129.04, 128.85, 127.79, 127.54, 127.04, 126.46, 119.66, 118.56, 118.02, 114.72, 114.41, 112.79, 69.80, 67.67, 57.39, 43.95, 21.55. IR (neat): 3028, 2865, 1598, 1504, 1398, 1337, 1249, 1147, 1103, 938, 739, 695 cm^{-1}. HRMS (EI) calcd for $C_{42}H_{38}N_4O_2S$ $[M+Na]^+$: 685.2613, found: 685.2638.

5-(4-ethoxyphenyl)-1,7,9-triphenyl-3-tosyloctahydro-1H-purine(3ga):

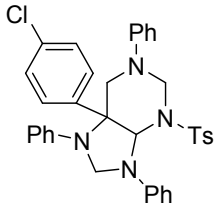


3ga

White solid, 63 mg, 50 %, m.p.: 138-140 ℃. ^1H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.0 Hz, 2H), 7.35 – 7.26 (m, 4H), 7.20 (d, *J* = 8.1 Hz, 2H), 7.09 – 7.00 (m, 6H), 6.95 – 6.85 (m, 3H), 6.72 (t, *J* = 7.4 Hz, 1H), 6.66 (t, *J* = 7.3 Hz, 1H), 6.44 (d, *J* = 8.1 Hz, 2H), 6.26 (d, *J* = 8.1 Hz, 2H), 6.17 (s, 1H), 5.11 (d, *J* = 2.3 Hz, 1H), 5.07 (d, *J* = 2.4 Hz, 1H), 4.85 (d, *J* = 11.3 Hz, 1H), 4.42 (d, *J* = 11.3 Hz, 1H), 4.26 (d, *J* = 13.5 Hz, 1H), 4.06 (q, *J* = 7.0 Hz, 2H), 3.80 – 3.72 (m, 1H), 2.42 (s, 3H), 1.44 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.60, 146.77, 143.96, 142.98, 142.76, 136.99, 133.38, 129.75, 129.31, 129.01, 127.77, 127.24, 119.57, 118.49, 117.98, 115.03, 114.78, 114.38, 112.82, 78.89, 69.55, 67.65, 63.48, 57.38, 44.04, 21.56, 14.86. IR (neat): 3042,

2868, 1599, 1505, 1397, 1338, 1245, 1148, 942, 743, 696, 666 cm^{-1}. HRMS (EI) calcd for $C_{38}H_{38}N_4O_3S$ $[M+Na]^+$: 653.2562, found: 653.2564.

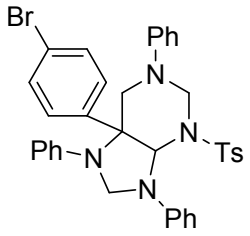
5-(4-chlorophenyl)-1,7,9-triphenyl-3-tosyloctahydro-1H-purine (3ha):



3ha

White solid, 66 mg, 53 %, m.p.: 139-141 ℃. ^1H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.3 Hz, 2H), 7.38 – 7.34 (m, 2H), 7.34 – 7.28 (m, 4H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.10 – 7.02 (m, 6H), 6.94 (t, *J* = 7.4 Hz, 1H), 6.74 (t, *J* = 7.3 Hz, 1H), 6.69 (t, *J* = 7.3 Hz, 1H), 6.39 (d, *J* = 8.0 Hz, 2H), 6.31 (d, *J* = 8.0 Hz, 2H), 6.12 (s, 1H), 5.09 (dd, *J* = 6.5, 3.0 Hz, 2H), 4.87 (d, *J* = 11.4 Hz, 1H), 4.39 (d, *J* = 11.4 Hz, 1H), 4.22 (d, *J* = 13.5 Hz, 1H), 3.90 (d, *J* = 13.5 Hz, 1H), 2.43 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.58, 144.11, 142.65, 140.04, 136.85, 133.97, 129.78, 129.24, 127.62, 119.96, 118.74, 118.50, 114.66, 113.25, 78.49, 69.00, 67.74, 57.65, 44.39, 21.57. IR (neat): 3061, 3029, 2986, 2869, 1598, 1493, 1397, 1329, 1156, 1104, 1093, 937, 741, 689 cm^{-1}. HRMS (EI) calcd for $C_{36}H_{33}ClN_4O_2S$ $[M+Na]^+$: 643.1910; found: 643.1913.

5-(4-bromophenyl)-1,7,9-triphenyl-3-tosyloctahydro-1H-purine (3ia):

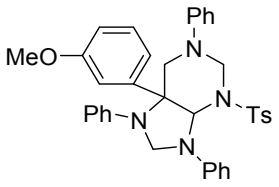


3ia

White solid, 60 mg, 45 %, m.p.: 138-140 ℃. ^1H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.3 Hz, 2H), 7.47 (d, *J* = 8.6 Hz, 2H), 7.32 (dd, *J* = 8.0, 6.5 Hz, 4H), 7.21 (d, *J* = 8.1 Hz, 2H), 7.14 – 7.02 (m, 6H), 6.95 (t, *J* = 7.3 Hz, 1H), 6.75 (t, *J* = 7.3 Hz, 1H), 6.70 (t, *J* = 7.3 Hz, 1H), 6.41 (d, *J* = 8.1 Hz, 2H), 6.33 (d, *J* = 8.1 Hz, 2H), 6.12 (s, 1H), 5.10 (dd, *J* = 7.8, 3.0 Hz, 2H), 4.89 (d, *J* = 11.3 Hz, 1H), 4.41 (d, *J* = 11.4 Hz, 1H), 4.22 (d, *J* = 13.5 Hz, 1H), 3.91 (d, *J* = 13.5 Hz, 1H), 2.44 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.58, 144.09, 142.65, 140.58, 136.87, 132.33, 129.77, 129.32, 129.13, 129.09, 127.96, 127.59, 122.20, 119.98, 118.75, 118.53, 114.68, 113.28, 78.42, 69.00,

67.75, 57.66, 44.41, 21.57. IR (neat): 3029, 2869, 1598, 1504, 1334, 1249, 1156, 1143, 936, 741, 691 cm^{-1}. HRMS (EI) calcd for $C_{36}H_{33}BrN_4O_2S$ $[M+Na]^+$: 687.1405; found: 687.1373.

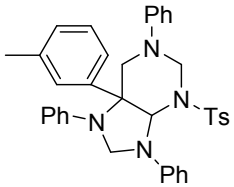
5-(3-methoxyphenyl)-1,7,9-triphenyl-3-tosyloctahydro-1H-purine (3ja):



3ja

White solid, 77 mg, 55 %, m.p.: 150-152 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.3 Hz, 2H), 7.31 (q, *J* = 8.1 Hz, 3H), 7.20 (d, *J* = 8.1 Hz, 2H), 7.09 – 6.96 (m, 7H), 6.91 (ddd, *J* = 10.3, 7.4, 3.3 Hz, 3H), 6.72 (t, *J* = 7.3 Hz, 1H), 6.65 (t, *J* = 7.3 Hz, 1H), 6.45 (d, *J* = 8.0 Hz, 2H), 6.27 – 6.18 (m, 3H), 5.10 (dd, *J* = 12.7, 2.9 Hz, 2H), 4.88 – 4.81 (m, 1H), 4.42 (d, *J* = 11.3 Hz, 1H), 4.29 (d, *J* = 13.6 Hz, 1H), 3.79 – 3.70 (m, 4H), 2.43 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.17, 146.60, 144.03, 143.26, 142.85, 142.62, 136.77, 130.28, 129.79, 129.30, 129.00, 127.73, 119.59, 118.50, 118.24, 117.94, 114.66, 114.35, 112.97, 112.72, 112.22, 78.68, 69.86, 67.67, 57.33, 55.23, 43.87, 21.56. IR (neat): 3028, 2874, 1599, 1501, 1397, 1336, 1164, 1104, 1034, 973, 746, 690 cm^{-1}. HRMS (EI) calcd for $C_{37}H_{36}N_4O_3S$ $[M+H]^+$: 617.2586, found: 617.2560.

1,7,9-triphenyl-5-(m-tolyl)-3-tosyloctahydro-1H-purine (3ka):

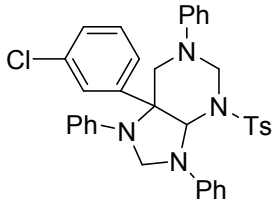


3ka

White solid, 90 mg, 75 %, m.p.: 155-157 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.3 Hz, 2H), 7.32 (dd, *J* = 8.5, 7.5 Hz, 2H), 7.28 – 7.19 (m, 3H), 7.18 – 7.12 (m, 3H), 7.08 – 6.98 (m, 6H), 6.92 (t, *J* = 7.3 Hz, 1H), 6.71 (t, *J* = 7.3 Hz, 1H), 6.64 (t, *J* = 7.3 Hz, 1H), 6.43 (d, *J* = 8.0 Hz, 2H), 6.21 (d, *J* = 10.1 Hz, 3H), 5.13 (d, *J* = 2.8 Hz, 1H), 5.09 (d, *J* = 2.8 Hz, 1H), 4.84 (dd, *J* = 11.3, 1.0 Hz, 1H), 4.41 (d, *J* = 11.3 Hz, 1H), 4.32 (d, *J* = 13.6 Hz, 1H), 3.70 (d, *J* = 13.7 Hz, 1H), 2.43 (s, 3H), 2.36 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 146.61, 143.98, 142.90, 142.50, 141.73, 138.86, 136.91, 129.75, 129.29, 128.95, 127.79, 126.46, 123.02, 119.48, 118.34, 117.76, 114.55, 114.24, 112.54, 78.83, 70.17, 67.60, 57.28, 43.52, 21.79, 21.57. IR (neat): 3028, 2875, 1600, 1501, 1398,

1342, 1158, 1112, 1096, 974, 749, 692 cm^{-1}. HRMS (EI) calcd for $C_{37}H_{36}N_4O_2S$ $[M+Na]^+$: 623.2457; found: 623.2448.

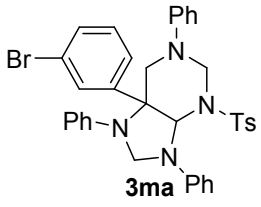
5-(3-chlorophenyl)-1,7,9-triphenyl-3-tosyloctahydro-1H-purine (3la):



3la

White solid, 83 mg, 67 %, m.p.: 163-165 ℃. ^1H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.3 Hz, 2H), 7.48 (dd, *J* = 10.6, 4.8 Hz, 2H), 7.39 – 7.30 (m, 3H), 7.29 – 7.23 (m, 3H), 7.09 – 6.99 (m, 6H), 6.94 (s, 1H), 6.74 (s, 1H), 6.66 (s, 1H), 6.39 (d, *J* = 8.1 Hz, 2H), 6.23 (d, *J* = 8.1 Hz, 2H), 6.14 (s, 1H), 5.10 (dd, *J* = 5.6, 2.9 Hz, 2H), 4.87 (d, *J* = 11.3 Hz, 1H), 4.40 (d, *J* = 11.3 Hz, 1H), 4.27 (d, *J* = 13.6 Hz, 1H), 3.63 (d, *J* = 13.6 Hz, 1H), 2.45 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.40, 144.29, 142.44, 136.84, 131.31, 131.00, 129.98, 129.11, 127.67, 124.99, 123.40, 119.86, 118.74, 118.18, 114.51, 112.83, 78.66, 69.64, 67.67, 57.45, 43.53, 21.63. IR (neat): 3046, 2873, 1598, 1501, 1349, 1164, 1110, 1096, 971, 800, 749, 695 cm^{-1}. HRMS (EI) calcd for $C_{36}H_{33}ClN_4O_2S$ $[M+Na]^+$: 643.1910; found: 643.1908.

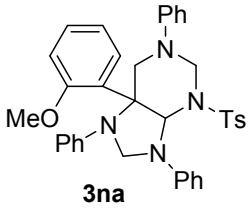
5-(3-bromophenyl)-1,7,9-triphenyl-3-tosyloctahydro-1H-purine (3ma):



3ma

White solid, 86 mg, 65 %, m.p.: 173-175 ℃. ^1H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.3 Hz, 2H), 7.48 (dd, *J* = 11.2, 4.8 Hz, 2H), 7.38 – 7.30 (m, 3H), 7.27 – 7.24 (m, 3H), 7.04 (ddd, *J* = 21.6, 10.1, 8.0 Hz, 6H), 6.94 (t, *J* = 7.3 Hz, 1H), 6.73 (t, *J* = 7.3 Hz, 1H), 6.66 (t, *J* = 7.3 Hz, 1H), 6.38 (d, *J* = 8.1 Hz, 2H), 6.22 (d, *J* = 8.1 Hz, 2H), 6.13 (s, 1H), 5.10 (dd, *J* = 5.5, 2.9 Hz, 2H), 4.87 (d, *J* = 11.3 Hz, 1H), 4.39 (d, *J* = 11.3 Hz, 1H), 4.27 (d, *J* = 13.6 Hz, 1H), 3.63 (d, *J* = 13.6 Hz, 1H), 2.45 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.43, 144.32, 142.47, 136.86, 131.34, 131.03, 130.01, 129.14, 127.70, 125.01, 123.42, 119.89, 118.77, 118.22, 114.54, 112.86, 78.69, 69.67, 67.70, 57.48, 43.56, 21.66. IR (neat): 3061, 2875, 1598, 1500, 1397, 1348, 1163, 1110, 1096, 969, 748, 695 cm^{-1}. HRMS (EI) calcd for $C_{36}H_{33}BrN_4O_2S$ $[M+H]^+$: 665.1586; found: 665.1578.

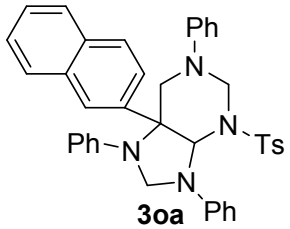
5-(2-methoxyphenyl)-1,7,9-triphenyl-3-tosyloctahydro-1H-purine (3na):



3na

White solid, 58 mg, 47 %, m.p.: 124-126 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 8.3 Hz, 2H), 7.33 (t, *J* = 7.9 Hz, 3H), 7.18 (d, *J* = 8.1 Hz, 3H), 7.11 (d, *J* = 8.1 Hz, 2H), 7.07 – 7.01 (m, 2H), 6.95 (ddd, *J* = 22.3, 15.2, 7.5 Hz, 5H), 6.66 – 6.57 (m, 2H), 6.57 – 6.51 (m, 3H), 6.26 (d, *J* = 8.2 Hz, 2H), 5.17 (d, *J* = 2.4 Hz, 1H), 4.87 (d, *J* = 2.5 Hz, 1H), 4.71 (d, *J* = 10.8 Hz, 1H), 4.54 (d, *J* = 10.9 Hz, 1H), 4.43 (d, *J* = 13.6 Hz, 1H), 4.01 (d, *J* = 13.7 Hz, 1H), 3.71 (s, 3H), 2.42 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.08, 146.90, 143.72, 143.13, 137.03, 129.72, 129.25, 128.93, 128.84, 128.68, 128.25, 127.84, 120.28, 119.12, 117.45, 117.24, 113.93, 113.40, 112.33, 111.99, 77.44, 69.88, 67.77, 57.07, 55.60, 44.03, 21.53. IR (neat): 3029, 2953, 2918, 2838, 1598, 1501, 1401, 1331, 1251, 1169, 1104, 966, 743, 693 cm^{-1}. HRMS (EI) calcd for $C_{37}H_{36}N_4O_3S$ $[M+Na]^+$: 639.2406, found: 639.2438.

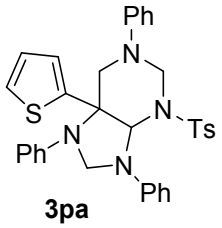
5-(naphthalen-2-yl)-1,7,9-triphenyl-3-tosyloctahydro-1H-purine (3oa):



3oa

White solid, 59 mg, 46 %, m.p.: 190-192 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 – 7.83 (m, 2H), 7.79 – 7.74 (m, 1H), 7.72 (s, 1H), 7.54 (ddd, *J* = 12.3, 7.8, 5.7 Hz, 5H), 7.33 (dd, *J* = 8.5, 7.5 Hz, 2H), 7.10 (t, *J* = 7.5 Hz, 4H), 7.03 (ddd, *J* = 14.3, 8.6, 7.5 Hz, 4H), 6.94 (t, *J* = 7.3 Hz, 1H), 6.69 (t, *J* = 7.0 Hz, 2H), 6.44 (d, *J* = 8.1 Hz, 2H), 6.33 – 6.25 (m, 3H), 5.16 (dd, *J* = 10.3, 2.9 Hz, 2H), 4.93 (d, *J* = 10.7 Hz, 1H), 4.46 (d, *J* = 11.3 Hz, 1H), 4.37 (d, *J* = 13.5 Hz, 1H), 3.91 (d, *J* = 13.6 Hz, 1H), 2.41 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.59, 143.91, 142.99, 142.64, 139.57, 137.07, 133.24, 132.90, 129.64, 129.34, 129.08, 128.38, 127.70, 126.45, 124.96, 124.06, 119.75, 118.46, 118.22, 114.56, 114.33, 113.05, 78.83, 69.73, 67.87, 57.61, 44.09, 21.59. IR (neat): 3037, 2949, 2861, 2734, 1598, 1503, 1396, 1342, 1160, 1111, 1088, 946, 741, 688 cm^{-1}. HRMS (EI) calcd for $C_{40}H_{36}N_4O_2S$ $[M+Na]^+$: 659.2457, found: 659.2456.

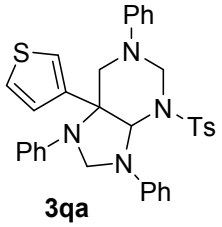
1,7,9-triphenyl-5-(thiophen-3-yl)-3-tosyloctahydro-1H-purine (3pa):



3pa

White solid, 77 mg, 65 %, m.p.: 118-120 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.3 Hz, 2H), 7.34 – 7.28 (m, 3H), 7.19 (d, *J* = 8.1 Hz, 2H), 7.11 – 7.03 (m, 7H), 6.99 (dd, *J* = 5.1, 1.3 Hz, 1H), 6.92 (dd, *J* = 9.8, 4.9 Hz, 1H), 6.76 (t, *J* = 7.3 Hz, 1H), 6.67 (t, *J* = 7.3 Hz, 1H), 6.48 (d, *J* = 8.0 Hz, 2H), 6.27 (d, *J* = 8.0 Hz, 2H), 6.17 (s, 1H), 5.04 (d, *J* = 2.9 Hz, 1H), 4.98 (d, *J* = 3.0 Hz, 1H), 4.89 – 4.84 (m, 1H), 4.51 (d, *J* = 11.4 Hz, 1H), 4.23 (d, *J* = 13.4 Hz, 1H), 3.56 (d, *J* = 13.5 Hz, 1H), 2.40 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.79, 144.05, 142.92, 142.61, 136.83, 129.76, 129.35, 129.07, 127.75, 127.03, 126.04, 121.58, 119.60, 119.32, 118.09, 115.65, 114.23, 112.76, 77.77, 67.99, 67.41, 57.15, 44.91, 21.56. IR (neat): 3064, 2867, 1597, 1502, 1397, 1335, 1248, 1211, 1190, 1104, 942, 743, 665 cm^{-1}. HRMS (EI) calcd for $C_{34}H_{32}N_4O_2S_2$ $[M+Na]^+$: 615.1864, found: 615.1832.

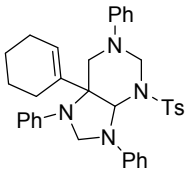
1,7,9-triphenyl-5-(thiophen-3-yl)-3-tosyloctahydro-1H-purine(3qa):



3qa

White solid, 69 mg, 58 %, m.p.: 124-126 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 8.3 Hz, 2H), 7.37 – 7.31 (m, 3H), 7.21 (d, *J* = 8.0 Hz, 2H), 7.13 – 7.05 (m, 7H), 7.01 (dd, *J* = 5.1, 1.4 Hz, 1H), 6.94 (t, *J* = 7.3 Hz, 1H), 6.79 (t, *J* = 7.3 Hz, 1H), 6.70 (t, *J* = 7.3 Hz, 1H), 6.53 – 6.48 (m, 2H), 6.30 (d, *J* = 7.9 Hz, 2H), 6.20 (d, *J* = 0.8 Hz, 1H), 5.07 (d, *J* = 3.0 Hz, 1H), 5.01 (d, *J* = 3.0 Hz, 1H), 4.90 (dd, *J* = 11.4, 1.2 Hz, 1H), 4.54 (d, *J* = 11.4 Hz, 1H), 4.26 (d, *J* = 13.5 Hz, 1H), 3.59 (d, *J* = 13.5 Hz, 1H), 2.43 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.85, 144.06, 142.97, 142.65, 136.90, 129.78, 129.37, 129.10, 127.77, 127.04, 126.07, 121.62, 119.65, 119.37, 118.14, 115.73, 114.30, 112.81, 77.82, 68.02, 67.46, 57.19, 44.99, 21.57. IR (neat): 2869, 1599, 1504, 1398, 1336, 1250, 1211, 1160, 1146, 943, 791, 744, 666 cm^{-1}. HRMS (EI) calcd for $C_{34}H_{32}N_4O_2S_2$ $[M+H]^+$: 593.2045, found: 593.2008.

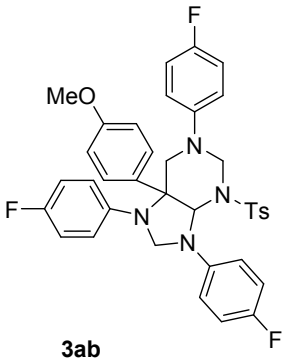
5-(cyclohex-1-en-1-yl)-1,7,9-triphenyl-3-tosyloctahydro-1H-purine (3ra):



3ra

White solid, 59 mg, 50 %, m.p.: 187-189 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.2 Hz, 2H), 7.33 (t, *J* = 8.0 Hz, 2H), 7.24 (d, *J* = 8.1 Hz, 2H), 7.17 (dd, *J* = 8.3, 7.6 Hz, 2H), 7.05 (d, *J* = 8.0 Hz, 2H), 6.96 (dd, *J* = 8.5, 7.5 Hz, 2H), 6.92 (t, *J* = 7.3 Hz, 1H), 6.76 (t, *J* = 7.3 Hz, 1H), 6.72 (d, *J* = 8.1 Hz, 2H), 6.59 (t, *J* = 7.3 Hz, 1H), 6.13 (d, *J* = 8.2 Hz, 2H), 6.08 (s, 1H), 5.63 (s, 1H), 4.89 (d, *J* = 2.6 Hz, 1H), 4.84 (d, *J* = 2.6 Hz, 1H), 4.72 (d, *J* = 10.6 Hz, 1H), 4.31 (d, *J* = 10.7 Hz, 1H), 4.09 (d, *J* = 13.7 Hz, 1H), 3.35 (d, *J* = 13.8 Hz, 1H), 2.42 (s, 3H), 2.18 (d, *J* = 3.8 Hz, 2H), 1.97 (d, *J* = 4.6 Hz, 2H), 1.67 – 1.63 (m, 2H), 1.60 – 1.54 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 146.46, 144.06, 143.76, 142.44, 139.16, 137.19, 129.67, 129.31, 128.95, 127.87, 124.78, 119.27, 117.82, 117.49, 113.78, 112.91, 112.42, 76.30, 70.89, 67.49, 57.21, 42.87, 25.49, 24.07, 22.82, 22.00, 21.58. IR (neat): 3060, 2948, 2921, 2859, 1600, 1503, 1403, 1343, 1158, 1105, 1094, 974, 744, 690 cm^{-1}. HRMS (EI) calcd for $C_{36}H_{38}N_4O_2S$ $[M+H]^+$: 591.2794, found: 591.2788.

1,7,9-tris(4-fluorophenyl)-5-(4-methoxyphenyl)-3-tosyloctahydro-1H-purine (3ab):

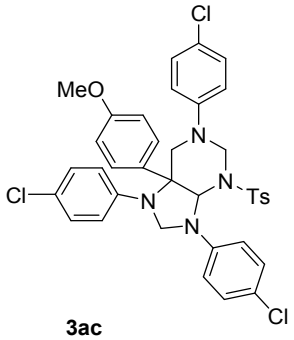


3ab

White solid, 99 mg, 74 %, m.p.: 157-159 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 8.3 Hz, 2H), 7.18 (dd, *J* = 15.4, 8.4 Hz, 4H), 7.03 – 7.01 (m, 3H), 6.87 – 6.72 (m, 7H), 6.37 – 6.28 (m, 4H), 6.05 (s, 1H), 5.03 (d, *J* = 2.8 Hz, 1H), 4.90 (d, *J* = 2.8 Hz, 1H), 4.82 (d, *J* = 11.6 Hz, 1H), 4.47 (d, *J* = 11.6 Hz, 1H), 3.91 (d, *J* = 13.2 Hz, 1H), 3.83 (s, 3H), 3.61 (d, *J* = 13.2 Hz, 1H), 2.42 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.33, 144.03, 143.56, 139.35, 139.08, 136.89, 132.60, 129.72, 127.57, 127.29, 116.82, 116.35, 115.84, 114.82, 78.77, 68.69, 68.26, 57.98, 55.28, 45.69,

21.54. IR (neat): 3029, 2953, 2918, 2838, 1598, 1501, 1401, 1331, 1251, 1169, 1104, 966, 743, 693 cm^{-1}. HRMS (EI) calcd for $C_{37}H_{33}F_3N_4O_3S$ $[M+Na]^+$: 693.2123 , found: 693.2097.

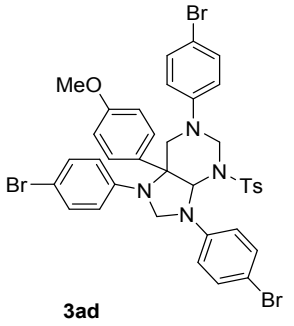
1,7,9-tris(4-chlorophenyl)-5-(4-methoxyphenyl)-3-tosyloctahydro-1H-purine (3ac):



3ac

White solid, 124 mg, 86 %, m.p.: 165-167 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 8.3 Hz, 2H), 7.26 – 7.16 (m, 6H), 7.00 (dt, *J* = 10.2, 4.0 Hz, 4H), 6.97 – 6.86 (m, 4H), 6.33 (d, *J* = 9.0 Hz, 2H), 6.18 (d, *J* = 9.0 Hz, 2H), 6.08 (s, 1H), 5.02 (d, *J* = 2.9 Hz, 1H), 4.95 (d, *J* = 2.9 Hz, 1H), 4.81 (d, *J* = 11.5 Hz, 1H), 4.37 (d, *J* = 11.5 Hz, 1H), 4.12 (d, *J* = 13.6 Hz, 1H), 3.83 (s, 3H), 3.65 (d, *J* = 13.6 Hz, 1H), 2.44 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.42, 145.17, 144.42, 141.17, 140.97, 136.51, 132.50, 129.88, 129.24, 128.99, 127.64, 126.99, 124.98, 124.10, 123.08, 116.02, 115.47, 114.68, 113.71, 78.66, 69.63, 67.55, 57.23, 55.31, 43.89, 21.59. IR (neat): 2876, 1595, 1493, 1328, 1246, 1160, 1095, 1029, 952, 816, 680 cm^{-1}. HRMS (EI) calcd for $C_{37}H_{33}Cl_3N_4O_3S$ $[M+Na]^+$: 741.1237, found: 741.1212.

1,7,9-tris(4-bromophenyl)-5-(4-methoxyphenyl)-3-tosyloctahydro-1H-purine (3ad):

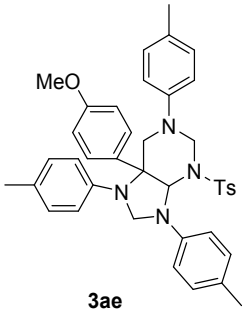


3ad

White solid, 102 mg, 60 %, m.p.: 195-197 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 8.3 Hz, 2H), 7.37 (d, *J* = 8.9 Hz, 2H), 7.17 (ddd, *J* = 16.0, 12.6, 7.6 Hz, 8H), 6.88 (dd, *J* = 8.8, 6.6 Hz, 4H), 6.28 (d, *J* = 9.0 Hz, 2H), 6.12 (d, *J* = 9.0 Hz, 2H), 6.07 (s, 1H), 5.01 (d, *J* = 2.9 Hz, 1H), 4.95 (d, *J* = 2.9 Hz, 1H), 4.80 (d, *J* = 11.5 Hz, 1H), 4.35 (d, *J* = 11.5 Hz, 1H), 4.13 (d, *J* = 13.6 Hz, 1H), 3.83 (s, 3H), 3.65 (d, *J* = 13.7 Hz, 1H), 2.44 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.43, 145.55,

144.46, 141.57, 141.33, 136.45, 132.43, 132.12, 131.86, 129.89, 127.63, 126.94, 116.37, 115.86, 114.70, 114.11, 112.26, 111.34, 110.23, 78.62, 69.68, 67.41, 57.12, 55.31, 43.66, 21.60. IR (neat): 2972, 2929, 2840, 1591, 1416, 1360, 1275, 1180, 1163, 982, 798, 664 cm^{-1}. HRMS (EI) calcd for $C_{37}H_{33}Br_3N_4O_3S$ $[M+Na]^+$: 872.9721, found: 872.9743.

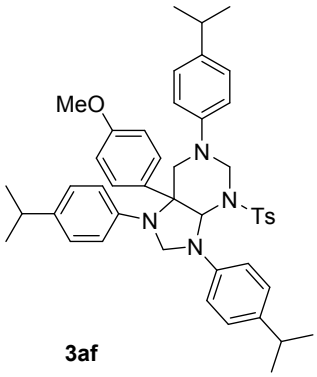
5-(4-methoxyphenyl)-1,7,9-tri-p-tolyl-3-tosyloctahydro-1H-purine (3ae):



3ae

White solid, 82 mg, 62 %, m.p.: 132-134 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.2 Hz, 2H), 7.27 (d, *J* = 8.4 Hz, 2H), 7.19 – 7.10 (m, 4H), 7.01 (d, *J* = 8.4 Hz, 2H), 6.93 – 6.81 (m, 6H), 6.32 (dd, *J* = 14.1, 8.5 Hz, 4H), 6.08 (s, 1H), 5.07 (d, *J* = 2.7 Hz, 1H), 4.99 (d, *J* = 2.8 Hz, 1H), 4.86 (d, *J* = 11.3 Hz, 1H), 4.44 (d, *J* = 11.5 Hz, 1H), 4.00 (d, *J* = 13.2 Hz, 1H), 3.83 (s, 3H), 3.71 (d, *J* = 13.2 Hz, 1H), 2.42 (s, 3H), 2.31 (s, 3H), 2.21 (s, 3H), 2.18 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.01, 145.00, 143.59, 140.94, 140.72, 137.22, 133.50, 129.77, 129.61, 129.57, 129.51, 129.06, 127.83, 127.72, 127.64, 127.52, 114.98, 114.33, 113.82, 78.90, 68.26, 68.10, 58.00, 55.23, 45.54, 21.54, 20.49, 20.28. IR (neat): 3037, 2920, 1616, 1511, 1340, 1246, 1162, 1145, 958, 797, 664 cm^{-1}. HRMS (EI) calcd for $C_{40}H_{42}N_4O_3S$ $[M+Na]^+$: 681.2875, found: 681.2874.

1,7,9-tris(4-isopropylphenyl)-5-(4-methoxyphenyl)-3-tosyloctahydro-1H-purine (3af):

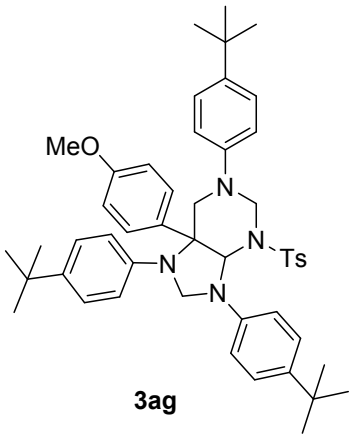


3af

White solid, 82 mg, 55 %, m.p.: 180-182 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 8.3 Hz, 2H), 7.34 – 7.31 (m, 2H), 7.18 (dd, *J* = 10.3, 8.4 Hz, 4H), 7.04 – 7.02 (m, 2H), 6.93 – 6.89 (m, 4H), 6.86 (d, *J* = 8.9 Hz, 2H), 6.37 (d, *J* = 8.7 Hz, 2H), 6.26 (d, *J* = 8.7 Hz, 2H), 6.11 (s, 1H), 5.09

(d, *J* = 2.9 Hz, 1H), 5.04 (d, *J* = 2.9 Hz, 1H), 4.85 (d, *J* = 11.1 Hz, 1H), 4.40 (d, *J* = 11.4 Hz, 1H), 4.09 (d, *J* = 13.3 Hz, 1H), 3.84 (s, 3H), 3.75 (d, *J* = 13.3 Hz, 1H), 2.89 (dt, *J* = 13.8, 6.9 Hz, 1H), 2.76 (dtd, *J* = 13.8, 6.9, 2.6 Hz, 2H), 2.42 (s, 3H), 1.27 (d, *J* = 6.9 Hz, 6H), 1.20 – 1.15 (m, 12H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.01, 144.98, 143.59, 141.08, 140.08, 138.75, 137.25, 133.93, 129.60, 127.59, 127.12, 126.79, 114.75, 114.35, 113.53, 79.02, 68.69, 68.03, 57.91, 55.23, 45.16, 33.25, 33.01, 32.98, 24.19, 24.09, 24.07, 21.55. IR (neat): 2956, 2867, 1612, 1513, 1335, 1249, 1160, 1101, 960, 811, 663 cm^{-1}. HRMS (EI) calcd for $C_{46}H_{54}N_4O_3S$ $[M+Na]^+$: 765.3814, found: 765.3816.

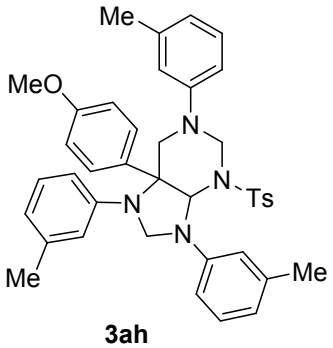
1,7,9-tris(4-(tert-butyl)phenyl)-5-(4-methoxyphenyl)-3-tosyloctahydro-1H-purine(3ag):



3ag

White solid, 94 mg, 60 %, m.p.: 176-178 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 8.2 Hz, 2H), 7.39 (dd, *J* = 8.6, 3.1 Hz, 4H), 7.21 (d, *J* = 8.1 Hz, 2H), 7.14 – 7.07 (m, 6H), 6.91 (d, *J* = 8.7 Hz, 2H), 6.43 (d, *J* = 8.6 Hz, 2H), 6.28 (d, *J* = 8.6 Hz, 2H), 6.18 (s, 1H), 5.12 (dd, *J* = 12.5, 2.3 Hz, 2H), 4.92 (d, *J* = 11.3 Hz, 1H), 4.45 (d, *J* = 11.3 Hz, 1H), 4.18 (d, *J* = 13.4 Hz, 1H), 3.88 (s, 3H), 3.83 (d, *J* = 5.6 Hz, 1H), 2.46 (s, 3H), 1.38 (s, 9H), 1.29 (s, 18H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.06, 144.49, 143.59, 142.28, 140.94, 140.64, 137.33, 134.09, 129.61, 127.60, 126.04, 125.68, 114.40, 113.06, 79.08, 68.87, 67.97, 57.83, 55.22, 44.88, 33.99, 33.76, 31.71, 31.30, 21.54. IR (neat): 2960, 2903, 2867, 1613, 1517, 1363, 1339, 1250, 1162, 961, 826, 662 cm^{-1}. HRMS (EI) calcd for $C_{49}H_{60}N_4O_3S$ $[M+Na]^+$: 807.4284, found: 807.4261.

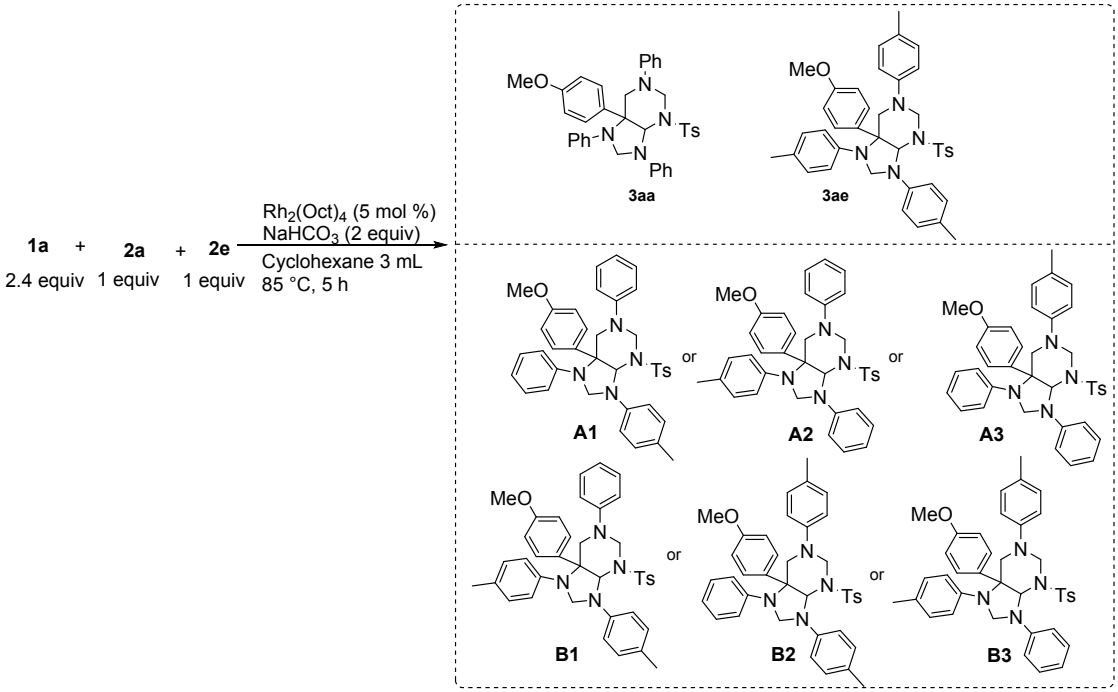
5-(4-methoxyphenyl)-1,7,9-tri-m-tolyl-3-tosyloctahydro-1H-purine(3ah):



3ah

White solid, 90 mg, 68 %, m.p.: 170-172 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.3 Hz, 2H), 7.32 (d, *J* = 8.8 Hz, 2H), 7.24 – 7.18 (m, 3H), 6.95 (td, *J* = 7.8, 4.0 Hz, 2H), 6.91 (t, *J* = 5.9 Hz, 2H), 6.89 – 6.85 (m, 2H), 6.75 (d, *J* = 7.5 Hz, 1H), 6.57 (d, *J* = 7.4 Hz, 1H), 6.49 (d, *J* = 7.4 Hz, 1H), 6.30 (s, 1H), 6.24 (dd, *J* = 8.3, 1.9 Hz, 1H), 6.18 (s, 1H), 6.09 (dd, *J* = 8.2, 2.1 Hz, 1H), 5.99 (s, 1H), 5.06 (dd, *J* = 6.6, 2.8 Hz, 2H), 4.84 (d, *J* = 11.0 Hz, 1H), 4.39 (d, *J* = 11.0 Hz, 1H), 4.30 (d, *J* = 13.6 Hz, 1H), 3.85 (s, 3H), 3.78 (d, *J* = 13.3 Hz, 1H), 2.44 (s, 3H), 2.36 (s, 3H), 2.18 (s, 3H), 2.08 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 159.09, 146.58, 143.86, 143.09, 142.74, 139.09, 138.80, 138.70, 137.08, 133.84, 129.72, 129.13, 128.71, 127.72, 127.28, 120.30, 119.26, 118.85, 115.31, 114.95, 114.44, 114.03, 111.91, 111.39, 109.75, 79.00, 69.79, 67.67, 57.38, 55.27, 44.08, 21.77, 21.69, 21.58, 21.55. IR (neat): 2914, 1602, 1494, 1405, 1342, 1249, 1181, 1031, 947, 819, 759, 667 cm^{-1}. HRMS (EI) calcd for $C_{40}H_{42}N_4O_3S$ $[M+Na]^+$: 681.2875, found: 681.2872.

4. Control Experiments



Inseparable mixed products were detected by HRMS

Scheme S1 Control experiment.

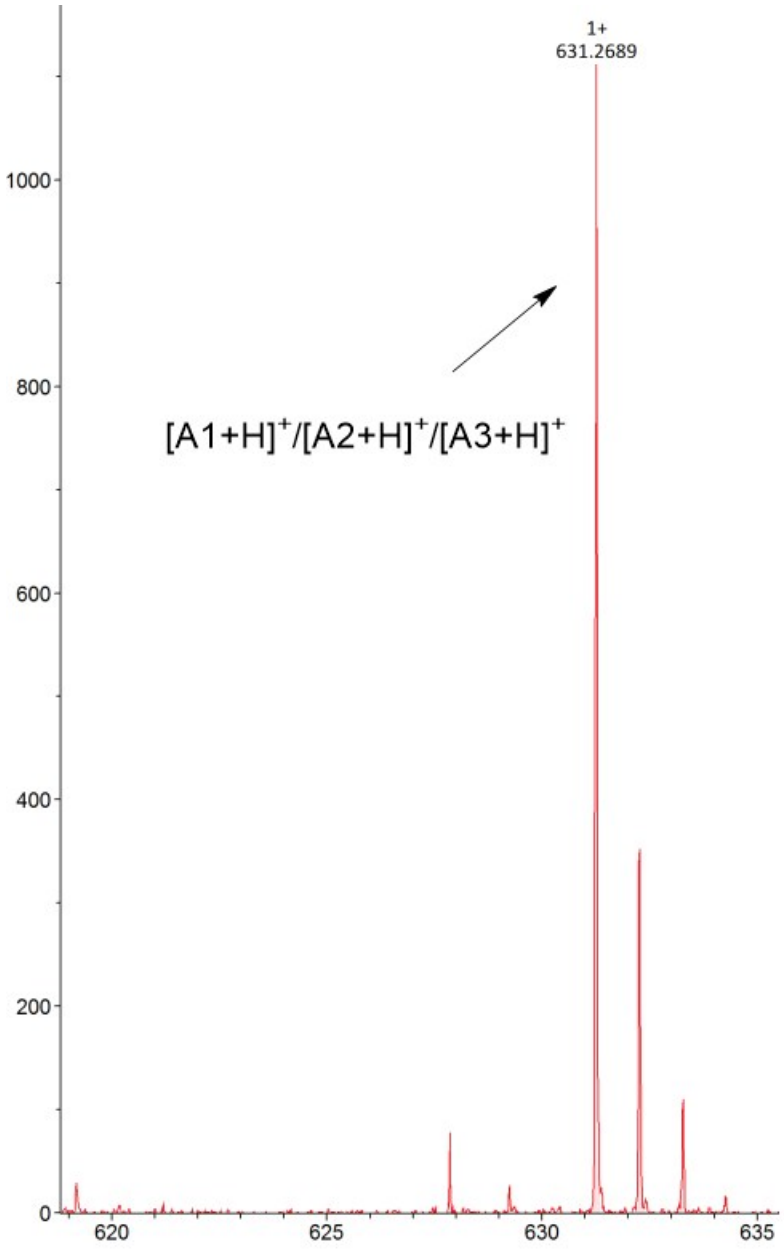
A dry tube equipped with a magnetic stirrer bar was charged with **1a** (0.24 mmol, 80 mg), **2a** (0.1 mmol, 32 mg), **2e** (0.1 mmol, 36 mg), $Rh_2(OAc)_4$ (5 mol %, 7.8 mg), $NaHCO_3$ (2 equiv, 33.6 mg), and cyclohexane (3 mL). The mixture was stirred under air at 85 ℃ for 5 hours. After cooling to room temperature, the crude residue was filtered by diatomite. The signals of mixed products were found by Bruker micrOTOF–Q instrument.

HRMS (EI) calcd for **A1**/**A2**/**A3** $C_{38}H_{38}N_4O_3S$ $[M+H]^+$: 631.2743; found: 631.2689.

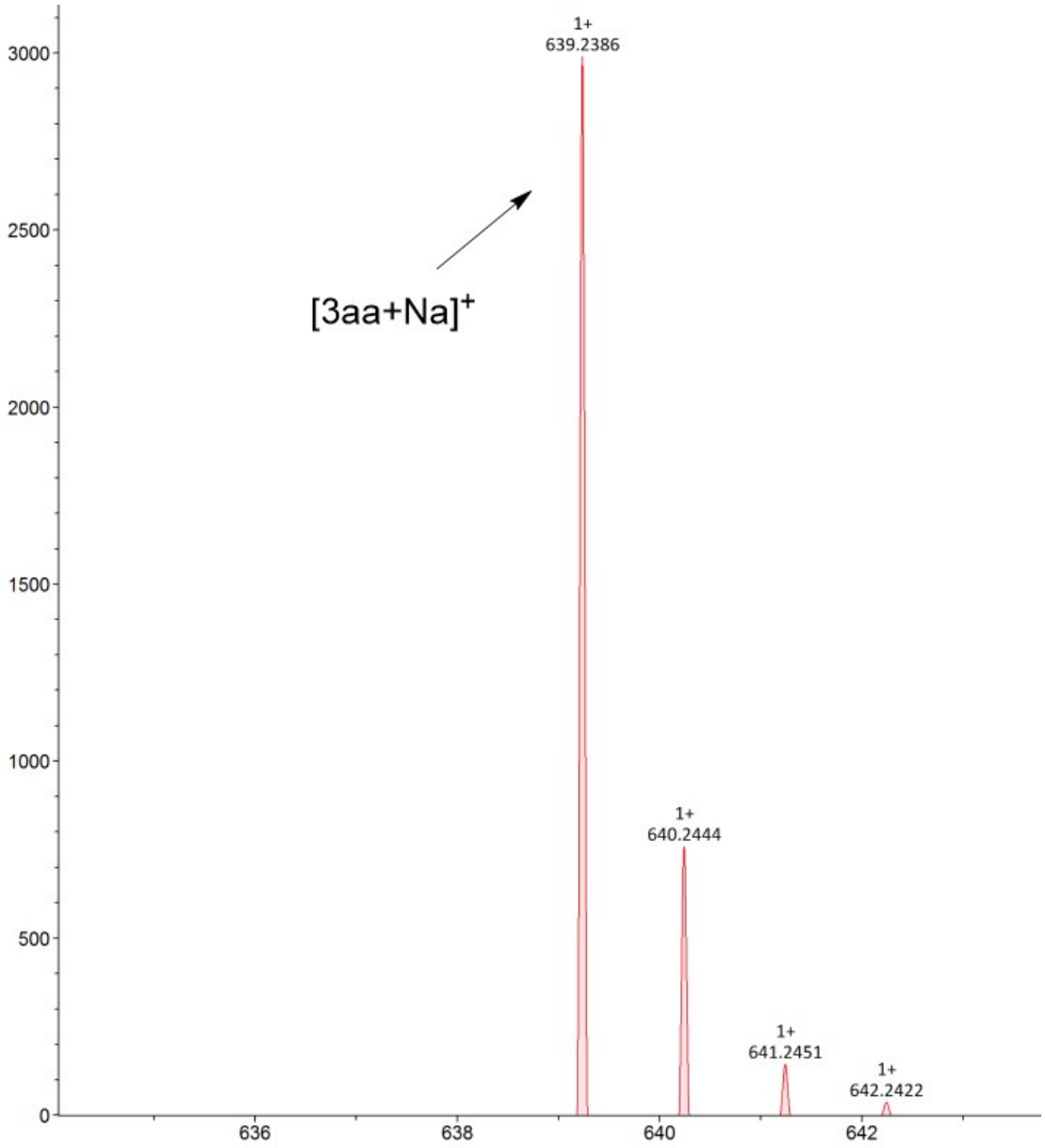
HRMS (EI) calcd for **3aa** $C_{37}H_{36}N_4O_3S$ $[M+Na]^+$: 639.2406; found: 639.2386.

HRMS (EI) calcd for **B1**/**B2**/**B3** $C_{39}H_{40}N_4O_3S$ $[M+Na]^+$: 667.2719, found: 667.2719.

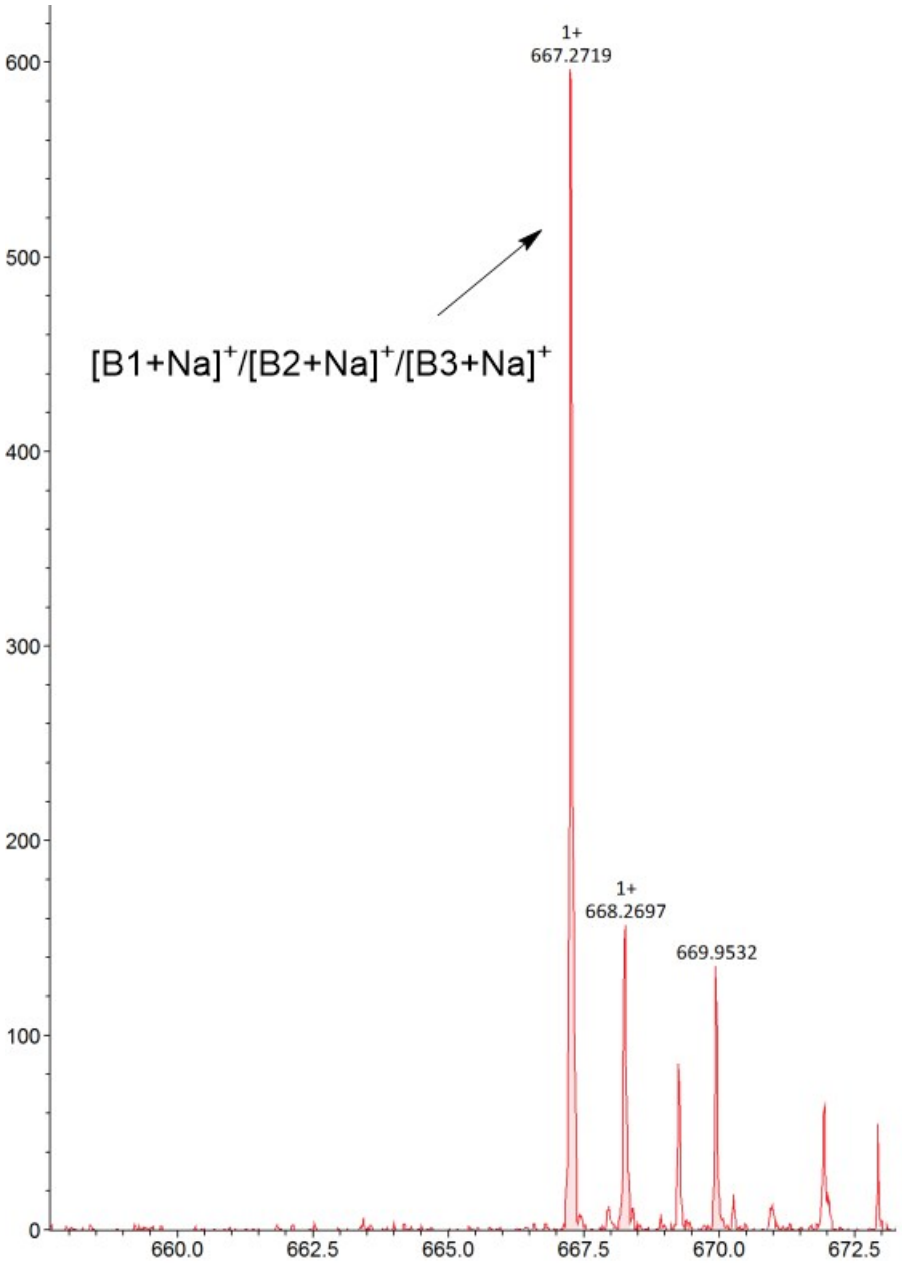
HRMS (EI) calcd for **3ae** $C_{40}H_{42}N_4O_3S$ $[M+Na]^+$: 681.2875, found: 681.2874.



