Supporting information for:

A Homodinuclear Cobalt Complex for Catalytic Asymmetric Michael Reaction of β-Ketoesters to Nitroolefins

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1. ESI-MS charts

1.1 ESI-MS analysis of the complexes

1.1.1 ESI-MS of **2a**/Co(acac)$_2$ = 1:1 mixture without the additive of *N*-methyl morpholine

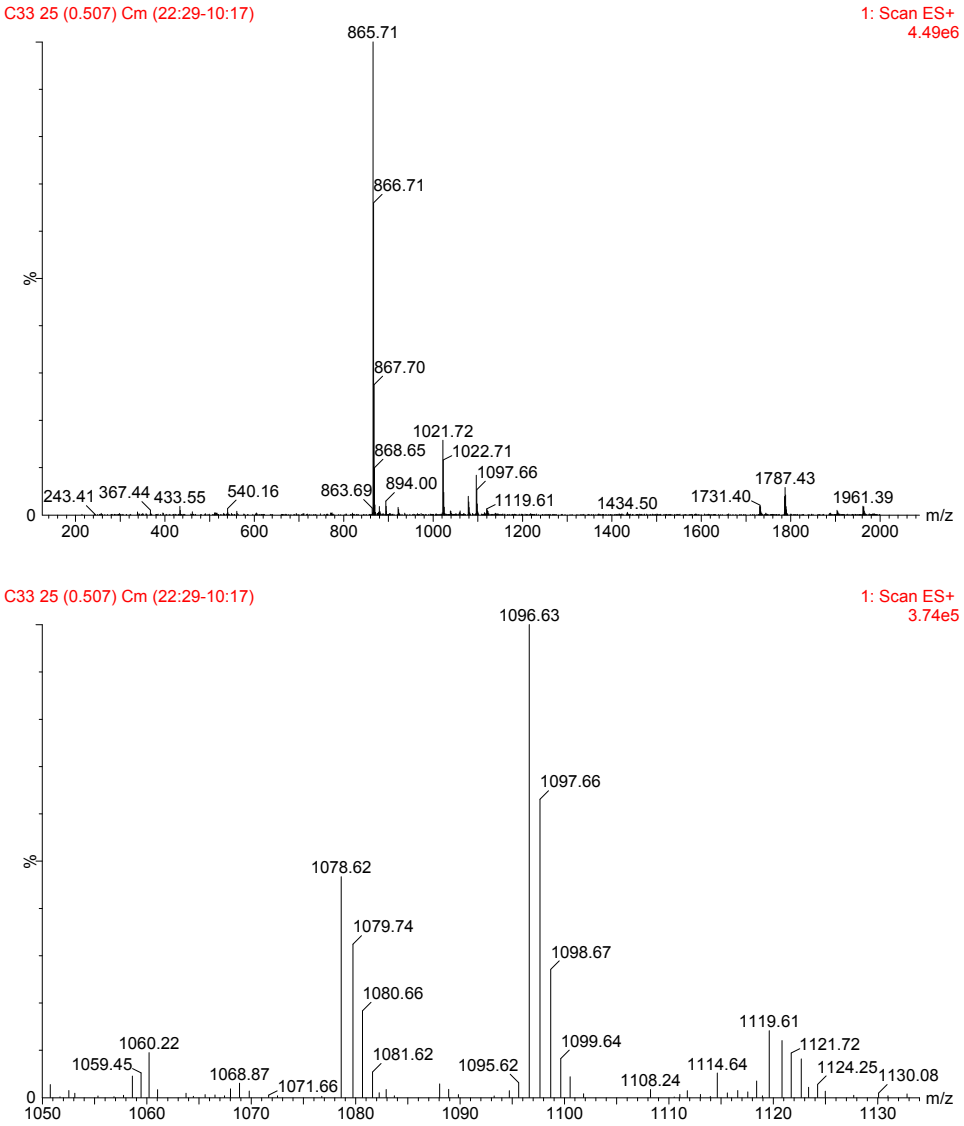


Figure S1.

Calcd. $C_{56}H_{57}Co_2N_4O_7S_2^+$ [$M_{\mathbf{2a}}$ – 3H + Co_2(acac) + H]$^+$: 1079.23, Found: 1079.74;

Calcd. $C_{56}H_{60}Co_2N_5O_7S_2^+$ [$M_{\mathbf{2a}}$ – 3H + Co_2(acac) + NH_4]$^+$: 1096.26,Found: 1096.63.

1.1.2 ESI-MS of **2a**/Co(acac)$_2$ = 1:1 mixture with the additive of *N*-methyl morpholine