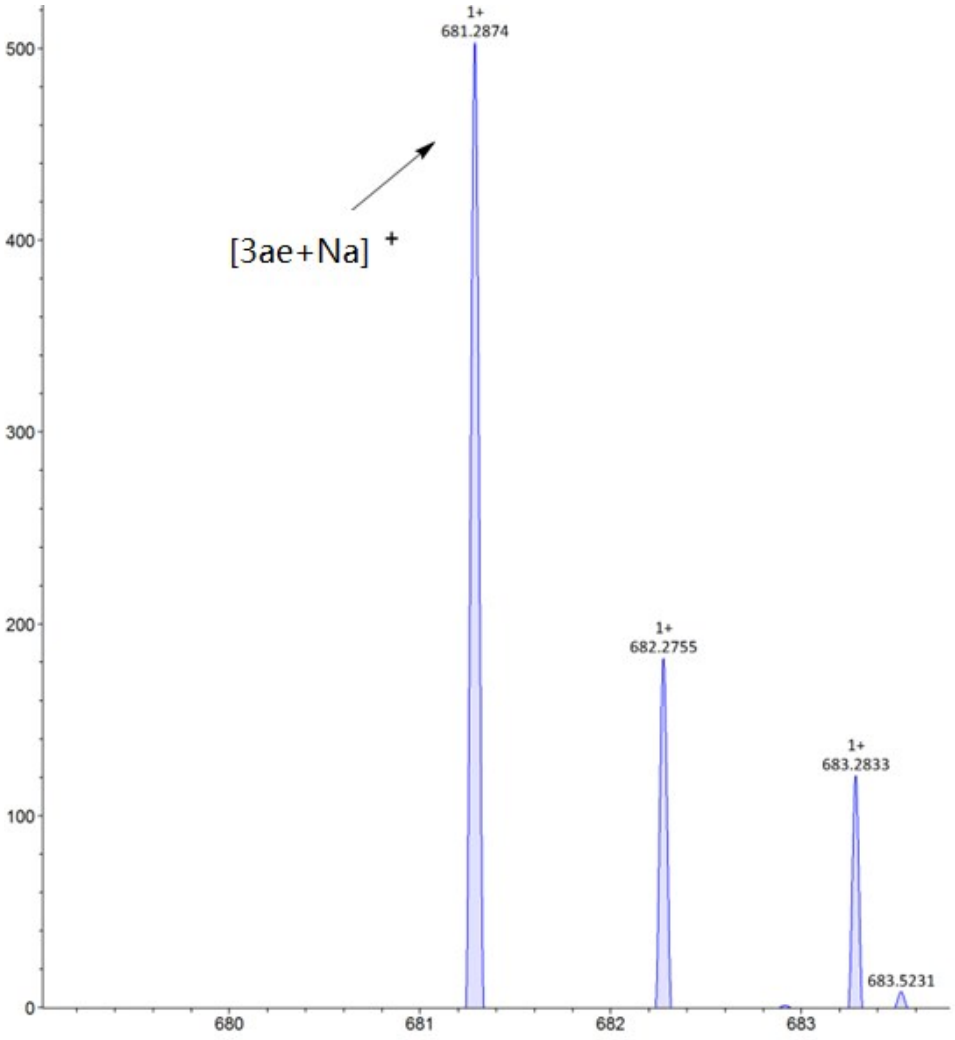
HRMS (EI) calcd for **A1/A2/A3** $C_{38}H_{38}N_4O_3S$ $[M+H]^+$: 631.2743; found: 631.2689.



HRMS (EI) calcd for **3aa** $C_{37}H_{36}N_4O_3S$ $[M+Na]^+$: 639.2406; found: 639.2386.



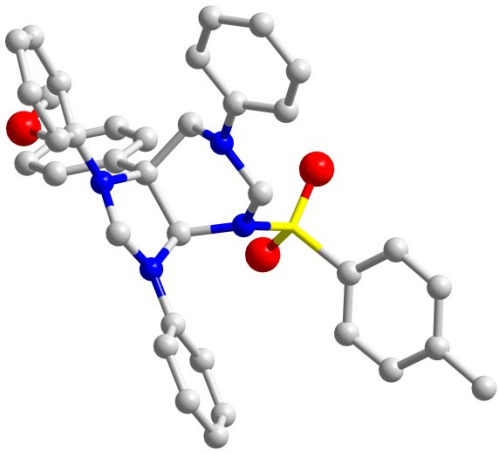
HRMS (EI) calcd for **B1/B2/B3** $C_{39}H_{40}N_4O_3S$ $[M+Na]^+$: 667.2719, found: 667.2719.

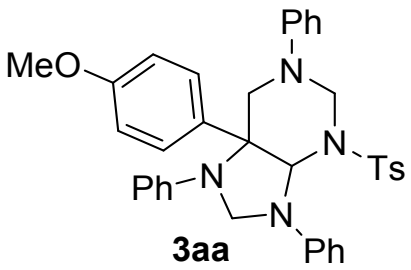


HRMS (EI) calcd for **3ae** $C_{40}H_{42}N_4O_3S$ $[M+Na]^+$: 681.2875, found: 681.2874.

5. X-ray Structure of 3aa

The crystallographic data of **3aa** (CCDC 1903355) can be obtained free of charge from the Cambridge Crystallographic Data Centre via http://www.ccdc.cam.ac.uk/data_request/cif.





3aa

6. Computational Methods

The ωB97XD density functional method[1] was employed to carry out all the calculations. The LANL2DZ basis set[2] in conjunction with LANL2DZ pseudopotential was used for Rh atom and the 6-31G(d) basis set[3] was employed for other atoms. Vibrational frequency analyses were performed on the optimized geometries at the same level of theory to characterize them as local minima (no imaginary frequency) or transition states (one imaginary frequency). In addition, intrinsic reaction coordinate (IRC) calculations were used to verify that the transition states connect with appropriate reactants and products.[4] The gas-phase Gibbs free energies for all species were obtained at 298.15 K and 1 atm at their respective optimized structures. To consider solvation effects, single-point energy computations using the SMD solvation model[5] with cyclohexane as solvent were performed based on the optimized gas-phase geometries. The basis set, SDD[6] for Rh and atom and 6-311++G(d,p) for other atoms, was utilized for single-point energy calculation. The solution-phase Gibbs free energy was determined by adding the solvation single-point energy and the gas-phase thermal correction to the Gibbs free energy obtained from the vibrational frequency analyses. All calculations were carried out with the Gaussian 09 suite of programs.[7]

References

1. J.-D. Chai and M. Head-Gordon, *Phys. Chem. Chem. Phys.*, 2008, **10**, 6615－6620.
2. P. J. Hay and W. R. Wadt, *J. Chem. Phys*., 1985, **82**, 270-283.
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7. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K.

N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian 09, Revision C.01, Gaussian, Inc., Wallingford CT, 2010.

7. Additional Computational Results and Discussion

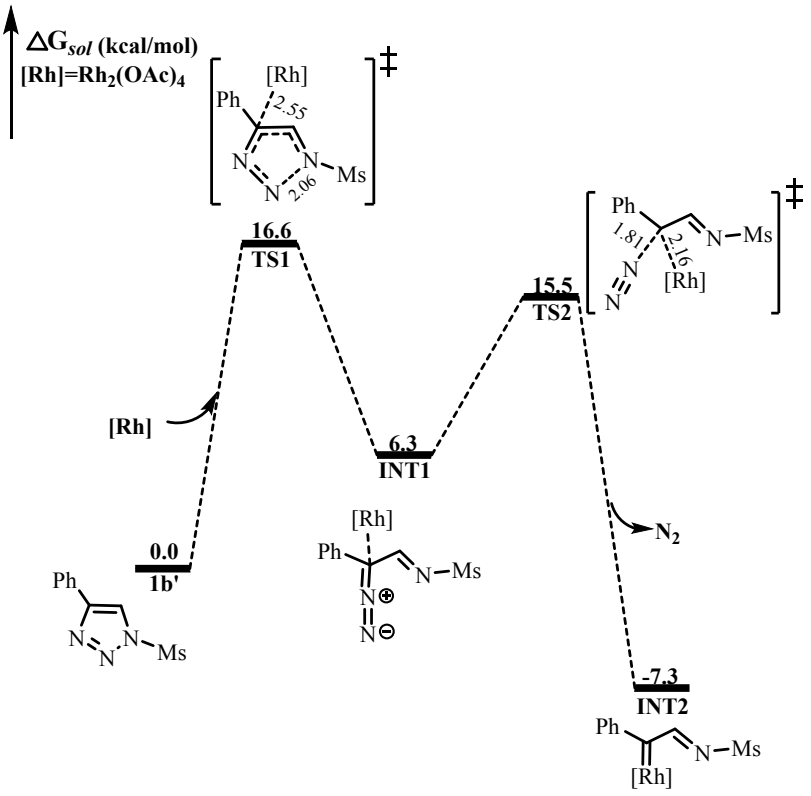


Figure S1. Energy profile (in kcal · mol^{-1}) for the formation of the Rh_2(II)-azavinyl carbene **INT2**. Bond lengths are shown in Å.

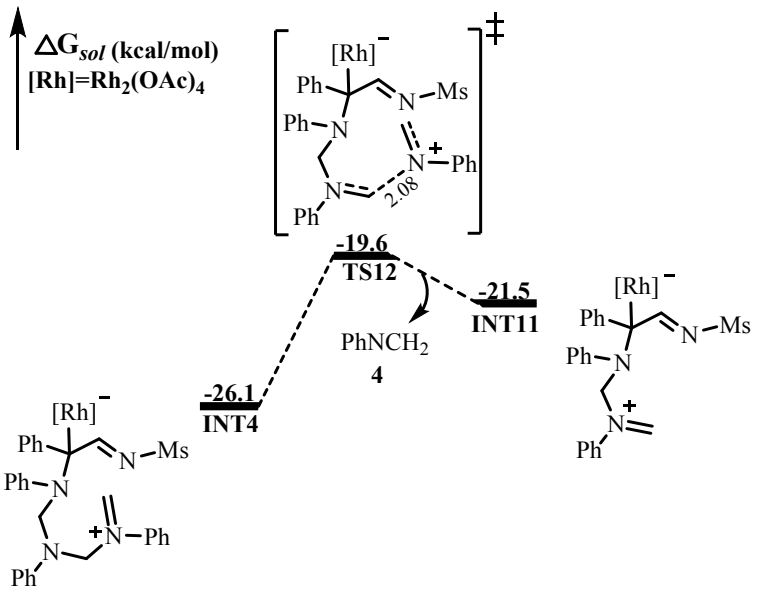


Figure S2. Energy profile (in kcal · mol^{-1}) for the fragmentation of **INT4**. Bond lengths are shown in Å.

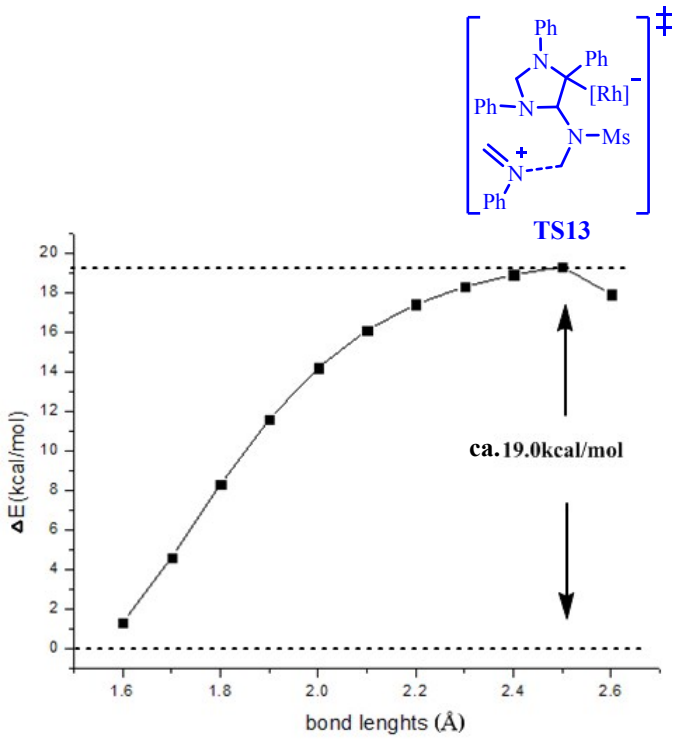


Figure S3. The potential energy surface scan for **INT7** to undergo the fragmentation. An approximate energy barrier (19 kcal/mol) was estimated to break the C–N bond.

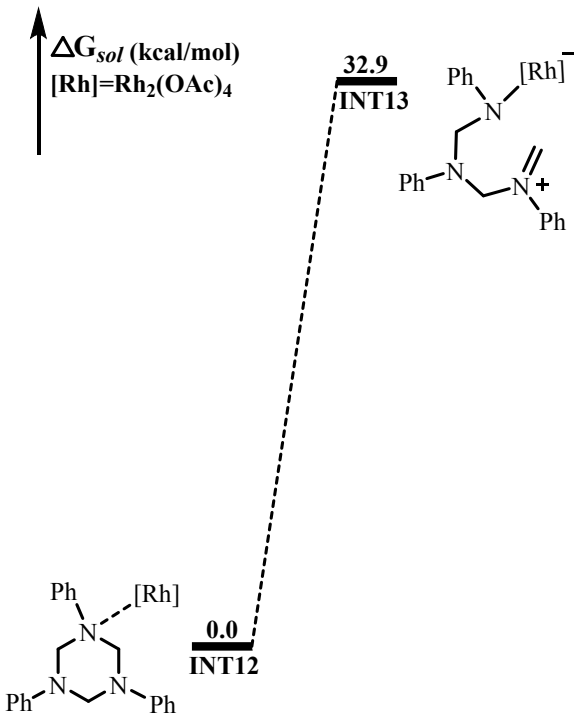


Figure S4. Energy profile for the Rh_2(II) catalyst assisted C–N bond cleavage of triazinane, which exhibits a thermodynamically very unfavorable process.

8. Cartesian Coordinates and Energies

1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.745588	-0.277243	-0.035392
2	6	0	-0.294060	0.620199	-0.016062
3	7	0	-1.401630	-0.166914	-0.057736
4	7	0	-1.074322	-1.477313	-0.102477
5	7	0	0.211205	-1.540978	-0.082423
6	16	0	-3.060043	0.329512	-0.112825
7	8	0	-3.011599	1.738580	0.217390
8	8	0	-3.631960	-0.149260	-1.347965
9	6	0	-3.704474	-0.621267	1.245439
10	1	0	-0.361619	1.695040	0.025387
11	1	0	-3.501837	-1.674993	1.048594
12	1	0	-3.223951	-0.288579	2.165978
13	1	0	-4.779145	-0.430263	1.275758
14	6	0	2.196811	-0.050226	-0.007119
15	6	0	3.071820	-1.140377	-0.021063
16	6	0	2.722032	1.244714	0.033860
17	6	0	4.446100	-0.934948	0.006239
18	1	0	2.663619	-2.144892	-0.054462
19	6	0	4.096635	1.446514	0.061209
20	1	0	2.057072	2.104113	0.042753
21	6	0	4.963523	0.356995	0.047724
22	1	0	5.115856	-1.789497	-0.005480
23	1	0	4.490993	2.457668	0.092226
24	1	0	6.037545	0.514920	0.068476

Zero-point correction= 0.180440 (Hartree/Particle)
Thermal correction to Energy= 0.193255
Thermal correction to Enthalpy= 0.194200
Thermal correction to Gibbs Free Energy= 0.138732
Sum of electronic and zero-point Energies= -1060.746958
Sum of electronic and thermal Energies= -1060.734143
Sum of electronic and thermal Enthalpies= -1060.733199
Sum of electronic and thermal Free Energies= -1060.788666
ωB97XD /6-311++G (d, p)/SMD// ωB97XD /6-31G(d) energy= -1061.12954697

2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.330767	-1.273140	-0.397508
2	6	0	-1.157393	0.234177	-1.506353
3	6	0	1.147141	0.758574	-1.414201
4	1	0	0.440443	-1.920524	0.472903
5	1	0	-2.169518	0.634148	-1.502339
6	1	0	1.309347	0.295218	-2.404625
7	7	0	-0.189923	1.306609	-1.421465
8	7	0	-0.992810	-0.692797	-0.387992
9	7	0	1.329313	-0.210049	-0.338389
10	1	0	1.869729	1.568298	-1.290842
11	1	0	-0.997789	-0.289362	-2.465971
12	1	0	0.497279	-1.891987	-1.309402
13	6	0	-0.497248	2.317124	-0.464792
14	6	0	-1.623764	3.114844	-0.698402
15	6	0	0.283386	2.567228	0.666156
16	6	0	-1.968639	4.129916	0.183992

17	1	0	-2.213475	2.949230	-1.595965
18	6	0	-0.054449	3.603609	1.533261
19	1	0	1.132716	1.931952	0.888845
20	6	0	-1.181090	4.384980	1.304720
21	1	0	-2.845781	4.738360	-0.016932
22	1	0	0.564604	3.784661	2.407340
23	1	0	-1.443778	5.185098	1.989864
24	6	0	2.646194	-0.623360	-0.043371
25	6	0	2.894939	-1.297469	1.162535
26	6	0	3.727713	-0.352112	-0.889612
27	6	0	4.179301	-1.696802	1.499448
28	1	0	2.074522	-1.478351	1.850676
29	6	0	5.018456	-0.738711	-0.533027
30	1	0	3.574130	0.153006	-1.837063
31	6	0	5.253516	-1.418042	0.654888
32	1	0	4.346272	-2.213535	2.440160
33	1	0	5.842486	-0.513018	-1.203822
34	1	0	6.259475	-1.722699	0.925606
35	6	0	-2.085941	-1.526800	-0.080333
36	6	0	-3.306785	-0.929527	0.269028
37	6	0	-1.998349	-2.923049	-0.079830
38	6	0	-4.407122	-1.709111	0.591538
39	1	0	-3.369253	0.154030	0.319763
40	6	0	-3.103294	-3.698027	0.268270
41	1	0	-1.073861	-3.416717	-0.361833
42	6	0	-4.313441	-3.100870	0.596566
43	1	0	-5.341011	-1.225623	0.863467
44	1	0	-3.012684	-4.780545	0.266980
45	1	0	-5.173293	-3.708571	0.860266

Zero-point correction= 0.383776 (Hartree/Particle)
Thermal correction to Energy= 0.402461
Thermal correction to Enthalpy= 0.403405
Thermal correction to Gibbs Free Energy= 0.334633
Sum of electronic and zero-point Energies= -976.411786
Sum of electronic and thermal Energies= -976.393101
Sum of electronic and thermal Enthalpies= -976.392157
Sum of electronic and thermal Free Energies= -976.460929

ωB97XD /6-311++G (d, p)/SMD// ωB97XD /6-31G(d) energy= -977.04999295

3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.094744	2.165573	-0.030480
2	6	0	0.319439	0.750199	0.018993
3	6	0	-1.380001	2.228580	-0.698720
4	6	0	-1.060213	0.121113	0.369733
5	6	0	0.765477	0.237118	-1.400567
6	7	0	-1.977787	0.940518	-0.400851
7	1	0	-1.973216	3.055732	-0.286594
8	1	0	-1.305097	2.385564	-1.791150
9	1	0	-1.265388	0.186076	1.439994
10	7	0	-1.168419	-1.277727	-0.024069
11	1	0	1.806967	0.492269	-1.598085
12	7	0	0.551363	-1.172091	-1.679764
13	1	0	0.167057	0.788090	-2.137077
14	16	0	-1.310314	-2.526513	1.057418
15	6	0	-0.812280	-1.556518	-1.411825
16	8	0	-2.124511	-3.552724	0.428418
17	8	0	-1.705713	-1.923281	2.326247
18	1	0	-0.988263	-2.611011	-1.611792
19	1	0	-1.488039	-0.965936	-2.038638
20	6	0	0.316576	-3.234251	1.281135

21	1	0	1.019271	-2.456007	1.579601
22	1	0	0.215144	-3.985757	2.067133
23	1	0	0.636415	-3.702975	0.349746
24	6	0	1.398353	0.561154	1.083150
25	6	0	2.694220	1.033680	0.831356
26	6	0	1.151257	-0.012499	2.333080
27	6	0	3.704592	0.922902	1.778485
28	1	0	2.926508	1.510619	-0.115743
29	6	0	2.166187	-0.136853	3.280817
30	1	0	0.169371	-0.389563	2.596460
31	6	0	3.446612	0.328003	3.009822
32	1	0	4.695233	1.304376	1.550207
33	1	0	1.942635	-0.599243	4.237564
34	1	0	4.234890	0.232383	3.750313
35	6	0	-3.369327	0.852703	-0.261441
36	6	0	-3.983266	0.002072	0.666368
37	6	0	-4.179184	1.642449	-1.091732
38	6	0	-5.370688	-0.052037	0.747626
39	1	0	-3.394978	-0.612224	1.336442
40	6	0	-5.563264	1.587251	-0.989419
41	1	0	-3.723141	2.292743	-1.832554
42	6	0	-6.171810	0.736321	-0.071656
43	1	0	-5.824487	-0.720471	1.473380
44	1	0	-6.168348	2.210681	-1.641609
45	1	0	-7.253578	0.688208	0.002731
46	6	0	1.574063	-2.133579	-1.624020
47	6	0	2.793284	-1.914525	-0.972497
48	6	0	1.380283	-3.371180	-2.261918
49	6	0	3.769881	-2.905721	-0.942054
50	1	0	2.974847	-0.985273	-0.448951
51	6	0	2.350985	-4.362269	-2.204912
52	1	0	0.469766	-3.552481	-2.824434
53	6	0	3.556570	-4.140313	-1.543020
54	1	0	4.700731	-2.707094	-0.418405
55	1	0	2.167455	-5.310825	-2.701210
56	1	0	4.316188	-4.914308	-1.504117
57	6	0	0.840423	3.201881	-0.324438
58	6	0	1.389518	3.909035	0.746652
59	6	0	1.224594	3.532700	-1.627555
60	6	0	2.325494	4.912640	0.524424
61	1	0	1.077844	3.642580	1.751088
62	6	0	2.154596	4.544541	-1.849571
63	1	0	0.801666	2.998221	-2.472929
64	6	0	2.710916	5.232667	-0.775013
65	1	0	2.751239	5.448729	1.367268
66	1	0	2.446933	4.792381	-2.865689
67	1	0	3.438561	6.019276	-0.950520

Zero-point correction= 0.559119 (Hartree/Particle)
Thermal correction to Energy= 0.589146
Thermal correction to Enthalpy= 0.590090
Thermal correction to Gibbs Free Energy= 0.498105
Sum of electronic and zero-point Energies= -1927.770308
Sum of electronic and thermal Energies= -1927.740281
Sum of electronic and thermal Enthalpies= -1927.739337
Sum of electronic and thermal Free Energies= -1927.831322
ωB97XD /6-311++G (d, p)/SMD// ωB97XD /6-31G(d) energy= -1928.75119521

4 ($PhNCH_2$)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.760462	0.227434	0.334810
2	7	0	-1.927077	-0.464189	-0.324575

3	6	0	-0.548581	-0.196665	-0.164791
4	6	0	-0.028404	1.101026	-0.175982
5	6	0	0.318856	-1.285160	-0.037666
6	6	0	1.341379	1.303739	-0.035906
7	1	0	-0.695731	1.945116	-0.326031
8	6	0	1.682384	-1.074785	0.122118
9	1	0	-0.096468	-2.287708	-0.057344
10	6	0	2.199335	0.219927	0.123060
11	1	0	1.738327	2.314495	-0.055942
12	1	0	2.347554	-1.925750	0.235371
13	1	0	3.267386	0.380906	0.232940
14	1	0	-3.825685	0.045531	0.192671
15	1	0	-2.472885	1.003644	1.056501

Zero-point correction= 0.123308 (Hartree/Particle)
Thermal correction to Energy= 0.129688
Thermal correction to Enthalpy= 0.130632
Thermal correction to Gibbs Free Energy= 0.092793
Sum of electronic and zero-point Energies= -325.444599
Sum of electronic and thermal Energies= -325.438218
Sum of electronic and thermal Enthalpies= -325.437274
Sum of electronic and thermal Free Energies= -325.475114
ωB97XD /6-311++G (d, p)/SMD// ωB97XD /6-31G(d) energy= -325.65509775

N2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.000000	0.550870
2	7	0	0.000000	0.000000	-0.550870

Zero-point correction= 0.005700 (Hartree/Particle)
Thermal correction to Energy= 0.008061
Thermal correction to Enthalpy= 0.009005
Thermal correction to Gibbs Free Energy= -0.012743
Sum of electronic and zero-point Energies= -109.479351
Sum of electronic and thermal Energies= -109.476991
Sum of electronic and thermal Enthalpies= -109.476046
Sum of electronic and thermal Free Energies= -109.497794
ωB97XD /6-311++G (d, p)/SMD// ωB97XD /6-31G(d) energy= -109.51212332

$Rh_2(OAc)_4$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.814242	-1.901838	0.000356
2	8	0	-1.411356	-1.487166	-1.127407
3	8	0	-1.412303	-1.486290	1.128033
4	6	0	-2.887731	-2.958142	-0.000699
5	1	0	-2.795312	-3.589756	-0.885648
6	1	0	-3.863575	-2.462007	-0.032833
7	1	0	-2.833392	-3.555063	0.910814
8	6	0	-1.901839	1.814233	0.000333
9	8	0	-1.487149	1.411353	-1.127425
10	8	0	-1.486305	1.412291	1.128015
11	6	0	-2.958137	2.887728	-0.000725
12	1	0	-3.555259	2.833187	0.910645
13	1	0	-3.589554	2.795514	-0.885834
14	1	0	-2.461987	3.863576	-0.032506
15	6	0	1.814231	1.901834	0.000372
16	8	0	1.411369	1.487149	-1.127395
17	8	0	1.412276	1.486292	1.128044
18	6	0	2.887714	2.958145	-0.000693
19	1	0	2.794970	3.590052	-0.885401

20	1	0	3.863550	2.462031	-0.033374
21	1	0	2.833696	3.554763	0.911034
22	6	0	1.901837	-1.814237	0.000411
23	8	0	1.487172	-1.411363	-1.127365
24	8	0	1.486271	-1.412296	1.128075
25	6	0	2.958206	-2.887662	-0.000758
26	1	0	2.462238	-3.863445	-0.037023
27	1	0	3.552854	-2.835750	0.912364
28	1	0	3.592024	-2.792787	-0.883888
29	45	0	0.000008	-0.000009	-1.187543
30	45	0	-0.000015	-0.000001	1.187976

Zero-point correction= 0.214198 (Hartree/Particle)
Thermal correction to Energy= 0.232054
Thermal correction to Enthalpy= 0.232998
Thermal correction to Gibbs Free Energy= 0.168018
Sum of electronic and zero-point Energies= -1132.578352
Sum of electronic and thermal Energies= -1132.560496
Sum of electronic and thermal Enthalpies= -1132.559552
Sum of electronic and thermal Free Energies= -1132.624531
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)-LANL2DZ energy= -1132.83755973

TS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.760795	0.501387	0.080242
2	6	0	-0.422344	-0.261820	0.010849
3	7	0	-1.550078	0.391281	0.082358
4	7	0	-0.680380	2.275256	0.262489
5	7	0	0.375487	1.795047	0.203428
6	16	0	-3.013559	-0.446927	0.076038
7	8	0	-2.779190	-1.820357	-0.352287
8	8	0	-3.687984	-0.178975	1.331592
9	6	0	-3.857439	0.431184	-1.224680
10	1	0	-0.394364	-1.341497	-0.112124
11	1	0	-3.899955	1.488419	-0.960052
12	1	0	-3.320347	0.281020	-2.161895
13	1	0	-4.863327	0.011366	-1.288933
14	6	0	2.165760	0.096880	0.022889
15	6	0	3.173741	1.053159	-0.144827
16	6	0	2.525835	-1.250818	0.133720
17	6	0	4.507715	0.669361	-0.199249
18	1	0	2.909960	2.103170	-0.236450
19	6	0	3.861196	-1.630218	0.068278
20	1	0	1.765800	-2.011934	0.284273
21	6	0	4.858627	-0.673937	-0.097142
22	1	0	5.276009	1.425811	-0.327278
23	1	0	4.120883	-2.680649	0.157113
24	1	0	5.901154	-0.972382	-0.144113

Zero-point correction= 0.177594 (Hartree/Particle)
Thermal correction to Energy= 0.190531
Thermal correction to Enthalpy= 0.191476
Thermal correction to Gibbs Free Energy= 0.135838
Sum of electronic and zero-point Energies= -1060.709410
Sum of electronic and thermal Energies= -1060.696473
Sum of electronic and thermal Enthalpies= -1060.695529
Sum of electronic and thermal Free Energies= -1060.751167
ωB97XD /6-311++G (d, p)/SMD// ωB97XD /6-31G(d) energy= -1061.08961391

INT1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.523514	-1.707165	2.055986
2	8	0	0.585300	-2.305988	1.973084
3	8	0	-0.899102	-0.741865	1.318890
4	6	0	-1.497458	-2.168102	3.107993
5	1	0	-1.641876	-3.248449	3.020948
6	1	0	-1.072474	-1.972864	4.097204
7	1	0	-2.447490	-1.641793	3.001218
8	6	0	2.235069	0.803377	1.876946
9	8	0	2.745951	-0.351565	1.808864
10	8	0	1.245316	1.220244	1.202429
11	6	0	2.830144	1.771780	2.865581
12	1	0	3.895306	1.573529	2.995760
13	1	0	2.660332	2.797680	2.534635
14	1	0	2.334170	1.632556	3.831978
15	6	0	2.793430	-0.079751	-1.715083
16	8	0	3.162832	-1.043498	-0.990718
17	8	0	1.687611	0.542130	-1.620256
18	6	0	3.748205	0.407055	-2.774505
19	1	0	3.202962	0.641817	-3.691387
20	1	0	4.225282	1.326966	-2.420576
21	1	0	4.518111	-0.340584	-2.966967
22	6	0	0.025822	-2.563009	-1.520591
23	8	0	0.992389	-2.989646	-0.829122
24	8	0	-0.469289	-1.393771	-1.469395
25	6	0	-0.585044	-3.512563	-2.518876
26	1	0	-0.086023	-3.373195	-3.483701
27	1	0	-0.437989	-4.545240	-2.199681
28	1	0	-1.645982	-3.293700	-2.652239
29	45	0	1.919173	-1.720309	0.511762
30	45	0	0.349148	-0.033772	-0.154616
31	6	0	-2.339742	1.126698	-0.196345
32	6	0	-1.204513	1.762548	-0.844384
33	1	0	-2.403052	1.270213	0.885044
34	6	0	-0.609383	3.054955	-0.395759
35	6	0	0.640572	3.468910	-0.866093
36	6	0	-1.299500	3.852917	0.519154
37	6	0	1.189255	4.664951	-0.421985
38	1	0	1.199114	2.829768	-1.543303
39	6	0	-0.732417	5.037495	0.978579
40	1	0	-2.283687	3.562586	0.873728
41	6	0	0.510143	5.449499	0.507784
42	1	0	2.160570	4.977466	-0.793713
43	1	0	-1.275563	5.646392	1.694599
44	1	0	0.946865	6.378646	0.860881
45	7	0	-1.140302	1.515228	-2.172558
46	7	0	-1.036090	1.255906	-3.254501
47	7	0	-3.163608	0.386977	-0.842921
48	16	0	-4.301951	-0.419079	0.116577
49	8	0	-4.145667	-0.075815	1.528658
50	8	0	-5.596030	-0.252655	-0.520543
51	6	0	-3.731556	-2.091531	-0.125434
52	1	0	-4.377386	-2.740725	0.469704
53	1	0	-3.810119	-2.332303	-1.185957
54	1	0	-2.695841	-2.145568	0.211924

Zero-point correction= 0.394763 (Hartree/Particle)
Thermal correction to Energy= 0.431091
Thermal correction to Enthalpy= 0.432035
Thermal correction to Gibbs Free Energy= 0.324769
Sum of electronic and zero-point Energies= -2193.323203
Sum of electronic and thermal Energies= -2193.286875
Sum of electronic and thermal Enthalpies= -2193.285931
Sum of electronic and thermal Free Energies= -2193.393197

ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)- LANL2DZ energy= -2193.97513237

TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.596678	0.878175	1.794950
2	8	0	-3.280098	-0.004851	1.218001
3	8	0	-1.377025	1.164364	1.552948
4	6	0	-3.276524	1.708368	2.855014
5	1	0	-4.114370	1.158921	3.285863
6	1	0	-3.663776	2.620979	2.389044
7	1	0	-2.563299	1.996527	3.629379
8	6	0	-2.192457	1.248964	-1.911556
9	8	0	-2.978558	0.292817	-1.677881
10	8	0	-1.067461	1.454239	-1.353200
11	6	0	-2.595498	2.242768	-2.972130
12	1	0	-3.670363	2.193753	-3.149758
13	1	0	-2.071382	1.994480	-3.900999
14	1	0	-2.295540	3.250758	-2.677842
15	6	0	-0.227814	-1.933937	-2.000060
16	8	0	-1.438065	-2.195524	-1.773848
17	8	0	0.466874	-1.042353	-1.411895
18	6	0	0.483485	-2.725068	-3.068560
19	1	0	0.144280	-2.375294	-4.049022
20	1	0	0.221111	-3.782166	-2.984035
21	1	0	1.562825	-2.582915	-2.991539
22	6	0	-0.619183	-2.292705	1.665487
23	8	0	-1.735241	-2.490104	1.118105
24	8	0	0.162825	-1.310741	1.450973
25	6	0	-0.130045	-3.332221	2.643678
26	1	0	0.379209	-4.125293	2.084800
27	1	0	-0.975205	-3.780211	3.168847
28	1	0	0.577342	-2.895076	3.350273
29	45	0	-2.433113	-1.142591	-0.293253
30	45	0	-0.387186	0.122162	0.066390
31	6	0	1.435631	1.241763	0.337662
32	6	0	2.472822	0.338487	-0.120127
33	1	0	2.505391	0.253488	-1.213570
34	6	0	1.539043	2.687681	0.093515
35	6	0	0.422885	3.514813	0.290604
36	6	0	2.742813	3.248410	-0.362522
37	6	0	0.514980	4.875657	0.033172
38	1	0	-0.501268	3.076936	0.650131
39	6	0	2.822063	4.605909	-0.641926
40	1	0	3.616521	2.616697	-0.498524
41	6	0	1.708126	5.419151	-0.440307
42	1	0	-0.348262	5.514427	0.191585
43	1	0	3.751224	5.031362	-1.007002
44	1	0	1.772532	6.482764	-0.650206
45	7	0	3.169963	-0.416734	0.641960
46	16	0	4.026527	-1.638415	-0.174074
47	8	0	3.947584	-1.459637	-1.622077
48	8	0	5.321880	-1.755506	0.469557
49	7	0	1.607335	1.076351	2.128264
50	7	0	1.299414	1.046044	3.185754
51	6	0	2.999652	-3.027518	0.275990
52	1	0	3.448839	-3.917615	-0.169619
53	1	0	2.975021	-3.106172	1.363406
54	1	0	1.999683	-2.845842	-0.121834

Zero-point correction= 0.391778 (Hartree/Particle)
Thermal correction to Energy= 0.428378
Thermal correction to Enthalpy= 0.429322

Thermal correction to Gibbs Free Energy= 0.321305
Sum of electronic and zero-point Energies= -2193.307555
Sum of electronic and thermal Energies= -2193.270955
Sum of electronic and thermal Enthalpies= -2193.270011
Sum of electronic and thermal Free Energies= -2193.378028
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)- LANL2DZ energy= -2193.95689021

INT2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.028273	0.881789	2.249172
2	8	0	-2.921806	0.127224	1.791188
3	8	0	-0.882767	1.101177	1.730280
4	6	0	-2.300695	1.589200	3.553738
5	1	0	-1.934594	2.617408	3.509072
6	1	0	-1.755075	1.075582	4.352004
7	1	0	-3.367019	1.569802	3.780622
8	6	0	-2.517603	1.605112	-1.373185
9	8	0	-3.298974	0.673680	-1.057729
10	8	0	-1.277721	1.684765	-1.082817
11	6	0	-3.069049	2.739725	-2.200802
12	1	0	-2.785359	2.580264	-3.246318
13	1	0	-2.636163	3.688823	-1.877501
14	1	0	-4.156863	2.766978	-2.129489
15	6	0	-0.931914	-1.672455	-2.226570
16	8	0	-2.053639	-1.895084	-1.707050
17	8	0	-0.047550	-0.862282	-1.789071
18	6	0	-0.565527	-2.410902	-3.488760
19	1	0	-0.415910	-1.690097	-4.298033
20	1	0	-1.351975	-3.115090	-3.760523
21	1	0	0.380701	-2.938206	-3.338466
22	6	0	-0.454887	-2.394937	1.363907
23	8	0	-1.687926	-2.436636	1.128031
24	8	0	0.351879	-1.467445	1.022970
25	6	0	0.155587	-3.558033	2.107912
26	1	0	-0.625925	-4.185733	2.536756
27	1	0	0.821769	-3.192193	2.893491
28	1	0	0.748836	-4.155536	1.407379
29	45	0	-2.577442	-0.921927	0.039794
30	45	0	-0.378294	0.158866	-0.030185
31	6	0	1.428598	1.029233	-0.194671
32	6	0	2.417213	0.010651	-0.503498
33	1	0	2.220593	-0.618398	-1.380633
34	6	0	1.774098	2.404570	-0.107171
35	6	0	0.811379	3.345247	0.336158
36	6	0	3.075190	2.860301	-0.445553
37	6	0	1.144328	4.685102	0.438478
38	1	0	-0.175383	2.992950	0.605967
39	6	0	3.393254	4.201747	-0.348339
40	1	0	3.823780	2.147755	-0.773592
41	6	0	2.427566	5.110514	0.093322
42	1	0	0.409006	5.403445	0.785597
43	1	0	4.387853	4.547001	-0.609839
44	1	0	2.681790	6.163911	0.170679
45	7	0	3.366564	-0.227375	0.326049
46	16	0	4.288939	-1.615142	-0.045251
47	8	0	3.755793	-2.305216	-1.216165
48	8	0	5.682507	-1.203424	-0.019106
49	6	0	3.916045	-2.580886	1.404405
50	1	0	4.272249	-2.041601	2.282742
51	1	0	2.834400	-2.718046	1.445077
52	1	0	4.432251	-3.537338	1.298744

Zero-point correction= 0.383907 (Hartree/Particle)
Thermal correction to Energy= 0.418499
Thermal correction to Enthalpy= 0.419443
Thermal correction to Gibbs Free Energy= 0.313721
Sum of electronic and zero-point Energies= -2083.848844
Sum of electronic and thermal Energies= -2083.814253
Sum of electronic and thermal Enthalpies= -2083.813308
Sum of electronic and thermal Free Energies= -2083.919030
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)- LANL2DZ energy= -2084.46082529

TS3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.290571	-1.364143	-2.316736
2	8	0	3.426207	-1.624785	-1.851422
3	8	0	1.403957	-0.625578	-1.772996
4	6	0	1.906458	-2.001092	-3.630606
5	1	0	1.293675	-1.317014	-4.222304
6	1	0	1.315999	-2.901208	-3.426570
7	1	0	2.799186	-2.292281	-4.185333
8	6	0	4.072178	1.732277	-1.203031
9	8	0	4.799629	0.759677	-0.871242
10	8	0	2.815423	1.829361	-1.027543
11	6	0	4.742523	2.920928	-1.845995
12	1	0	4.972115	3.654598	-1.065923
13	1	0	4.069705	3.392076	-2.565119
14	1	0	5.674230	2.618049	-2.325635
15	6	0	3.525450	0.769673	2.343015
16	8	0	4.314205	-0.092533	1.877027
17	8	0	2.460620	1.188810	1.783254
18	6	0	3.855712	1.391626	3.676096
19	1	0	2.963638	1.839491	4.118604
20	1	0	4.603952	2.175823	3.519444
21	1	0	4.292285	0.641464	4.339025
22	6	0	1.720747	-2.304786	1.218389
23	8	0	2.918612	-2.474843	0.871516
24	8	0	1.055615	-1.224383	1.106178
25	6	0	0.971933	-3.483395	1.787158
26	1	0	0.243293	-3.149519	2.528792
27	1	0	1.665160	-4.204339	2.222471
28	1	0	0.421470	-3.970147	0.973147
29	45	0	3.934214	-0.891715	0.013163
30	45	0	1.823784	0.351569	0.009714
31	6	0	0.047576	1.565379	0.065381
32	6	0	-0.147371	1.760547	1.484104
33	1	0	0.507481	2.551381	1.879819
34	6	0	-0.268555	2.618022	-0.861826
35	6	0	0.199231	2.548940	-2.187362
36	6	0	-1.101281	3.696377	-0.490109
37	6	0	-0.146927	3.531417	-3.105269
38	1	0	0.828416	1.717062	-2.475466
39	6	0	-1.429611	4.682539	-1.404094
40	1	0	-1.481905	3.751866	0.526966
41	6	0	-0.953175	4.596090	-2.714801
42	1	0	0.204740	3.460960	-4.129201
43	1	0	-2.060001	5.514234	-1.105923
44	1	0	-1.219134	5.364562	-3.434853
45	7	0	-0.821082	1.017794	2.283583
46	16	0	-0.595069	1.327734	3.926372
47	8	0	0.318149	2.447929	4.147744
48	8	0	-1.917948	1.349686	4.532109
49	6	0	0.243869	-0.181749	4.372461
50	1	0	-0.423509	-1.020696	4.172970

51	1	0	1.146152	-0.258153	3.763930
52	1	0	0.484687	-0.120183	5.435719
53	6	0	-3.744474	-1.674668	0.221622
54	6	0	-1.486174	-1.052422	-0.285481
55	6	0	-3.030210	0.606759	0.327265
56	1	0	-4.566579	-2.324546	-0.085499
57	1	0	-0.597771	-1.305864	-0.850724
58	1	0	-2.649444	0.461719	1.341898
59	7	0	-1.909144	0.316177	-0.577905
60	7	0	-2.569534	-1.989394	-0.570707
61	7	0	-4.128762	-0.282635	-0.002340
62	1	0	-3.342125	1.647238	0.234832
63	1	0	-1.206306	-1.067855	0.773571
64	1	0	-3.554023	-1.838179	1.306551
65	6	0	-2.167495	0.609579	-1.956576
66	6	0	-1.400648	0.011069	-2.962249
67	6	0	-3.124397	1.558504	-2.334783
68	6	0	-1.592190	0.340957	-4.298044
69	1	0	-0.610160	-0.677931	-2.703549
70	6	0	-3.296926	1.898148	-3.671165
71	1	0	-3.762777	2.036112	-1.604246
72	6	0	-2.537693	1.291279	-4.665768
73	1	0	-0.983882	-0.147017	-5.054666
74	1	0	-4.045871	2.639989	-3.931549
75	1	0	-2.684370	1.552219	-5.709247
76	6	0	-5.395149	0.059579	0.540698
77	6	0	-6.543081	-0.430068	-0.094024
78	6	0	-5.534633	0.870070	1.671474
79	6	0	-7.803976	-0.119953	0.396304
80	1	0	-6.428762	-1.035431	-0.988755
81	6	0	-6.805062	1.196025	2.144317
82	1	0	-4.660088	1.235328	2.201931
83	6	0	-7.941671	0.701094	1.515735
84	1	0	-8.685266	-0.504867	-0.108586
85	1	0	-6.898507	1.829310	3.021615
86	1	0	-8.928644	0.952403	1.891718
87	6	0	-2.148709	-3.336221	-0.595667
88	6	0	-1.146462	-3.708423	-1.507159
89	6	0	-2.677074	-4.318957	0.248782
90	6	0	-0.669498	-5.009591	-1.548252
91	1	0	-0.761439	-2.966589	-2.199799
92	6	0	-2.204926	-5.630000	0.187754
93	1	0	-3.448295	-4.072065	0.970248
94	6	0	-1.193631	-5.983146	-0.696469
95	1	0	0.108281	-5.271332	-2.260265
96	1	0	-2.629443	-6.375382	0.854097
97	1	0	-0.822546	-7.002344	-0.731492

Zero-point correction= 0.770431 (Hartree/Particle)
Thermal correction to Energy= 0.824256
Thermal correction to Enthalpy= 0.825200
Thermal correction to Gibbs Free Energy= 0.678340
Sum of electronic and zero-point Energies= -3060.278981
Sum of electronic and thermal Energies= -3060.225156
Sum of electronic and thermal Enthalpies= -3060.224212
Sum of electronic and thermal Free Energies= -3060.371072

ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)- LANL2DZ energy= -3061.53721910

INT3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.137971	-1.749638	-2.427580
2	8	0	2.362720	-2.034605	-2.415621
3	8	0	0.570267	-0.856606	-1.718274

4	6	0	0.229232	-2.542461	-3.333755
5	1	0	-0.452896	-1.865950	-3.855483
6	1	0	-0.374775	-3.219959	-2.718601
7	1	0	0.809682	-3.126029	-4.048698
8	6	0	3.093655	1.493354	-2.434170
9	8	0	3.850227	0.485303	-2.518692
10	8	0	2.141797	1.644805	-1.611137
11	6	0	3.353155	2.640945	-3.376256
12	1	0	4.172669	3.244835	-2.972736
13	1	0	2.464419	3.268377	-3.461245
14	1	0	3.661723	2.262437	-4.352828
15	6	0	4.185277	0.831948	1.010557
16	8	0	4.769353	0.058952	0.200420
17	8	0	2.933406	1.040141	1.064927
18	6	0	5.025676	1.589644	2.004345
19	1	0	4.393747	1.987767	2.800584
20	1	0	5.514016	2.421878	1.486556
21	1	0	5.807948	0.940357	2.404181
22	6	0	2.310658	-2.378662	1.046577
23	8	0	3.321554	-2.464071	0.300508
24	8	0	1.437645	-1.454510	1.021212
25	6	0	2.123150	-3.453659	2.088956
26	1	0	2.683706	-3.169147	2.986271
27	1	0	2.521472	-4.403529	1.728317
28	1	0	1.069494	-3.553634	2.356681
29	45	0	3.626264	-1.012054	-1.133133
30	45	0	1.669117	0.154743	-0.286871
31	6	0	-0.395389	1.388530	0.437879
32	6	0	0.263733	1.551257	1.691169
33	1	0	1.047793	2.312112	1.667993
34	6	0	-0.487627	2.627843	-0.401830
35	6	0	-0.438603	2.580721	-1.801324
36	6	0	-0.656129	3.875795	0.210251
37	6	0	-0.566741	3.736502	-2.558139
38	1	0	-0.307531	1.623449	-2.292582
39	6	0	-0.766603	5.041056	-0.546032
40	1	0	-0.706456	3.939695	1.294667
41	6	0	-0.727960	4.972816	-1.934057
42	1	0	-0.536706	3.672770	-3.642156
43	1	0	-0.890644	5.997270	-0.046496
44	1	0	-0.822053	5.877152	-2.528328
45	7	0	0.062443	0.873657	2.792751
46	16	0	1.070821	1.219120	4.070305
47	8	0	1.919309	2.382952	3.806885
48	8	0	0.247286	1.203398	5.271871
49	6	0	2.117512	-0.228214	4.095679
50	1	0	1.485042	-1.111185	4.195940
51	1	0	2.675962	-0.255645	3.160216
52	1	0	2.785396	-0.131671	4.954406
53	6	0	-3.390109	-1.189711	2.005826
54	6	0	-1.353135	-0.878505	0.790840
55	6	0	-2.643703	1.027388	1.613548
56	1	0	-4.281507	-1.805393	2.103315
57	1	0	-0.720572	-1.231503	-0.010886
58	1	0	-2.007033	0.970411	2.495407
59	7	0	-1.710798	0.557564	0.444791
60	7	0	-2.536156	-1.675693	0.928622
61	7	0	-3.776695	0.182504	1.761076
62	1	0	-2.915268	2.060158	1.415954
63	1	0	-0.762371	-0.813325	1.706625
64	1	0	-2.841143	-1.214572	2.959993
65	6	0	-2.468921	0.626918	-0.842705
66	6	0	-2.455255	-0.431273	-1.744054
67	6	0	-3.219468	1.764600	-1.132561
68	6	0	-3.201132	-0.353169	-2.916232
69	1	0	-1.876129	-1.323589	-1.566355
70	6	0	-3.964580	1.834898	-2.301193

71	1	0	-3.220913	2.621771	-0.472838
72	6	0	-3.964093	0.773030	-3.198095
73	1	0	-3.185784	-1.193281	-3.603752
74	1	0	-4.546102	2.728038	-2.502019
75	1	0	-4.552045	0.824010	-4.109125
76	6	0	-4.956969	0.453886	1.010997
77	6	0	-5.467597	-0.436352	0.064515
78	6	0	-5.619807	1.661631	1.243459
79	6	0	-6.618387	-0.110794	-0.646086
80	1	0	-4.931667	-1.349748	-0.167511
81	6	0	-6.755514	1.990431	0.513293
82	1	0	-5.242828	2.336204	2.007212
83	6	0	-7.262652	1.104247	-0.434304
84	1	0	-6.996074	-0.805635	-1.390278
85	1	0	-7.257223	2.935196	0.700644
86	1	0	-8.154314	1.357616	-0.999156
87	6	0	-2.482961	-3.033107	0.571183
88	6	0	-1.273423	-3.648415	0.208826
89	6	0	-3.656620	-3.802731	0.520129
90	6	0	-1.251693	-4.973912	-0.218075
91	1	0	-0.336556	-3.107722	0.280195
92	6	0	-3.617531	-5.129239	0.110890
93	1	0	-4.614309	-3.365283	0.782149
94	6	0	-2.418653	-5.726775	-0.270890
95	1	0	-0.299442	-5.419780	-0.491871
96	1	0	-4.542735	-5.697270	0.079521
97	1	0	-2.395950	-6.761822	-0.595549

Zero-point correction= 0.774626 (Hartree/Particle)
Thermal correction to Energy= 0.827723
Thermal correction to Enthalpy= 0.828667
Thermal correction to Gibbs Free Energy= 0.685840
Sum of electronic and zero-point Energies= -3060.310658
Sum of electronic and thermal Energies= -3060.257560
Sum of electronic and thermal Enthalpies= -3060.256616
Sum of electronic and thermal Free Energies= -3060.399444

ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)- LANL2DZ energy= -3061.57238543

TS4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.402659	1.831964	-2.282460
2	8	0	-2.586349	2.218227	-2.100096
3	8	0	-0.826357	0.870471	-1.679986
4	6	0	-0.553719	2.581086	-3.280163
5	1	0	-0.003137	1.871667	-3.903552
6	1	0	0.180742	3.183257	-2.732542
7	1	0	-1.168533	3.235766	-3.898378
8	6	0	-3.572273	-1.262853	-2.103798
9	8	0	-4.245070	-0.192548	-2.094307
10	8	0	-2.563471	-1.515836	-1.380463
11	6	0	-4.011983	-2.361991	-3.036186
12	1	0	-4.728687	-3.000510	-2.508761
13	1	0	-3.152846	-2.972094	-3.322307
14	1	0	-4.506742	-1.940119	-3.912782
15	6	0	-4.184789	-0.621756	1.463473
16	8	0	-4.810666	0.197409	0.733849
17	8	0	-2.950175	-0.905503	1.373668
18	6	0	-4.952197	-1.341092	2.542283
19	1	0	-4.262848	-1.869427	3.203116
20	1	0	-5.629159	-2.061808	2.072537
21	1	0	-5.563488	-0.627931	3.101058
22	6	0	-2.110100	2.443177	1.338175

23	8	0	-3.196699	2.618122	0.725881
24	8	0	-1.302246	1.476571	1.172273
25	6	0	-1.730265	3.456585	2.391115
26	1	0	-2.261086	4.395464	2.228970
27	1	0	-0.649835	3.620057	2.391863
28	1	0	-2.010897	3.059607	3.372872
29	45	0	-3.764228	1.240598	-0.702511
30	45	0	-1.813322	-0.088184	-0.122362
31	6	0	0.335094	-1.509921	0.132438
32	6	0	-0.204661	-1.733944	1.407416
33	1	0	-1.065208	-2.402457	1.461964
34	6	0	0.108993	-2.536193	-0.926870
35	6	0	0.028259	-2.197117	-2.285628
36	6	0	-0.016414	-3.885016	-0.578776
37	6	0	-0.159724	-3.170660	-3.254311
38	1	0	0.087475	-1.153588	-2.572906
39	6	0	-0.234288	-4.862270	-1.548456
40	1	0	0.066037	-4.180602	0.463593
41	6	0	-0.298450	-4.510760	-2.891260
42	1	0	-0.214319	-2.881185	-4.300238
43	1	0	-0.335892	-5.901405	-1.248715
44	1	0	-0.451604	-5.271967	-3.651039
45	7	0	0.267490	-1.182139	2.522470
46	16	0	-0.516662	-1.501566	3.929549
47	8	0	-1.467637	-2.609195	3.808417
48	8	0	0.513354	-1.565350	4.964872
49	6	0	-1.465262	-0.010558	4.208283
50	1	0	-0.779901	0.838065	4.228017
51	1	0	-2.178675	0.089818	3.390300
52	1	0	-1.974060	-0.118112	5.168898
53	6	0	3.344407	1.051079	1.843988
54	6	0	1.364421	0.683068	0.472279
55	6	0	3.106942	-1.298986	1.803095
56	1	0	4.152036	1.757238	2.029587
57	1	0	0.768968	1.186493	-0.282893
58	1	0	2.185493	-1.193013	2.385759
59	7	0	1.579048	-0.719345	0.049856
60	7	0	2.609371	1.410157	0.665830
61	7	0	3.927582	-0.297719	1.661484
62	1	0	3.445612	-2.278583	1.484109
63	1	0	0.786350	0.647123	1.395197
64	1	0	2.700813	0.984939	2.732929
65	6	0	2.383751	-0.862906	-1.130206
66	6	0	2.525633	0.164910	-2.066169
67	6	0	3.073460	-2.059956	-1.338189
68	6	0	3.363681	0.002728	-3.166180
69	1	0	1.975321	1.091189	-1.956283
70	6	0	3.896859	-2.224219	-2.443365
71	1	0	2.930860	-2.882580	-0.644590
72	6	0	4.058849	-1.186986	-3.358556
73	1	0	3.463681	0.815755	-3.879581
74	1	0	4.417309	-3.166125	-2.586019
75	1	0	4.710205	-1.310128	-4.218324
76	6	0	5.222862	-0.450138	1.053041
77	6	0	5.494687	0.089089	-0.201795
78	6	0	6.192572	-1.154997	1.760902
79	6	0	6.760929	-0.086423	-0.748310
80	1	0	4.713923	0.593727	-0.757947
81	6	0	7.454293	-1.328894	1.199748
82	1	0	5.959902	-1.552855	2.744184
83	6	0	7.739986	-0.792248	-0.052644
84	1	0	6.970096	0.313992	-1.734988
85	1	0	8.213289	-1.879189	1.746322
86	1	0	8.724243	-0.929365	-0.489271
87	6	0	2.674133	2.754979	0.223500
88	6	0	1.512871	3.507591	0.000955
89	6	0	3.917988	3.351956	-0.019449

90	6	0	1.601738	4.812825	-0.476483
91	1	0	0.537210	3.084479	0.215944
92	6	0	3.996113	4.663488	-0.472439
93	1	0	4.830410	2.781157	0.127230
94	6	0	2.839621	5.400868	-0.714043
95	1	0	0.687737	5.375839	-0.642740
96	1	0	4.971681	5.104170	-0.655537
97	1	0	2.903809	6.420971	-1.078624

Zero-point correction= 0.770602 (Hartree/Particle)
Thermal correction to Energy= 0.824240
Thermal correction to Enthalpy= 0.825184
Thermal correction to Gibbs Free Energy= 0.680393
Sum of electronic and zero-point Energies= -3060.293025
Sum of electronic and thermal Energies= -3060.239388
Sum of electronic and thermal Enthalpies= -3060.238444
Sum of electronic and thermal Free Energies= -3060.383235
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)- LANL2DZ energy= -3061.55516242

INT4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.896205	-2.228157	-2.023442
2	8	0	2.719971	-2.833085	-1.286165
3	8	0	1.389341	-1.085950	-1.793971
4	6	0	1.443051	-2.908014	-3.291180
5	1	0	0.361390	-3.071484	-3.243914
6	1	0	1.958414	-3.859452	-3.424684
7	1	0	1.640760	-2.251446	-4.143071
8	6	0	4.402789	0.346984	-1.178220
9	8	0	4.739260	-0.811739	-0.796730
10	8	0	3.297306	0.918695	-0.942307
11	6	0	5.408894	1.147395	-1.964073
12	1	0	6.041766	1.700427	-1.261741
13	1	0	4.891963	1.863083	-2.606304
14	1	0	6.046605	0.482431	-2.549275
15	6	0	3.439779	0.214232	2.383042
16	8	0	4.084324	-0.812425	2.033178
17	8	0	2.423176	0.689009	1.787302
18	6	0	3.893124	0.950589	3.617069
19	1	0	3.201214	1.762713	3.847318
20	1	0	4.894185	1.355881	3.440676
21	1	0	3.964996	0.251506	4.455020
22	6	0	0.826550	-2.332452	1.598698
23	8	0	1.992232	-2.803004	1.554703
24	8	0	0.414882	-1.280694	1.011128
25	6	0	-0.206325	-3.087356	2.402004
26	1	0	0.262299	-3.882043	2.982821
27	1	0	-0.940946	-3.523635	1.715770
28	1	0	-0.733129	-2.396232	3.066213
29	45	0	3.429874	-1.861007	0.387267
30	45	0	1.797156	-0.106281	-0.006886
31	6	0	0.123176	1.699216	-0.599933
32	6	0	0.302043	2.078516	0.739545
33	1	0	1.230656	2.574397	1.021492
34	6	0	0.897076	2.350947	-1.696435
35	6	0	0.803328	1.848536	-3.000684
36	6	0	1.731296	3.455818	-1.482482
37	6	0	1.538074	2.403524	-4.040458
38	1	0	0.169590	0.990955	-3.199077
39	6	0	2.470564	4.009823	-2.521163
40	1	0	1.811331	3.898176	-0.494478

41	6	0	2.383970	3.485340	-3.807436
42	1	0	1.449650	1.986629	-5.040068
43	1	0	3.108612	4.866652	-2.322974
44	1	0	2.955184	3.923342	-4.620869
45	7	0	-0.612125	1.851115	1.671339
46	16	0	-0.294113	2.260500	3.224810
47	8	0	0.888984	3.108447	3.376535
48	8	0	-1.570902	2.716141	3.781371
49	6	0	0.060966	0.680301	3.987110
50	1	0	-0.818850	0.043123	3.880293
51	1	0	0.919231	0.242834	3.478845
52	1	0	0.272318	0.860678	5.043373
53	6	0	-2.493720	-0.540061	0.804734
54	6	0	-1.464507	-0.071906	-1.407727
55	6	0	-3.595869	1.529857	1.466328
56	1	0	-2.574455	-1.462681	1.381115
57	1	0	-1.846308	-0.094725	-2.439026
58	1	0	-2.587721	1.948577	1.552249
59	7	0	-1.215901	1.266781	-0.967754
60	7	0	-2.482055	-0.785855	-0.590547
61	7	0	-3.722082	0.290310	1.162647
62	1	0	-4.489652	2.119822	1.644823
63	1	0	-0.519592	-0.605567	-1.399436
64	1	0	-1.639905	0.044678	1.149929
65	6	0	-2.187565	2.244797	-1.213919
66	6	0	-3.431621	1.911158	-1.785000
67	6	0	-1.975818	3.592602	-0.865978
68	6	0	-4.398308	2.887841	-2.014351
69	1	0	-3.659092	0.882849	-2.038866
70	6	0	-2.955526	4.550454	-1.087088
71	1	0	-1.036008	3.896266	-0.424428
72	6	0	-4.178092	4.214597	-1.664587
73	1	0	-5.337023	2.594733	-2.479483
74	1	0	-2.751628	5.578827	-0.803527
75	1	0	-4.935577	4.971021	-1.842656
76	6	0	-5.010655	-0.317116	0.961047
77	6	0	-5.931637	0.301405	0.122075
78	6	0	-5.296168	-1.531048	1.579324
79	6	0	-7.161242	-0.311283	-0.100695
80	1	0	-5.668733	1.229937	-0.374485
81	6	0	-6.527891	-2.132240	1.350474
82	1	0	-4.571556	-2.001700	2.235081
83	6	0	-7.458758	-1.527091	0.508571
84	1	0	-7.881617	0.160678	-0.760922
85	1	0	-6.758704	-3.077428	1.830442
86	1	0	-8.416084	-2.005084	0.327254
87	6	0	-2.694153	-2.136944	-1.016346
88	6	0	-1.636829	-3.052901	-1.024282
89	6	0	-3.957813	-2.544038	-1.441628
90	6	0	-1.847487	-4.363564	-1.440944
91	1	0	-0.654685	-2.725365	-0.697986
92	6	0	-4.168689	-3.859302	-1.849698
93	1	0	-4.770913	-1.824466	-1.446453
94	6	0	-3.116074	-4.770287	-1.851228
95	1	0	-1.019553	-5.066754	-1.441172
96	1	0	-5.157784	-4.169193	-2.173879
97	1	0	-3.281498	-5.793624	-2.174422

Zero-point correction= 0.770250 (Hartree/Particle)
Thermal correction to Energy= 0.824778
Thermal correction to Enthalpy= 0.825723
Thermal correction to Gibbs Free Energy= 0.679002
Sum of electronic and zero-point Energies= -3060.310662
Sum of electronic and thermal Energies= -3060.256134
Sum of electronic and thermal Enthalpies= -3060.255190
Sum of electronic and thermal Free Energies= -3060.401910

ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)- LANL2DZ energy= -3061.57140563

TS5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.998393	-1.707997	-2.634354
2	8	0	2.059463	-2.348514	-2.408117
3	8	0	0.526986	-0.770728	-1.918434
4	6	0	0.224737	-2.063175	-3.880019
5	1	0	0.242931	-3.143745	-4.035760
6	1	0	0.712625	-1.592680	-4.740297
7	1	0	-0.802725	-1.698611	-3.817215
8	6	0	3.744785	0.688832	-1.904219
9	8	0	4.223466	-0.479013	-1.805752
10	8	0	2.656989	1.091768	-1.397918
11	6	0	4.514561	1.696095	-2.718850
12	1	0	5.585589	1.496631	-2.651793
13	1	0	4.279631	2.705435	-2.375187
14	1	0	4.213527	1.604144	-3.767977
15	6	0	3.729152	-0.429561	1.687596
16	8	0	4.184057	-1.364863	0.972188
17	8	0	2.711613	0.278980	1.419678
18	6	0	4.431164	-0.112602	2.981160
19	1	0	5.300524	-0.755964	3.117619
20	1	0	3.722553	-0.253298	3.802814
21	1	0	4.738111	0.937372	2.980893
22	6	0	1.020795	-2.749934	0.997657
23	8	0	2.052096	-3.177158	0.405730
24	8	0	0.540774	-1.577604	0.901214
25	6	0	0.275819	-3.708529	1.886561
26	1	0	0.893241	-4.580337	2.105551
27	1	0	-0.639311	-4.033076	1.380603
28	1	0	-0.010671	-3.193925	2.806596
29	45	0	3.165735	-1.877466	-0.732284
30	45	0	1.548610	-0.163126	-0.215015
31	6	0	-0.044394	1.953675	0.379654
32	6	0	-0.047583	1.342355	1.626000
33	1	0	0.884596	1.370286	2.190034
34	6	0	0.976767	2.973477	-0.000879
35	6	0	0.780181	3.742403	-1.154749
36	6	0	2.138264	3.221849	0.748484
37	6	0	1.710430	4.692420	-1.562393
38	1	0	-0.119461	3.604980	-1.744605
39	6	0	3.068514	4.167056	0.339501
40	1	0	2.349961	2.645523	1.640866
41	6	0	2.867103	4.909821	-0.822359
42	1	0	1.522300	5.268803	-2.464068
43	1	0	3.960118	4.327391	0.939813
44	1	0	3.593593	5.653796	-1.135820
45	7	0	-1.109248	0.752477	2.206183
46	16	0	-0.878608	0.324148	3.771876
47	8	0	-2.113173	-0.343735	4.202532
48	8	0	0.397821	-0.346133	4.016831
49	6	0	-0.829613	1.890589	4.645017
50	1	0	0.058565	2.445722	4.335246
51	1	0	-1.733503	2.451010	4.400877
52	1	0	-0.783591	1.675053	5.714295
53	6	0	-2.096552	-0.793677	-0.637134
54	6	0	-1.538237	1.425139	-1.546838
55	6	0	-3.193728	0.035568	1.323862
56	1	0	-2.100297	-1.735195	-1.184018
57	1	0	-1.971543	2.137300	-2.258025
58	7	0	-1.317309	2.063892	-0.281253
59	7	0	-2.490697	0.305209	-1.451478

60	7	0	-2.943924	-0.999274	0.589300
61	1	0	-3.660599	-0.093010	2.292856
62	1	0	-0.574774	1.088093	-1.932821
63	1	0	-1.099685	-0.642764	-0.230672
64	6	0	-2.240735	3.021976	0.168095
65	6	0	-3.516357	3.128139	-0.415822
66	6	0	-1.935235	3.881906	1.237861
67	6	0	-4.432954	4.070121	0.044988
68	1	0	-3.814681	2.463211	-1.218008
69	6	0	-2.861119	4.812415	1.686994
70	1	0	-0.959065	3.835332	1.704436
71	6	0	-4.119462	4.919754	1.097897
72	1	0	-5.408333	4.126158	-0.430328
73	1	0	-2.587409	5.469310	2.508048
74	1	0	-4.838439	5.649876	1.455284
75	6	0	-3.162076	-2.350284	1.036995
76	6	0	-3.599320	-3.298283	0.109424
77	6	0	-2.969803	-2.694295	2.371044
78	6	0	-3.835638	-4.603006	0.526427
79	1	0	-3.776505	-3.022961	-0.925324
80	6	0	-3.224444	-4.001834	2.775752
81	1	0	-2.603465	-1.960543	3.083910
82	6	0	-3.649198	-4.959121	1.860487
83	1	0	-4.175547	-5.339349	-0.194836
84	1	0	-3.067323	-4.269571	3.815720
85	1	0	-3.834334	-5.979153	2.182173
86	6	0	-3.298311	0.001434	-2.569968
87	6	0	-2.912323	0.323565	-3.876463
88	6	0	-4.520563	-0.654065	-2.369245
89	6	0	-3.736782	-0.000794	-4.951228
90	1	0	-1.956717	0.803955	-4.059634
91	6	0	-5.325165	-0.996776	-3.449347
92	1	0	-4.847258	-0.870557	-1.356214
93	6	0	-4.940701	-0.667219	-4.747280
94	1	0	-3.421604	0.256992	-5.958047
95	1	0	-6.268681	-1.504757	-3.272251
96	1	0	-5.574742	-0.924819	-5.589598
97	1	0	-3.110162	1.013462	0.878570

Zero-point correction= 0.771347 (Hartree/Particle)
Thermal correction to Energy= 0.824940
Thermal correction to Enthalpy= 0.825884
Thermal correction to Gibbs Free Energy= 0.680380
Sum of electronic and zero-point Energies= -3060.312405
Sum of electronic and thermal Energies= -3060.258813
Sum of electronic and thermal Enthalpies= -3060.257868
Sum of electronic and thermal Free Energies= -3060.403372

ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)- LANL2DZ energy= -3061.57075327

INT5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.550631	0.234037	2.861572
2	8	0	2.794189	0.457384	2.877565
3	8	0	0.858821	-0.024830	1.829822
4	6	0	0.812544	0.310309	4.172907
5	1	0	-0.083230	-0.313487	4.145567
6	1	0	0.501519	1.348057	4.337382
7	1	0	1.469725	0.017787	4.993383
8	6	0	3.324545	-2.384954	0.797714
9	8	0	4.149819	-1.577918	1.318818
10	8	0	2.271311	-2.062888	0.171625
11	6	0	3.618337	-3.857078	0.899747
12	1	0	4.111674	-4.178782	-0.023549

13	1	0	2.682621	-4.411998	0.995957
14	1	0	4.283289	-4.056189	1.741280
15	6	0	4.071074	0.136659	-1.756179
16	8	0	4.763372	0.382238	-0.725457
17	8	0	2.823309	-0.083405	-1.773445
18	6	0	4.781389	0.102633	-3.083307
19	1	0	4.069043	-0.095275	-3.884914
20	1	0	5.545042	-0.680157	-3.061051
21	1	0	5.292683	1.055446	-3.247873
22	6	0	2.304024	2.756087	0.287555
23	8	0	3.388640	2.428970	0.840961
24	8	0	1.435222	1.955434	-0.182243
25	6	0	1.989471	4.228478	0.200049
26	1	0	2.907736	4.816523	0.226189
27	1	0	1.375777	4.503848	1.065195
28	1	0	1.419100	4.444013	-0.706150
29	45	0	3.820589	0.431431	1.098430
30	45	0	1.766102	-0.099101	-0.028586
31	6	0	-0.984909	-1.186134	-0.463912
32	6	0	-0.516204	-0.906273	-1.730363
33	1	0	0.130807	-1.649756	-2.181408
34	6	0	-0.719956	-2.577304	0.022383
35	6	0	-0.320281	-2.837808	1.338166
36	6	0	-0.889261	-3.654294	-0.850302
37	6	0	-0.085604	-4.137392	1.760707
38	1	0	-0.180569	-2.009079	2.019768
39	6	0	-0.644749	-4.959693	-0.430406
40	1	0	-1.236356	-3.473992	-1.862644
41	6	0	-0.244269	-5.205671	0.877473
42	1	0	0.223838	-4.319570	2.785901
43	1	0	-0.783632	-5.782569	-1.125138
44	1	0	-0.066114	-6.223481	1.212725
45	7	0	-0.926600	0.146120	-2.610691
46	16	0	0.137999	0.475389	-3.902437
47	8	0	1.068270	-0.629449	-4.056729
48	8	0	-0.682257	0.884619	-5.035804
49	6	0	1.009166	1.924825	-3.347050
50	1	0	0.278053	2.726618	-3.232147
51	1	0	1.511348	1.713787	-2.406062
52	1	0	1.730939	2.172290	-4.128999
53	6	0	-3.285870	1.751750	-1.360856
54	6	0	-1.520910	1.106298	0.187381
55	6	0	-2.361806	0.229261	-3.024183
56	1	0	-4.296371	2.178086	-1.368482
57	1	0	-1.014652	1.510775	1.064620
58	1	0	-2.422656	1.067612	-3.717294
59	7	0	-1.695162	-0.328039	0.358878
60	7	0	-2.793468	1.782763	0.020496
61	7	0	-3.266317	0.433651	-1.937420
62	1	0	-2.648107	-0.662965	-3.579511
63	1	0	-0.850025	1.269795	-0.655718
64	1	0	-2.659084	2.389267	-2.004690
65	6	0	-2.476247	-0.747195	1.469659
66	6	0	-2.500063	0.016074	2.642071
67	6	0	-3.261267	-1.901703	1.410607
68	6	0	-3.268152	-0.383440	3.731026
69	1	0	-1.922648	0.929103	2.719412
70	6	0	-4.013423	-2.302890	2.505903
71	1	0	-3.296273	-2.482259	0.497909
72	6	0	-4.023460	-1.550193	3.676654
73	1	0	-3.270768	0.229052	4.628399
74	1	0	-4.614581	-3.203653	2.426363
75	1	0	-4.621225	-1.860395	4.528264
76	6	0	-4.174764	-0.550307	-1.525354
77	6	0	-5.210134	-0.232029	-0.632246
78	6	0	-4.086976	-1.878968	-1.974952
79	6	0	-6.135503	-1.191621	-0.243427

80	1	0	-5.273046	0.756729	-0.197656
81	6	0	-5.022257	-2.829043	-1.580413
82	1	0	-3.273649	-2.197332	-2.615593
83	6	0	-6.060902	-2.497202	-0.717068
84	1	0	-6.916176	-0.910483	0.457238
85	1	0	-4.920755	-3.845975	-1.948665
86	1	0	-6.785857	-3.243056	-0.407780
87	6	0	-2.864758	3.088470	0.580946
88	6	0	-1.756280	3.941768	0.611029
89	6	0	-4.083860	3.537697	1.095005
90	6	0	-1.864706	5.214025	1.166663
91	1	0	-0.808802	3.605475	0.198593
92	6	0	-4.193432	4.816539	1.628614
93	1	0	-4.933574	2.861258	1.093114
94	6	0	-3.082875	5.658116	1.672039
95	1	0	-0.995517	5.865971	1.190136
96	1	0	-5.145479	5.151704	2.029559
97	1	0	-3.167675	6.652473	2.099570

Zero-point correction= 0.774106 (Hartree/Particle)
Thermal correction to Energy= 0.826621
Thermal correction to Enthalpy= 0.827565
Thermal correction to Gibbs Free Energy= 0.686281
Sum of electronic and zero-point Energies= -3060.335709
Sum of electronic and thermal Energies= -3060.283195
Sum of electronic and thermal Enthalpies= -3060.282250
Sum of electronic and thermal Free Energies= -3060.423534
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)- LANL2DZ energy= -3061.59214285

TS6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.614953	2.473694	-0.015760
2	8	0	-3.763592	1.977513	-0.097721
3	8	0	-1.514375	1.835573	-0.134371
4	6	0	-2.475433	3.956547	0.221535
5	1	0	-3.448390	4.412427	0.405964
6	1	0	-2.010611	4.419458	-0.655025
7	1	0	-1.801181	4.126871	1.065684
8	6	0	-2.590340	0.124964	-2.997745
9	8	0	-3.734095	0.221111	-2.485237
10	8	0	-1.496670	-0.071552	-2.378381
11	6	0	-2.490733	0.303699	-4.495403
12	1	0	-3.375057	-0.112038	-4.981490
13	1	0	-1.585087	-0.166873	-4.882765
14	1	0	-2.456960	1.375501	-4.722056
15	6	0	-2.916818	-2.751034	-0.701727
16	8	0	-3.997210	-2.104360	-0.754097
17	8	0	-1.755960	-2.268089	-0.522452
18	6	0	-2.988532	-4.252387	-0.833645
19	1	0	-2.140021	-4.618046	-1.415886
20	1	0	-3.931913	-4.552565	-1.291342
21	1	0	-2.925381	-4.691738	0.167849
22	6	0	-2.961452	-0.392228	2.229898
23	8	0	-4.044690	-0.388349	1.586616
24	8	0	-1.798214	-0.259509	1.736244
25	6	0	-3.016040	-0.596650	3.721470
26	1	0	-2.345782	0.109171	4.218321
27	1	0	-2.644115	-1.602533	3.943085
28	1	0	-4.036415	-0.486854	4.090187
29	45	0	-3.962906	-0.066114	-0.447880
30	45	0	-1.516463	-0.240459	-0.296287
31	7	0	1.031886	-0.571425	1.486529
32	6	0	0.771376	-0.519655	0.056868

33	6	0	2.320824	0.025341	1.791470
34	6	0	1.149470	0.863062	-0.326486
35	6	0	3.650084	1.576346	0.369211
36	7	0	2.367715	1.313042	1.083849
37	1	0	2.442306	0.189777	2.859915
38	1	0	3.151422	-0.584268	1.426239
39	1	0	0.457713	1.646765	-0.037573
40	7	0	1.816583	1.168089	-1.515299
41	1	0	4.474638	1.674570	1.077344
42	7	0	3.916473	0.539406	-0.571261
43	1	0	3.521364	2.539607	-0.132099
44	16	0	1.556254	2.748904	-2.148233
45	6	0	3.119144	0.555485	-1.789301
46	8	0	2.566159	2.939610	-3.176170
47	8	0	1.461270	3.687004	-1.039505
48	1	0	2.968663	-0.467061	-2.129281
49	1	0	3.587956	1.137227	-2.587137
50	6	0	-0.038555	2.589894	-2.904094
51	1	0	-0.763976	2.350503	-2.125031
52	1	0	-0.251571	3.556468	-3.366668
53	1	0	0.007757	1.793919	-3.646212
54	6	0	1.359760	-1.652006	-0.753355
55	6	0	2.279810	-2.555660	-0.206986
56	6	0	1.000552	-1.826270	-2.098409
57	6	0	2.854130	-3.561690	-0.978970
58	1	0	2.555032	-2.491070	0.839334
59	6	0	1.576278	-2.827528	-2.871616
60	1	0	0.264772	-1.163710	-2.537775
61	6	0	2.514426	-3.698399	-2.319856
62	1	0	3.579367	-4.231091	-0.526019
63	1	0	1.282206	-2.932705	-3.912605
64	1	0	2.964777	-4.479719	-2.925135
65	6	0	1.837186	2.411646	1.873190
66	6	0	2.571067	3.575488	2.095232
67	6	0	0.554078	2.280719	2.417219
68	6	0	2.023571	4.605543	2.855310
69	1	0	3.565266	3.706341	1.685643
70	6	0	0.025083	3.314277	3.180805
71	1	0	-0.031743	1.383605	2.241692
72	6	0	0.751425	4.481780	3.400970
73	1	0	2.602984	5.509069	3.016817
74	1	0	-0.970821	3.200617	3.598934
75	1	0	0.329034	5.288204	3.992160
76	6	0	4.978792	-0.365113	-0.446670
77	6	0	5.419846	-1.092617	-1.562986
78	6	0	5.619684	-0.593005	0.782499
79	6	0	6.436183	-2.032434	-1.440552
80	1	0	4.976643	-0.933963	-2.538541
81	6	0	6.645809	-1.524695	0.886529
82	1	0	5.318017	-0.061275	1.678740
83	6	0	7.059886	-2.260141	-0.218826
84	1	0	6.745763	-2.585331	-2.322465
85	1	0	7.116559	-1.679605	1.852938
86	1	0	7.855592	-2.992272	-0.130044
87	6	0	0.540020	-1.539932	2.388260
88	6	0	-0.077514	-2.718596	1.955247
89	6	0	0.641562	-1.315097	3.770049
90	6	0	-0.571200	-3.635093	2.876620
91	1	0	-0.209004	-2.904016	0.898585
92	6	0	0.165477	-2.248524	4.682824
93	1	0	1.053974	-0.384688	4.147851
94	6	0	-0.444154	-3.421327	4.246584
95	1	0	-1.051066	-4.538331	2.509232
96	1	0	0.257955	-2.042976	5.745751
97	1	0	-0.817493	-4.149907	4.959575

Zero-point correction= 0.774535 (Hartree/Particle)

Thermal correction to Energy= 0.826794
Thermal correction to Enthalpy= 0.827739
Thermal correction to Gibbs Free Energy= 0.687557
Sum of electronic and zero-point Energies= -3060.311521
Sum of electronic and thermal Energies= -3060.259262
Sum of electronic and thermal Enthalpies= -3060.258317
Sum of electronic and thermal Free Energies= -3060.398499
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)- LANL2DZ energy= -3061.56997496

INT6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.519392	2.471630	0.401569
2	8	0	-3.685837	2.041570	0.253636
3	8	0	-1.443199	1.816320	0.181734
4	6	0	-2.321004	3.881737	0.901944
5	1	0	-3.209310	4.486096	0.713753
6	1	0	-1.436090	4.326082	0.439922
7	1	0	-2.138449	3.844239	1.981476
8	6	0	-2.616890	0.689452	-2.910577
9	8	0	-3.757067	0.697452	-2.384781
10	8	0	-1.520805	0.371204	-2.347433
11	6	0	-2.515978	1.146218	-4.348846
12	1	0	-3.439072	0.915424	-4.882821
13	1	0	-1.661263	0.679597	-4.842929
14	1	0	-2.378096	2.233570	-4.365736
15	6	0	-3.002185	-2.553731	-1.155986
16	8	0	-4.063654	-1.884041	-1.058410
17	8	0	-1.820348	-2.142425	-0.932147
18	6	0	-3.122246	-4.006504	-1.549969
19	1	0	-2.313121	-4.278544	-2.231326
20	1	0	-4.093838	-4.200978	-2.005705
21	1	0	-3.024170	-4.620441	-0.647992
22	6	0	-2.950842	-0.764255	2.145571
23	8	0	-4.038278	-0.582224	1.542284
24	8	0	-1.785337	-0.600733	1.661672
25	6	0	-2.992139	-1.246909	3.573716
26	1	0	-2.283831	-0.677105	4.180997
27	1	0	-2.661154	-2.290675	3.592716
28	1	0	-4.000840	-1.168334	3.980604
29	45	0	-3.976846	0.079632	-0.418966
30	45	0	-1.515536	-0.199048	-0.335649
31	7	0	1.019812	-0.910949	1.283925
32	6	0	0.698929	-0.515583	-0.092501
33	6	0	2.278052	-0.358792	1.674290
34	6	0	1.254596	0.933641	-0.120988
35	6	0	3.597139	1.505777	0.685685
36	7	0	2.230194	1.056260	1.178397
37	1	0	2.433311	-0.345566	2.751246
38	1	0	3.131189	-0.838406	1.184986
39	1	0	0.478948	1.651699	0.129478
40	7	0	1.940698	1.399812	-1.286780
41	1	0	4.292952	1.460481	1.520757
42	7	0	4.020689	0.693515	-0.390129
43	1	0	3.468927	2.547453	0.385729
44	16	0	1.682131	3.042708	-1.687823
45	6	0	3.244579	0.839211	-1.618911
46	8	0	2.688017	3.383263	-2.681145
47	8	0	1.591008	3.819952	-0.455712
48	1	0	3.112821	-0.140931	-2.073259
49	1	0	3.725222	1.509724	-2.335556
50	6	0	0.082912	2.998998	-2.449721
51	1	0	-0.642494	2.634867	-1.720388

52	1	0	-0.138426	4.024937	-2.753001
53	1	0	0.128527	2.329617	-3.307954
54	6	0	1.305337	-1.433080	-1.137317
55	6	0	2.219724	-2.439424	-0.797956
56	6	0	0.992756	-1.275190	-2.495901
57	6	0	2.837348	-3.219276	-1.772389
58	1	0	2.459102	-2.632345	0.241778
59	6	0	1.610239	-2.050915	-3.469825
60	1	0	0.261199	-0.531765	-2.784419
61	6	0	2.546746	-3.021660	-3.117333
62	1	0	3.555384	-3.976651	-1.471783
63	1	0	1.353039	-1.898240	-4.514739
64	1	0	3.030546	-3.624716	-3.880217
65	6	0	1.641062	1.946490	2.209511
66	6	0	2.336315	3.049775	2.695223
67	6	0	0.371762	1.635709	2.700411
68	6	0	1.757072	3.845029	3.680952
69	1	0	3.313783	3.327515	2.324130
70	6	0	-0.187679	2.436451	3.688891
71	1	0	-0.184451	0.783825	2.323932
72	6	0	0.496854	3.543301	4.182214
73	1	0	2.302072	4.708099	4.049221
74	1	0	-1.174951	2.186162	4.065326
75	1	0	0.050345	4.168245	4.949185
76	6	0	5.082411	-0.219798	-0.327120
77	6	0	5.586409	-0.776449	-1.512476
78	6	0	5.662250	-0.615953	0.888527
79	6	0	6.613259	-1.711759	-1.473809
80	1	0	5.184287	-0.484073	-2.474953
81	6	0	6.698737	-1.542345	0.910378
82	1	0	5.308813	-0.222796	1.836124
83	6	0	7.180659	-2.104692	-0.266389
84	1	0	6.975493	-2.129507	-2.408348
85	1	0	7.123619	-1.830534	1.867337
86	1	0	7.984604	-2.832708	-0.242613
87	6	0	0.529044	-2.024809	1.993859
88	6	0	-0.106035	-3.090113	1.347140
89	6	0	0.657244	-2.073326	3.390222
90	6	0	-0.603944	-4.160037	2.081531
91	1	0	-0.249330	-3.063519	0.275920
92	6	0	0.176601	-3.159253	4.111878
93	1	0	1.093020	-1.240717	3.934359
94	6	0	-0.459676	-4.215094	3.465446
95	1	0	-1.100983	-4.969725	1.554043
96	1	0	0.287247	-3.166811	5.192735
97	1	0	-0.837362	-5.062157	4.029650

Zero-point correction= 0.775335 (Hartree/Particle)
Thermal correction to Energy= 0.828184
Thermal correction to Enthalpy= 0.829128
Thermal correction to Gibbs Free Energy= 0.687110
Sum of electronic and zero-point Energies= -3060.313867
Sum of electronic and thermal Energies= -3060.261018
Sum of electronic and thermal Enthalpies= -3060.260074
Sum of electronic and thermal Free Energies= -3060.402092
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)- LANL2DZ energy= -3061.57403485

TS7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.245459	-1.834920	2.006530
2	8	0	3.453501	-1.520780	1.865759
3	8	0	1.257006	-1.381489	1.339454

4	6	0	1.923815	-2.872869	3.053753
5	1	0	2.765246	-2.987819	3.738004
6	1	0	1.729587	-3.829716	2.559773
7	1	0	1.017058	-2.597362	3.595920
8	6	0	2.943456	-1.917319	-1.640399
9	8	0	3.995095	-1.640332	-1.023208
10	8	0	1.801304	-1.358648	-1.495953
11	6	0	2.996843	-3.025897	-2.669321
12	1	0	4.008614	-3.423115	-2.752192
13	1	0	2.669605	-2.642011	-3.640885
14	1	0	2.310652	-3.828074	-2.378352
15	6	0	3.384604	1.887714	-1.542131
16	8	0	4.369078	1.291125	-1.038026
17	8	0	2.155203	1.661425	-1.305975
18	6	0	3.658958	3.009182	-2.517431
19	1	0	2.933366	2.978636	-3.333773
20	1	0	4.678305	2.943247	-2.900180
21	1	0	3.537985	3.965116	-1.996447
22	6	0	2.643494	1.795006	2.109299
23	8	0	3.799832	1.386624	1.831759
24	8	0	1.554778	1.414726	1.571349
25	6	0	2.488542	2.831244	3.196860
26	1	0	2.039047	2.359053	4.076631
27	1	0	1.806256	3.615884	2.857657
28	1	0	3.458175	3.249552	3.469637
29	45	0	4.016142	-0.136055	0.431958
30	45	0	1.590474	0.136527	-0.024986
31	7	0	-1.276676	1.135493	0.545213
32	6	0	-0.514885	0.449494	-0.517901
33	6	0	-1.493980	0.174599	1.602119
34	6	0	-1.145343	-0.973655	-0.470598
35	6	0	-3.820979	-1.598012	0.576006
36	7	0	-1.649905	-1.117948	0.921280
37	1	0	-0.639687	0.132127	2.293519
38	1	0	-2.409795	0.405670	2.156890
39	1	0	-0.382242	-1.724480	-0.673784
40	7	0	-2.229387	-1.196259	-1.472963
41	1	0	-3.371502	-2.487142	0.149252
42	7	0	-4.184689	-0.615756	-0.189092
43	1	0	-4.215391	-1.640931	1.586340
44	16	0	-2.252780	-2.578239	-2.441514
45	6	0	-3.407490	-0.392483	-1.451885
46	8	0	-3.426757	-2.449632	-3.292336
47	8	0	-2.114714	-3.760333	-1.598057
48	1	0	-3.143731	0.663158	-1.450940
49	1	0	-4.039810	-0.612136	-2.311614
50	6	0	-0.783236	-2.439112	-3.427651
51	1	0	0.091483	-2.317967	-2.781566
52	1	0	-0.717210	-3.367920	-3.998724
53	1	0	-0.892751	-1.575927	-4.084060
54	6	0	-0.685478	1.110365	-1.874508
55	6	0	-1.574300	2.171898	-2.100405
56	6	0	0.055851	0.665900	-2.977707
57	6	0	-1.735963	2.740276	-3.362016
58	1	0	-2.143733	2.589567	-1.277925
59	6	0	-0.107964	1.222876	-4.240235
60	1	0	0.795385	-0.110610	-2.833017
61	6	0	-1.009819	2.264247	-4.446030
62	1	0	-2.432584	3.564368	-3.488280
63	1	0	0.491052	0.849810	-5.067303
64	1	0	-1.131850	2.705305	-5.430848
65	6	0	-1.412455	-2.270386	1.727610
66	6	0	-1.015778	-3.495535	1.190674
67	6	0	-1.736729	-2.207945	3.090449
68	6	0	-0.951870	-4.626651	1.997504
69	1	0	-0.769399	-3.588031	0.143688
70	6	0	-1.658721	-3.343598	3.890322

71	1	0	-2.049709	-1.273194	3.542888
72	6	0	-1.271160	-4.564828	3.349760
73	1	0	-0.642850	-5.567412	1.551994
74	1	0	-1.908024	-3.265029	4.944385
75	1	0	-1.216400	-5.451941	3.972216
76	6	0	-5.044276	0.434479	0.288073
77	6	0	-6.389171	0.147990	0.502928
78	6	0	-4.523895	1.701768	0.534104
79	6	0	-7.224674	1.151632	0.985290
80	1	0	-6.773881	-0.843446	0.283672
81	6	0	-5.367600	2.695296	1.016737
82	1	0	-3.465397	1.888112	0.382722
83	6	0	-6.715797	2.422800	1.240758
84	1	0	-8.274900	0.938649	1.156331
85	1	0	-4.957216	3.677689	1.227464
86	1	0	-7.371436	3.201955	1.616446
87	6	0	-1.010735	2.457389	0.974010
88	6	0	-0.117437	3.302930	0.297478
89	6	0	-1.707520	2.981919	2.074426
90	6	0	0.050146	4.618514	0.704381
91	1	0	0.482060	2.922125	-0.518767
92	6	0	-1.524173	4.302529	2.477245
93	1	0	-2.404297	2.368512	2.635886
94	6	0	-0.649357	5.137095	1.793671
95	1	0	0.756411	5.243287	0.164556
96	1	0	-2.075282	4.672201	3.337802
97	1	0	-0.506750	6.167015	2.105652

Zero-point correction= 0.773924 (Hartree/Particle)
Thermal correction to Energy= 0.826151
Thermal correction to Enthalpy= 0.827095
Thermal correction to Gibbs Free Energy= 0.688016
Sum of electronic and zero-point Energies= -3060.293909
Sum of electronic and thermal Energies= -3060.241682
Sum of electronic and thermal Enthalpies= -3060.240738
Sum of electronic and thermal Free Energies= -3060.379817

ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)- LANL2DZ energy= -3061.55352382

INT7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.508172	-1.969581	-2.268295
2	8	0	-2.760102	-1.945381	-2.344086
3	8	0	-0.784698	-1.337308	-1.431280
4	6	0	-0.749682	-2.846026	-3.239528
5	1	0	-1.407200	-3.193024	-4.037432
6	1	0	-0.347967	-3.709111	-2.698476
7	1	0	0.102369	-2.298147	-3.651816
8	6	0	-2.640412	-2.456819	1.210360
9	8	0	-3.613119	-2.425659	0.423548
10	8	0	-1.713147	-1.581290	1.315271
11	6	0	-2.519625	-3.632171	2.154818
12	1	0	-3.271469	-4.387936	1.926161
13	1	0	-2.658386	-3.284303	3.184287
14	1	0	-1.514899	-4.058481	2.076181
15	6	0	-4.013563	1.121387	1.201408
16	8	0	-4.728133	0.337599	0.527984
17	8	0	-2.745398	1.224412	1.161658
18	6	0	-4.712370	2.071505	2.147368
19	1	0	-4.104992	2.229691	3.041338
20	1	0	-5.699896	1.689672	2.410651
21	1	0	-4.833823	3.037410	1.645046
22	6	0	-2.788700	1.529622	-2.253734

23	8	0	-3.821995	0.814687	-2.203787
24	8	0	-1.721710	1.373936	-1.578212
25	6	0	-2.767219	2.697237	-3.212558
26	1	0	-2.091471	2.465196	-4.042361
27	1	0	-2.371132	3.578771	-2.700299
28	1	0	-3.765859	2.891491	-3.605727
29	45	0	-3.844214	-0.842693	-0.941526
30	45	0	-1.661672	-0.023297	-0.080589
31	7	0	0.937209	1.570033	-0.250895
32	6	0	0.270726	0.622602	0.661152
33	6	0	1.383019	0.814030	-1.392466
34	6	0	1.115697	-0.679512	0.452282
35	6	0	4.517957	-1.738470	0.172097
36	7	0	1.816780	-0.436313	-0.797350
37	1	0	0.580576	0.647706	-2.126381
38	1	0	2.227841	1.307033	-1.880244
39	1	0	0.461461	-1.549050	0.390574
40	7	0	2.102172	-1.041647	1.517875
41	1	0	4.121376	-2.560347	0.753382
42	7	0	4.270507	-0.528605	0.541200
43	1	0	5.163728	-1.922956	-0.677693
44	16	0	1.921626	-2.429807	2.453274
45	6	0	3.285229	-0.274707	1.662608
46	8	0	3.229163	-2.636252	3.072769
47	8	0	1.346927	-3.487262	1.634702
48	1	0	3.061244	0.786236	1.639015
49	1	0	3.796536	-0.520549	2.592318
50	6	0	0.723252	-2.043734	3.697767
51	1	0	-0.226096	-1.873913	3.184318
52	1	0	0.665597	-2.922425	4.344544
53	1	0	1.036671	-1.159542	4.252480
54	6	0	0.295142	1.152986	2.085796
55	6	0	1.221370	2.130786	2.484643
56	6	0	-0.619620	0.718115	3.051039
57	6	0	1.269552	2.609064	3.789859
58	1	0	1.893925	2.560580	1.748772
59	6	0	-0.578648	1.195187	4.358177
60	1	0	-1.382478	0.005901	2.768586
61	6	0	0.372195	2.135624	4.742158
62	1	0	1.999969	3.368264	4.055891
63	1	0	-1.307727	0.832790	5.078350
64	1	0	0.398781	2.511677	5.760798
65	6	0	2.314219	-1.429246	-1.621079
66	6	0	2.329119	-2.780675	-1.236235
67	6	0	2.918427	-1.089364	-2.852286
68	6	0	2.916640	-3.747602	-2.053862
69	1	0	1.825924	-3.097962	-0.333279
70	6	0	3.497115	-2.063407	-3.651170
71	1	0	2.927754	-0.062426	-3.196514
72	6	0	3.509246	-3.403800	-3.260119
73	1	0	2.890236	-4.784511	-1.731282
74	1	0	3.944195	-1.769296	-4.596454
75	1	0	3.958943	-4.160318	-3.894877
76	6	0	4.925392	0.599936	-0.066997
77	6	0	6.276909	0.496889	-0.396340
78	6	0	4.223403	1.783318	-0.292282
79	6	0	6.918720	1.575694	-0.993323
80	1	0	6.834815	-0.404186	-0.160748
81	6	0	4.880582	2.857248	-0.882407
82	1	0	3.169399	1.868373	-0.038907
83	6	0	6.222188	2.756024	-1.240199
84	1	0	7.970358	1.496406	-1.248236
85	1	0	4.326601	3.773257	-1.061307
86	1	0	6.728321	3.599034	-1.699302
87	6	0	0.465916	2.876071	-0.493075
88	6	0	-0.608441	3.430897	0.217216
89	6	0	1.123029	3.683015	-1.435807

90	6	0	-1.000587	4.742234	-0.016446
91	1	0	-1.174341	2.826125	0.913418
92	6	0	0.716034	4.993610	-1.664347
93	1	0	1.954593	3.292489	-2.014392
94	6	0	-0.347668	5.539343	-0.954669
95	1	0	-1.845350	5.139150	0.539903
96	1	0	1.239806	5.587888	-2.408510
97	1	0	-0.666253	6.561807	-1.132474

Zero-point correction= 0.773367 (Hartree/Particle)
Thermal correction to Energy= 0.826720
Thermal correction to Enthalpy= 0.827664
Thermal correction to Gibbs Free Energy= 0.684661
Sum of electronic and zero-point Energies= -3060.304158
Sum of electronic and thermal Energies= -3060.250805
Sum of electronic and thermal Enthalpies= -3060.249861
Sum of electronic and thermal Free Energies= -3060.392863
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)- LANL2DZ energy= -3061.56618896

INT8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.763628	2.449738	0.032323
2	8	0	-3.821412	2.020225	-0.497355
3	8	0	-1.685757	1.795647	0.206806
4	6	0	-2.739282	3.884031	0.500475
5	1	0	-3.736858	4.321137	0.445715
6	1	0	-2.050789	4.452414	-0.132216
7	1	0	-2.347437	3.936809	1.519629
8	6	0	-1.697656	0.822488	-3.073057
9	8	0	-2.951288	0.804539	-2.998587
10	8	0	-0.879924	0.425582	-2.181513
11	6	0	-1.067982	1.335321	-4.347273
12	1	0	-1.781954	1.937242	-4.910948
13	1	0	-0.767050	0.478955	-4.960877
14	1	0	-0.172711	1.914519	-4.109578
15	6	0	-2.698713	-2.546964	-1.649972
16	8	0	-3.704573	-1.860489	-1.960715
17	8	0	-1.691236	-2.159946	-0.976001
18	6	0	-2.670093	-3.993352	-2.089308
19	1	0	-1.661570	-4.266639	-2.408359
20	1	0	-3.389639	-4.164085	-2.891106
21	1	0	-2.935751	-4.625729	-1.235141
22	6	0	-3.774107	-0.777965	1.497096
23	8	0	-4.582843	-0.616519	0.546940
24	8	0	-2.513802	-0.620552	1.453603
25	6	0	-4.325647	-1.186064	2.842943
26	1	0	-4.275699	-0.327839	3.521264
27	1	0	-3.705324	-1.980899	3.266689
28	1	0	-5.363152	-1.509875	2.751565
29	45	0	-3.861130	0.096239	-1.265689
30	45	0	-1.591925	-0.190555	-0.338377
31	7	0	0.523567	-0.636530	1.930394
32	6	0	0.477254	-0.480570	0.460070
33	6	0	0.215993	0.682219	2.470935
34	6	0	1.074741	0.928351	0.270575
35	6	0	3.466817	-1.372051	1.959129
36	7	0	0.800252	1.588672	1.507919
37	1	0	-0.870391	0.835951	2.557293
38	1	0	0.681019	0.814840	3.455510
39	1	0	0.646835	1.428584	-0.596151
40	7	0	2.601804	0.981430	0.000023
41	1	0	3.896921	-2.365731	2.013222

42	7	0	4.065237	-0.469164	1.266116
43	1	0	2.517182	-1.120259	2.438320
44	16	0	3.196468	1.844409	-1.326060
45	6	0	3.455641	0.897482	1.132310
46	8	0	4.220987	2.762851	-0.841424
47	8	0	2.045031	2.331401	-2.068118
48	1	0	4.272298	1.615819	1.073935
49	1	0	2.871542	1.080661	2.036204
50	6	0	4.021842	0.664163	-2.380519
51	1	0	3.404807	-0.228299	-2.480402
52	1	0	4.135973	1.167330	-3.343268
53	1	0	4.999652	0.427249	-1.963249
54	6	0	1.165410	-1.558210	-0.304357
55	6	0	1.614939	-2.765057	0.261811
56	6	0	1.357778	-1.407874	-1.693209
57	6	0	2.164595	-3.786669	-0.521019
58	1	0	1.456825	-2.973268	1.312024
59	6	0	1.920238	-2.412792	-2.464000
60	1	0	0.991260	-0.507603	-2.175007
61	6	0	2.325006	-3.621577	-1.888244
62	1	0	2.455812	-4.719090	-0.043644
63	1	0	2.023933	-2.261646	-3.535752
64	1	0	2.738815	-4.417038	-2.500979
65	6	0	0.598912	2.963822	1.648921
66	6	0	0.867669	3.862364	0.607422
67	6	0	0.149751	3.479922	2.874812
68	6	0	0.697839	5.227778	0.796909
69	1	0	1.177187	3.506377	-0.365995
70	6	0	-0.021151	4.850108	3.047149
71	1	0	-0.086903	2.818445	3.700679
72	6	0	0.253874	5.738508	2.013832
73	1	0	0.910450	5.898311	-0.030807
74	1	0	-0.378086	5.219256	4.004614
75	1	0	0.119565	6.806634	2.151097
76	6	0	5.201944	-0.782265	0.441142
77	6	0	5.125005	-1.876276	-0.414354
78	6	0	6.325534	0.040189	0.478429
79	6	0	6.205063	-2.156500	-1.244588
80	1	0	4.214711	-2.465242	-0.468206
81	6	0	7.396598	-0.251995	-0.358304
82	1	0	6.371311	0.893748	1.146243
83	6	0	7.337866	-1.347508	-1.219058
84	1	0	6.145109	-2.998537	-1.926131
85	1	0	8.277132	0.381191	-0.338479
86	1	0	8.174661	-1.563738	-1.875356
87	6	0	-0.083843	-1.702857	2.651266
88	6	0	-0.816315	-2.732439	2.045994
89	6	0	0.117903	-1.758274	4.037963
90	6	0	-1.332218	-3.768542	2.813705
91	1	0	-1.001051	-2.714756	0.979150
92	6	0	-0.418045	-2.791550	4.800964
93	1	0	0.697454	-0.986527	4.536968
94	6	0	-1.147844	-3.807570	4.194740
95	1	0	-1.902367	-4.549923	2.318753
96	1	0	-0.253220	-2.799739	5.874747
97	1	0	-1.564146	-4.617488	4.785787

Zero-point correction= 0.771904 (Hartree/Particle)
Thermal correction to Energy= 0.825464
Thermal correction to Enthalpy= 0.826408
Thermal correction to Gibbs Free Energy= 0.683112
Sum of electronic and zero-point Energies= -3060.294773
Sum of electronic and thermal Energies= -3060.241214
Sum of electronic and thermal Enthalpies= -3060.240269
Sum of electronic and thermal Free Energies= -3060.383565

ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)- LANL2DZ energy= -3061.55673884

TS8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.667477	2.476388	-0.106066
2	8	0	-3.701539	2.046222	-0.691615
3	8	0	-1.615175	1.805216	0.129697
4	6	0	-2.657820	3.915349	0.336528
5	1	0	-3.672179	4.315733	0.353111
6	1	0	-2.051970	4.493929	-0.367724
7	1	0	-2.182721	4.003860	1.316434
8	6	0	-1.437461	0.709907	-3.099657
9	8	0	-2.699386	0.765760	-3.094314
10	8	0	-0.709290	0.291397	-2.148851
11	6	0	-0.711426	1.149891	-4.344304
12	1	0	-1.363210	1.755271	-4.975325
13	1	0	-0.403242	0.259313	-4.902671
14	1	0	0.187522	1.702420	-4.062206
15	6	0	-2.610279	-2.547113	-1.667302
16	8	0	-3.566699	-1.832086	-2.079917
17	8	0	-1.673360	-2.169443	-0.900437
18	6	0	-2.577671	-3.992864	-2.094440
19	1	0	-1.542431	-4.326178	-2.192158
20	1	0	-3.121911	-4.126306	-3.030535
21	1	0	-3.062611	-4.598026	-1.320766
22	6	0	-3.869735	-0.676040	1.349367
23	8	0	-4.596641	-0.536547	0.325063
24	8	0	-2.611813	-0.525418	1.393424
25	6	0	-4.536166	-1.038404	2.651783
26	1	0	-4.556967	-0.152735	3.295311
27	1	0	-3.946376	-1.805989	3.160267
28	1	0	-5.557740	-1.379714	2.480506
29	45	0	-3.704463	0.118271	-1.416924
30	45	0	-1.567005	-0.192039	-0.346451
31	7	0	0.459944	-0.570437	2.169587
32	6	0	0.896778	-0.562109	0.800882
33	6	0	0.147530	0.794064	2.558708
34	6	0	1.243592	0.897301	0.431155
35	6	0	3.176425	-1.039492	1.874964
36	7	0	0.904105	1.617420	1.635908
37	1	0	-0.932210	0.996908	2.478859
38	1	0	0.470356	0.976619	3.588879
39	1	0	0.702356	1.256964	-0.445755
40	7	0	2.689265	1.173931	0.073203
41	1	0	3.307938	-2.114354	1.864041
42	7	0	4.092387	-0.288229	1.312678
43	1	0	2.454897	-0.604038	2.560340
44	16	0	3.142702	1.870952	-1.381867
45	6	0	3.676739	1.121433	1.104662
46	8	0	4.065915	2.957860	-1.085746
47	8	0	1.917824	2.118645	-2.127419
48	1	0	4.537268	1.734862	0.846642
49	1	0	3.241760	1.478529	2.042328
50	6	0	4.077670	0.647554	-2.288188
51	1	0	3.534477	-0.296698	-2.300267
52	1	0	4.181808	1.052109	-3.297579
53	1	0	5.059102	0.530126	-1.828636
54	6	0	1.273323	-1.703101	-0.032533
55	6	0	1.410618	-3.042111	0.412334
56	6	0	1.524991	-1.481478	-1.407974
57	6	0	1.770114	-4.066250	-0.454961
58	1	0	1.253783	-3.287605	1.455667
59	6	0	1.888000	-2.511293	-2.262846
60	1	0	1.340759	-0.501212	-1.829407
61	6	0	2.024863	-3.820986	-1.803044

62	1	0	1.862753	-5.074345	-0.058514
63	1	0	2.047090	-2.284335	-3.314773
64	1	0	2.304743	-4.625876	-2.475339
65	6	0	0.678589	3.002176	1.657961
66	6	0	0.882428	3.812509	0.533553
67	6	0	0.260088	3.615526	2.849569
68	6	0	0.698560	5.187338	0.612947
69	1	0	1.141526	3.381032	-0.422601
70	6	0	0.065905	4.991885	2.911370
71	1	0	0.080365	3.025945	3.741618
72	6	0	0.290458	5.793458	1.797476
73	1	0	0.867313	5.786339	-0.277296
74	1	0	-0.262343	5.435515	3.847191
75	1	0	0.143677	6.867531	1.849312
76	6	0	5.132673	-0.838719	0.498855
77	6	0	4.900218	-1.979302	-0.268021
78	6	0	6.371372	-0.198371	0.467506
79	6	0	5.918452	-2.474014	-1.075261
80	1	0	3.923661	-2.452619	-0.275523
81	6	0	7.377967	-0.697041	-0.352302
82	1	0	6.551700	0.679387	1.080371
83	6	0	7.153933	-1.834053	-1.126641
84	1	0	5.725682	-3.352227	-1.683031
85	1	0	8.340739	-0.197037	-0.380462
86	1	0	7.940270	-2.216849	-1.769290
87	6	0	-0.224566	-1.594443	2.861541
88	6	0	-0.941478	-2.618274	2.229000
89	6	0	-0.184527	-1.577902	4.264053
90	6	0	-1.585551	-3.591227	2.984968
91	1	0	-1.021977	-2.645518	1.150724
92	6	0	-0.855129	-2.538774	5.010889
93	1	0	0.388229	-0.812390	4.779410
94	6	0	-1.558667	-3.559190	4.376831
95	1	0	-2.134141	-4.374386	2.468708
96	1	0	-0.809782	-2.496456	6.095439
97	1	0	-2.073739	-4.318209	4.957589

Zero-point correction= 0.771815 (Hartree/Particle)
Thermal correction to Energy= 0.824664
Thermal correction to Enthalpy= 0.825608
Thermal correction to Gibbs Free Energy= 0.684345
Sum of electronic and zero-point Energies= -3060.257861
Sum of electronic and thermal Energies= -3060.205012
Sum of electronic and thermal Enthalpies= -3060.204068
Sum of electronic and thermal Free Energies= -3060.345330

ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)- LANL2DZ energy= -3061.51484255

TS9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.787073	2.406631	-0.051257
2	8	0	-3.838198	1.954122	-0.580290
3	8	0	-1.702955	1.765910	0.128414
4	6	0	-2.786727	3.843197	0.403941
5	1	0	-3.791876	4.262166	0.347568
6	1	0	-2.109265	4.417528	-0.234978
7	1	0	-2.392617	3.911187	1.421296
8	6	0	-1.681833	0.743017	-3.126222
9	8	0	-2.937200	0.722505	-3.051616
10	8	0	-0.868891	0.350697	-2.229421
11	6	0	-1.052730	1.253550	-4.399907
12	1	0	-0.173320	1.855527	-4.159277

13	1	0	-1.773946	1.833451	-4.976975
14	1	0	-0.725638	0.397548	-5.000207
15	6	0	-2.664085	-2.613063	-1.651645
16	8	0	-3.668714	-1.931999	-1.984094
17	8	0	-1.664969	-2.208412	-0.977086
18	6	0	-2.637132	-4.066985	-2.061167
19	1	0	-1.618778	-4.366301	-2.318628
20	1	0	-3.315230	-4.240688	-2.897712
21	1	0	-2.965021	-4.676033	-1.211675
22	6	0	-3.780560	-0.798493	1.449487
23	8	0	-4.581175	-0.665435	0.485346
24	8	0	-2.523712	-0.623710	1.410721
25	6	0	-4.340418	-1.186960	2.795845
26	1	0	-4.320210	-0.311013	3.452599
27	1	0	-3.706797	-1.955679	3.246981
28	1	0	-5.368701	-1.537272	2.698744
29	45	0	-3.838478	0.026633	-1.318044
30	45	0	-1.594237	-0.224965	-0.379712
31	7	0	0.448531	-0.549190	1.994726
32	6	0	0.516390	-0.437415	0.544687
33	6	0	0.186648	0.781113	2.517545
34	6	0	1.066497	0.982627	0.310160
35	6	0	3.348005	-1.692091	1.606272
36	7	0	0.778763	1.665010	1.540378
37	1	0	-0.895874	0.960957	2.619218
38	1	0	0.667042	0.915627	3.494355
39	1	0	0.618969	1.462949	-0.558372
40	7	0	2.561378	0.985723	0.029025
41	1	0	3.894340	-2.620863	1.713513
42	7	0	4.025477	-0.657037	1.097308
43	1	0	2.604498	-1.436116	2.349402
44	16	0	3.186422	1.916675	-1.223169
45	6	0	3.431262	0.692831	1.139442
46	8	0	4.181506	2.830624	-0.676336
47	8	0	2.049291	2.415025	-1.985175
48	1	0	4.235536	1.425020	1.185937
49	1	0	2.843793	0.774427	2.055123
50	6	0	4.057289	0.796666	-2.308450
51	1	0	5.015257	0.525243	-1.867903
52	1	0	3.442984	-0.084235	-2.490474
53	1	0	4.213506	1.357581	-3.232608
54	6	0	1.208567	-1.487824	-0.168081
55	6	0	1.769241	-2.643353	0.467204
56	6	0	1.417037	-1.371732	-1.570233
57	6	0	2.292828	-3.711186	-0.325546
58	1	0	1.397253	-2.942388	1.439308
59	6	0	1.986324	-2.387178	-2.296181
60	1	0	1.028582	-0.498137	-2.081512
61	6	0	2.415080	-3.591506	-1.681560
62	1	0	2.590854	-4.628112	0.176831
63	1	0	2.084069	-2.274586	-3.372985
64	1	0	2.817273	-4.400411	-2.283470
65	6	0	0.542755	3.038093	1.649465
66	6	0	0.784949	3.923048	0.589888
67	6	0	0.071323	3.567495	2.861988
68	6	0	0.566583	5.285514	0.748043
69	1	0	1.120650	3.559122	-0.371459
70	6	0	-0.149394	4.934350	3.002559
71	1	0	-0.135728	2.920126	3.706646
72	6	0	0.096842	5.808243	1.950068
73	1	0	0.763275	5.944210	-0.093069
74	1	0	-0.519990	5.312025	3.951490
75	1	0	-0.074800	6.873940	2.062636
76	6	0	5.216174	-0.857665	0.332775
77	6	0	5.308931	-1.921578	-0.561491
78	6	0	6.288513	0.024473	0.484667
79	6	0	6.467697	-2.094837	-1.311485

80	1	0	4.462972	-2.583433	-0.702987
81	6	0	7.436895	-0.149681	-0.279297
82	1	0	6.236921	0.845045	1.191553
83	6	0	7.531526	-1.207320	-1.181114
84	1	0	6.526302	-2.919470	-2.014989
85	1	0	8.262490	0.544837	-0.162492
86	1	0	8.429119	-1.337054	-1.777123
87	6	0	-0.143485	-1.609815	2.715222
88	6	0	-0.791952	-2.693053	2.101957
89	6	0	-0.036794	-1.611738	4.115051
90	6	0	-1.314872	-3.726106	2.869077
91	1	0	-0.924343	-2.711221	1.027121
92	6	0	-0.577350	-2.644758	4.873741
93	1	0	0.473233	-0.801693	4.626196
94	6	0	-1.220218	-3.713759	4.259171
95	1	0	-1.820490	-4.545093	2.364749
96	1	0	-0.483690	-2.610931	5.955511
97	1	0	-1.638540	-4.522337	4.850357

Zero-point correction= 0.772204 (Hartree/Particle)
Thermal correction to Energy= 0.824946
Thermal correction to Enthalpy= 0.825890
Thermal correction to Gibbs Free Energy= 0.683989
Sum of electronic and zero-point Energies= -3060.286695
Sum of electronic and thermal Energies= -3060.233953
Sum of electronic and thermal Enthalpies= -3060.233009
Sum of electronic and thermal Free Energies= -3060.374910
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)- LANL2DZ energy= -3061.54340166

INT9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.719294	1.517229	-0.067085
2	6	0	-0.836929	0.960980	0.843158
3	6	0	-2.610140	0.521238	-0.627303
4	6	0	-1.138572	-0.524085	0.934724
5	6	0	1.349705	1.610686	-1.010172
6	7	0	-2.370778	-0.638756	0.190045
7	1	0	-3.652879	0.858231	-0.554383
8	1	0	-2.388323	0.338118	-1.695534
9	1	0	-1.247588	-0.911340	1.947950
10	7	0	0.017103	-1.224339	0.333145
11	1	0	2.147334	2.097725	-1.580497
12	7	0	1.643604	0.177543	-0.942835
13	1	0	0.425970	1.730935	-1.591519
14	16	0	0.673388	-2.581340	1.039965
15	6	0	0.549211	-0.773618	-0.962770
16	8	0	0.643919	-3.688177	0.094959
17	8	0	0.025080	-2.705045	2.344205
18	1	0	0.846932	-1.677585	-1.491181
19	1	0	-0.293803	-0.353073	-1.519422
20	6	0	2.392550	-2.197283	1.325874
21	1	0	2.473193	-1.226397	1.814429
22	1	0	2.769155	-2.995889	1.968712
23	1	0	2.926610	-2.198318	0.375784
24	6	0	0.352791	1.471345	1.256436
25	6	0	1.135262	2.394329	0.342107
26	6	0	1.042270	0.865413	2.373448
27	6	0	2.404424	2.904171	0.966797
28	1	0	0.555407	3.280057	0.047553
29	6	0	2.254220	1.296897	2.784538
30	1	0	0.537772	0.080544	2.931635
31	6	0	2.920748	2.387091	2.090303

32	1	0	2.894858	3.736972	0.467573
33	1	0	2.722264	0.860995	3.661801
34	1	0	3.841371	2.787341	2.506638
35	6	0	-3.025386	-1.840956	-0.088188
36	6	0	-2.800865	-2.984816	0.690326
37	6	0	-3.953642	-1.913816	-1.137526
38	6	0	-3.477894	-4.163614	0.410096
39	1	0	-2.097165	-2.966209	1.513605
40	6	0	-4.631613	-3.100378	-1.397945
41	1	0	-4.159566	-1.049537	-1.760069
42	6	0	-4.398219	-4.235763	-0.632066
43	1	0	-3.276229	-5.037765	1.021729
44	1	0	-5.346545	-3.129760	-2.215325
45	1	0	-4.923148	-5.161899	-0.842900
46	6	0	2.943597	-0.247907	-1.304237
47	6	0	4.057997	0.398920	-0.753443
48	6	0	3.173449	-1.299042	-2.204928
49	6	0	5.349159	0.009393	-1.087960
50	1	0	3.901446	1.195076	-0.034702
51	6	0	4.469542	-1.700315	-2.513699
52	1	0	2.348967	-1.809265	-2.690655
53	6	0	5.568395	-1.050409	-1.962472
54	1	0	6.190949	0.529787	-0.639774
55	1	0	4.613884	-2.521637	-3.209607
56	1	0	6.577205	-1.364332	-2.210857
57	6	0	-2.004041	2.879707	-0.252316
58	6	0	-1.715396	3.831588	0.733069
59	6	0	-2.618237	3.292845	-1.440787
60	6	0	-2.038466	5.166243	0.524746
61	1	0	-1.248785	3.517532	1.660349
62	6	0	-2.942889	4.630920	-1.633322
63	1	0	-2.835900	2.570871	-2.221778
64	6	0	-2.653045	5.576736	-0.655485
65	1	0	-1.811427	5.890816	1.301001
66	1	0	-3.419214	4.932859	-2.561200
67	1	0	-2.901306	6.621616	-0.811011

Zero-point correction= 0.557743 (Hartree/Particle)
Thermal correction to Energy= 0.588027
Thermal correction to Enthalpy= 0.588971
Thermal correction to Gibbs Free Energy= 0.496124
Sum of electronic and zero-point Energies= -1927.718215
Sum of electronic and thermal Energies= -1927.687931
Sum of electronic and thermal Enthalpies= -1927.686987
Sum of electronic and thermal Free Energies= -1927.779834

ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)- LANL2DZ energy= -1928.69825826

TS10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.933482	1.397100	-2.701424
2	8	0	-3.106891	0.950062	-2.823468
3	8	0	-1.170168	1.237348	-1.698529
4	6	0	-1.374950	2.220450	-3.835801
5	1	0	-2.004845	2.135136	-4.721558
6	1	0	-0.354938	1.898870	-4.062475
7	1	0	-1.334372	3.269018	-3.521858
8	6	0	-1.836533	-2.165872	-1.725082
9	8	0	-3.002349	-1.864190	-2.083746
10	8	0	-1.125155	-1.535595	-0.873929
11	6	0	-1.195317	-3.377508	-2.356785
12	1	0	-1.917060	-3.920793	-2.966808
13	1	0	-0.792191	-4.034131	-1.579315
14	1	0	-0.360354	-3.048892	-2.984757

15	6	0	-3.832579	-1.364476	1.364401
16	8	0	-4.557381	-1.283679	0.334177
17	8	0	-2.682744	-0.847215	1.517443
18	6	0	-4.391763	-2.128364	2.539575
19	1	0	-3.598952	-2.380179	3.245522
20	1	0	-4.901994	-3.028920	2.190234
21	1	0	-5.133240	-1.500678	3.044650
22	6	0	-3.922410	2.215474	0.338575
23	8	0	-4.657012	1.539143	-0.433863
24	8	0	-2.734896	1.928573	0.687083
25	6	0	-4.484923	3.499768	0.893858
26	1	0	-3.967262	4.342468	0.424683
27	1	0	-4.295467	3.552414	1.968714
28	1	0	-5.553608	3.570640	0.689891
29	45	0	-3.910211	-0.177916	-1.293206
30	45	0	-1.874335	0.217900	-0.043332
31	7	0	1.705899	-2.096749	1.230275
32	6	0	2.606119	-1.101048	1.489471
33	6	0	1.871425	-2.649032	-0.103520
34	6	0	3.437858	-0.874985	0.246658
35	6	0	0.121934	0.713088	1.273356
36	7	0	3.069727	-2.004267	-0.578182
37	1	0	1.997002	-3.738823	-0.044653
38	1	0	0.986018	-2.424530	-0.714748
39	1	0	4.512073	-0.844596	0.435022
40	7	0	3.089003	0.444559	-0.333478
41	1	0	-0.576051	1.285085	1.867612
42	7	0	0.936082	1.400641	0.396082
43	1	0	0.085822	-0.364797	1.186317
44	16	0	4.282042	1.496031	-0.847757
45	6	0	1.685305	0.722736	-0.646842
46	8	0	4.013259	1.886399	-2.223049
47	8	0	5.548761	0.865626	-0.481338
48	1	0	1.661518	1.310947	-1.562063
49	1	0	1.186133	-0.222036	-0.872035
50	6	0	4.149668	2.973307	0.148356
51	1	0	3.323890	3.585088	-0.211737
52	1	0	4.004793	2.701356	1.193949
53	1	0	5.098202	3.497196	0.009636
54	6	0	2.495713	-0.183765	2.524412
55	6	0	1.227820	0.040391	3.182065
56	6	0	3.575758	0.715857	2.816211
57	6	0	1.171394	1.016706	4.223607
58	1	0	0.492605	-0.750652	3.246218
59	6	0	3.457608	1.677078	3.775179
60	1	0	4.520283	0.590301	2.292167
61	6	0	2.237850	1.820980	4.507276
62	1	0	0.252152	1.104842	4.796146
63	1	0	4.301937	2.319511	4.006716
64	1	0	2.174255	2.559050	5.301379
65	6	0	3.497959	-2.218937	-1.889835
66	6	0	4.662162	-1.616767	-2.385868
67	6	0	2.778672	-3.083648	-2.730230
68	6	0	5.068471	-1.853966	-3.692496
69	1	0	5.257771	-0.964842	-1.759114
70	6	0	3.205841	-3.319286	-4.033141
71	1	0	1.886830	-3.588316	-2.375013
72	6	0	4.347826	-2.701792	-4.529572
73	1	0	5.967468	-1.364486	-4.054755
74	1	0	2.631578	-3.994094	-4.661767
75	1	0	4.674080	-2.880955	-5.548957
76	6	0	0.916390	2.818961	0.425255
77	6	0	1.039175	3.491915	1.642034
78	6	0	0.774560	3.557800	-0.754627
79	6	0	1.046629	4.882561	1.674982
80	1	0	1.159797	2.923368	2.556099
81	6	0	0.800299	4.946977	-0.713841

82	1	0	0.617034	3.049317	-1.697498
83	6	0	0.941238	5.618809	0.498884
84	1	0	1.154353	5.390041	2.629118
85	1	0	0.696065	5.506894	-1.638585
86	1	0	0.961958	6.703839	0.525362
87	6	0	0.967494	-2.850462	2.178798
88	6	0	1.536040	-3.215875	3.400793
89	6	0	-0.332850	-3.241194	1.858074
90	6	0	0.794565	-3.970174	4.301033
91	1	0	2.545336	-2.896511	3.639200
92	6	0	-1.058081	-4.012661	2.761275
93	1	0	-0.778957	-2.905238	0.926936
94	6	0	-0.501123	-4.376776	3.983478
95	1	0	1.235697	-4.250834	5.252535
96	1	0	-2.069374	-4.316751	2.508565
97	1	0	-1.073039	-4.971384	4.688998

Zero-point correction= 0.770571 (Hartree/Particle)
Thermal correction to Energy= 0.823075
Thermal correction to Enthalpy= 0.824020
Thermal correction to Gibbs Free Energy= 0.682741
Sum of electronic and zero-point Energies= -3060.269774
Sum of electronic and thermal Energies= -3060.217269
Sum of electronic and thermal Enthalpies= -3060.216325
Sum of electronic and thermal Free Energies= -3060.357603
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)- LANL2DZ energy= -3061.52495032

INT10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.109481	2.706551	-0.244071
2	8	0	-3.305084	2.476972	-0.544668
3	8	0	-1.263014	1.875795	0.226938
4	6	0	-1.581810	4.111766	-0.437391
5	1	0	-2.302889	4.722244	-0.982403
6	1	0	-0.626890	4.079447	-0.970667
7	1	0	-1.396609	4.562948	0.543117
8	6	0	-2.420277	-0.356977	-2.462423
9	8	0	-3.578958	0.021543	-2.201828
10	8	0	-1.437603	-0.452951	-1.640829
11	6	0	-2.099677	-0.740734	-3.893482
12	1	0	-3.006751	-0.751393	-4.498162
13	1	0	-1.624324	-1.726929	-3.916898
14	1	0	-1.392811	-0.020091	-4.320413
15	6	0	-3.712064	-2.289228	0.413071
16	8	0	-4.601519	-1.447410	0.139348
17	8	0	-2.461109	-2.080113	0.543567
18	6	0	-4.170883	-3.715436	0.638928
19	1	0	-3.327928	-4.408572	0.608619
20	1	0	-4.922940	-3.987897	-0.105186
21	1	0	-4.641309	-3.778931	1.625671
22	6	0	-3.428427	0.735695	2.619658
23	8	0	-4.340760	1.003609	1.797923
24	8	0	-2.291049	0.219212	2.369622
25	6	0	-3.695531	1.023795	4.080741
26	1	0	-2.780753	1.369345	4.567894
27	1	0	-4.009335	0.096407	4.571787
28	1	0	-4.492833	1.761470	4.183139
29	45	0	-4.108319	0.563707	-0.230550
30	45	0	-1.782949	-0.127236	0.419148
31	7	0	1.959383	-1.861820	-1.576859
32	6	0	2.859808	-1.333347	-0.800596
33	6	0	1.460393	-0.927957	-2.596635
34	6	0	3.167024	0.082158	-1.266653
35	6	0	0.079853	-0.792951	1.006507

36	7	0	2.375741	0.174807	-2.487944
37	1	0	1.523925	-1.423420	-3.573066
38	1	0	0.409412	-0.713802	-2.355196
39	1	0	4.235160	0.188280	-1.475869
40	7	0	2.848234	1.040071	-0.238300
41	1	0	-0.079454	-1.342087	1.939701
42	7	0	1.141867	0.172837	1.238493
43	1	0	0.399582	-1.509431	0.241517
44	16	0	3.918448	2.285792	0.076794
45	6	0	1.441669	1.127790	0.211052
46	8	0	3.300045	3.571343	-0.190721
47	8	0	5.164850	1.908651	-0.590380
48	1	0	1.259638	2.162151	0.508578
49	1	0	0.795660	0.947527	-0.647200
50	6	0	4.179678	2.178750	1.836976
51	1	0	4.503898	1.169349	2.091789
52	1	0	4.951918	2.913080	2.076719
53	1	0	3.251563	2.420275	2.357327
54	6	0	3.483592	-1.934866	0.370130
55	6	0	2.841289	-2.925884	1.129492
56	6	0	4.736737	-1.451348	0.780434
57	6	0	3.454533	-3.431394	2.266632
58	1	0	1.848428	-3.266478	0.864560
59	6	0	5.347260	-1.973759	1.912317
60	1	0	5.236685	-0.663967	0.224690
61	6	0	4.709239	-2.965343	2.654999
62	1	0	2.943050	-4.182715	2.858815
63	1	0	6.319556	-1.601107	2.217439
64	1	0	5.185122	-3.367200	3.544130
65	6	0	2.027312	1.453821	-2.997374
66	6	0	3.053778	2.327228	-3.361875
67	6	0	0.695959	1.864012	-3.114405
68	6	0	2.750736	3.600055	-3.829809
69	1	0	4.088507	2.015698	-3.257325
70	6	0	0.402520	3.129848	-3.613360
71	1	0	-0.114596	1.225190	-2.778231
72	6	0	1.425496	4.003418	-3.969126
73	1	0	3.558056	4.277303	-4.089760
74	1	0	-0.635987	3.436251	-3.698090
75	1	0	1.192016	4.995471	-4.342349
76	6	0	1.273679	0.638890	2.579170
77	6	0	2.123384	-0.034809	3.456194
78	6	0	0.572545	1.763755	3.023238
79	6	0	2.292672	0.422571	4.760176
80	1	0	2.660033	-0.907141	3.096758
81	6	0	0.754116	2.225609	4.323270
82	1	0	-0.126702	2.244775	2.345046
83	6	0	1.616611	1.560409	5.193767
84	1	0	2.961670	-0.104233	5.435061
85	1	0	0.208229	3.101232	4.663056
86	1	0	1.753830	1.923316	6.208146
87	6	0	1.437522	-3.203211	-1.594256
88	6	0	2.319377	-4.266106	-1.769403
89	6	0	0.062261	-3.393129	-1.483998
90	6	0	1.810589	-5.558782	-1.803141
91	1	0	3.384369	-4.081308	-1.867797
92	6	0	-0.427704	-4.695593	-1.517988
93	1	0	-0.615247	-2.552912	-1.352344
94	6	0	0.439211	-5.773832	-1.672926
95	1	0	2.486491	-6.397330	-1.934952
96	1	0	-1.495480	-4.856156	-1.413482
97	1	0	0.047018	-6.785601	-1.696313

Zero-point correction= 0.771759 (Hartree/Particle)
Thermal correction to Energy= 0.826004
Thermal correction to Enthalpy= 0.826948
Thermal correction to Gibbs Free Energy= 0.680095

Sum of electronic and zero-point Energies= -3060.311056
Sum of electronic and thermal Energies= -3060.256812
Sum of electronic and thermal Enthalpies= -3060.255868
Sum of electronic and thermal Free Energies= -3060.402720

ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)- LANL2DZ energy= -3061.57060287

TS11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.139148	-0.753574	1.951504
2	8	0	-4.201529	-0.780703	1.280387
3	8	0	-1.980582	-0.448564	1.518386
4	6	0	-3.227309	-1.080148	3.423912
5	1	0	-2.338614	-1.628244	3.745653
6	1	0	-4.130135	-1.655272	3.634293
7	1	0	-3.274085	-0.140368	3.985271
8	6	0	-3.372048	2.472133	0.141605
9	8	0	-4.402576	1.790883	-0.118073
10	8	0	-2.169944	2.068841	0.100224
11	6	0	-3.579273	3.913543	0.540671
12	1	0	-4.231023	3.958093	1.417956
13	1	0	-4.086602	4.440530	-0.272608
14	1	0	-2.622355	4.392068	0.754262
15	6	0	-2.803882	0.763571	-3.092130
16	8	0	-3.954166	0.458456	-2.670782
17	8	0	-1.718543	0.720616	-2.434815
18	6	0	-2.700308	1.262677	-4.513733
19	1	0	-2.685571	2.357703	-4.498197
20	1	0	-3.560076	0.931850	-5.097892
21	1	0	-1.768579	0.919247	-4.967748
22	6	0	-2.562035	-2.520058	-1.368712
23	8	0	-3.752409	-2.125715	-1.320919
24	8	0	-1.525014	-1.839412	-1.065838
25	6	0	-2.302632	-3.943393	-1.806020
26	1	0	-1.823731	-4.494469	-0.989243
27	1	0	-1.612060	-3.944837	-2.654319
28	1	0	-3.234093	-4.437149	-2.083279
29	45	0	-4.185868	-0.175943	-0.720547
30	45	0	-1.777752	0.141635	-0.461020
31	7	0	1.593327	-1.989703	1.039409
32	6	0	2.033613	-0.714874	1.107981
33	6	0	1.833959	-2.556488	-0.278297
34	6	0	3.152982	-0.588826	0.073822
35	6	0	0.419386	0.386563	-0.206565
36	7	0	2.811802	-1.652689	-0.848717
37	1	0	2.226679	-3.576485	-0.176623
38	1	0	0.893656	-2.589891	-0.853072
39	1	0	4.116075	-0.771347	0.570953
40	7	0	3.260905	0.712894	-0.570709
41	1	0	0.225643	0.437756	0.853305
42	7	0	0.995788	1.484567	-0.873872
43	1	0	0.562914	-0.545743	-0.729332
44	16	0	4.638547	1.638815	-0.423714
45	6	0	2.226981	1.128210	-1.530989
46	8	0	5.042146	2.093232	-1.743451
47	8	0	5.563584	0.867110	0.404352
48	1	0	2.624151	1.955736	-2.115515
49	1	0	2.043538	0.291354	-2.209440
50	6	0	4.146668	3.082472	0.502817
51	1	0	3.667095	2.773873	1.431997
52	1	0	5.062874	3.643450	0.700773
53	1	0	3.457940	3.678641	-0.097641
54	6	0	2.038592	0.028899	2.386375
55	6	0	0.866951	0.144689	3.153047
56	6	0	3.218677	0.616352	2.854965

57	6	0	0.879485	0.850127	4.346809
58	1	0	-0.066932	-0.282809	2.793452
59	6	0	3.221260	1.325517	4.054555
60	1	0	4.146618	0.524916	2.299126
61	6	0	2.054936	1.449111	4.800539
62	1	0	-0.038088	0.941919	4.919566
63	1	0	4.144434	1.779195	4.402000
64	1	0	2.058583	2.008468	5.731035
65	6	0	3.685611	-2.118319	-1.840711
66	6	0	4.997996	-1.646343	-1.960438
67	6	0	3.220817	-3.077848	-2.751706
68	6	0	5.816409	-2.126862	-2.977603
69	1	0	5.400011	-0.921539	-1.262971
70	6	0	4.055647	-3.558793	-3.752757
71	1	0	2.196730	-3.434710	-2.690639
72	6	0	5.358384	-3.084375	-3.876790
73	1	0	6.829737	-1.744947	-3.056110
74	1	0	3.676349	-4.302857	-4.447067
75	1	0	6.006253	-3.454335	-4.664861
76	6	0	0.885752	2.794748	-0.361086
77	6	0	0.622606	3.062134	0.985450
78	6	0	1.066183	3.873946	-1.236892
79	6	0	0.570917	4.374250	1.444648
80	1	0	0.457303	2.255304	1.687827
81	6	0	1.029277	5.181745	-0.768664
82	1	0	1.215105	3.681933	-2.295268
83	6	0	0.785719	5.442314	0.578956
84	1	0	0.371044	4.555992	2.496934
85	1	0	1.174007	6.001720	-1.466059
86	1	0	0.752511	6.463945	0.944453
87	6	0	0.834650	-2.720731	1.999119
88	6	0	1.404978	-3.029546	3.233855
89	6	0	-0.447553	-3.154345	1.675080
90	6	0	0.673541	-3.767311	4.156903
91	1	0	2.407996	-2.685253	3.464236
92	6	0	-1.163336	-3.910487	2.598792
93	1	0	-0.884826	-2.861154	0.726696
94	6	0	-0.608586	-4.213807	3.839376
95	1	0	1.110964	-4.004061	5.121668
96	1	0	-2.167172	-4.243072	2.351778
97	1	0	-1.173807	-4.796957	4.559880

Zero-point correction= 0.771030 (Hartree/Particle)
Thermal correction to Energy= 0.824701
Thermal correction to Enthalpy= 0.825645
Thermal correction to Gibbs Free Energy= 0.678416
Sum of electronic and zero-point Energies= -3060.292087
Sum of electronic and thermal Energies= -3060.238416
Sum of electronic and thermal Enthalpies= -3060.237472
Sum of electronic and thermal Free Energies= -3060.384701
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)- LANL2DZ energy= -3061.54923553

TS12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.921966	2.324354	-1.946971
2	8	0	-2.755878	2.886525	-1.190300
3	8	0	-1.371307	1.195907	-1.743885
4	6	0	-1.516148	3.037642	-3.213080
5	1	0	-0.428244	3.156457	-3.232969
6	1	0	-2.002096	4.011324	-3.279711
7	1	0	-1.796661	2.423966	-4.074207
8	6	0	-4.411874	-0.280363	-1.153578

9	8	0	-4.755796	0.851337	-0.705566
10	8	0	-3.289910	-0.842130	-0.979716
11	6	0	-5.427866	-1.060191	-1.947396
12	1	0	-6.050748	-1.632383	-1.251528
13	1	0	-4.920625	-1.756847	-2.617492
14	1	0	-6.074917	-0.379382	-2.503638
15	6	0	-3.383586	-0.279895	2.399912
16	8	0	-4.027654	0.765086	2.108205
17	8	0	-2.391248	-0.743322	1.755655
18	6	0	-3.806740	-1.058038	3.618842
19	1	0	-3.114183	-1.882235	3.799444
20	1	0	-4.815345	-1.450378	3.456494
21	1	0	-3.850250	-0.389236	4.483042
22	6	0	-0.820511	2.307195	1.696063
23	8	0	-1.979110	2.792401	1.648064
24	8	0	-0.411413	1.268160	1.084569
25	6	0	0.207139	3.026361	2.539023
26	1	0	-0.259731	3.823028	3.118359
27	1	0	0.972139	3.456622	1.882784
28	1	0	0.697181	2.314013	3.209272
29	45	0	-3.423405	1.868774	0.478401
30	45	0	-1.783242	0.132087	-0.002534
31	6	0	-0.177937	-1.668230	-0.666581
32	6	0	-0.299464	-2.130232	0.662897
33	1	0	-1.221864	-2.633342	0.951677
34	6	0	-0.967663	-2.302475	-1.765606
35	6	0	-0.846588	-1.815281	-3.073245
36	6	0	-1.846362	-3.373579	-1.552908
37	6	0	-1.592664	-2.349816	-4.116158
38	1	0	-0.172203	-0.990837	-3.279002
39	6	0	-2.593893	-3.909525	-2.594620
40	1	0	-1.958845	-3.803411	-0.562964
41	6	0	-2.478441	-3.398760	-3.884307
42	1	0	-1.478526	-1.944142	-5.117776
43	1	0	-3.264323	-4.740937	-2.395050
44	1	0	-3.057760	-3.822170	-4.699605
45	7	0	0.642332	-1.958452	1.568331
46	16	0	0.326880	-2.441370	3.110943
47	8	0	-0.900562	-3.230444	3.228791
48	8	0	1.575372	-2.994177	3.633841
49	6	0	0.055988	-0.876143	3.936367
50	1	0	0.968193	-0.282235	3.852799
51	1	0	-0.780370	-0.376287	3.447983
52	1	0	-0.163739	-1.087146	4.985204
53	6	0	2.211691	0.575241	0.800386
54	6	0	1.425732	0.070398	-1.480306
55	6	0	3.927027	-1.681352	1.510674
56	1	0	2.457973	1.363192	1.499424
57	1	0	2.036443	0.096553	-2.389392
58	1	0	2.960043	-2.162337	1.653814
59	7	0	1.161211	-1.251188	-1.055679
60	7	0	2.163218	0.902745	-0.465933
61	7	0	3.970634	-0.431701	1.272853
62	1	0	4.838182	-2.281150	1.581741
63	1	0	0.493374	0.594754	-1.680630
64	1	0	1.647771	-0.294157	1.133463
65	6	0	2.149559	-2.231816	-1.265150
66	6	0	3.444340	-1.883492	-1.687744
67	6	0	1.883561	-3.594106	-1.048414
68	6	0	4.410000	-2.860150	-1.918873
69	1	0	3.727095	-0.844880	-1.820245
70	6	0	2.862004	-4.554975	-1.261081
71	1	0	0.903606	-3.911344	-0.719015
72	6	0	4.134818	-4.204466	-1.704588
73	1	0	5.391581	-2.553849	-2.273113
74	1	0	2.616167	-5.597169	-1.080497
75	1	0	4.891209	-4.962489	-1.880031

76	6	0	5.182665	0.241766	0.993361
77	6	0	6.100438	-0.268724	0.073222
78	6	0	5.402805	1.489521	1.581310
79	6	0	7.231855	0.472794	-0.257008
80	1	0	5.906277	-1.227513	-0.396102
81	6	0	6.539273	2.218392	1.254341
82	1	0	4.684526	1.878989	2.296178
83	6	0	7.452849	1.716414	0.328579
84	1	0	7.939382	0.076537	-0.978977
85	1	0	6.708373	3.185383	1.717513
86	1	0	8.333916	2.293327	0.065683
87	6	0	2.540009	2.210758	-0.918319
88	6	0	1.553397	3.193952	-0.985676
89	6	0	3.845361	2.478852	-1.318109
90	6	0	1.884507	4.466452	-1.439627
91	1	0	0.541996	2.945548	-0.680169
92	6	0	4.169651	3.757599	-1.764518
93	1	0	4.599739	1.700190	-1.268149
94	6	0	3.193773	4.749034	-1.825949
95	1	0	1.119783	5.235519	-1.487834
96	1	0	5.189984	3.975083	-2.064212
97	1	0	3.452402	5.743278	-2.176915

Zero-point correction= 0.768355 (Hartree/Particle)
Thermal correction to Energy= 0.822935
Thermal correction to Enthalpy= 0.823879
Thermal correction to Gibbs Free Energy= 0.676441
Sum of electronic and zero-point Energies= -3060.300338
Sum of electronic and thermal Energies= -3060.245758
Sum of electronic and thermal Enthalpies= -3060.244814
Sum of electronic and thermal Free Energies= -3060.392252
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)- LANL2DZ energy= -3061.55858854

INT11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.310393	1.924575	-1.138862
2	8	0	-3.335602	1.462547	-0.574235
3	8	0	-1.145843	1.414442	-1.105346
4	6	0	-2.469166	3.181982	-1.957860
5	1	0	-1.534264	3.745003	-1.989967
6	1	0	-3.274342	3.798175	-1.554827
7	1	0	-2.735918	2.892226	-2.980078
8	6	0	-2.556685	-1.516557	-2.252805
9	8	0	-3.557095	-1.260811	-1.524432
10	8	0	-1.343532	-1.288685	-1.965006
11	6	0	-2.815984	-2.140726	-3.600172
12	1	0	-3.465873	-3.011442	-3.480499
13	1	0	-1.874523	-2.424830	-4.072464
14	1	0	-3.342589	-1.418932	-4.232195
15	6	0	-1.864006	-2.798440	1.173576
16	8	0	-3.010874	-2.274958	1.150236
17	8	0	-0.799830	-2.279016	0.710946
18	6	0	-1.712546	-4.165666	1.788402
19	1	0	-0.676626	-4.325118	2.095690
20	1	0	-1.974083	-4.917315	1.035805
21	1	0	-2.398962	-4.278470	2.629981
22	6	0	-1.571096	0.669596	2.448686
23	8	0	-2.767219	0.429311	2.155180
24	8	0	-0.558517	0.480734	1.697083
25	6	0	-1.317456	1.274370	3.811727
26	1	0	-1.903404	0.739297	4.562138
27	1	0	-1.658079	2.315703	3.813827
28	1	0	-0.259565	1.239011	4.075796

29	45	0	-3.231438	-0.405809	0.312791
30	45	0	-0.832980	-0.430698	-0.188903
31	6	0	1.560924	-0.596116	-0.742367
32	6	0	1.753509	-1.457233	0.384378
33	1	0	1.519962	-2.512440	0.256633
34	6	0	1.555476	-1.218499	-2.104098
35	6	0	1.971403	-0.485172	-3.221722
36	6	0	1.128481	-2.538838	-2.321116
37	6	0	1.958575	-1.037900	-4.499187
38	1	0	2.335050	0.529443	-3.093370
39	6	0	1.129356	-3.095399	-3.592151
40	1	0	0.750513	-3.132278	-1.495308
41	6	0	1.539553	-2.348663	-4.695313
42	1	0	2.291795	-0.439073	-5.342412
43	1	0	0.797187	-4.121884	-3.722001
44	1	0	1.537091	-2.785408	-5.689550
45	7	0	2.170843	-1.041601	1.549567
46	16	0	2.242230	-2.207131	2.739223
47	8	0	1.971521	-3.547569	2.214154
48	8	0	3.454086	-1.976968	3.511485
49	6	0	0.847066	-1.752823	3.761320
50	1	0	1.005619	-0.743459	4.141939
51	1	0	-0.054752	-1.802193	3.151122
52	1	0	0.804838	-2.467299	4.586110
53	6	0	1.423113	1.961014	1.571906
54	6	0	1.696297	1.873698	-0.862798
55	1	0	1.094145	2.474623	2.468265
56	1	0	2.364547	2.592799	-1.343000
57	7	0	2.319145	0.643103	-0.653327
58	7	0	1.253552	2.546190	0.445400
59	1	0	0.771609	1.780916	-1.429335
60	1	0	1.920047	0.984310	1.617974
61	6	0	3.730386	0.615185	-0.507035
62	6	0	4.426950	1.751514	-0.074656
63	6	0	4.462359	-0.543837	-0.793399
64	6	0	5.813939	1.733496	0.045134
65	1	0	3.897809	2.659303	0.200177
66	6	0	5.843452	-0.553849	-0.660088
67	1	0	3.954008	-1.438638	-1.130965
68	6	0	6.534091	0.582591	-0.245821
69	1	0	6.326489	2.628622	0.385825
70	1	0	6.384937	-1.467024	-0.887544
71	1	0	7.614116	0.565439	-0.142180
72	6	0	0.524479	3.777512	0.331344
73	6	0	-0.733990	3.876634	0.918696
74	6	0	1.069710	4.838637	-0.385567
75	6	0	-1.448108	5.062972	0.802294
76	1	0	-1.162140	3.014903	1.415989
77	6	0	0.342104	6.019662	-0.501903
78	1	0	2.056692	4.758708	-0.829393
79	6	0	-0.912567	6.134361	0.091361
80	1	0	-2.433271	5.138743	1.250777
81	1	0	0.763367	6.853726	-1.053472
82	1	0	-1.475215	7.057191	-0.005431

Zero-point correction= 0.642060 (Hartree/Particle)
Thermal correction to Energy= 0.689519
Thermal correction to Enthalpy= 0.690463
Thermal correction to Gibbs Free Energy= 0.559164
Sum of electronic and zero-point Energies= -2734.832338
Sum of electronic and thermal Energies= -2734.784880
Sum of electronic and thermal Enthalpies= -2734.783935
Sum of electronic and thermal Free Energies= -2734.915234

ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)- LANL2DZ energy= -2735.88204583

INT12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.431903	-2.581546	-0.550302
2	8	0	-3.520289	-1.980272	-0.752026
3	8	0	-1.321224	-2.037652	-0.250572
4	6	0	-2.431679	-4.086693	-0.645530
5	1	0	-3.337290	-4.438615	-1.140253
6	1	0	-2.391326	-4.503387	0.366308
7	1	0	-1.543468	-4.427187	-1.182844
8	6	0	-2.998834	-0.182518	2.246447
9	8	0	-3.976875	-0.131939	1.447467
10	8	0	-1.772041	-0.141130	1.929215
11	6	0	-3.307137	-0.272835	3.719387
12	1	0	-2.465273	-0.716092	4.253645
13	1	0	-4.220265	-0.849224	3.878865
14	1	0	-3.470607	0.739270	4.104469
15	6	0	-2.407052	2.664568	-0.055651
16	8	0	-3.509986	2.120113	-0.334362
17	8	0	-1.299899	2.066505	0.121203
18	6	0	-2.381486	4.169342	0.045638
19	1	0	-3.367681	4.547007	0.319104
20	1	0	-2.112260	4.580947	-0.933128
21	1	0	-1.630556	4.488608	0.770664
22	6	0	-1.845598	0.285623	-2.869288
23	8	0	-3.064216	0.273069	-2.549212
24	8	0	-0.861106	0.200868	-2.068124
25	6	0	-1.507230	0.381805	-4.336042
26	1	0	-1.230404	-0.613841	-4.698337
27	1	0	-0.648836	1.041437	-4.481151
28	1	0	-2.367057	0.739035	-4.903584
29	45	0	-3.593601	0.073906	-0.562597
30	45	0	-1.239432	0.013454	-0.044624
31	6	0	3.542982	0.238007	-0.903555
32	6	0	1.588782	-1.083358	-0.533723
33	6	0	1.514662	1.242946	-0.057755
34	1	0	4.627031	0.246253	-0.791428
35	1	0	1.218855	-2.070209	-0.273110
36	1	0	1.080851	1.410302	-1.055265
37	7	0	1.017960	-0.072304	0.380584
38	7	0	3.033550	-1.038766	-0.465057
39	7	0	2.963040	1.284186	-0.068511
40	1	0	1.120481	2.006523	0.611696
41	1	0	1.218607	-0.835905	-1.539547
42	1	0	3.301183	0.428836	-1.973199
43	6	0	1.253732	-0.402503	1.775590
44	6	0	0.763859	-1.622964	2.248769
45	6	0	1.899975	0.460398	2.657136
46	6	0	0.932343	-1.978285	3.579741
47	1	0	0.200709	-2.270738	1.584841
48	6	0	2.051097	0.102365	3.995399
49	1	0	2.316870	1.397997	2.313982
50	6	0	1.577178	-1.116414	4.463940
51	1	0	0.539935	-2.928519	3.930239
52	1	0	2.559998	0.785546	4.668917
53	1	0	1.706254	-1.392710	5.505949
54	6	0	3.565652	2.557876	-0.149638
55	6	0	4.931476	2.688214	0.146216
56	6	0	2.839399	3.709826	-0.476843
57	6	0	5.550048	3.928935	0.100913
58	1	0	5.499387	1.812006	0.444458
59	6	0	3.465624	4.954895	-0.498915
60	1	0	1.785058	3.646110	-0.725051
61	6	0	4.821020	5.074011	-0.219452
62	1	0	6.607385	4.005130	0.337619
63	1	0	2.882067	5.835696	-0.751152
64	1	0	5.305387	6.045025	-0.244532

65	6	0	3.745576	-2.213707	-0.770852
66	6	0	3.478069	-3.377450	-0.034199
67	6	0	4.732161	-2.255038	-1.761719
68	6	0	4.169606	-4.550640	-0.297774
69	1	0	2.750547	-3.338045	0.772028
70	6	0	5.438003	-3.432558	-2.002440
71	1	0	4.945476	-1.375457	-2.361213
72	6	0	5.157897	-4.586982	-1.281796
73	1	0	3.951362	-5.439656	0.286968
74	1	0	6.203197	-3.443641	-2.773396
75	1	0	5.704757	-5.503916	-1.477662

Zero-point correction= 0.600451 (Hartree/Particle)
Thermal correction to Energy= 0.640568
Thermal correction to Enthalpy= 0.641513
Thermal correction to Gibbs Free Energy= 0.522786
Sum of electronic and zero-point Energies= -2109.024115
Sum of electronic and thermal Energies= -2108.983997
Sum of electronic and thermal Enthalpies= -2108.983053
Sum of electronic and thermal Free Energies= -2109.101780
ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)- LANL2DZ energy= -2109.93130581

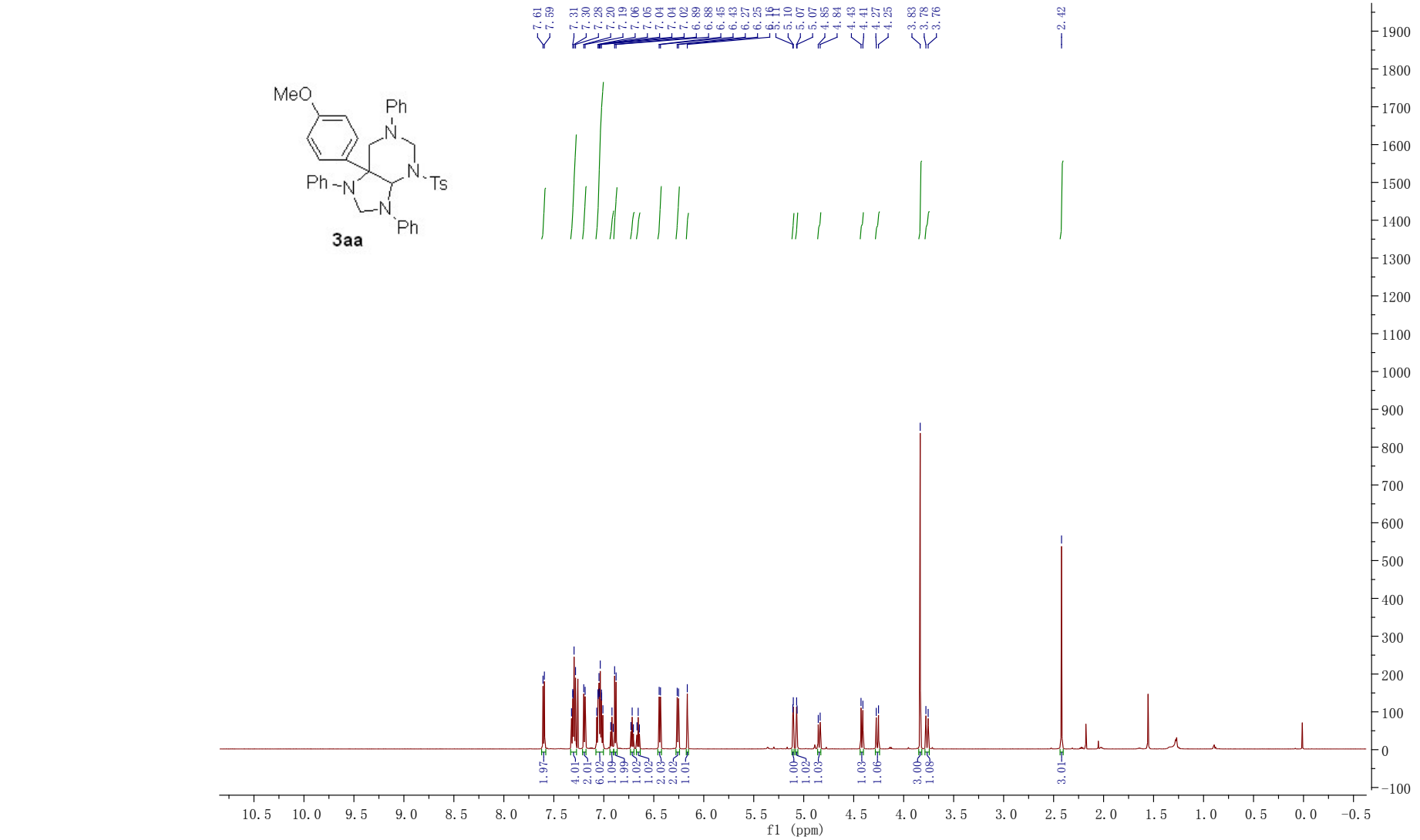
INT13

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.107098	0.578817	-2.043404
2	8	0	3.718845	-0.390639	-1.518062
3	8	0	1.966598	1.028624	-1.707524
4	6	0	3.798745	1.309911	-3.168616
5	1	0	4.572487	0.682477	-3.612869
6	1	0	4.265123	2.212927	-2.760781
7	1	0	3.071142	1.619199	-3.921880
8	6	0	3.155580	1.037520	1.620826
9	8	0	3.759629	-0.042135	1.368417
10	8	0	2.022713	1.389700	1.174654
11	6	0	3.841869	2.014178	2.544712
12	1	0	3.221493	2.899079	2.690936
13	1	0	4.804700	2.300338	2.111698
14	1	0	4.043487	1.527796	3.503489
15	6	0	0.762361	-1.765218	2.068670
16	8	0	1.863436	-2.240899	1.703641
17	8	0	0.130056	-0.806666	1.509790
18	6	0	0.086606	-2.388440	3.270205
19	1	0	0.750340	-3.105710	3.753328
20	1	0	-0.826191	-2.903545	2.949273
21	1	0	-0.199324	-1.606770	3.979734
22	6	0	0.786667	-2.287784	-1.725738
23	8	0	1.888021	-2.648027	-1.245730
24	8	0	0.145666	-1.225275	-1.432110
25	6	0	0.124823	-3.194287	-2.739361
26	1	0	-0.035082	-2.641653	-3.669912
27	1	0	-0.856646	-3.507617	-2.367553
28	1	0	0.742460	-4.071798	-2.931864
29	45	0	2.882242	-1.391787	0.084574
30	45	0	1.002754	0.177022	-0.118635
31	6	0	-2.754530	-0.526225	-1.265121
32	6	0	-1.343737	1.469915	-1.516915
33	6	0	-2.290636	-0.363501	1.149929
34	1	0	-3.674908	-0.953704	-1.673053
35	1	0	-1.501596	2.433327	-2.011910
36	1	0	-1.920495	0.652976	0.943081
37	7	0	-0.620159	1.585716	-0.276158
38	7	0	-2.690486	0.872981	-1.340047
39	7	0	-2.694594	-1.071297	0.160680

40	1	0	-2.295355	-0.807706	2.137134
41	1	0	-0.833755	0.824059	-2.239142
42	1	0	-1.889687	-0.968354	-1.761803
43	6	0	-0.199248	2.877511	0.077326
44	6	0	0.245168	3.839619	-0.845238
45	6	0	-0.206106	3.235079	1.436729
46	6	0	0.630664	5.110556	-0.425225
47	1	0	0.326365	3.576592	-1.895683
48	6	0	0.193647	4.495533	1.854015
49	1	0	-0.522310	2.488202	2.159484
50	6	0	0.607765	5.449940	0.923712
51	1	0	0.968202	5.835160	-1.162028
52	1	0	0.173606	4.741540	2.912832
53	1	0	0.912426	6.440637	1.248204
54	6	0	-2.995592	-2.470081	0.305878
55	6	0	-4.319069	-2.891235	0.363803
56	6	0	-1.935638	-3.370778	0.344151
57	6	0	-4.584164	-4.252825	0.478277
58	1	0	-5.122553	-2.161010	0.336820
59	6	0	-2.214308	-4.729404	0.458047
60	1	0	-0.918061	-3.000303	0.281145
61	6	0	-3.534986	-5.168767	0.524587
62	1	0	-5.611791	-4.596988	0.534001
63	1	0	-1.396097	-5.441351	0.493164
64	1	0	-3.748050	-6.229316	0.612838
65	6	0	-3.743248	1.638690	-0.798896
66	6	0	-3.554210	2.983666	-0.442546
67	6	0	-5.016916	1.079990	-0.596725
68	6	0	-4.605949	3.733131	0.071623
69	1	0	-2.584399	3.454414	-0.540583
70	6	0	-6.060058	1.841725	-0.081871
71	1	0	-5.219403	0.047302	-0.861020
72	6	0	-5.867073	3.175927	0.257830
73	1	0	-4.422202	4.769432	0.339468
74	1	0	-7.034143	1.379190	0.051420
75	1	0	-6.680795	3.767373	0.664875

Zero-point correction= 0.596634 (Hartree/Particle)
Thermal correction to Energy= 0.638208
Thermal correction to Enthalpy= 0.639152
Thermal correction to Gibbs Free Energy= 0.519241
Sum of electronic and zero-point Energies= -2108.967560
Sum of electronic and thermal Energies= -2108.925986
Sum of electronic and thermal Enthalpies= -2108.925042
Sum of electronic and thermal Free Energies= -2109.044953

ωB97XD /6-311++G (d, p)-SDD/SMD// ωB97XD /6-31G(d)- LANL2DZ energy= -2109.87530250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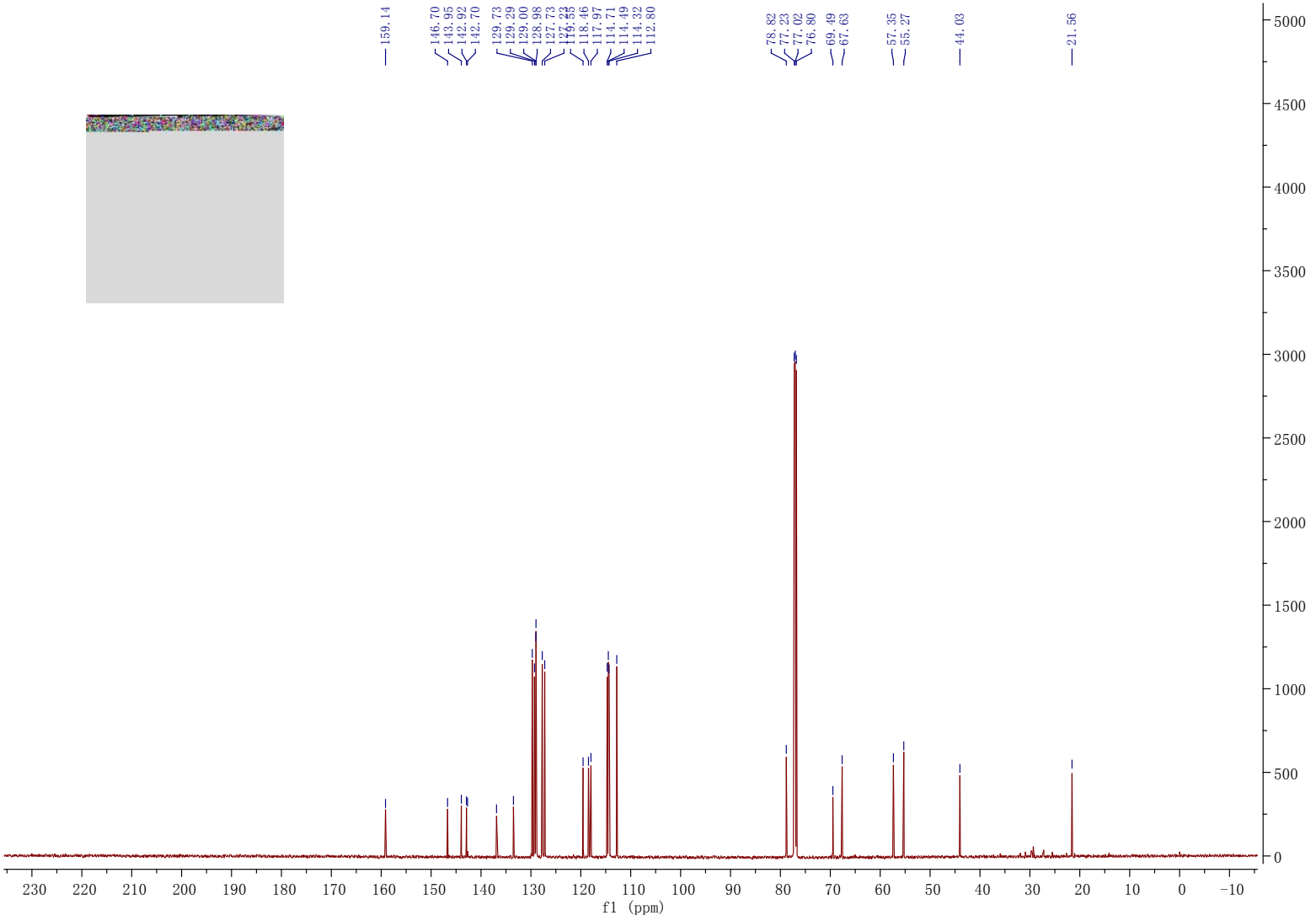
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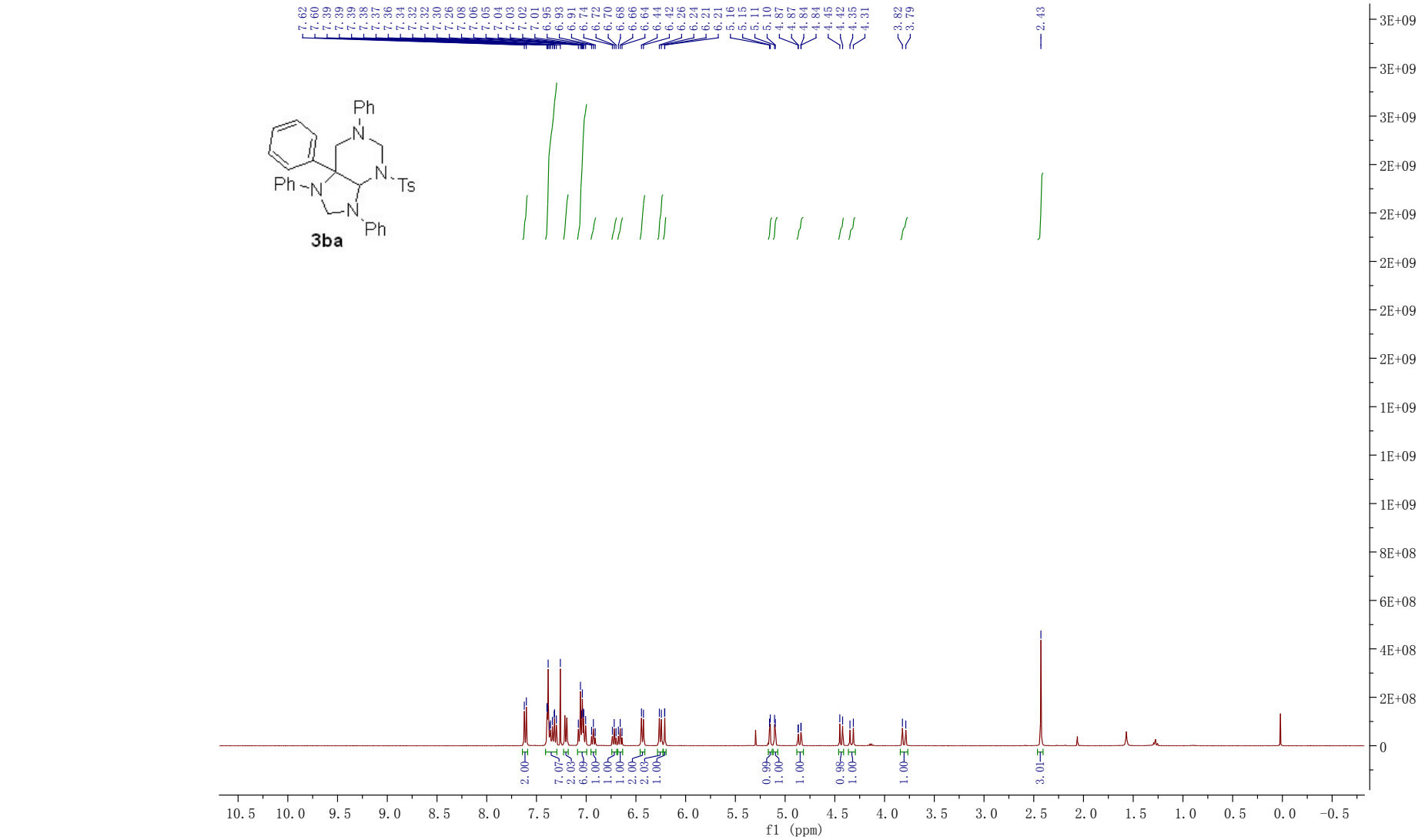
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Ph
N
Ts
N
Ph
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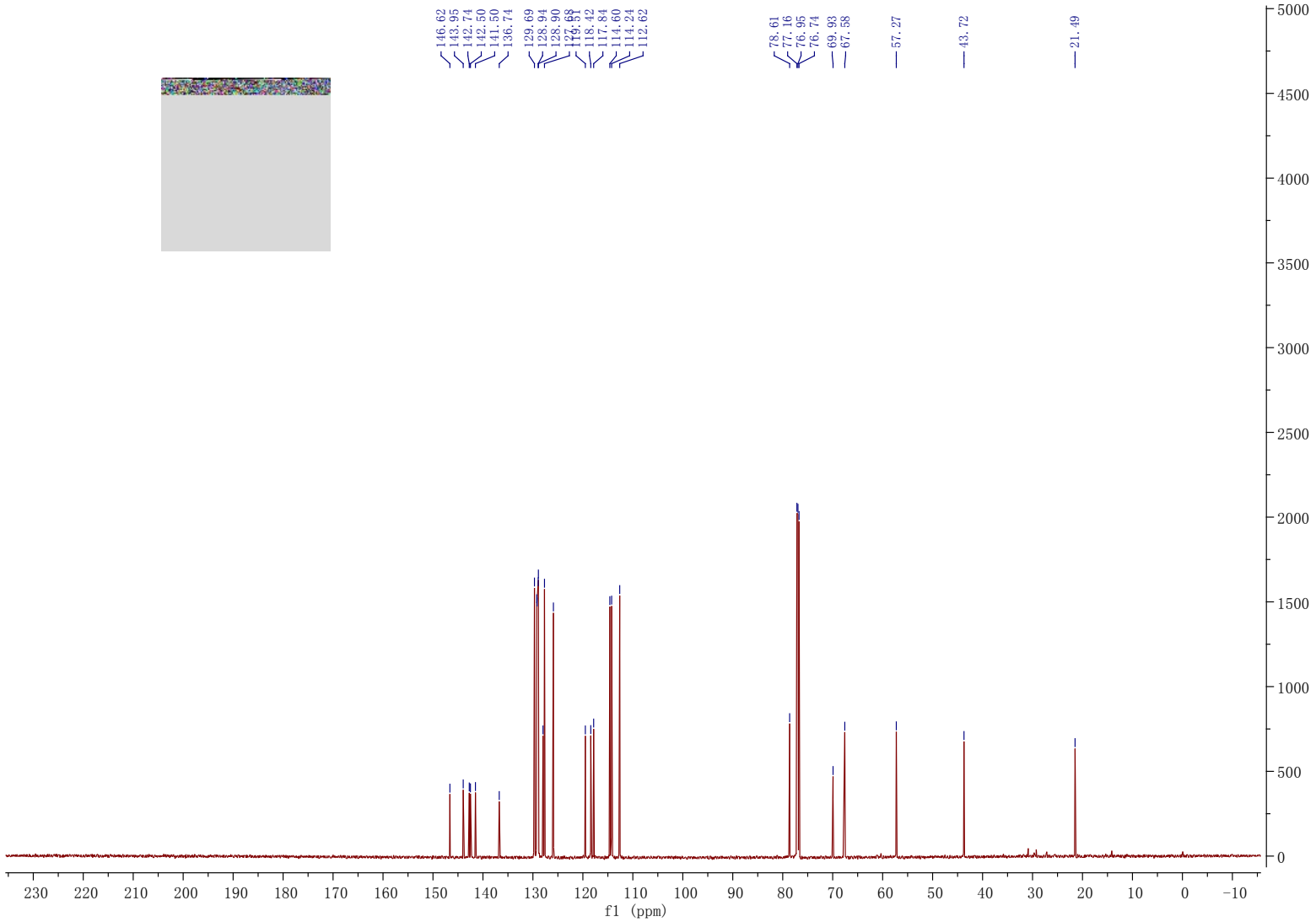
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76.74
69.93
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21.49
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4500
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1500
1000
500
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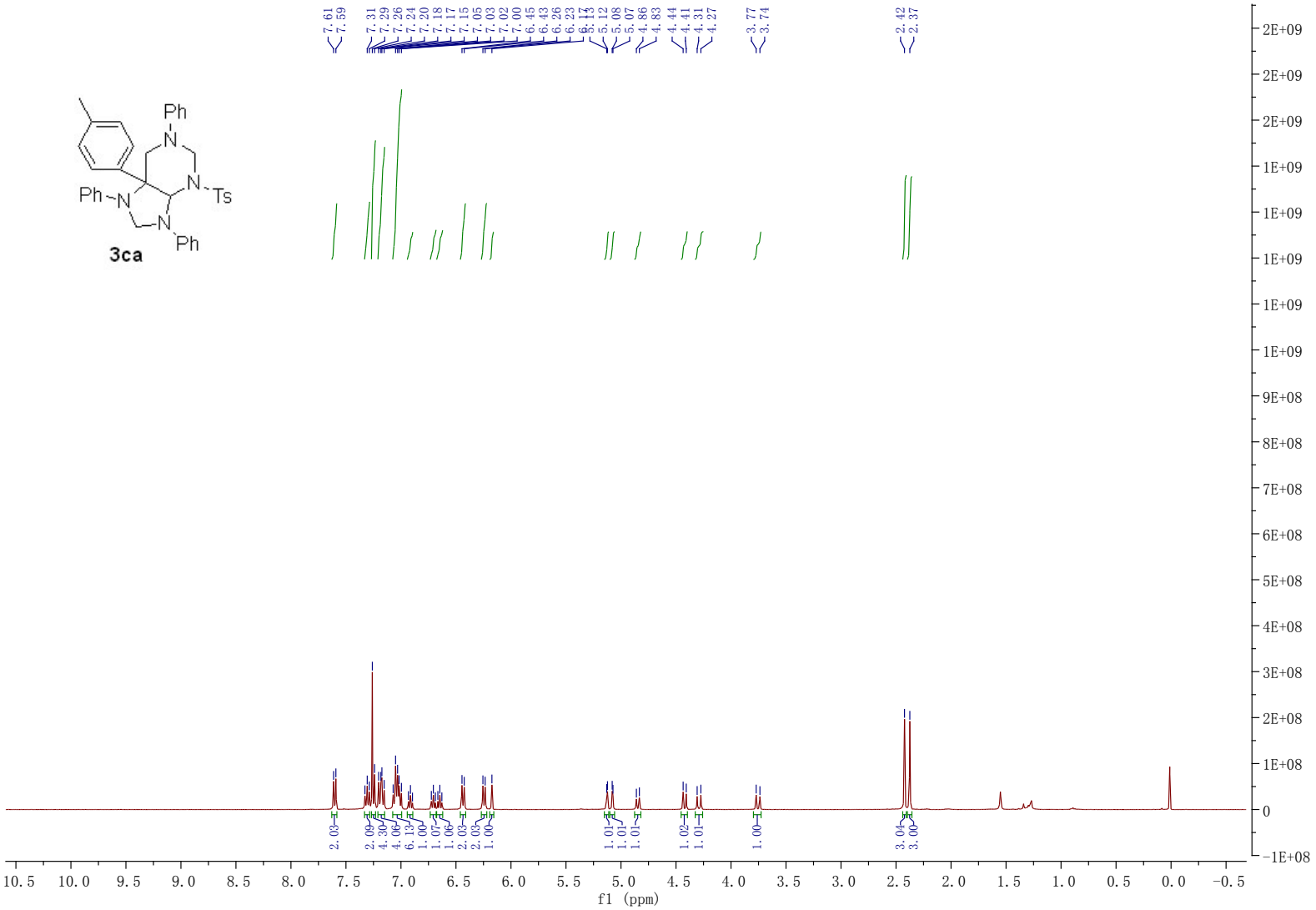
f1 (ppm)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6.43
6.26
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6.13
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5.08
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4.83
4.44
4.41
4.31
4.27
3.77
3.74
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9E+08
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6E+08
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3E+08
2E+08
1E+08
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2.09
4.30
4.06
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1.00
1.07
1.06
2.03
1.00
1.01
1.01
1.01
1.02
1.01
1.00
3.01
3.00
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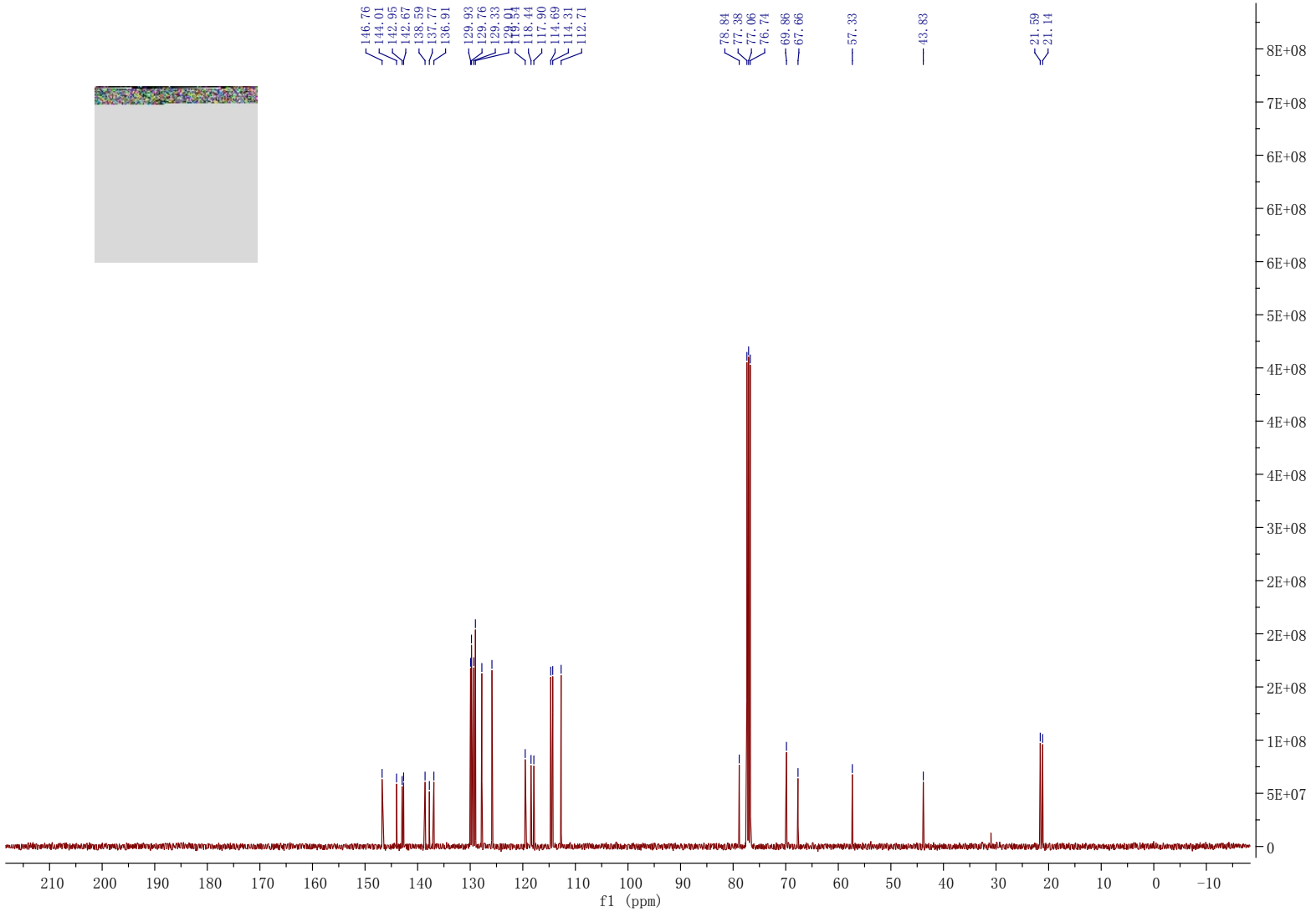
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5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
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200
190
180
170
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100
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80
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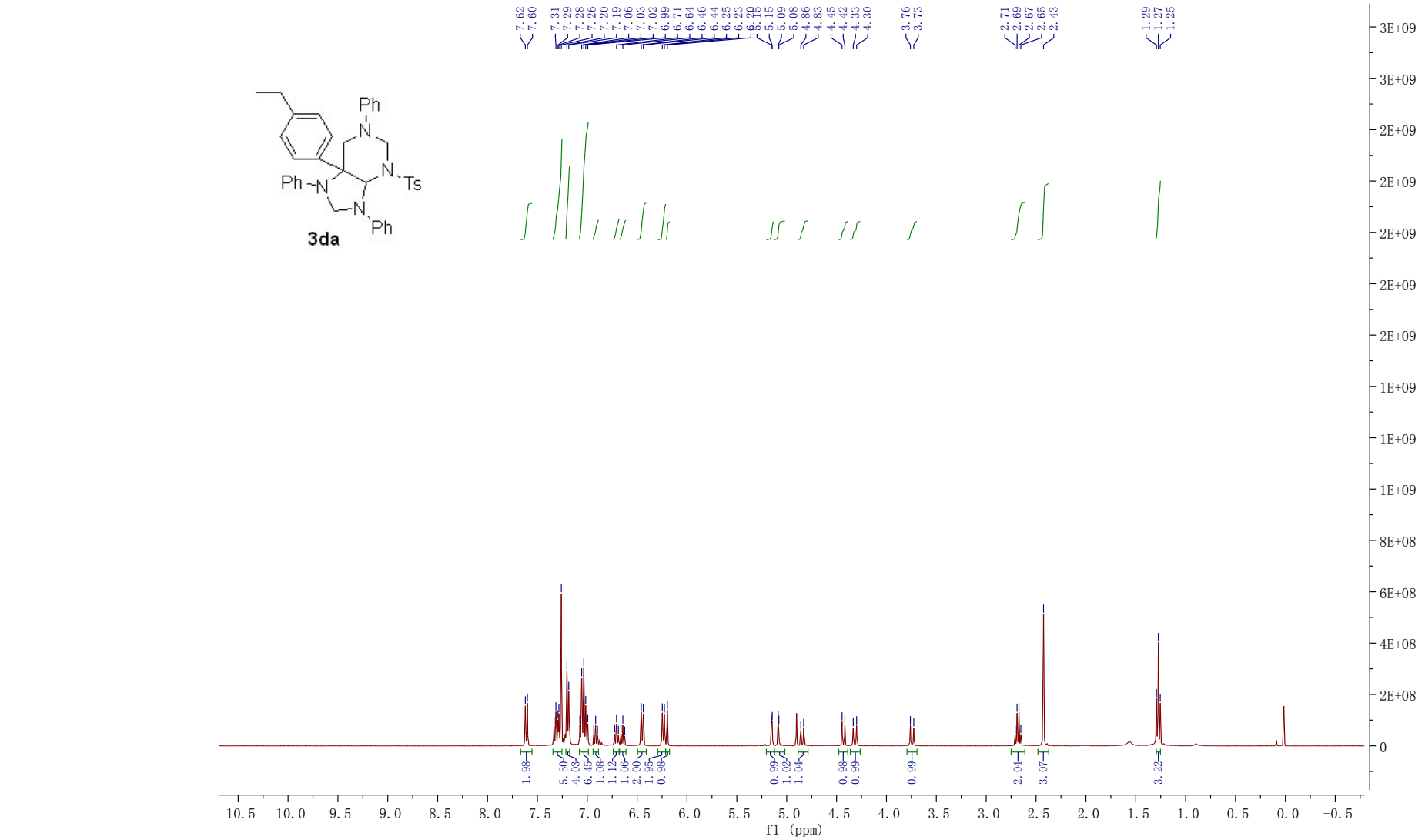
f1 (ppm)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7.19
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6.25
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6.20
5.15
5.09
5.08
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4.83
4.45
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0.99
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0.99
0.99
2.04
3.07
3.22
3E+09
3E+09
2E+09
2E+09
2E+09
2E+09
2E+09
1E+09
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6.0
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5.0
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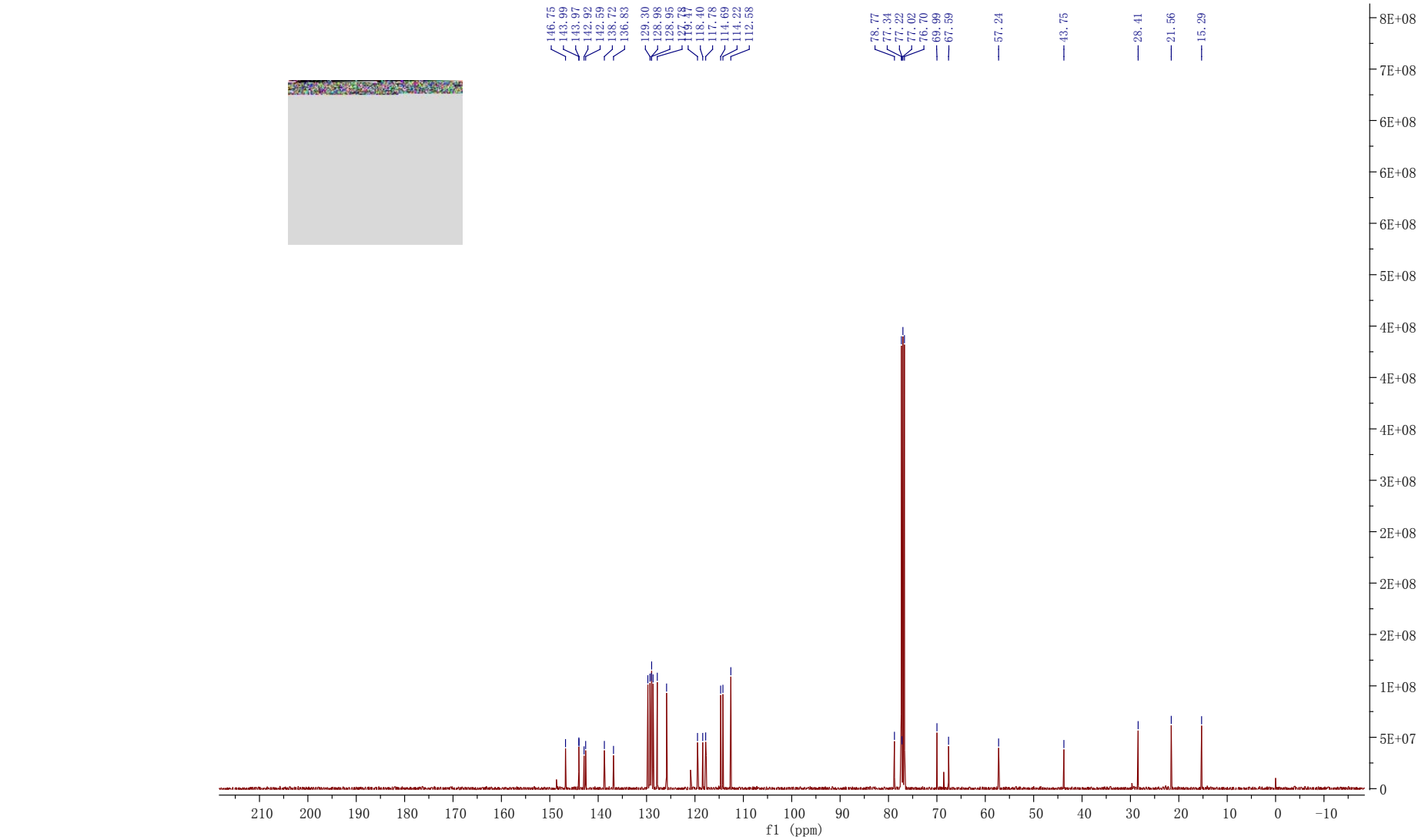
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15.29
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6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
210
200
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180
170
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100
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80
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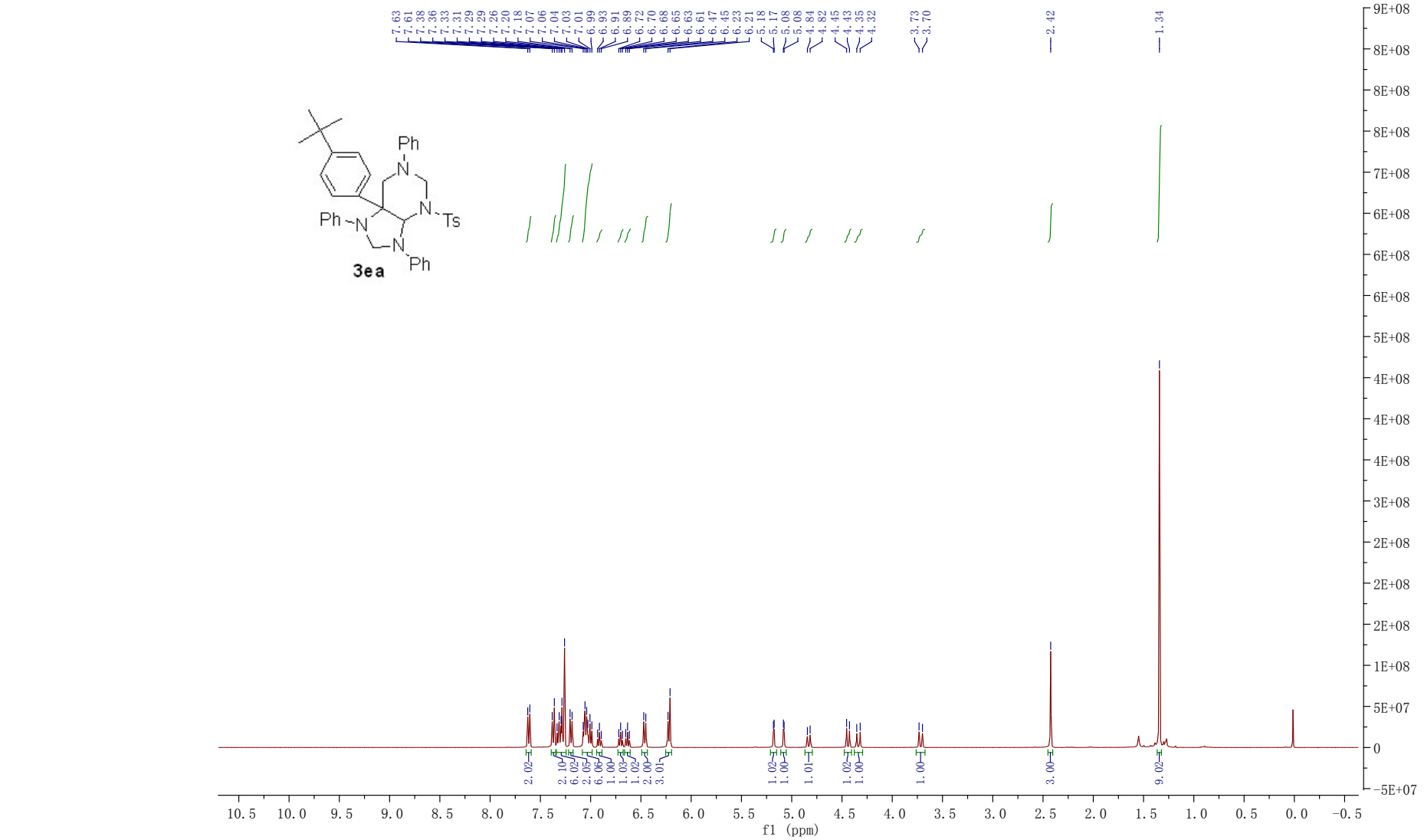
f1 (ppm)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7.03
7.01
6.99
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6.91
6.89
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6.70
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6.65
6.63
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5.17
5.08
5.08
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4.45
4.43
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Ph
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N
Ph
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3E+08
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2E+08
2E+08
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5E+07
0
-5E+07
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2.10
6.02
2.05
6.06
1.00
1.03
1.02
2.00
3.01
1.02
1.00
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1.00
3.00
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5.0
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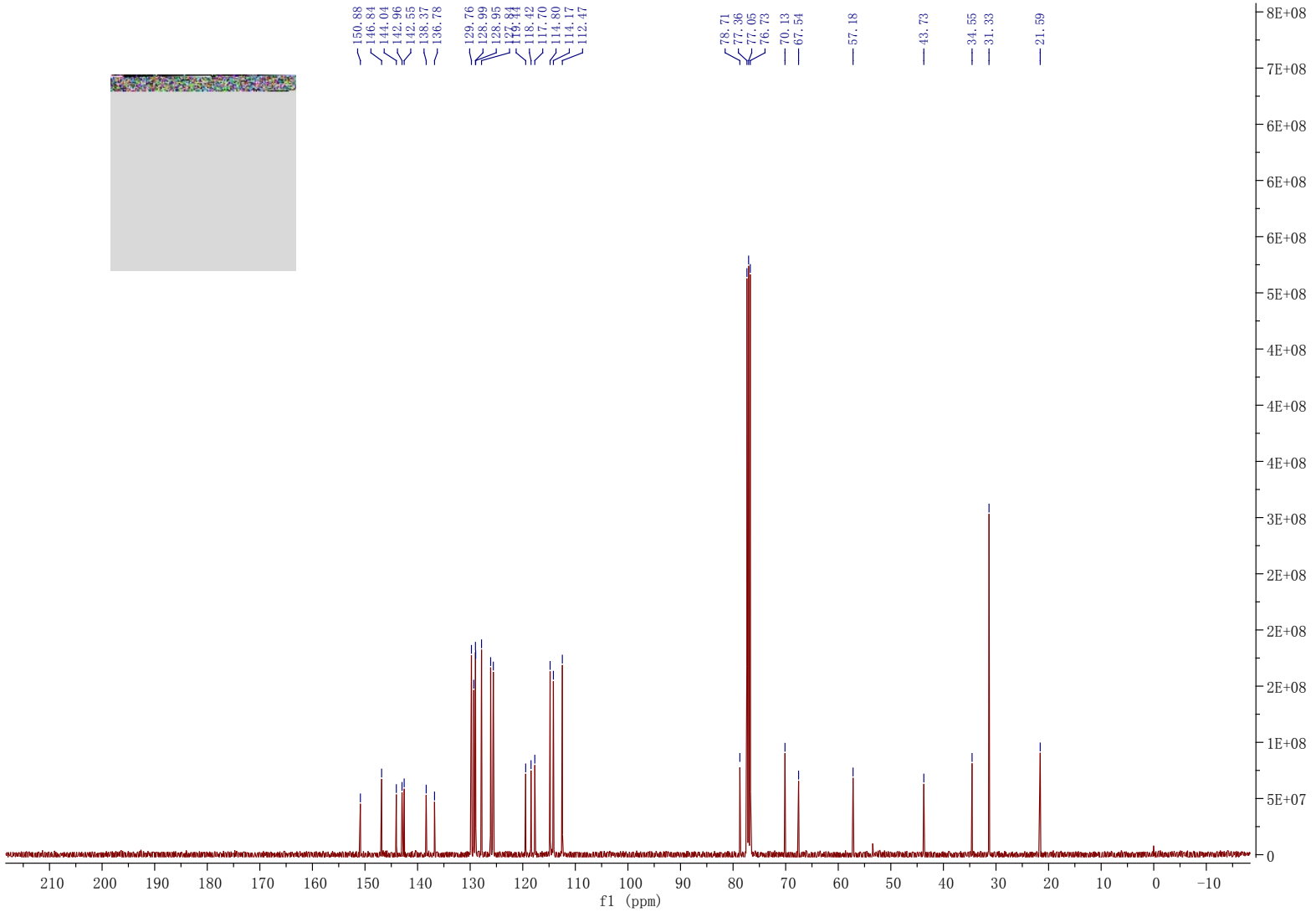
f1 (ppm)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21.59
8E+08
7E+08
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5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
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190
180
170
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100
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40
30
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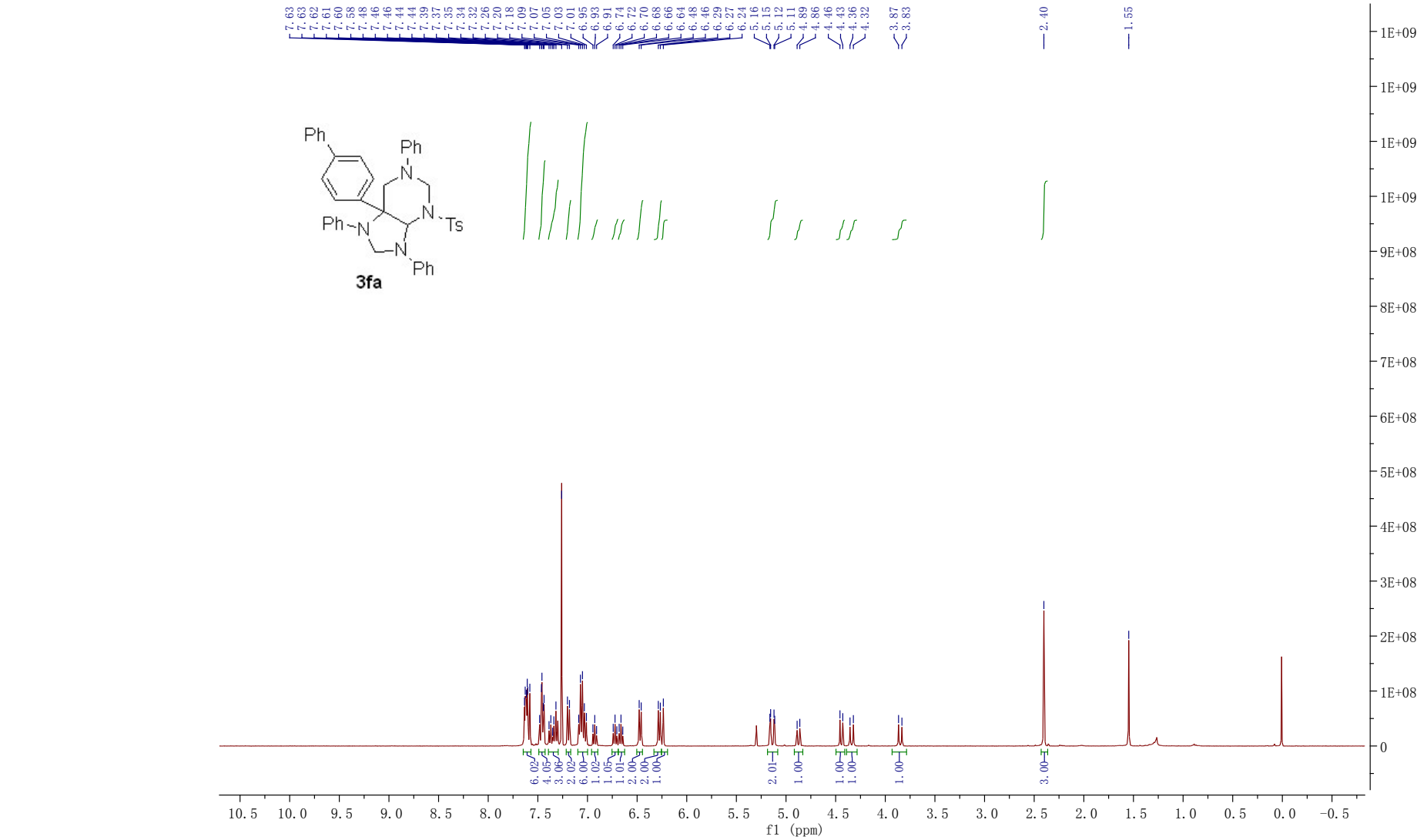
f1 (ppm)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N
Ts
Ph
N
N
Ph
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8E+08
7E+08
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3E+08
2E+08
1E+08
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5.0
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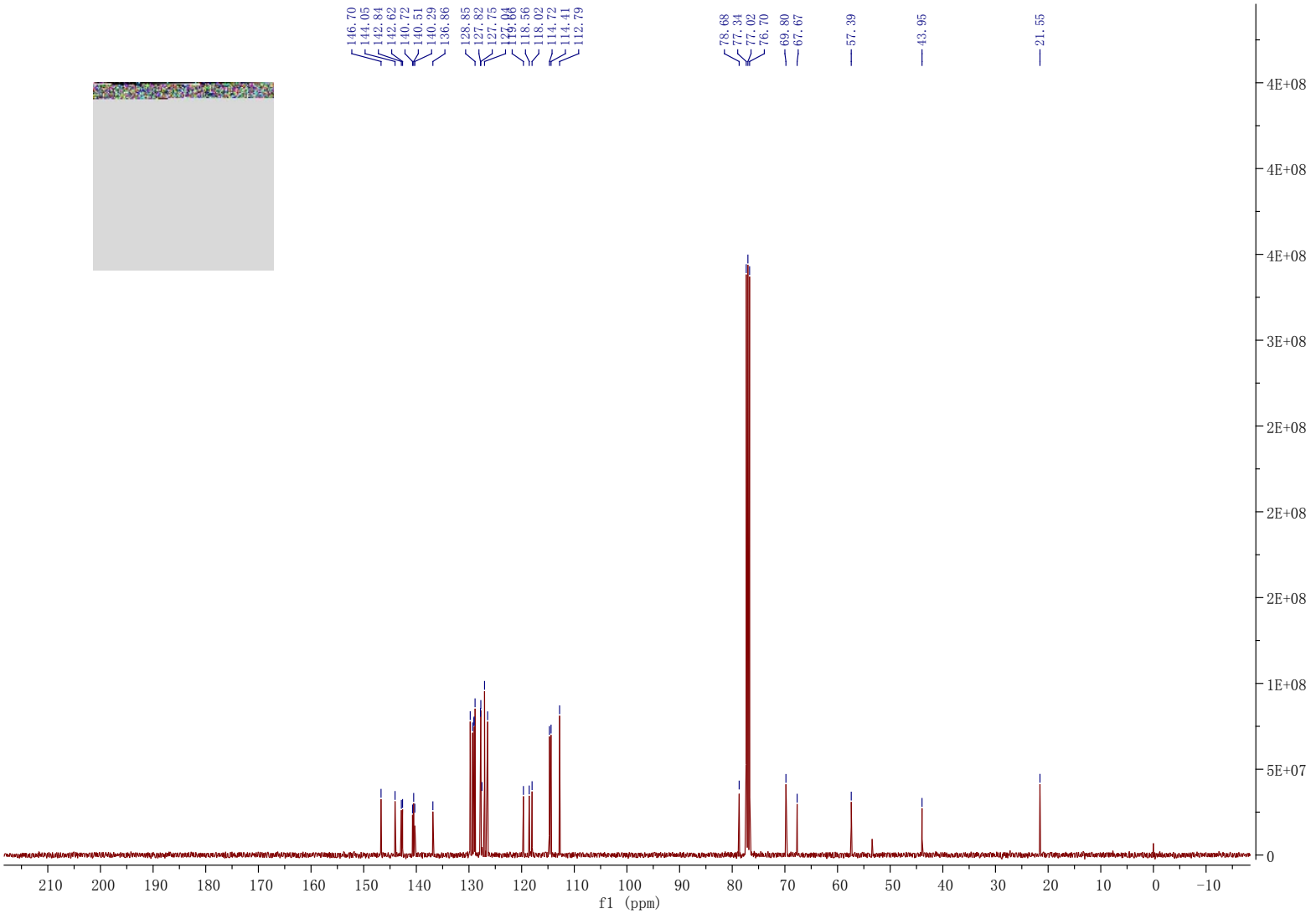
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114.41
112.79
78.68
77.34
77.02
76.70
69.80
67.67
57.39
43.95
21.55
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
210
200
190
180
170
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120
110
100
90
80
70
60
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40
30
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10
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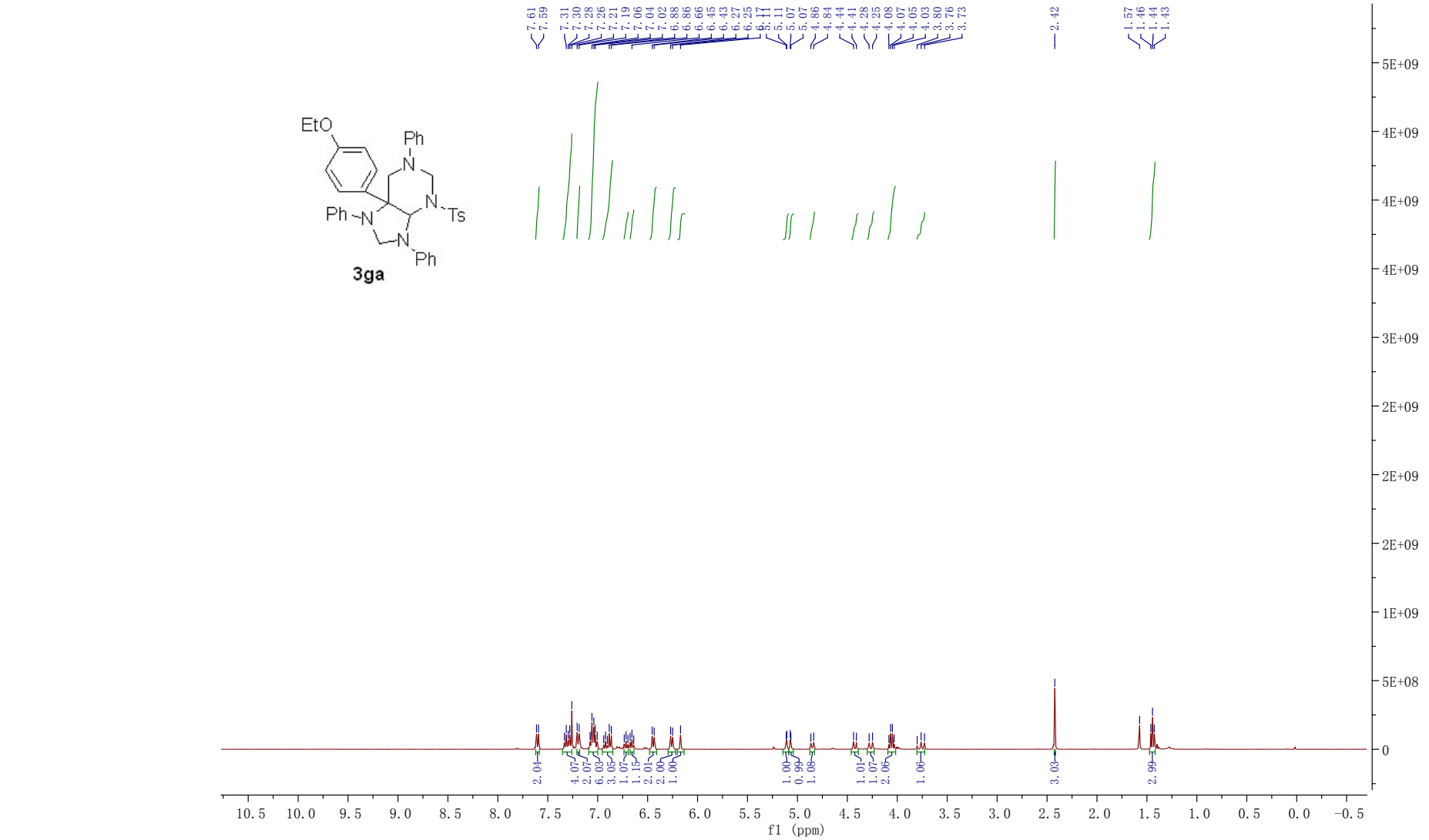
−10
f1 (ppm)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Ts
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5.11
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5.07
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1.46
1.44
1.43
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4E+09
4E+09
4E+09
3E+09
2E+09
2E+09
2E+09
1E+09
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4.07
2.07
6.03
3.05
1.07
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1.00
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1.08
1.01
1.07
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3.03
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6.0
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5.0
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2.0
1.5
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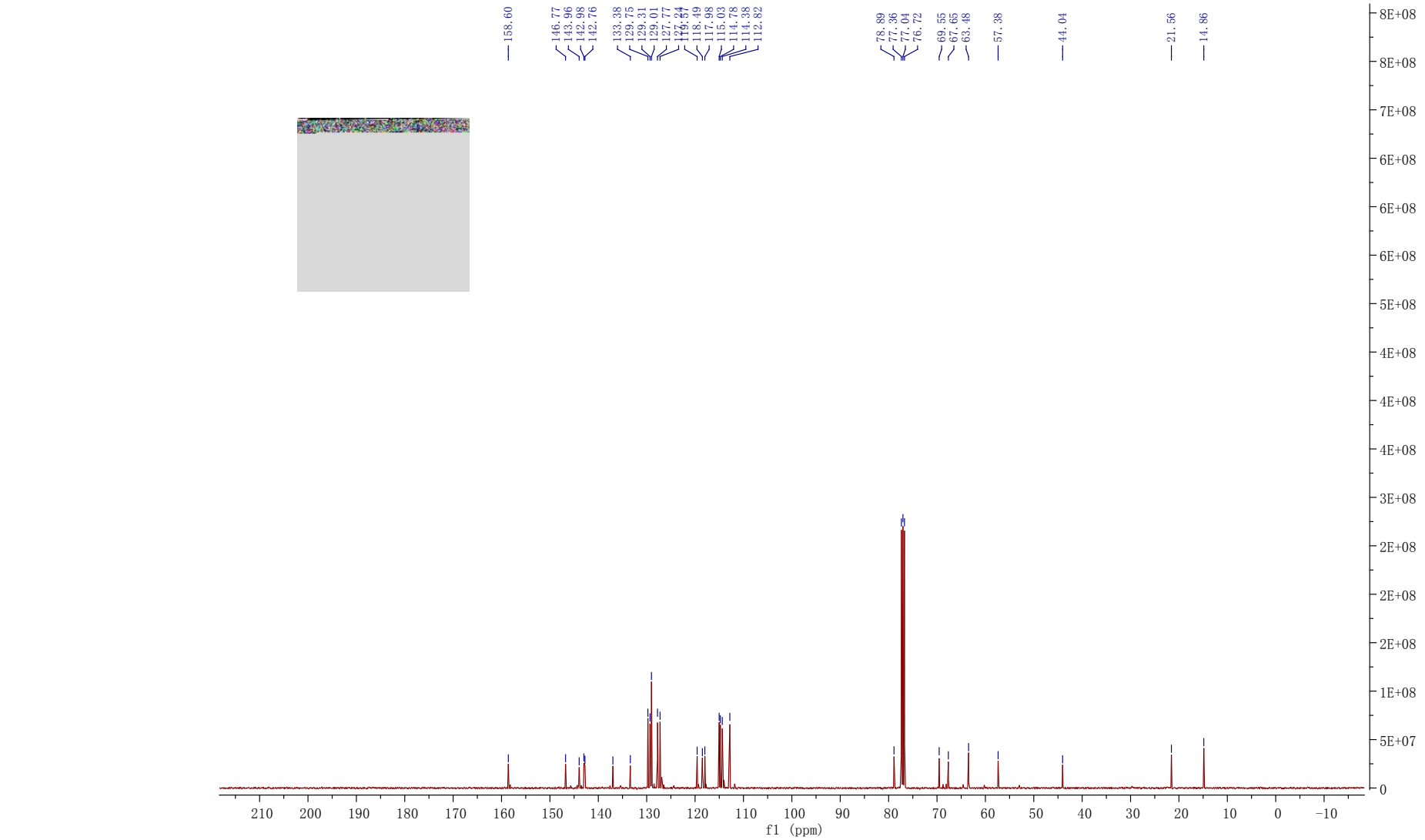
0.5
0.0
-0.5
f1 (ppm)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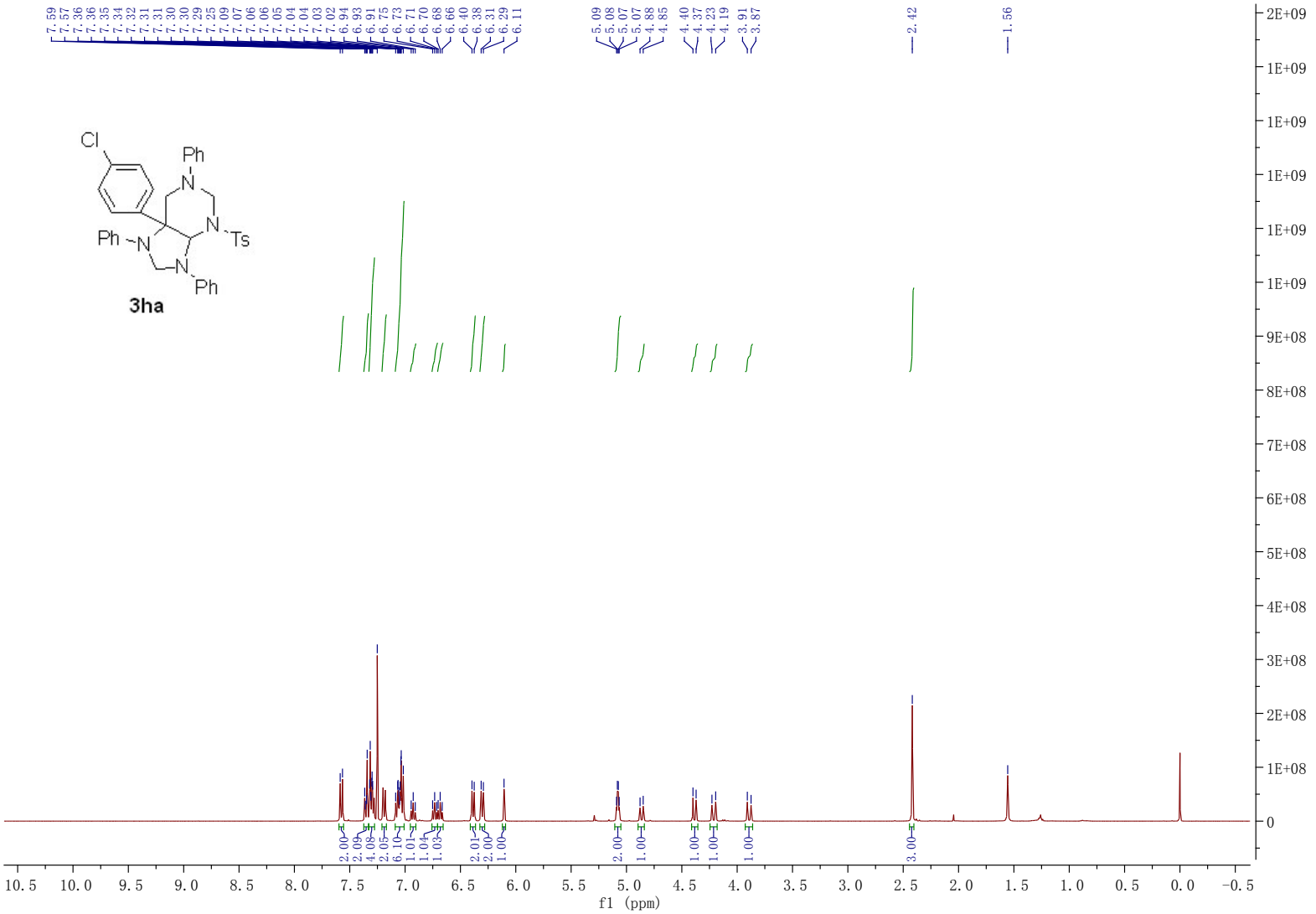
21.56
14.86
f1 (ppm)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7.04
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7.03
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Cl
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N
N
Ts
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N
Ph
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1E+09
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8E+08
7E+08
6E+08
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4E+08
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2E+08
1E+08
0
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4.08
2.05
6.10
1.01
1.04
1.03
2.01
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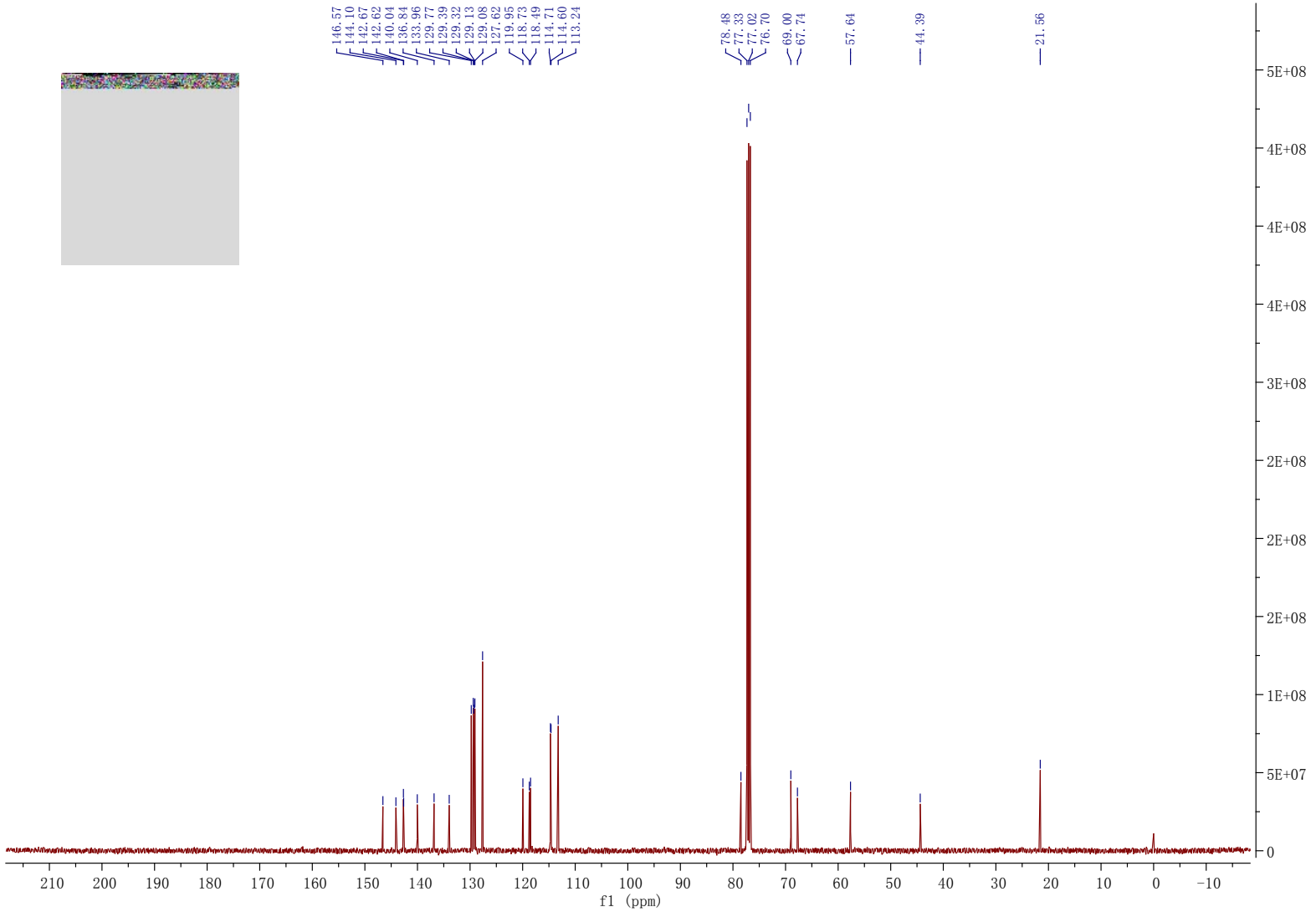
f1 (ppm)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113.24
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77.33
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67.74
57.64
44.39
21.56
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
210
200
190
180
170
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120
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100
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80
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60
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30
20
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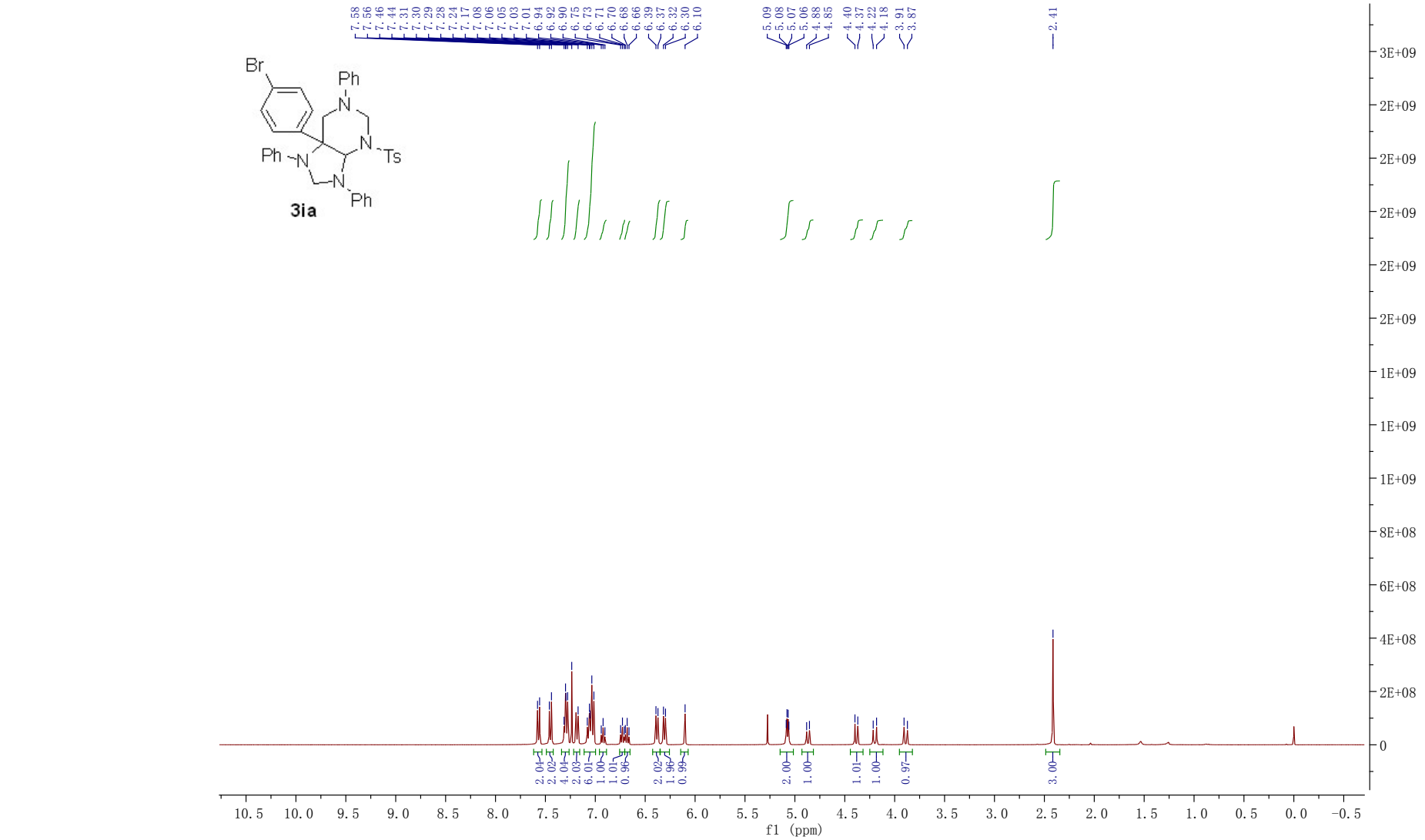
-10
f1 (ppm)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7.01
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5.07
5.06
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4.37
4.22
4.18
3.91
3.87
2.41
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Ph
N
N
Ts
Ph
N
N
Ph
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2E+09
2E+09
2E+09
2E+09
2E+09
1E+09
1E+09
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2E+08
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2.02
4.04
2.03
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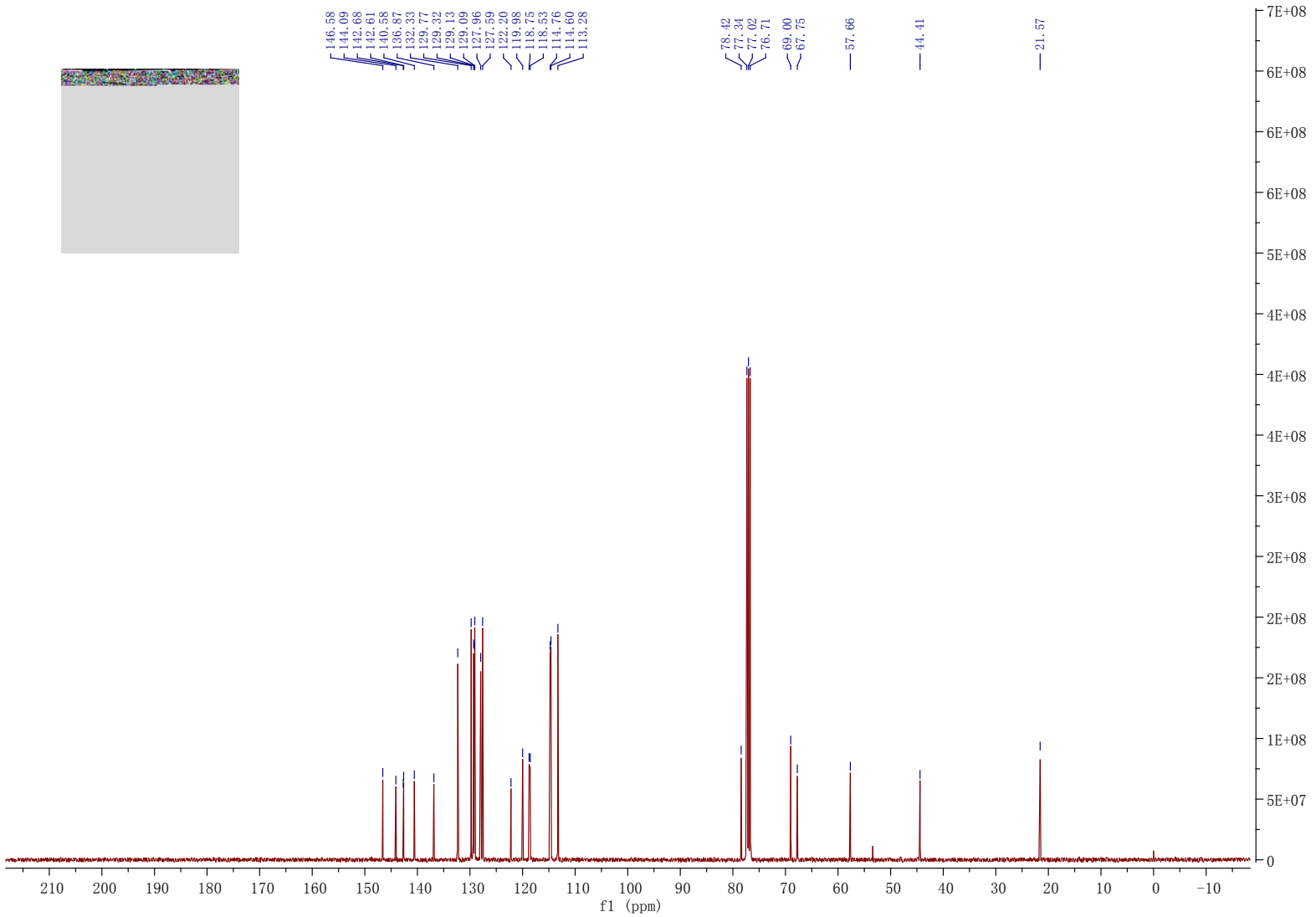
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129.13
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114.76
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113.28
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76.71
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67.75
57.66
44.41
21.57
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6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
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200
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180
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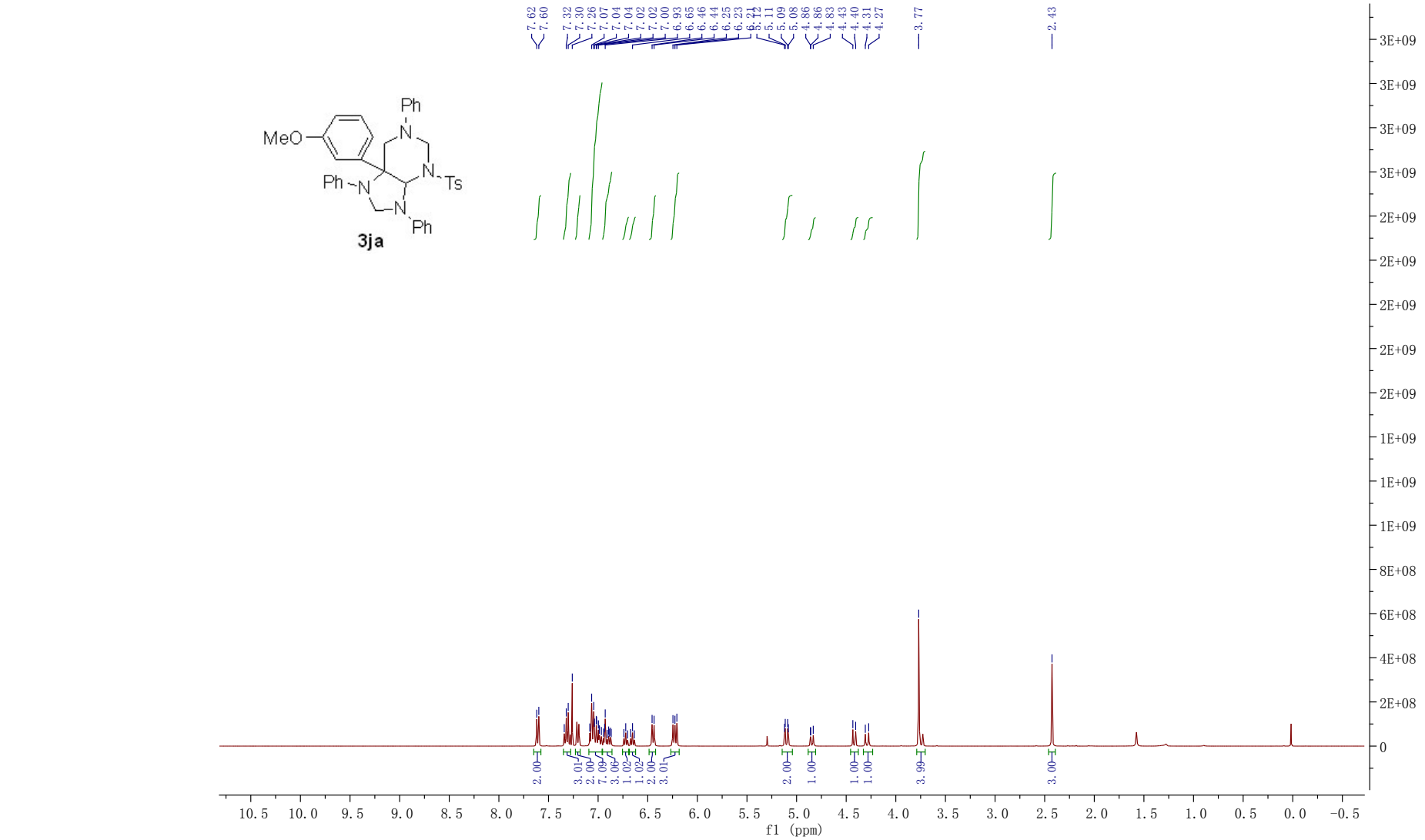
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Ts
Ph
N
N
Ph
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7.04
7.04
7.02
7.02
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6.23
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4.86
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4.31
4.27
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2.43
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3E+09
3E+09
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2E+09
2E+09
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1E+09
1E+09
1E+09
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6E+08
4E+08
2E+08
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2.00
2.09
3.06
1.02
1.02
2.00
3.01
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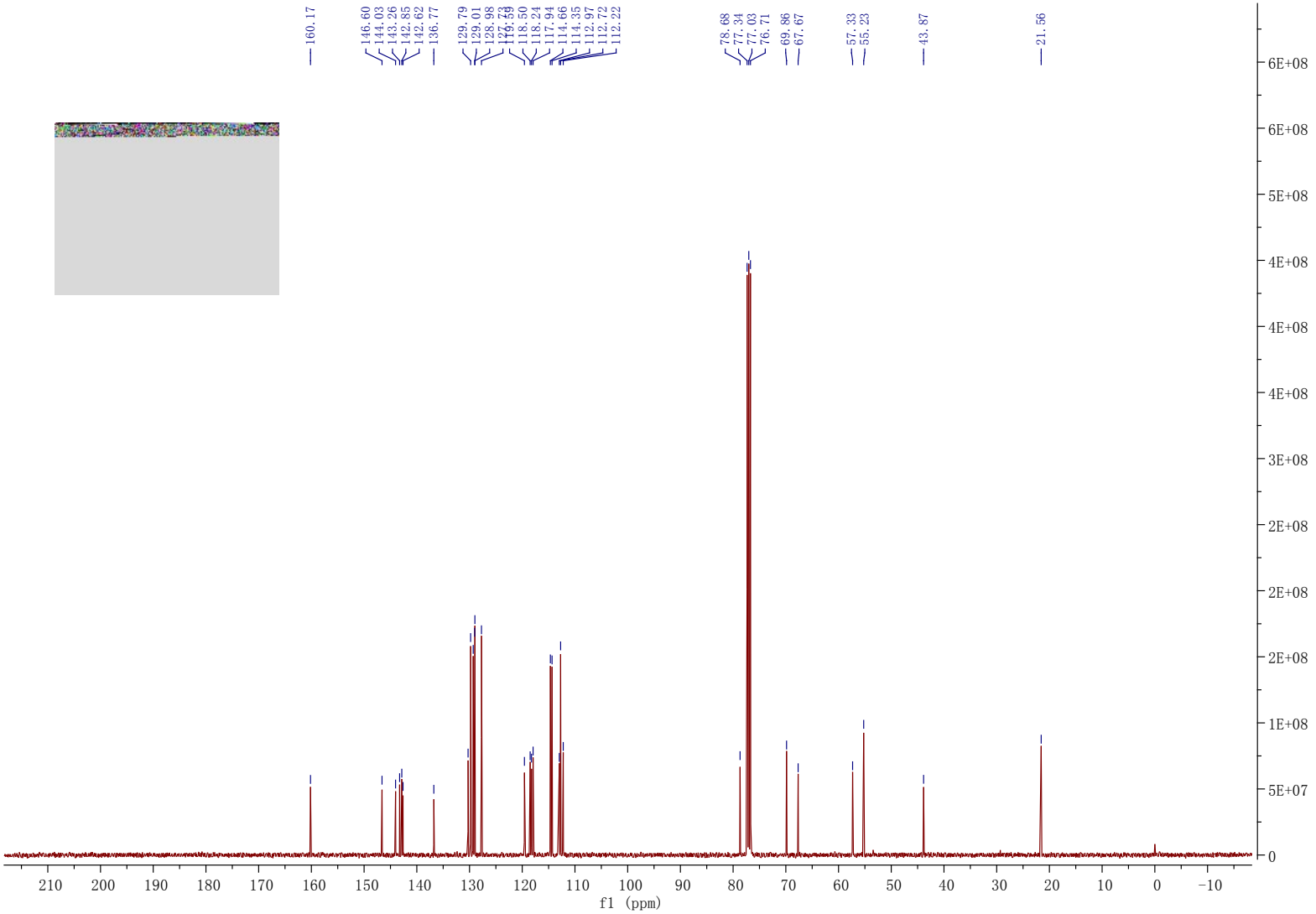
f1 (ppm)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77.34
77.03
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55.23
43.87
21.56
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6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
1E+08
5E+07
0
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200
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180
170
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100
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80
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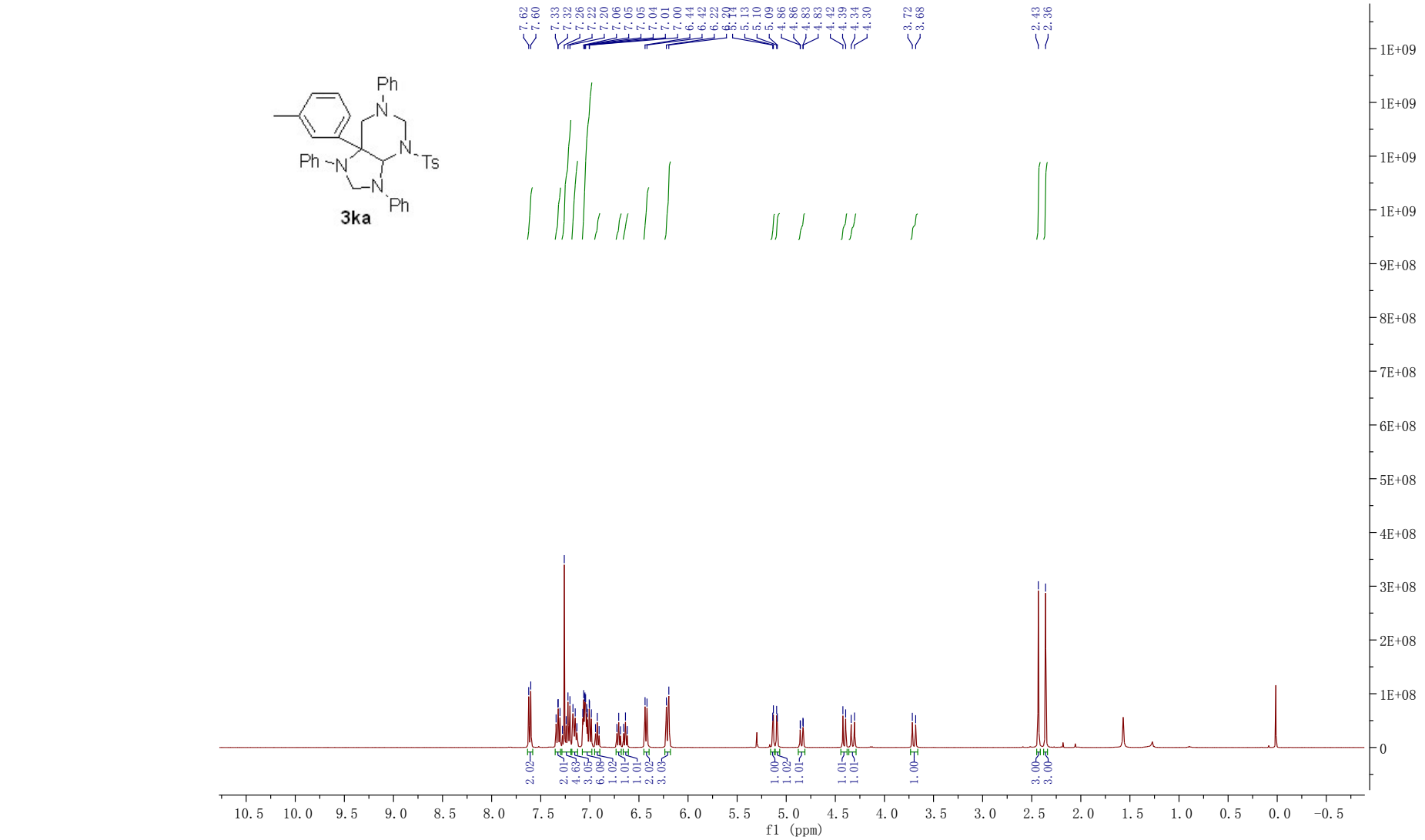
f1 (ppm)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Ph
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N
Ts
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Ph
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7.05
7.04
7.01
7.00
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6.22
6.20
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5.13
5.10
5.09
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4.86
4.83
4.42
4.39
4.34
4.30
3.72
3.68
2.43
2.36
1E+09
1E+09
1E+09
1E+09
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
2.02
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1.01
1.01
2.02
3.03
1.00
1.02
1.01
1.01
1.01
1.00
3.00
3.00
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9.0
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2.0
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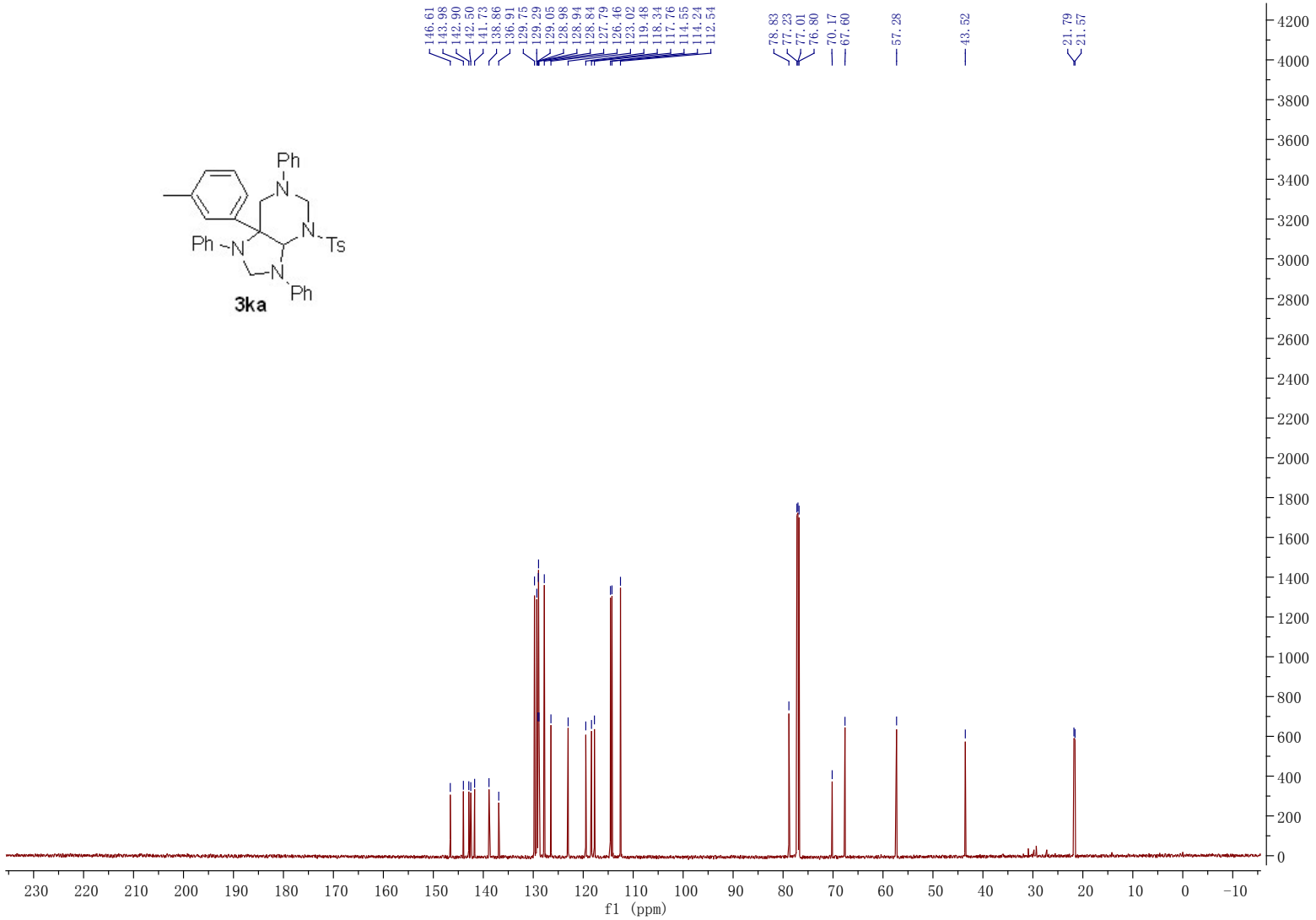
-0.5
f1 (ppm)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128.84
127.79
126.46
123.02
119.48
118.34
117.76
114.55
114.24
112.54
78.83
77.23
77.01
76.80
70.17
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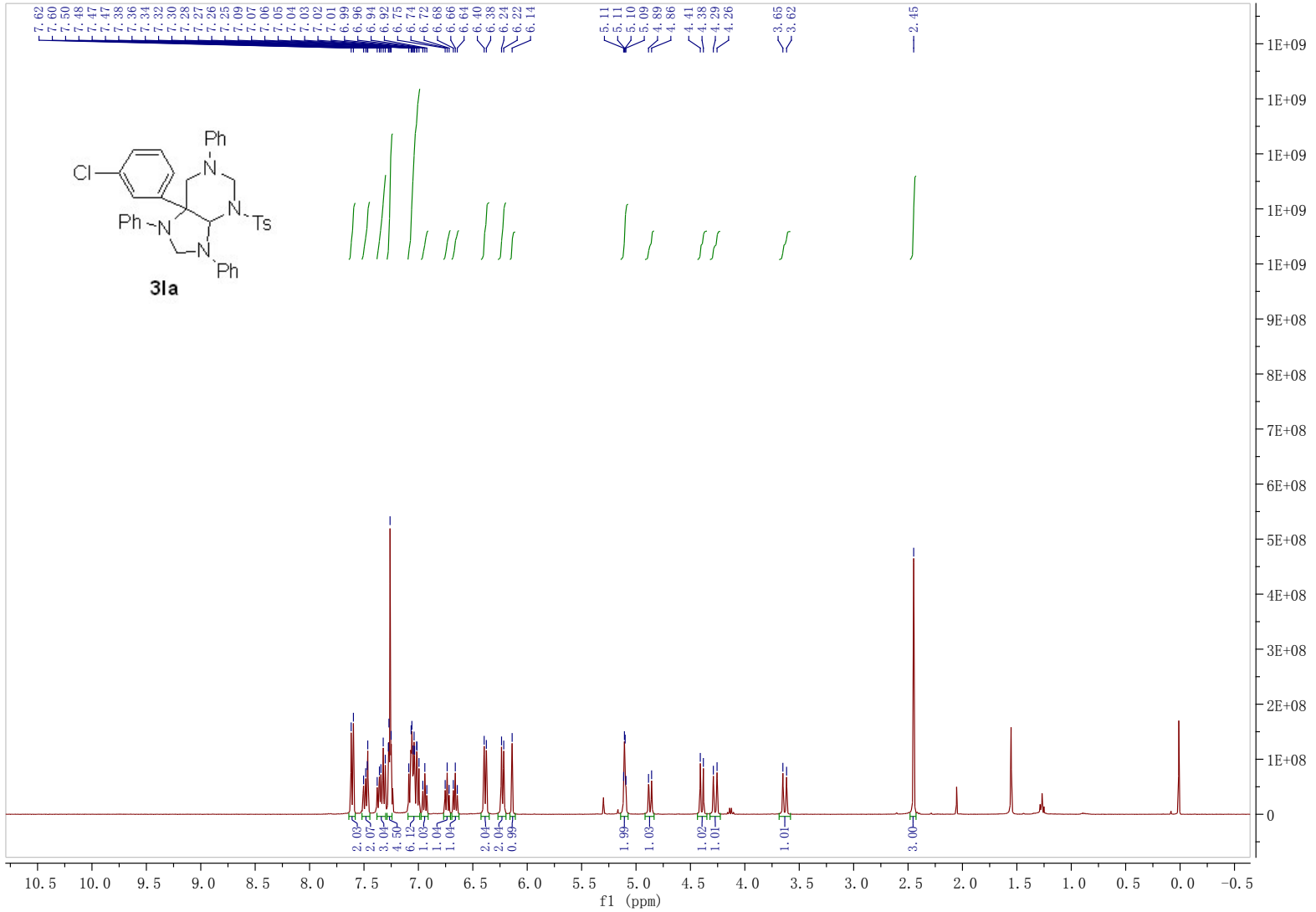
21.79
21.57
Ph
N
N
Ts
Ph
N
N
Ph
3ka
f1 (ppm)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7.27
7.26
7.25
7.09
7.07
7.06
7.05
7.04
7.03
7.02
7.01
6.99
6.96
6.94
6.92
6.75
6.74
6.72
6.68
6.66
6.64
6.40
6.38
6.24
6.22
6.14
5.11
5.11
5.10
5.09
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4.86
4.41
4.38
4.29
4.26
3.65
3.62
2.45
Cl
Ph
N
Ph
N
Ts
N
Ph
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1E+09
1E+09
1E+09
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6E+08
5E+08
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3E+08
2E+08
1E+08
0
2.03
2.07
3.04
4.50
6.12
1.03
1.04
1.04
2.04
2.04
0.99
1.99
1.03
1.02
1.01
1.01
3.00
10.5
10.0
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9.0
8.5
8.0
7.5
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6.5
6.0
5.5
5.0
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3.0
2.5
2.0
1.5
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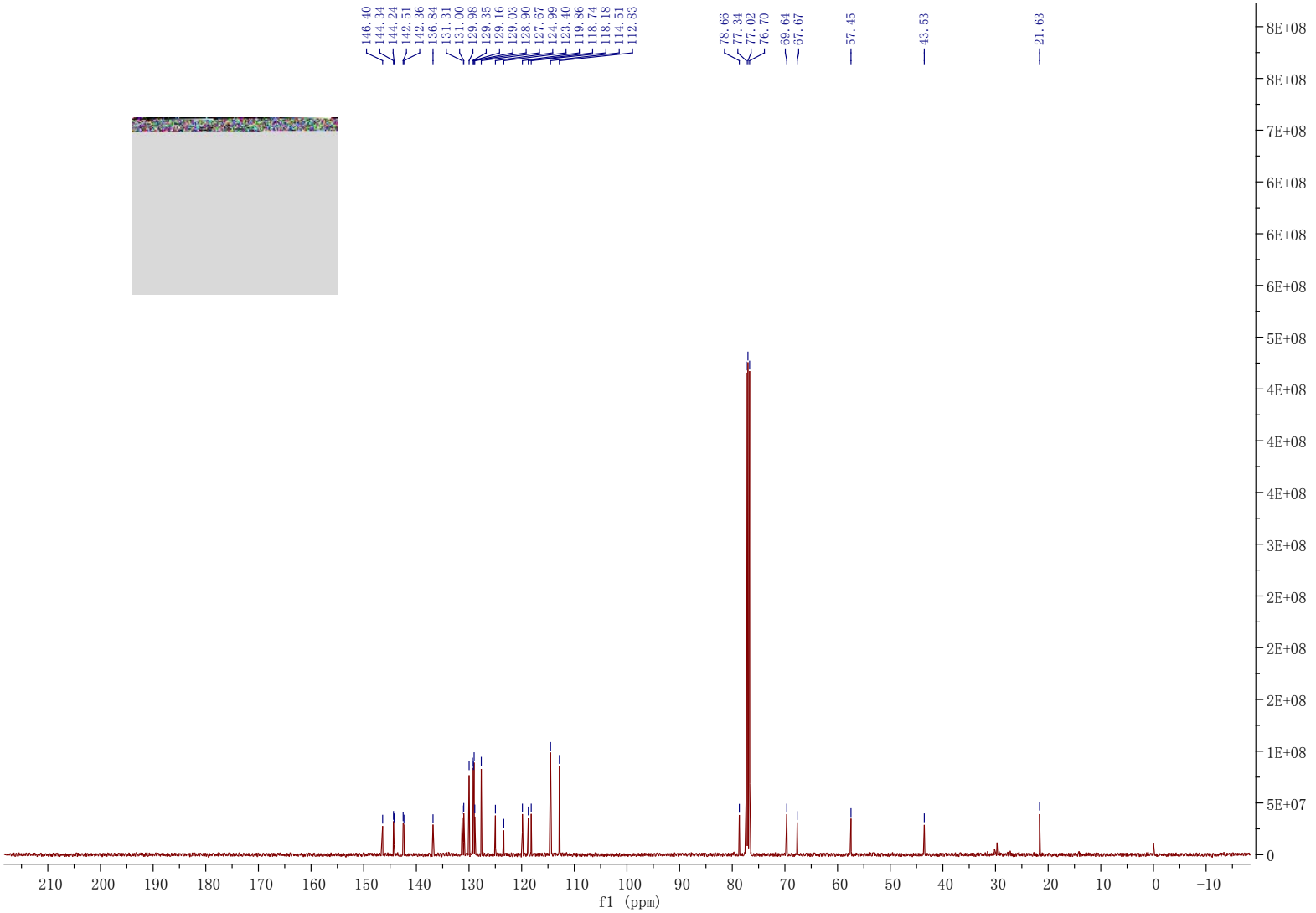
0.5
0.0
-0.5
f1 (ppm)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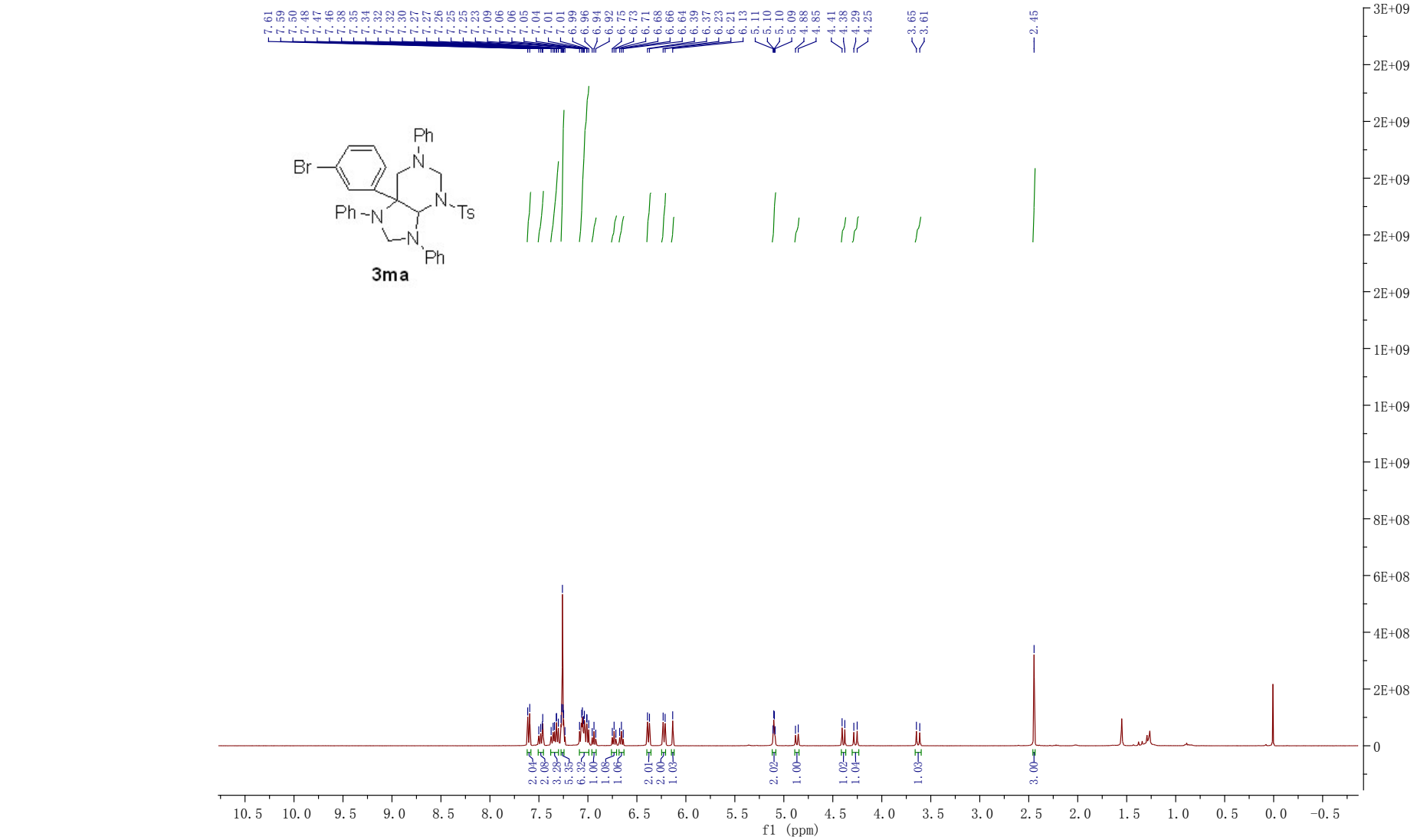
129.35
129.16
129.03
128.90
127.67
124.99
123.40
119.86
118.74
118.18
114.51
112.83
78.66
77.34
77.02
76.70
69.64
67.67
57.45
43.53
21.63
8E+08
8E+08
7E+08
6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.27
7.27
7.26
7.25
7.25
7.23
7.09
7.06
7.06
7.05
7.04
7.01
7.01
6.99
6.96
6.94
6.92
6.75
6.73
6.71
6.68
6.66
6.64
6.39
6.37
6.23
6.21
6.13
5.11
5.10
5.10
5.09
4.88
4.85
4.41
4.38
4.29
4.25
3.65
3.61
2.45
Br
Ph
N
Ph
N
N
Ts
N
Ph
3ma
3E+09
2E+09
2E+09
2E+09
2E+09
2E+09
1E+09
1E+09
1E+09
8E+08
6E+08
4E+08
2E+08
0
2.04
2.09
3.28
5.35
6.32
1.00
1.08
1.06
2.01
2.00
1.03
2.02
1.00
1.02
1.04
1.03
3.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.0
2.5
2.0
1.5
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0.5
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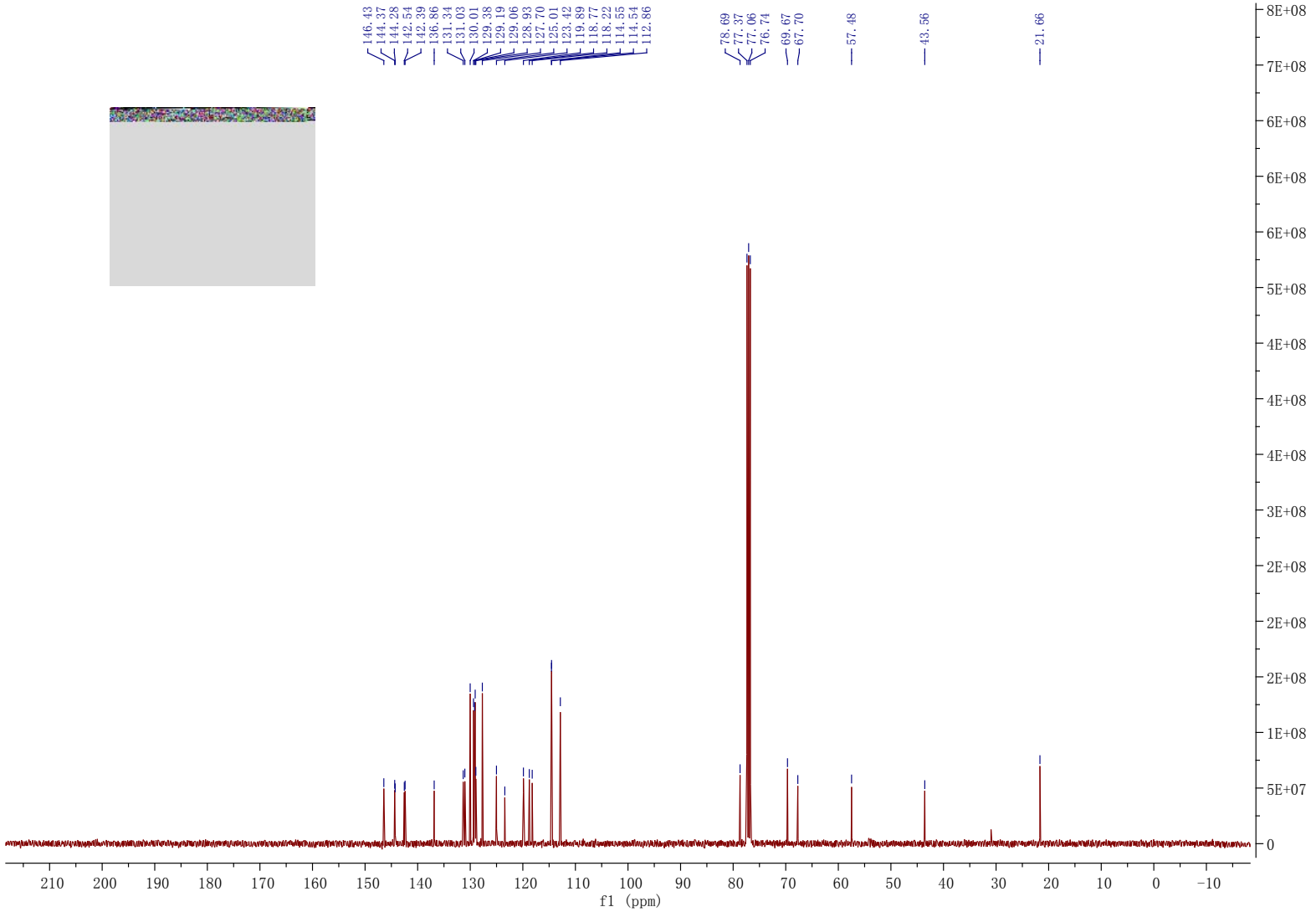
-0.5
f1 (ppm)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129.19
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127.70
125.01
123.42
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118.22
114.55
114.54
112.86
78.69
77.37
77.06
76.74
69.67
67.70
57.48
43.56
21.66
8E+08
7E+08
6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
210
200
190
180
170
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120
110
100
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80
70
60
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40
30
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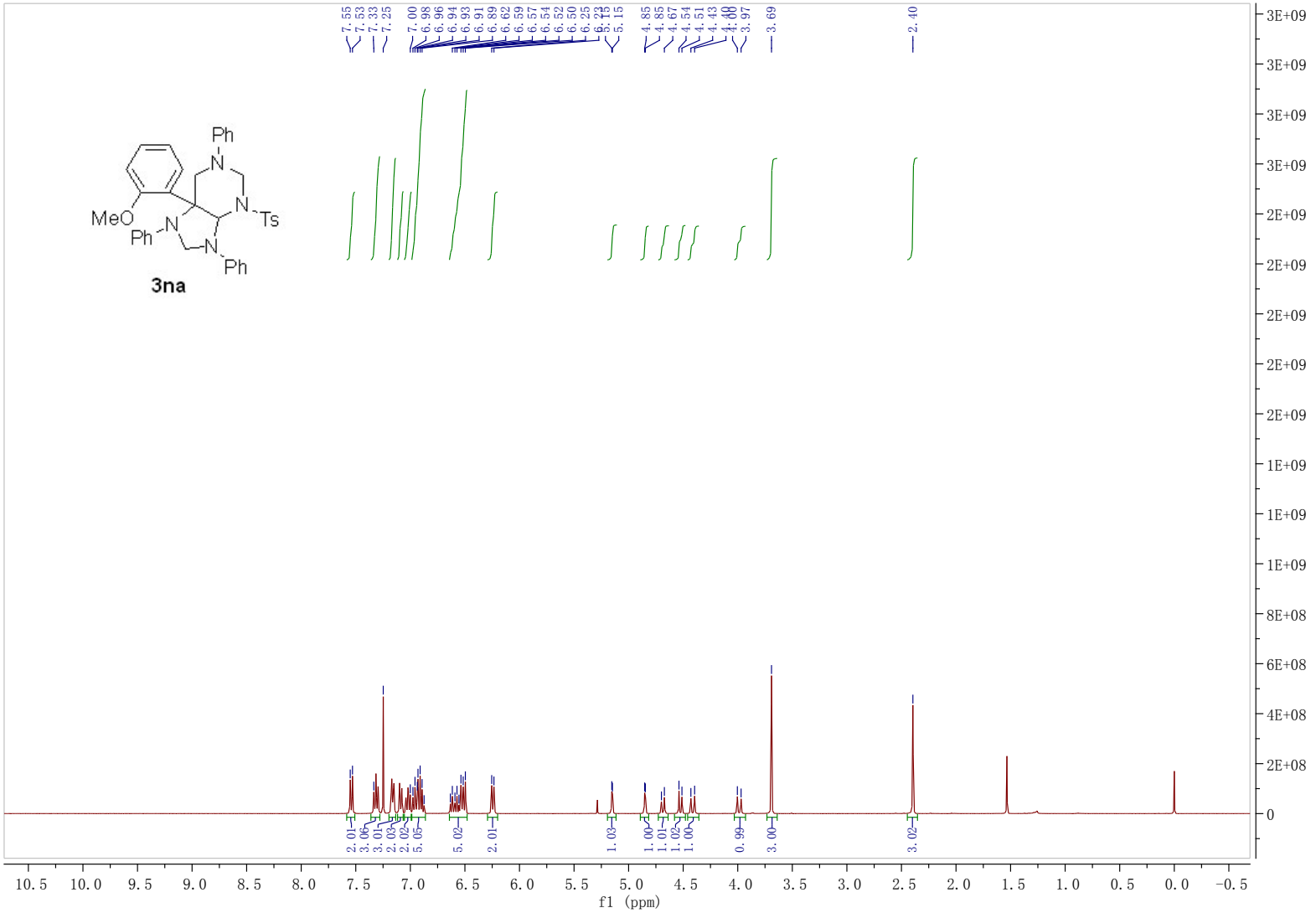
0
-10
f1 (ppm)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Ts
Ph
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Ph
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6.62
6.59
6.57
6.54
6.52
6.50
6.25
5.15
4.85
4.85
4.67
4.54
4.51
4.43
3.97
3.69
2.40
2.01
3.06
3.01
2.03
2.02
5.05
5.02
2.01
1.03
1.00
1.01
1.02
1.00
0.99
3.00
3.02
3E+09
2E+09
1E+09
8E+08
6E+08
4E+08
2E+08
0
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10.0
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9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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3.0
2.5
2.0
1.5
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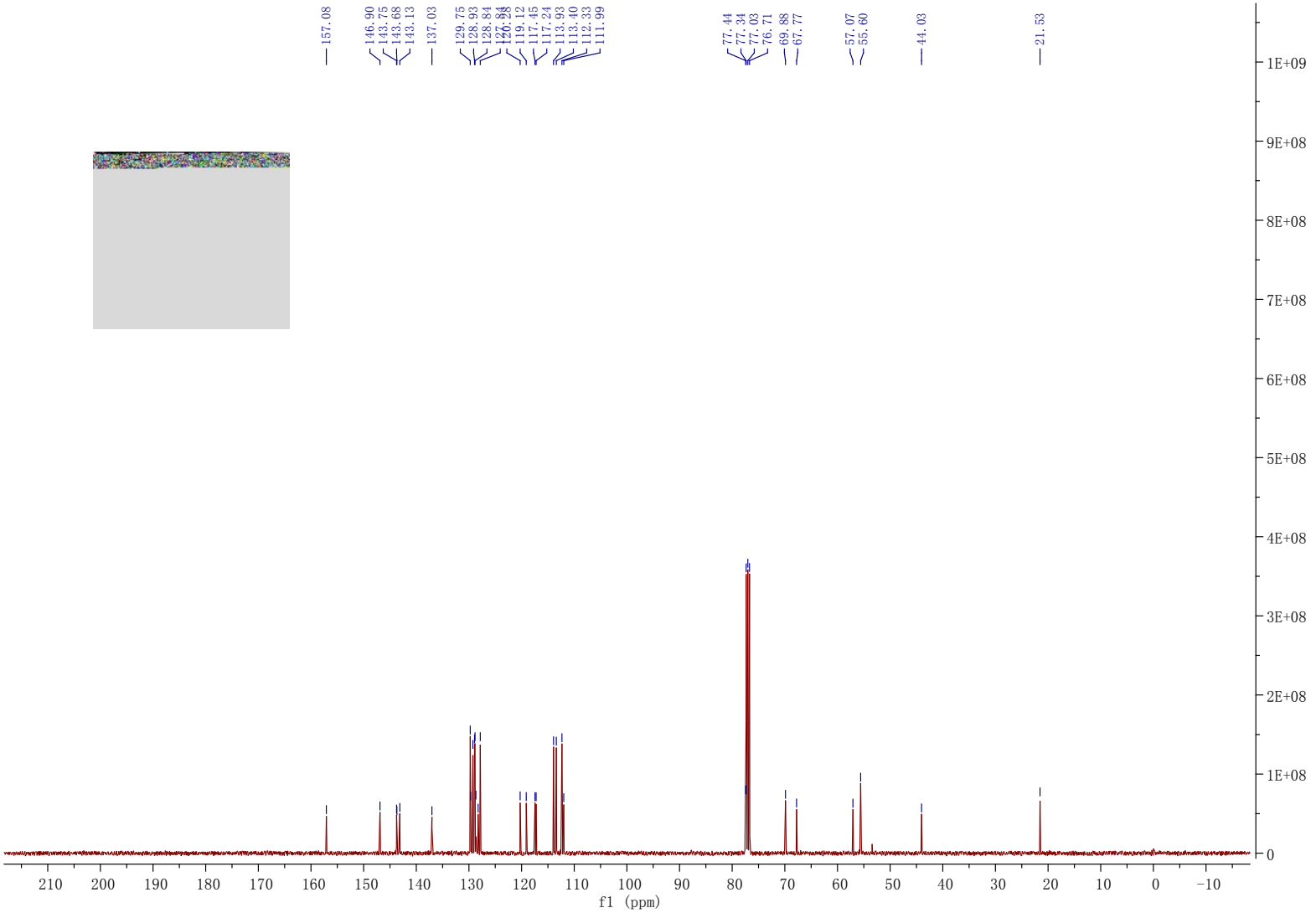
0.5
0.0
-0.5
f1 (ppm)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117.24
113.93
113.40
112.33
111.99
77.44
77.34
77.03
76.71
69.88
67.77
57.07
55.60
44.03
21.53
1E+09
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
210
200
190
180
170
160
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140
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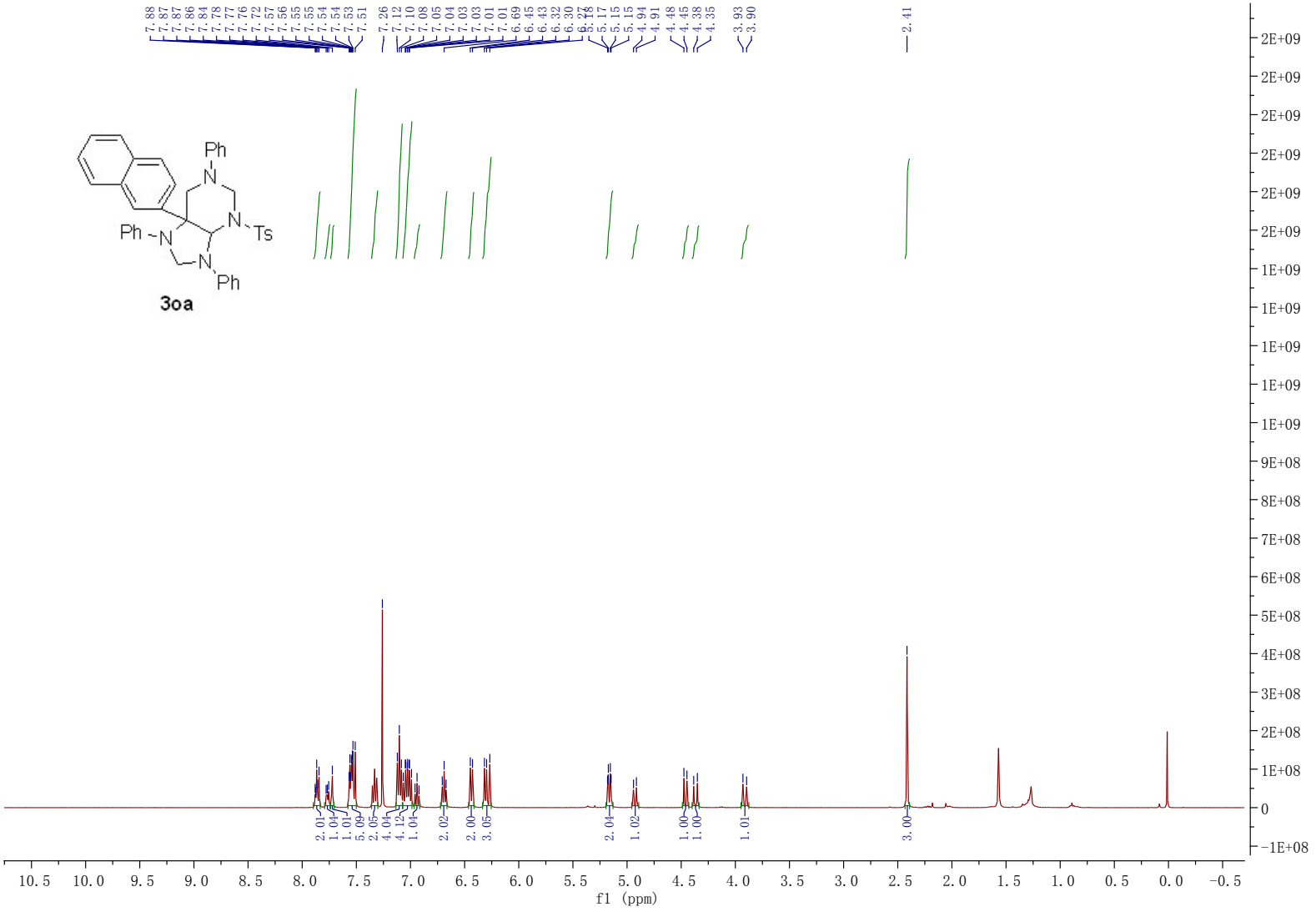
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.54
7.54
7.53
7.51
7.26
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7.08
7.05
7.04
7.03
7.03
7.01
7.01
6.69
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6.43
6.32
6.30
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5.15
5.15
4.94
4.91
4.48
4.45
4.38
4.35
3.93
3.90
2.41
Ph
N
Ph
N
Ts
N
N
Ph
3oa
2.01
1.04
1.01
5.09
2.05
4.04
4.12
1.04
2.02
2.00
3.05
2.04
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1.00
1.01
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1E+09
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
-1E+08
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9.0
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8.0
7.5
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6.5
6.0
5.5
5.0
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2.5
2.0
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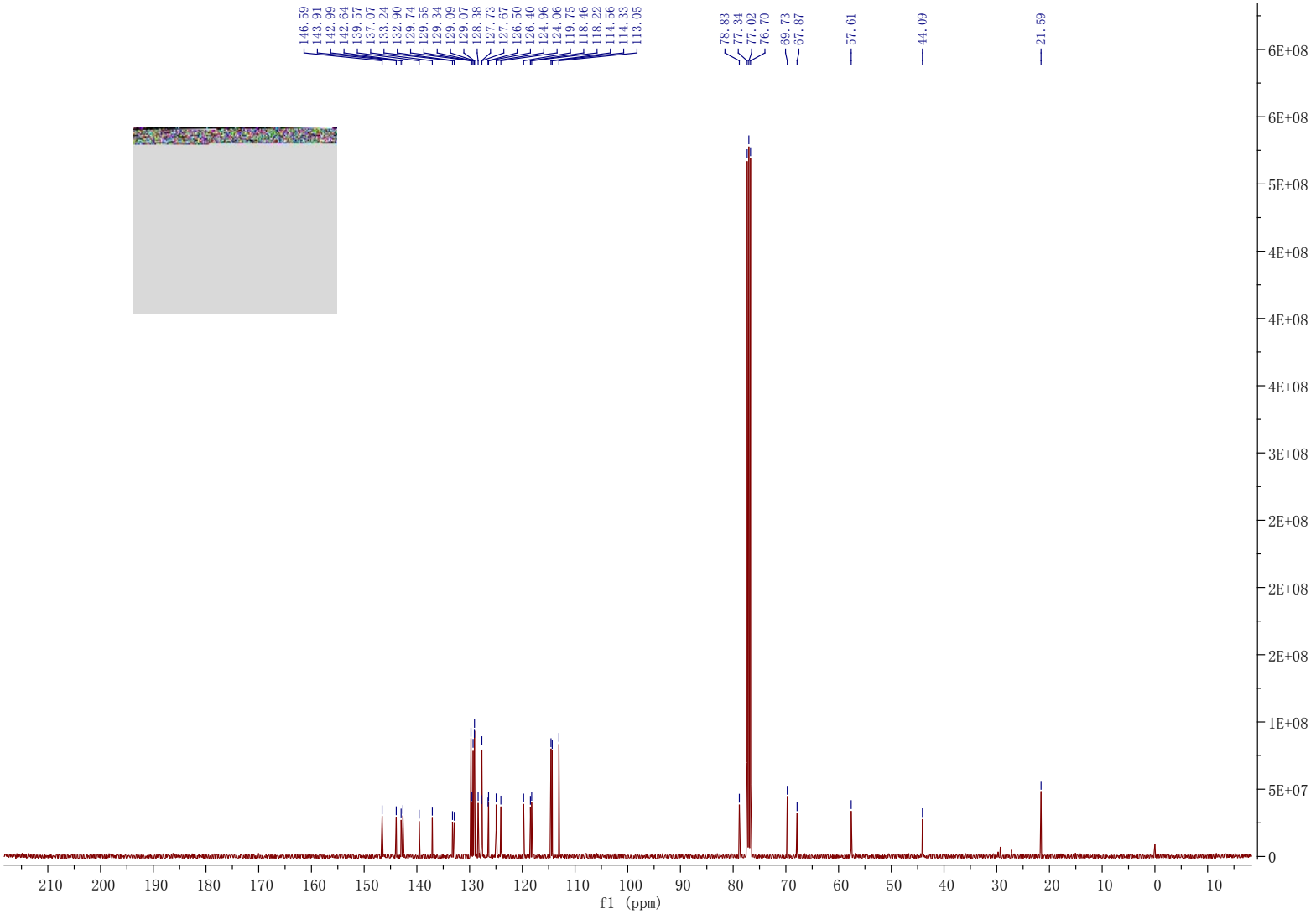
-0.5
f1 (ppm)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126.40
124.96
124.06
119.75
118.46
118.22
114.56
114.33
113.05
78.83
77.34
77.02
76.70
69.73
67.87
57.61
44.09
21.59
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
210
200
190
180
170
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140
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120
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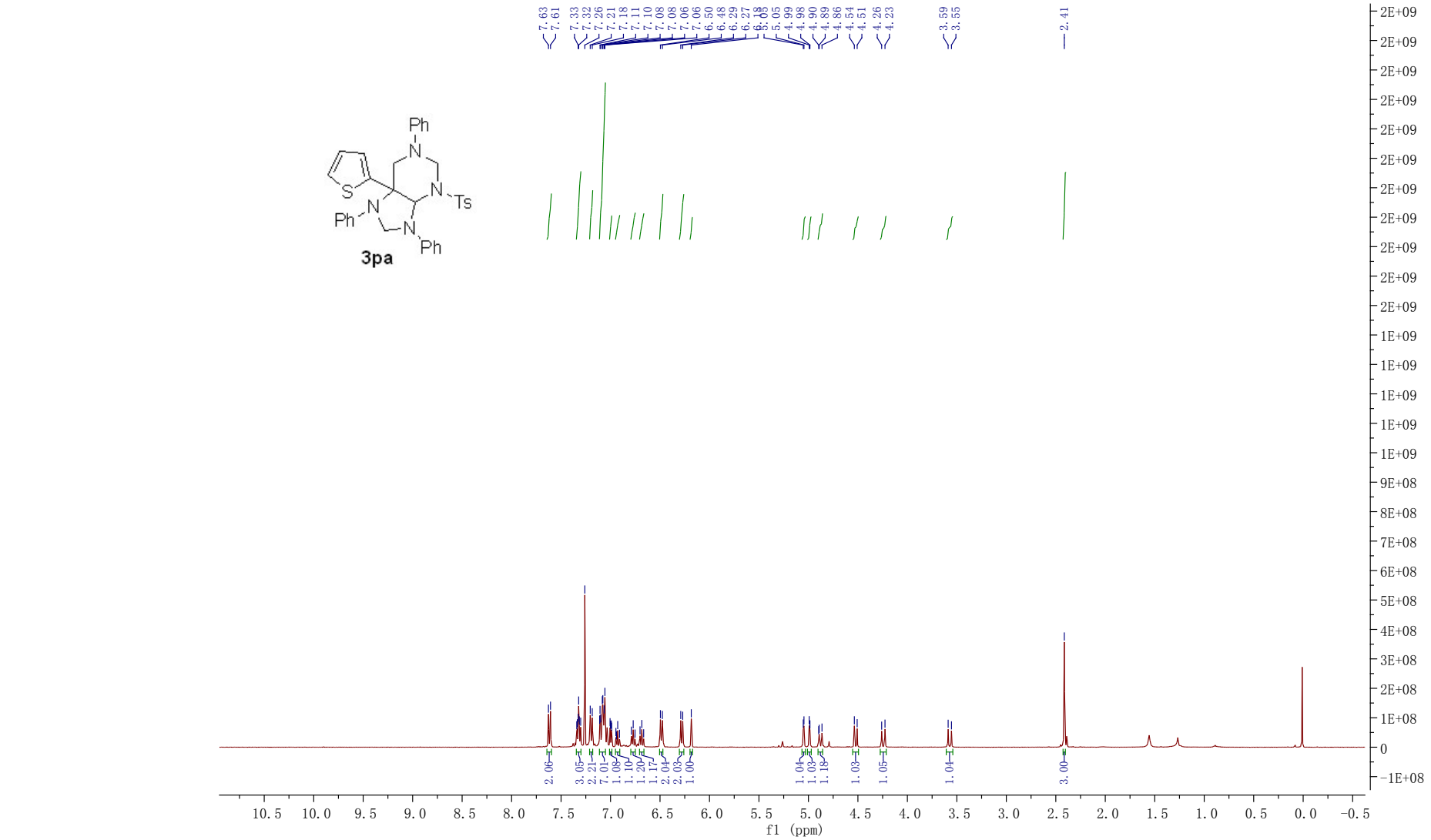
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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Ph
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Ph
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7.18
7.11
7.10
7.08
7.08
7.06
7.06
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6.48
6.29
6.27
5.05
4.99
4.98
4.90
4.89
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4.54
4.51
4.26
4.23
3.59
3.55
2.41
2.06
3.05
2.21
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1.08
1.10
1.20
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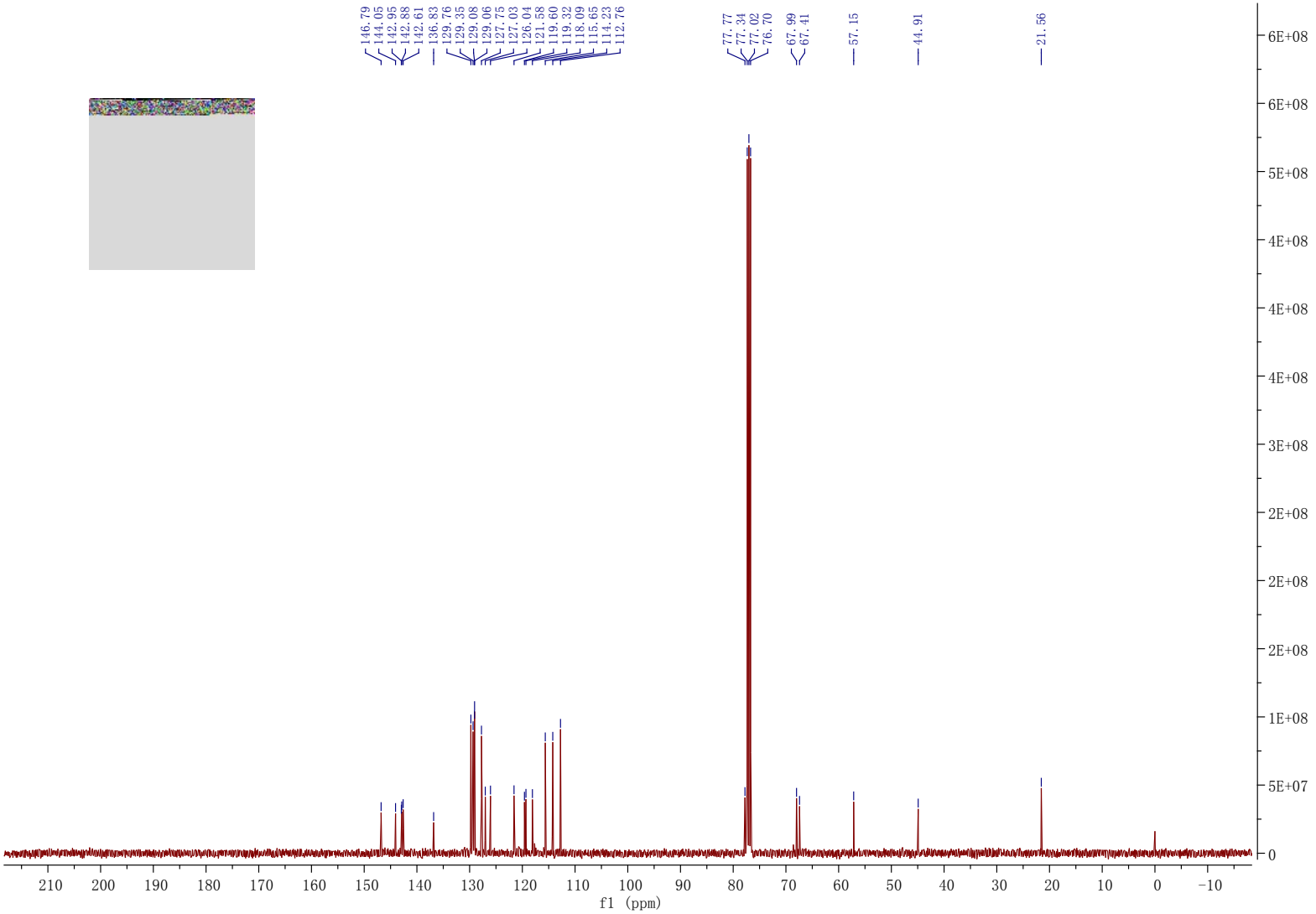
1.04
1.03
1.18
1.03
1.05
1.04
3.00
f1 (ppm)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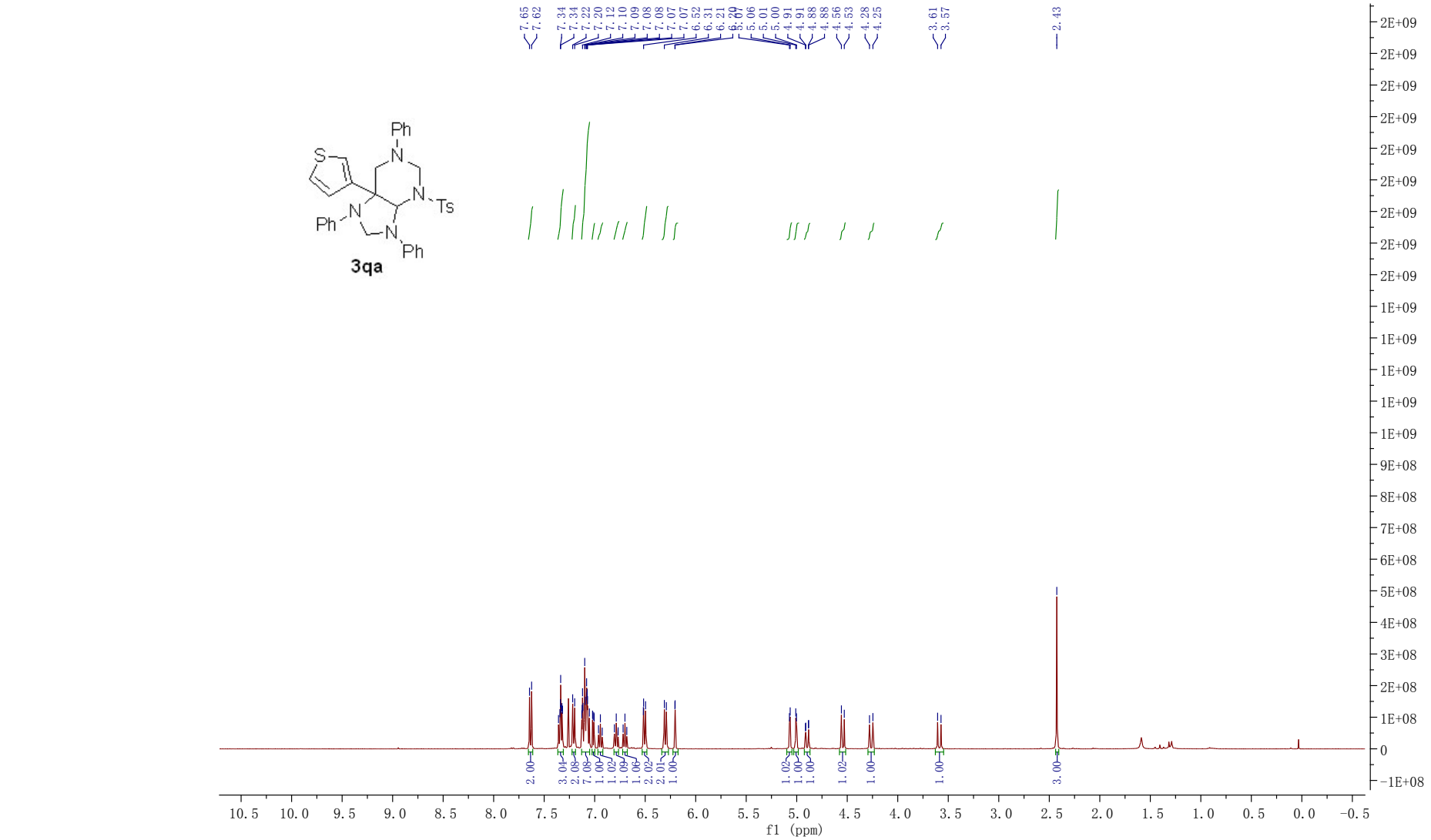
119.60
119.32
118.09
115.65
114.23
112.76
77.77
77.34
77.02
76.70
67.99
67.41
57.15
44.91
21.56
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.07
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6.21
5.06
5.01
5.00
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4.56
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4.25
3.61
3.57
2.43
Ph
N
S
N
Ts
Ph
N
N
Ph
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2.00
3.04
2.08
7.08
1.00
1.02
1.09
1.06
2.02
2.01
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1.00
1.02
1.00
1.00
3.00
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1E+09
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
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-1E+08
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7.0
6.5
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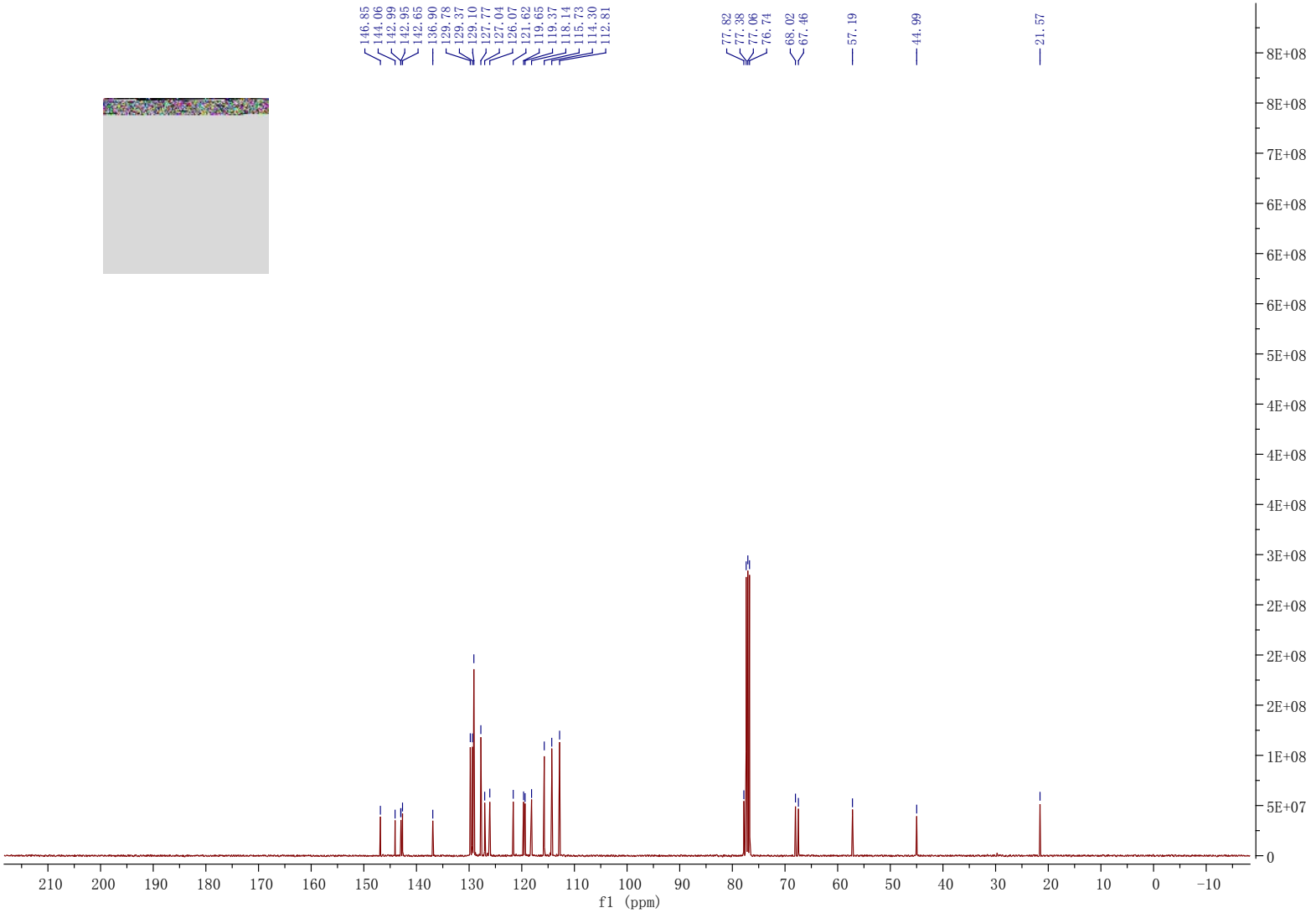
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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127.77
127.04
126.07
121.62
119.65
119.37
118.14
115.73
114.30
112.81
77.82
77.38
77.06
76.74
68.02
67.46
57.19
44.99
21.57
8E+08
8E+08
7E+08
6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
210
200
190
180
170
160
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140
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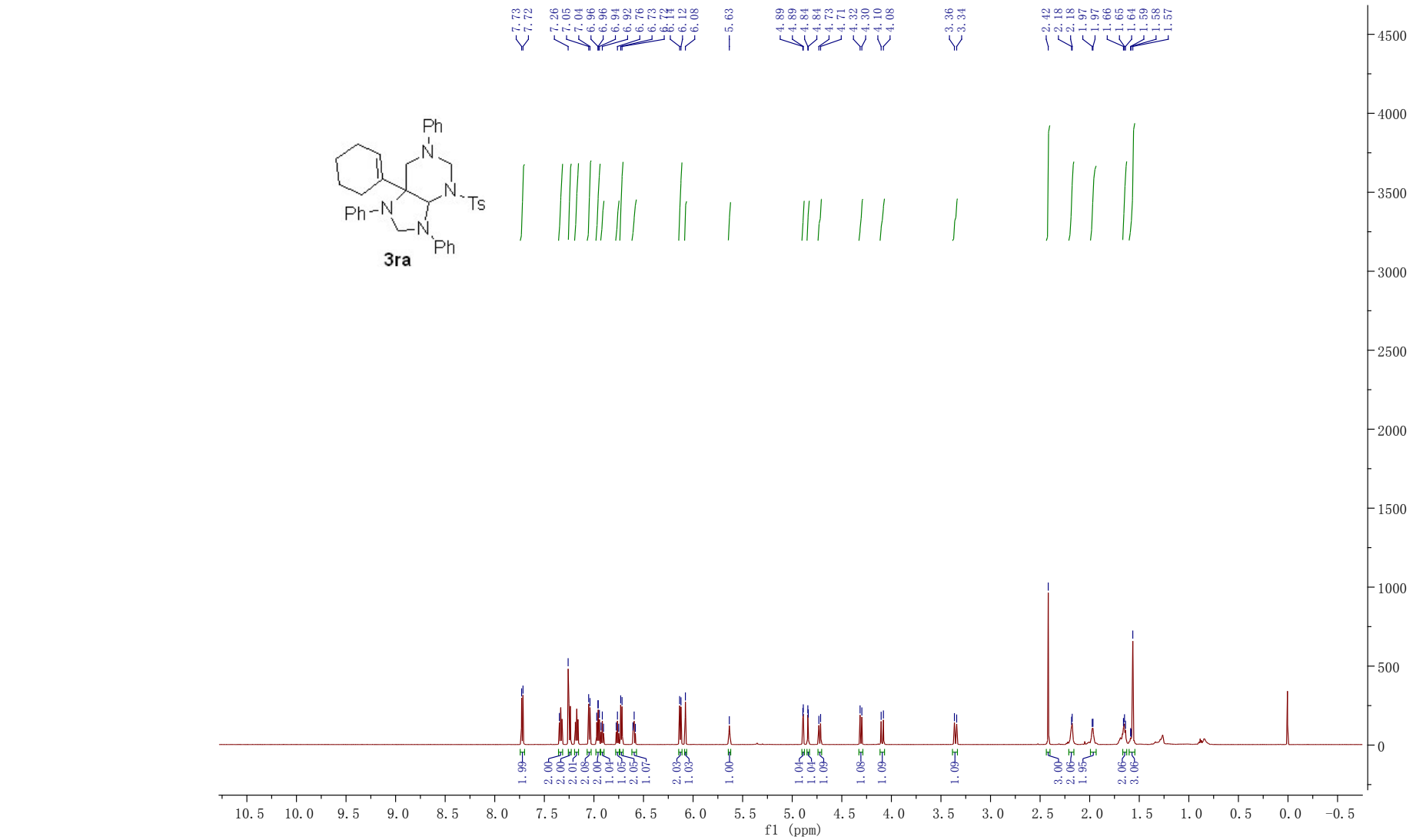
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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N
Ts
Ph
N
N
Ph
3ra
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7.72
7.26
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7.04
6.96
6.94
6.92
6.76
6.73
6.72
6.12
6.08
5.63
4.89
4.89
4.84
4.84
4.73
4.71
4.32
4.30
4.10
4.08
3.36
3.34
2.42
2.18
2.18
1.97
1.97
1.66
1.65
1.64
1.59
1.58
1.57
4500
4000
3500
3000
2500
2000
1500
1000
500
0
1.99
2.00
2.00
2.01
2.08
2.00
1.04
1.05
2.05
1.07
2.03
1.02
1.00
1.04
1.04
1.09
1.08
1.09
1.09
3.00
2.06
1.95
2.06
3.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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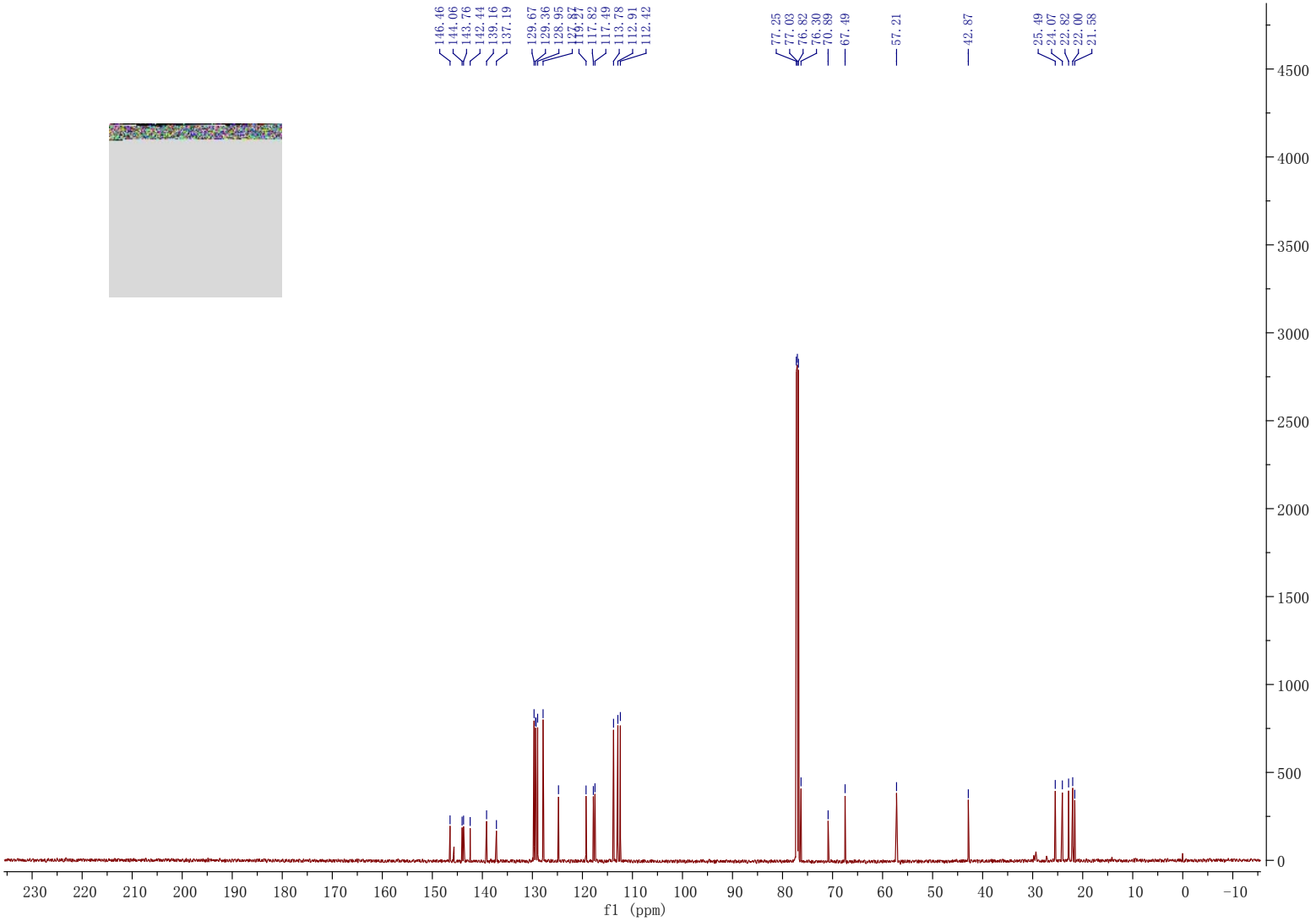
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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127.87
127.27
119.47
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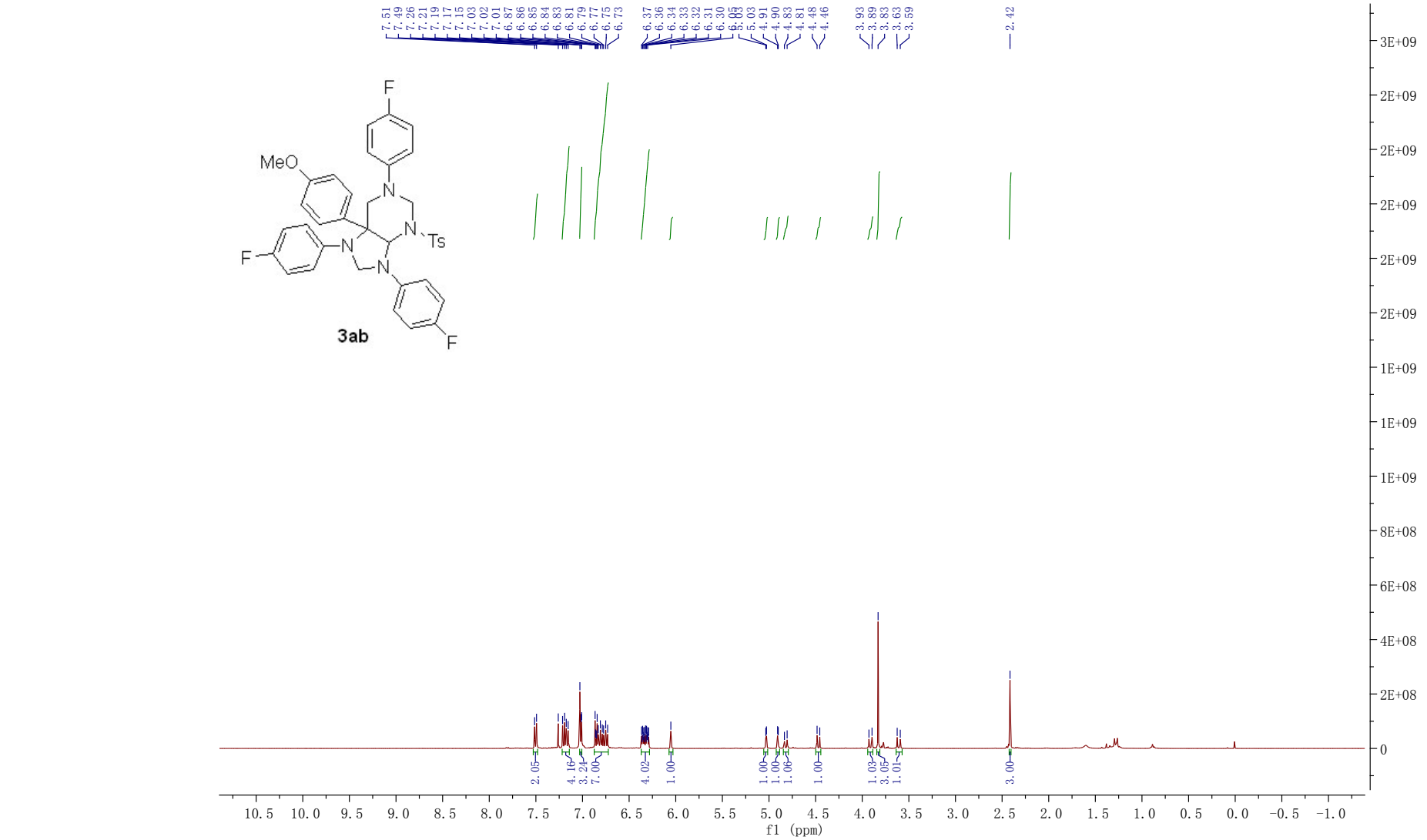
117.49
113.78
112.91
112.42
77.25
77.03
76.82
76.30
70.89
67.49
57.21
42.87
25.49
24.07
22.82
22.00
21.58
4500
4000
3500
3000
2500
2000
1500
1000
500
0
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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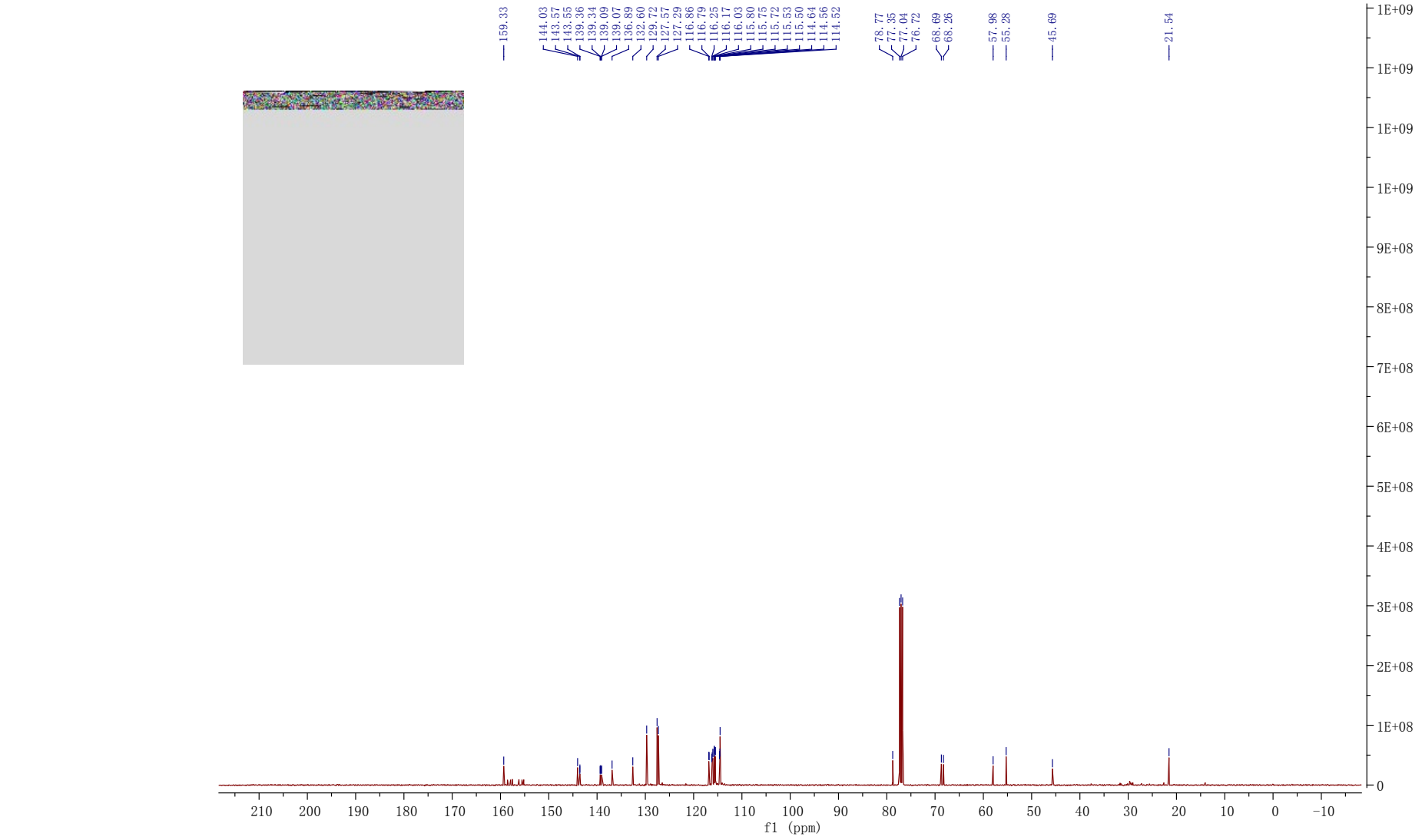
7.21
7.19
7.17
7.15
7.03
7.02
7.01
6.87
6.86
6.85
6.84
6.83
6.81
6.79
6.77
6.75
6.73
6.37
6.36
6.34
6.33
6.32
6.31
6.30
5.03
4.91
4.90
4.83
4.81
4.48
4.46
3.93
3.89
3.83
3.63
3.59
2.42
MeO
F
N
N
Ts
N
N
F
F
3ab
3E+09
2E+09
2E+09
2E+09
2E+09
2E+09
1E+09
1E+09
1E+09
8E+08
6E+08
4E+08
2E+08
0
2.05
4.16
3.24
7.00
4.02
1.00
1.00
1.00
1.06
1.00
1.08
3.05
1.01
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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139.34
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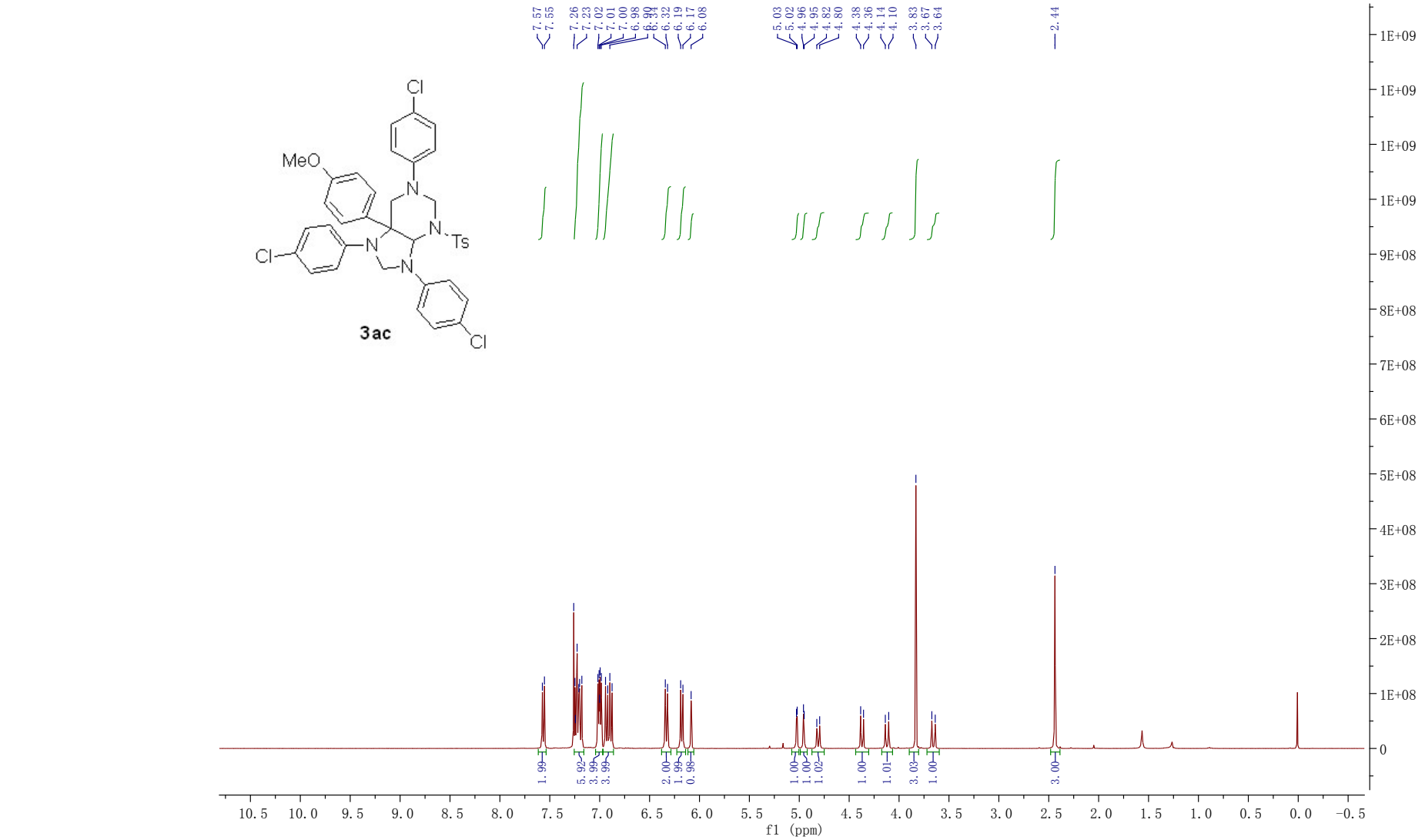
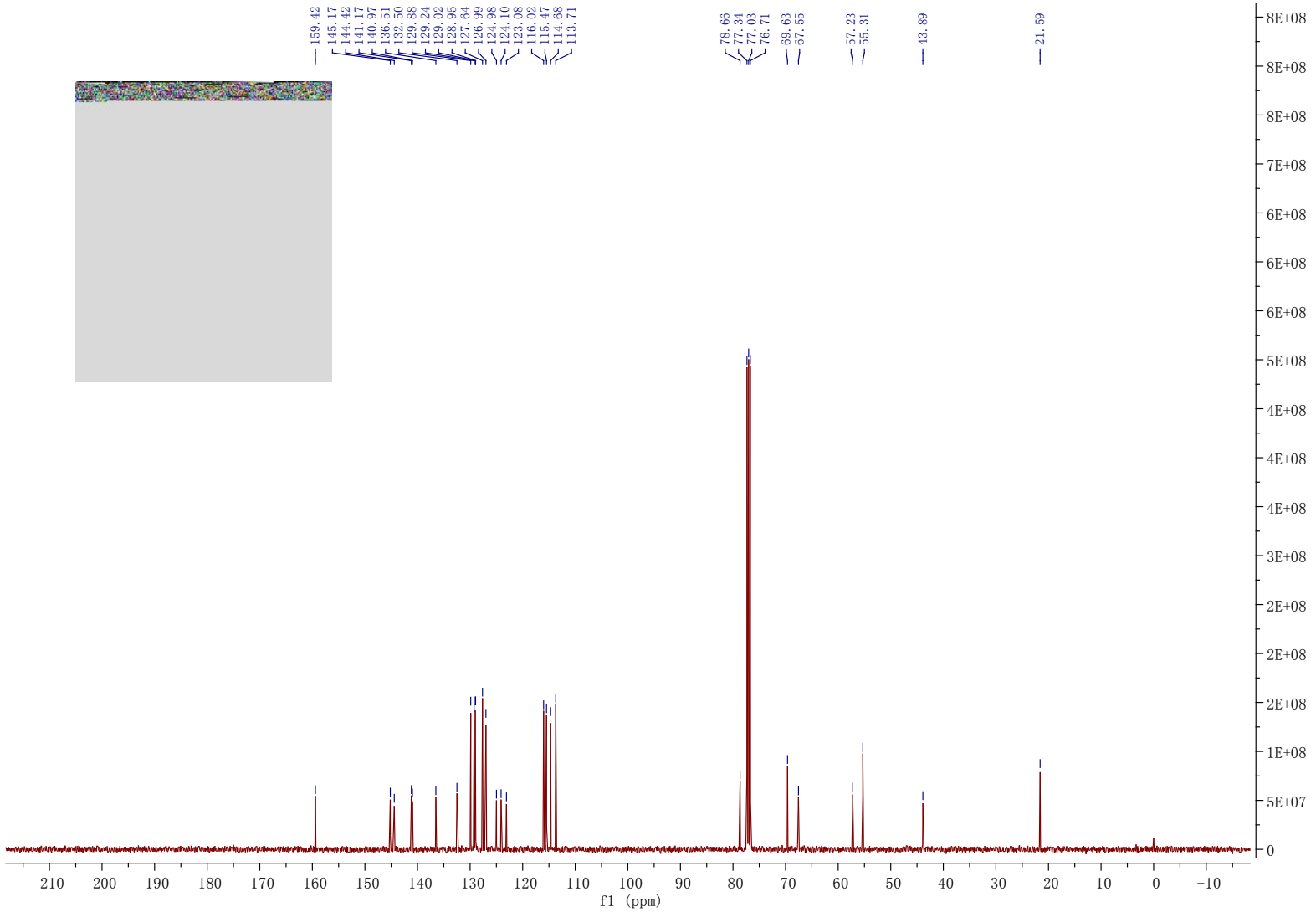
139.07
136.89
132.60
129.72
127.57
127.29
116.86
116.79
116.25
116.17
116.03
115.80
115.75
115.72
115.53
115.50
114.64
114.56
114.52
78.77
77.35
77.04
76.72
68.69
68.26
57.98
55.28
45.69
21.54
1E+09
1E+09
1E+09
1E+09
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


Cl
MeO
N
N
Ts
Cl
N
N
Cl
3ac
7.57
7.55
7.26
7.23
7.02
7.01
7.00
6.98
6.34
6.32
6.19
6.17
6.08
5.03
5.02
4.96
4.95
4.82
4.80
4.38
4.36
4.14
4.10
3.83
3.67
3.64
2.44
1E+09
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
1.99
5.92
3.99
3.99
2.00
1.99
0.98
1.00
1.00
1.02
1.00
1.01
3.03
1.00
3.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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144.42
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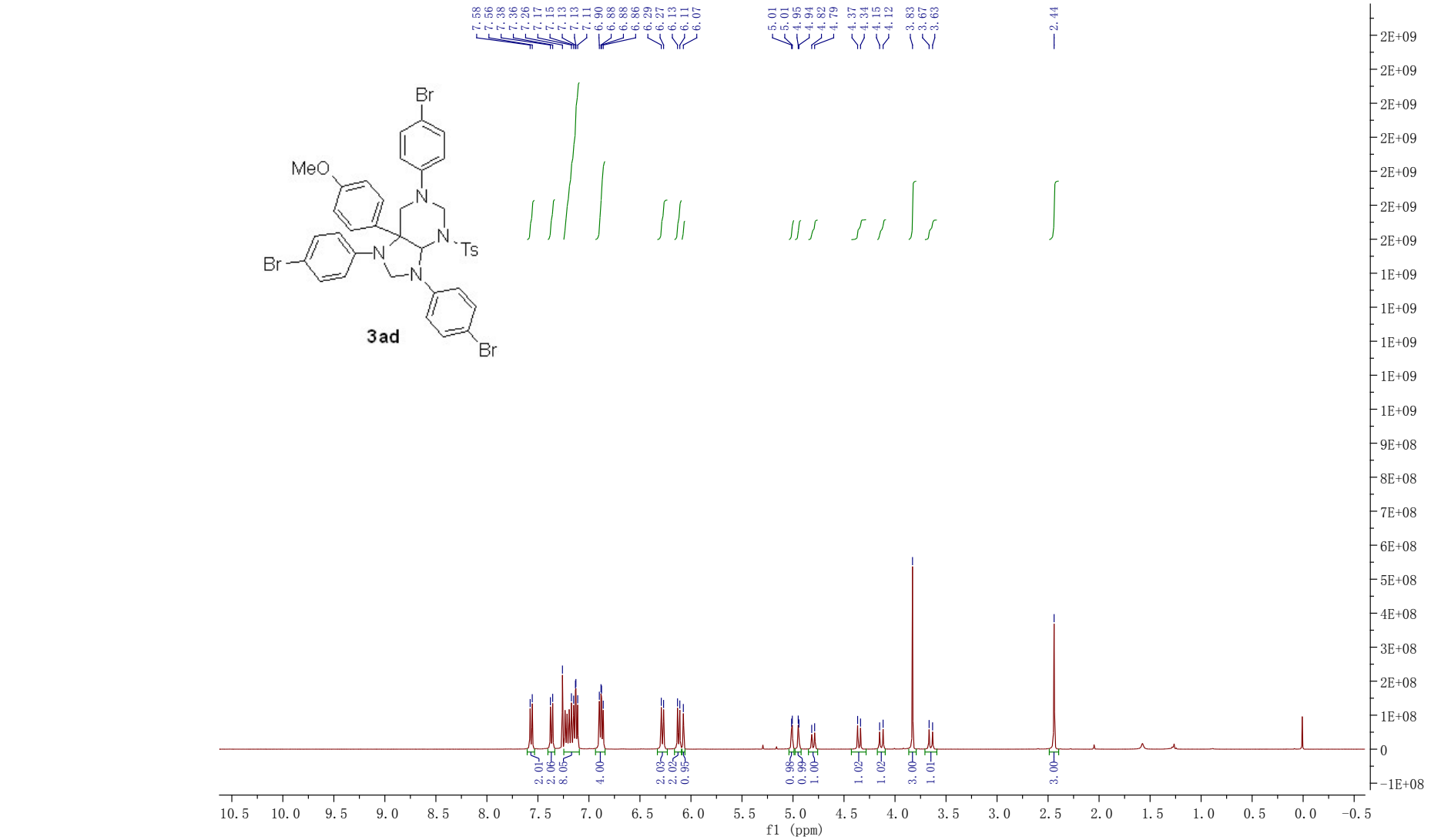
136.51
132.50
129.88
129.24
129.02
128.95
127.64
126.99
124.98
124.10
123.08
116.02
115.47
114.68
113.71
78.66
77.34
77.03
76.71
69.63
67.55
57.23
55.31
43.89
21.59
8E+08
8E+08
8E+08
7E+08
6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)


7.58
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7.38
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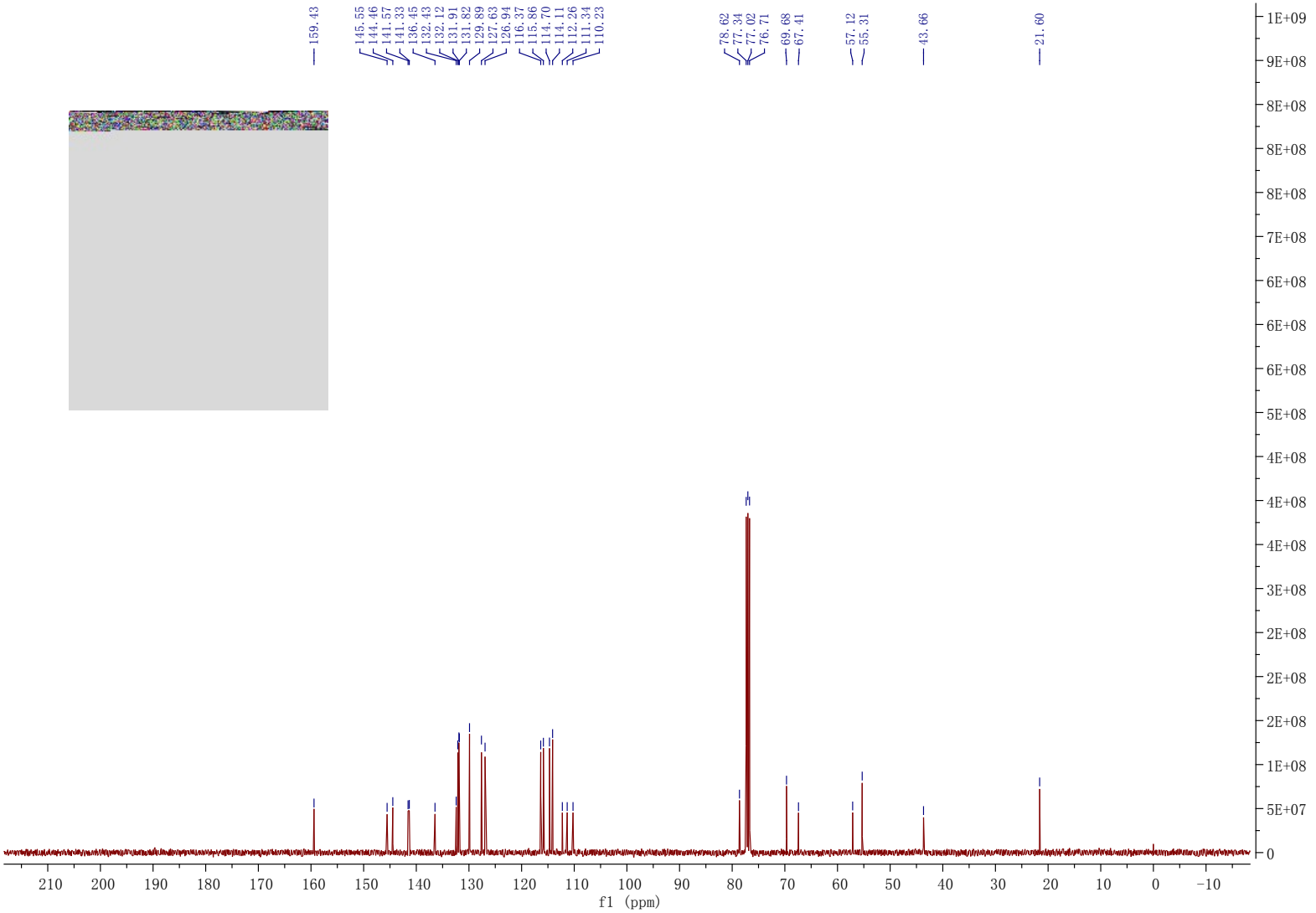
7.26
7.17
7.15
7.13
7.11
6.90
6.88
6.86
6.29
6.27
6.13
6.11
6.07
5.01
5.01
4.95
4.94
4.82
4.79
4.37
4.34
4.15
4.12
3.83
3.67
3.63
2.44
Br
MeO
N
N
N
Ts
Br
N
Br
3ad
2.01
2.06
8.05
4.00
2.03
2.02
0.95
0.98
0.99
1.00
1.02
1.02
3.00
1.01
3.00
f1 (ppm)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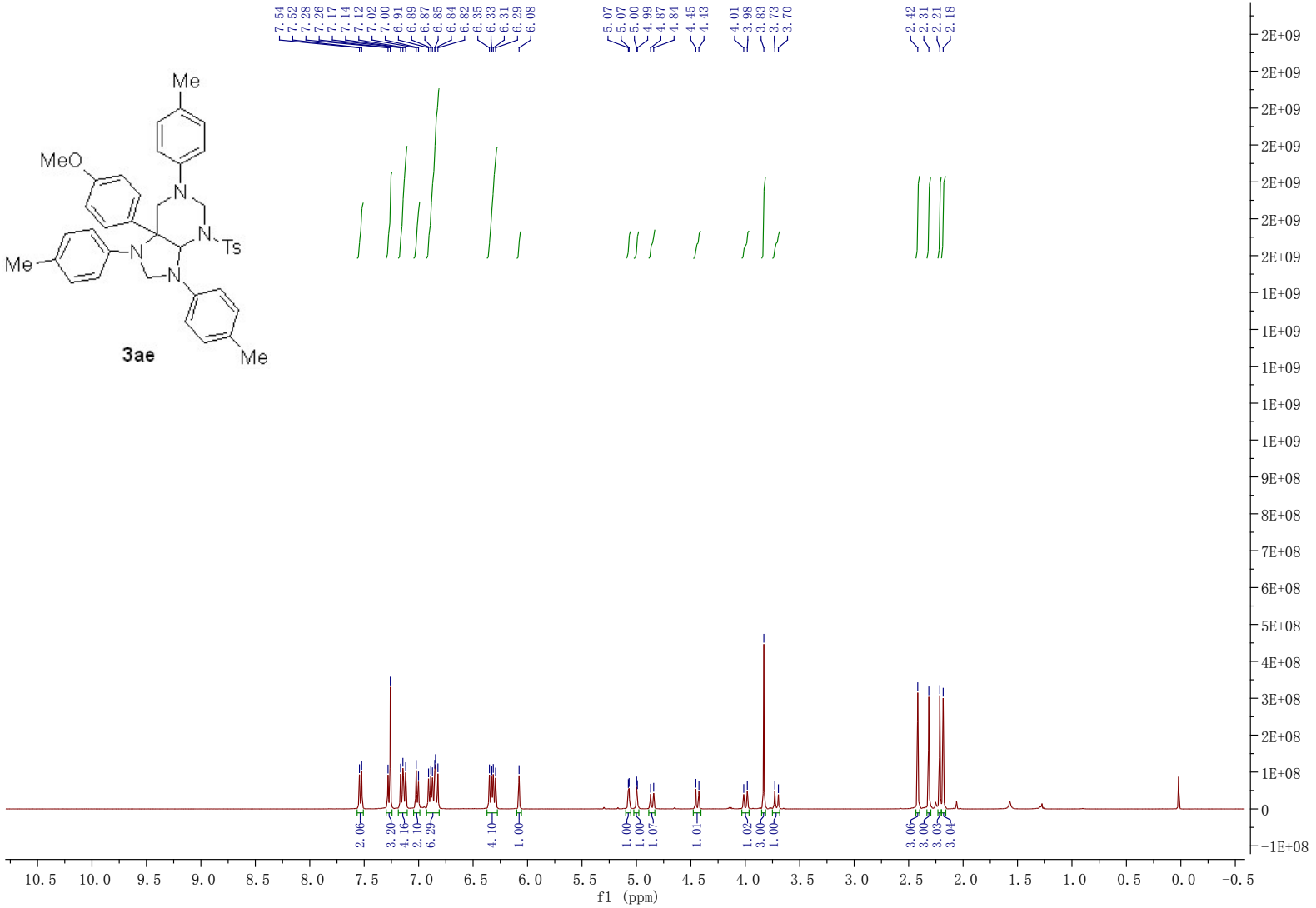
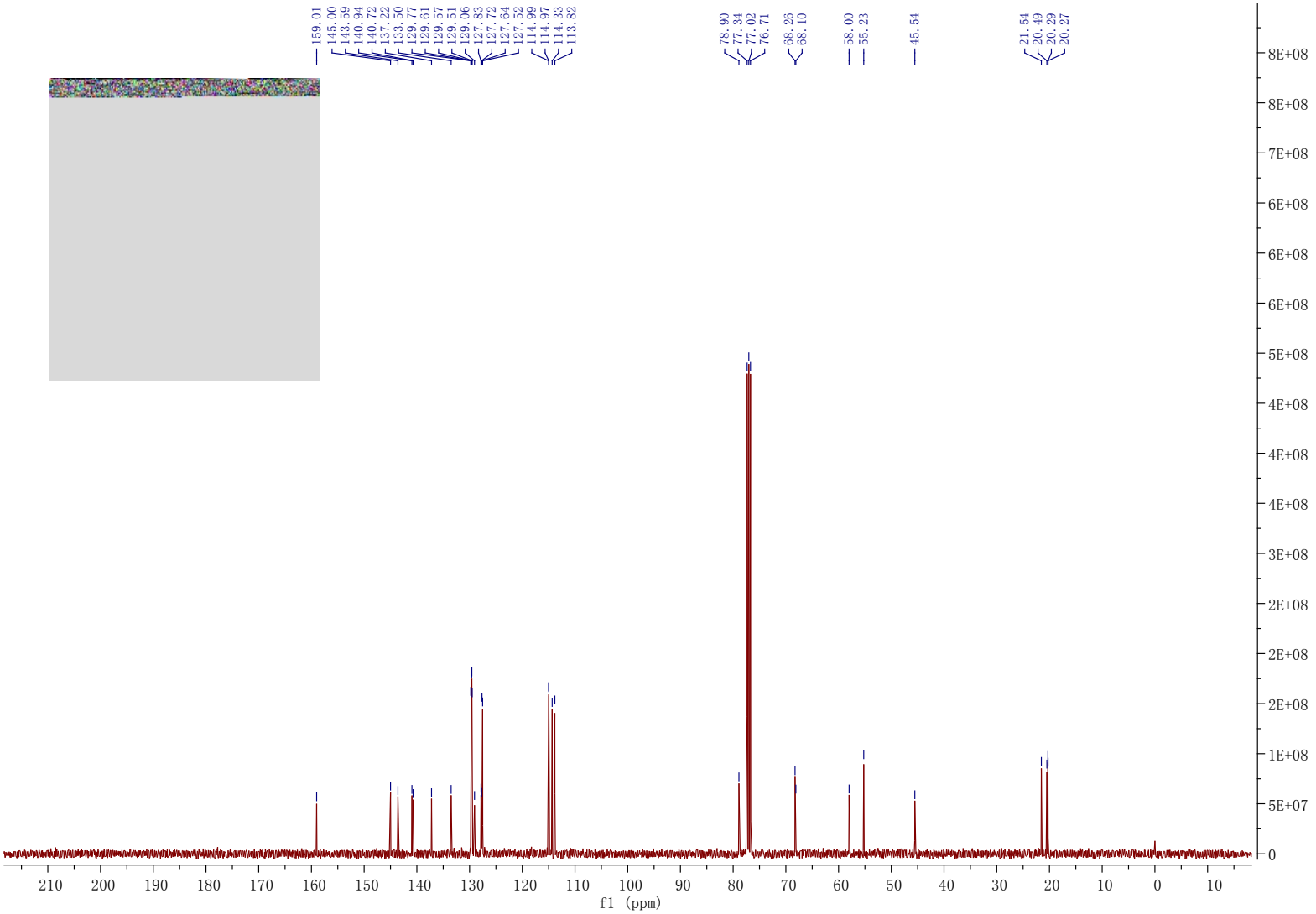
131.91
131.82
129.89
127.63
126.94
116.37
115.86
114.70
114.11
112.26
111.34
110.23
78.62
77.34
77.02
76.71
69.68
67.41
57.12
55.31
43.66
21.60
f1 (ppm)


Me
MeO
N
N
Ts
Me
N
N
Me
3ae
7.54
7.52
7.28
7.26
7.17
7.14
7.12
7.02
7.00
6.91
6.89
6.87
6.85
6.84
6.82
6.35
6.33
6.31
6.29
6.08
5.07
5.07
5.00
4.99
4.87
4.84
4.45
4.43
4.01
3.98
3.83
3.73
3.70
2.42
2.31
2.21
2.18
2.06
3.20
4.16
2.10
6.29
4.10
1.00
1.00
1.00
1.07
1.01
1.02
3.00
1.00
3.06
3.00
3.03
3.04
f1 (ppm)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140.72
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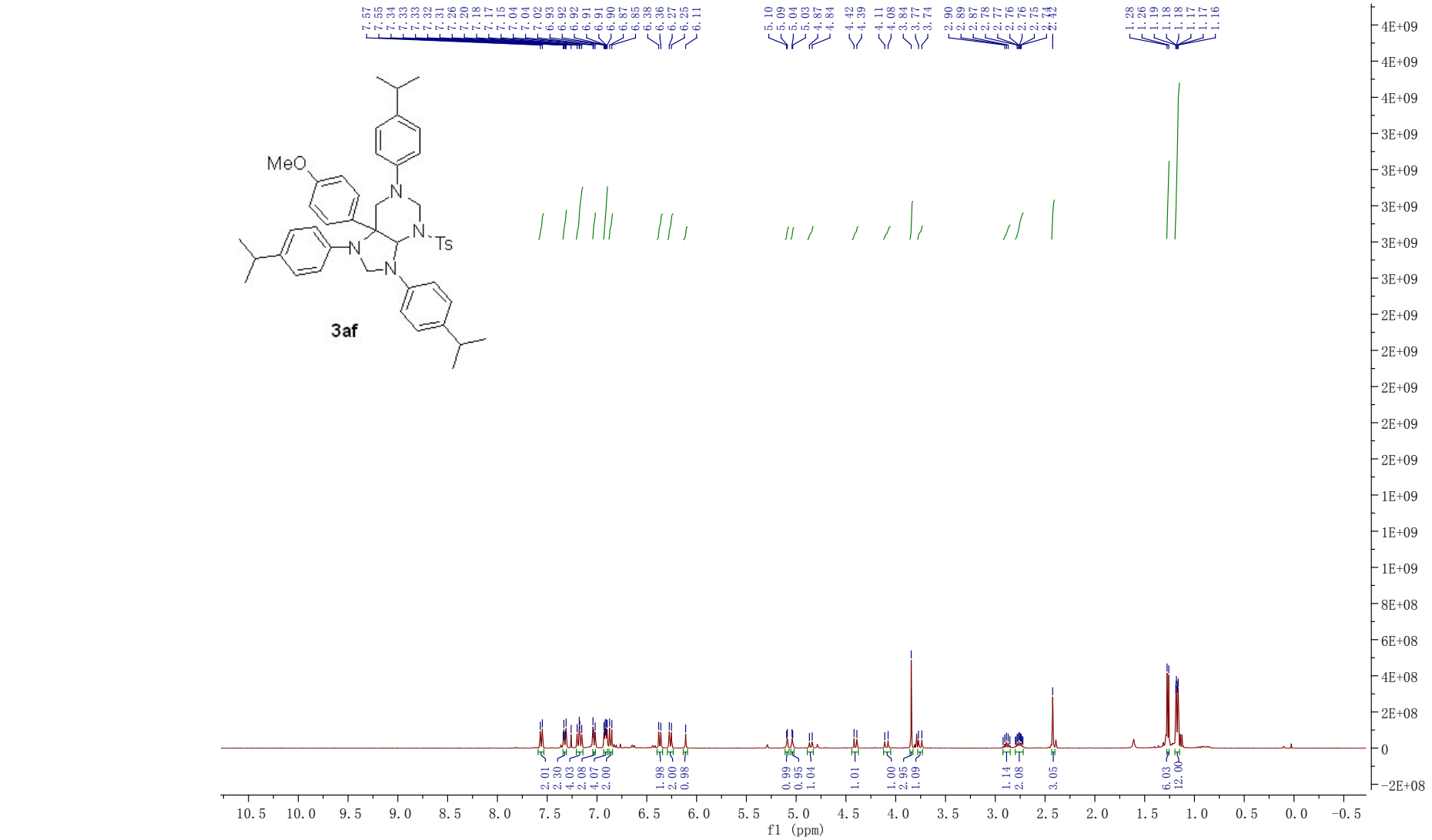
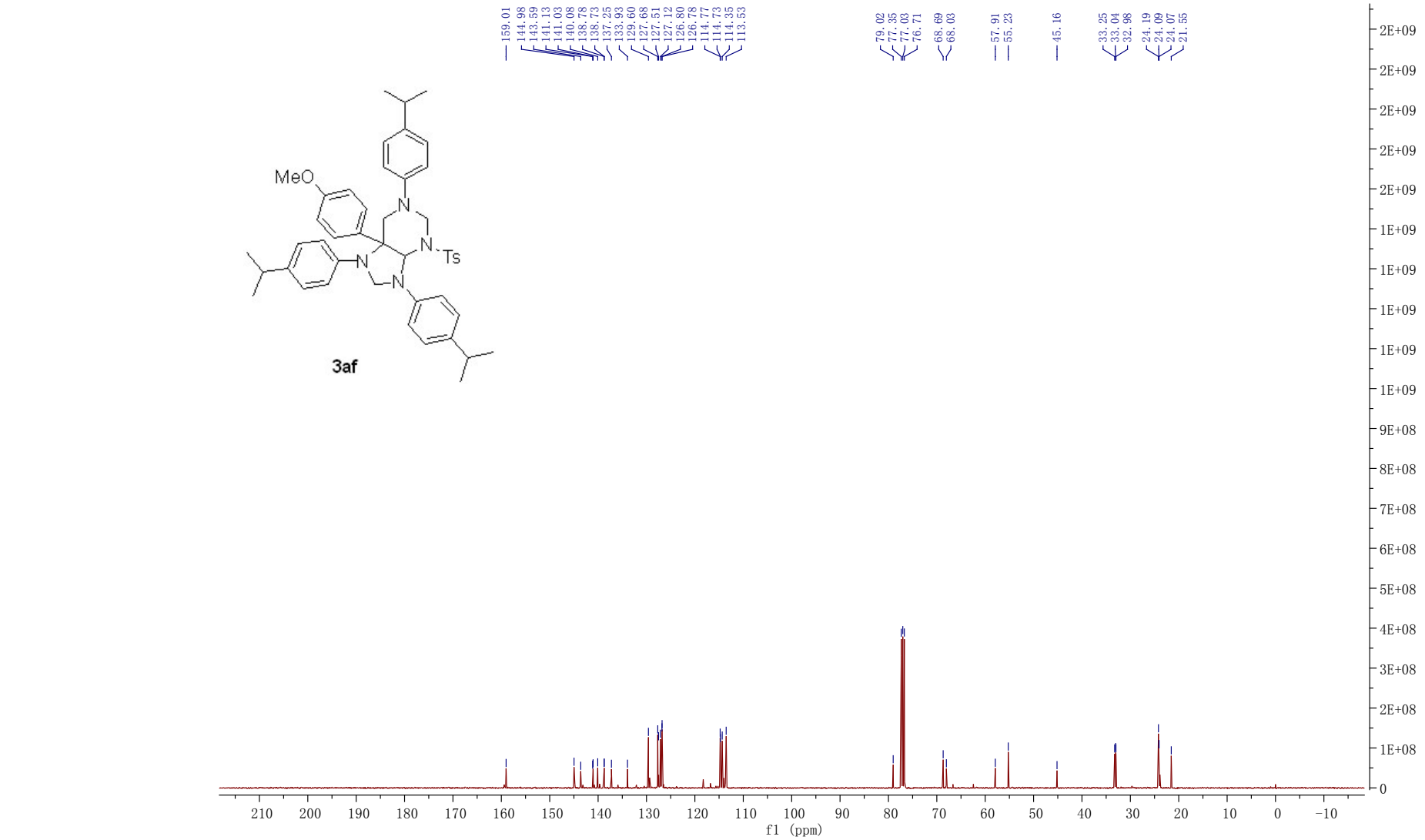
129.77
129.61
129.57
129.51
129.06
127.83
127.72
127.64
127.52
114.99
114.97
114.33
113.82
78.90
77.34
77.02
76.71
68.26
68.10
58.00
55.23
45.54
21.54
20.49
20.29
20.27
8E+08
8E+08
7E+08
6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)


MeO
N
N
Ts
N
N
3af
7.57 7.55 7.34 7.33 7.33 7.32 7.31 7.26 7.20 7.18 7.17 7.15 7.04 7.04 7.02 6.93 6.92 6.92 6.91 6.91 6.90 6.87 6.85 6.38 6.36 6.27 6.25 6.11
5.10 5.09 5.04 5.03 4.87 4.84 4.42 4.39 4.11 4.08 3.84 3.77 3.74 2.90 2.89 2.87 2.78 2.77 2.76 2.76 2.75 2.74 2.42 1.28 1.26 1.19 1.18 1.18 1.17 1.17 1.16
2.01 2.30 4.03 2.08 4.07 2.00 1.98 2.00 0.98 0.99 0.95 1.04 1.01 1.00 2.95 1.09 1.14 2.08 3.05 6.03 12.00
f1 (ppm)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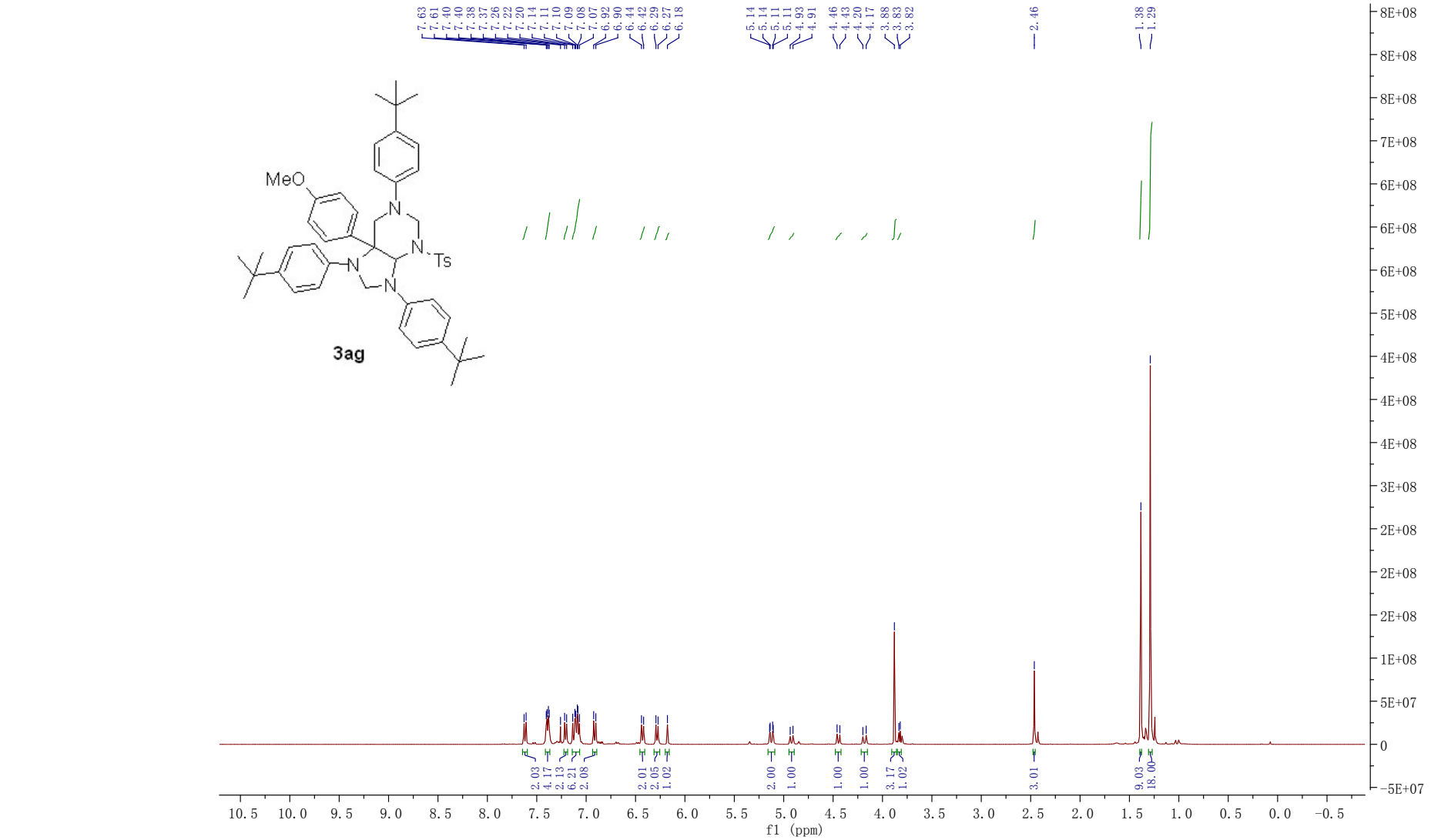
144.98
143.59
141.13
141.03
140.08
138.78
138.73
137.25
133.93
129.60
127.68
127.51
127.12
126.80
126.78
114.77
114.73
114.35
113.53
79.02
77.35
77.03
76.71
68.69
68.03
57.91
55.23
45.16
33.25
33.04
32.98
24.19
24.09
24.07
21.55
MeO
N
N
Ts
N
N
3af
2E+09
2E+09
2E+09
2E+09
2E+09
1E+09
1E+09
1E+09
1E+09
1E+09
1E+09
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.63
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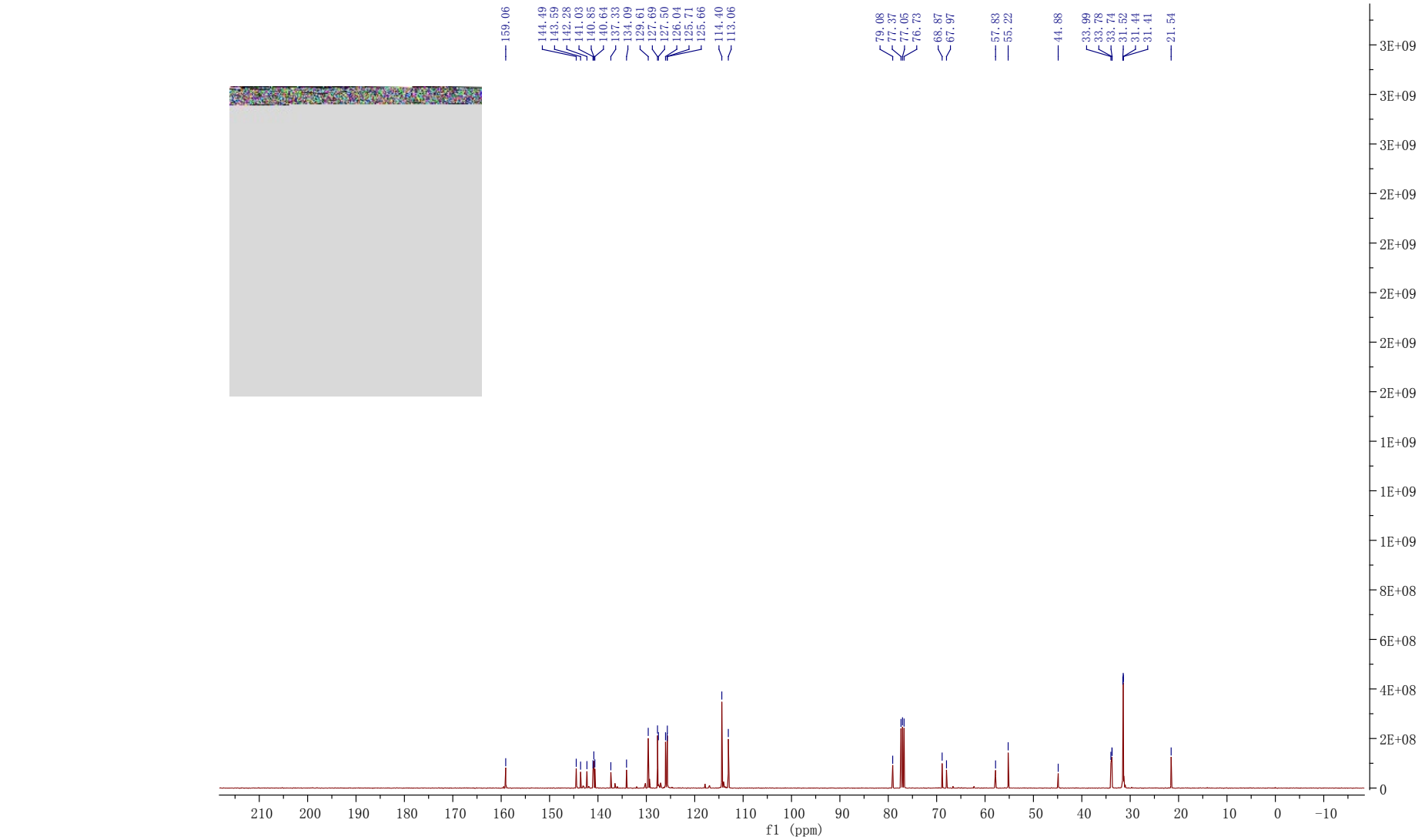
7.26
7.22
7.20
7.14
7.11
7.10
7.09
7.08
7.07
6.92
6.90
6.44
6.42
6.29
6.27
6.18
5.14
5.14
5.11
5.11
4.93
4.91
4.46
4.43
4.20
4.17
3.88
3.83
3.82
2.46
1.38
1.29
MeO
N
N
Ts
N
N
3ag
2.03
4.17
2.13
6.21
2.08
2.01
2.05
1.02
2.00
1.00
1.00
1.00
3.17
1.02
3.01
9.03
18.00
8E+08
8E+08
8E+08
7E+08
6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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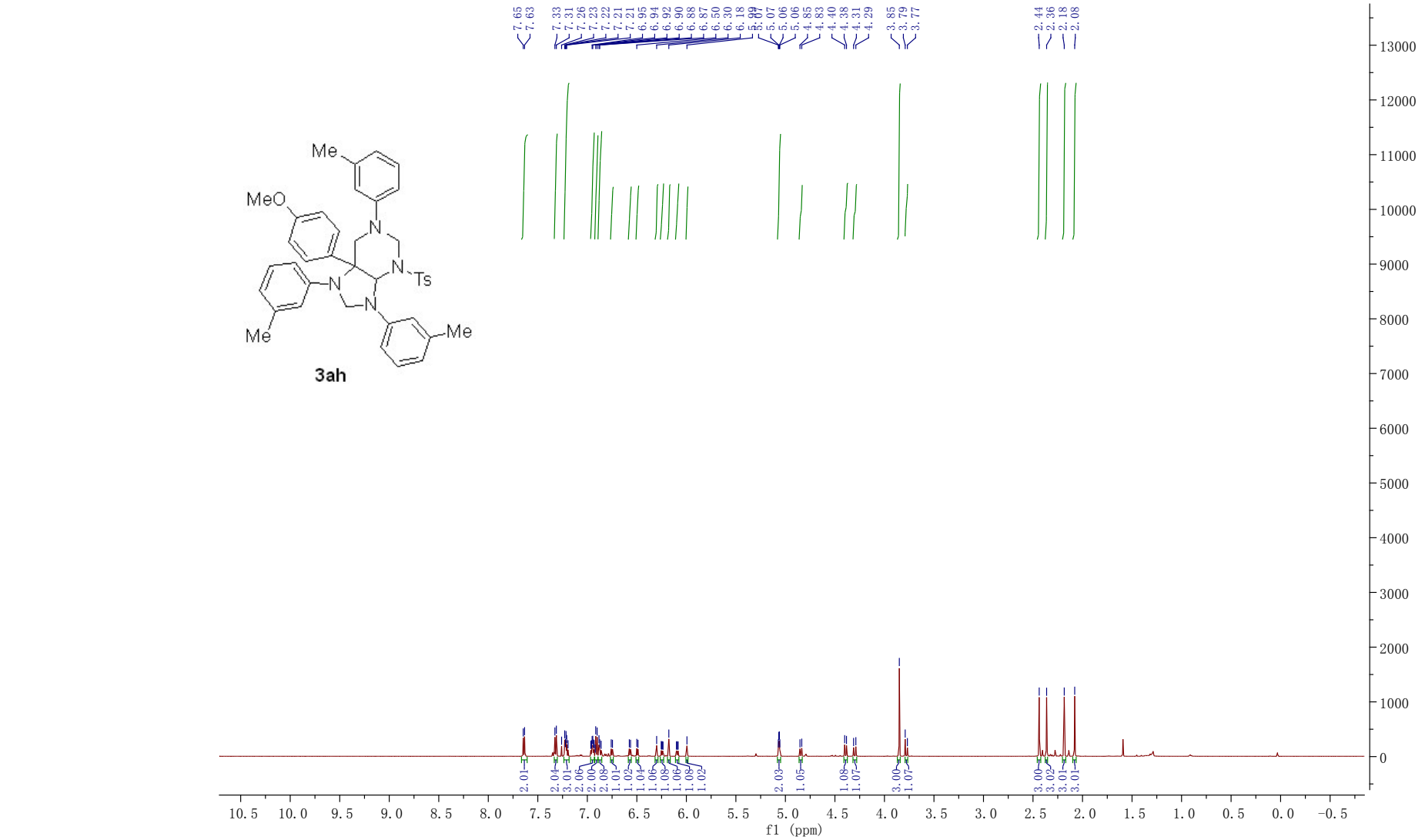
143.59
142.28
141.03
140.85
140.64
137.33
134.09
129.61
127.69
127.50
126.04
125.71
125.66
114.40
113.06
79.08
77.37
77.05
76.73
68.87
67.97
57.83
55.22
44.88
33.99
33.78
33.74
31.52
31.44
31.41
21.54
3E+09
3E+09
3E+09
2E+09
2E+09
2E+09
2E+09
2E+09
2E+09
1E+09
1E+09
1E+09
1E+09
8E+08
6E+08
4E+08
2E+08
0
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)


Me
MeO
N
N
Ts
N
N
Me
Me
3ah
7.65
7.63
7.33
7.31
7.26
7.23
7.22
7.21
7.21
6.95
6.94
6.92
6.90
6.88
6.87
6.50
6.30
6.18
5.07
5.06
5.06
4.85
4.83
4.40
4.38
4.31
4.29
3.85
3.79
3.77
2.44
2.36
2.18
2.08
2.01
2.04
3.01
2.06
2.00
2.09
1.01
1.02
1.04
1.06
1.08
1.06
1.09
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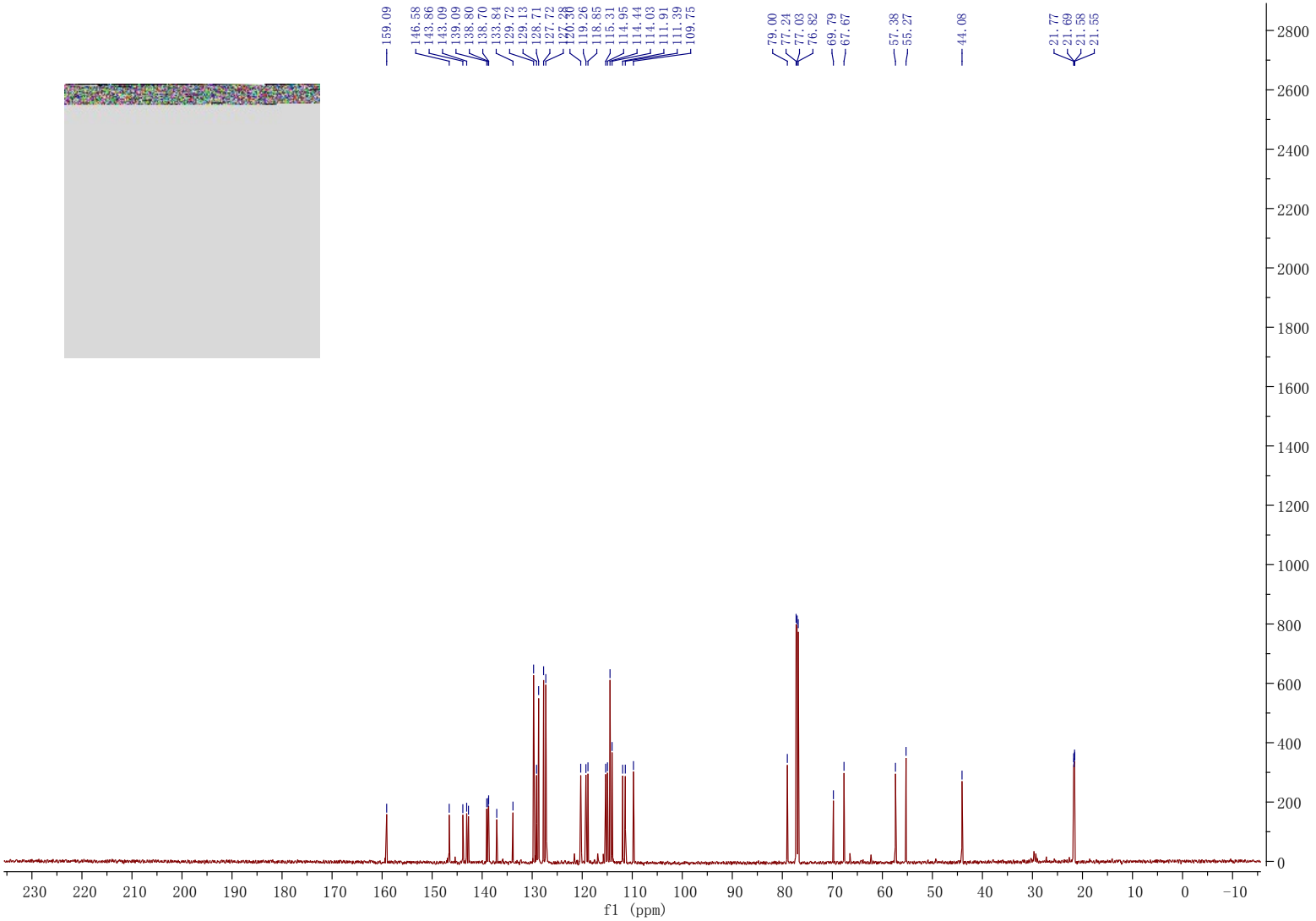
1.07
3.00
3.02
3.01
3.01
f1 (ppm)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143.86
143.09
139.09
138.80
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133.84
129.72
129.13
128.71
127.72
119.26
118.85
115.31
114.95
114.44
114.03
111.91
111.39
109.75
79.00
77.24
77.03
76.82
69.79
67.67
57.38
55.27
44.08
21.77
21.69
21.58
21.55
f1 (ppm)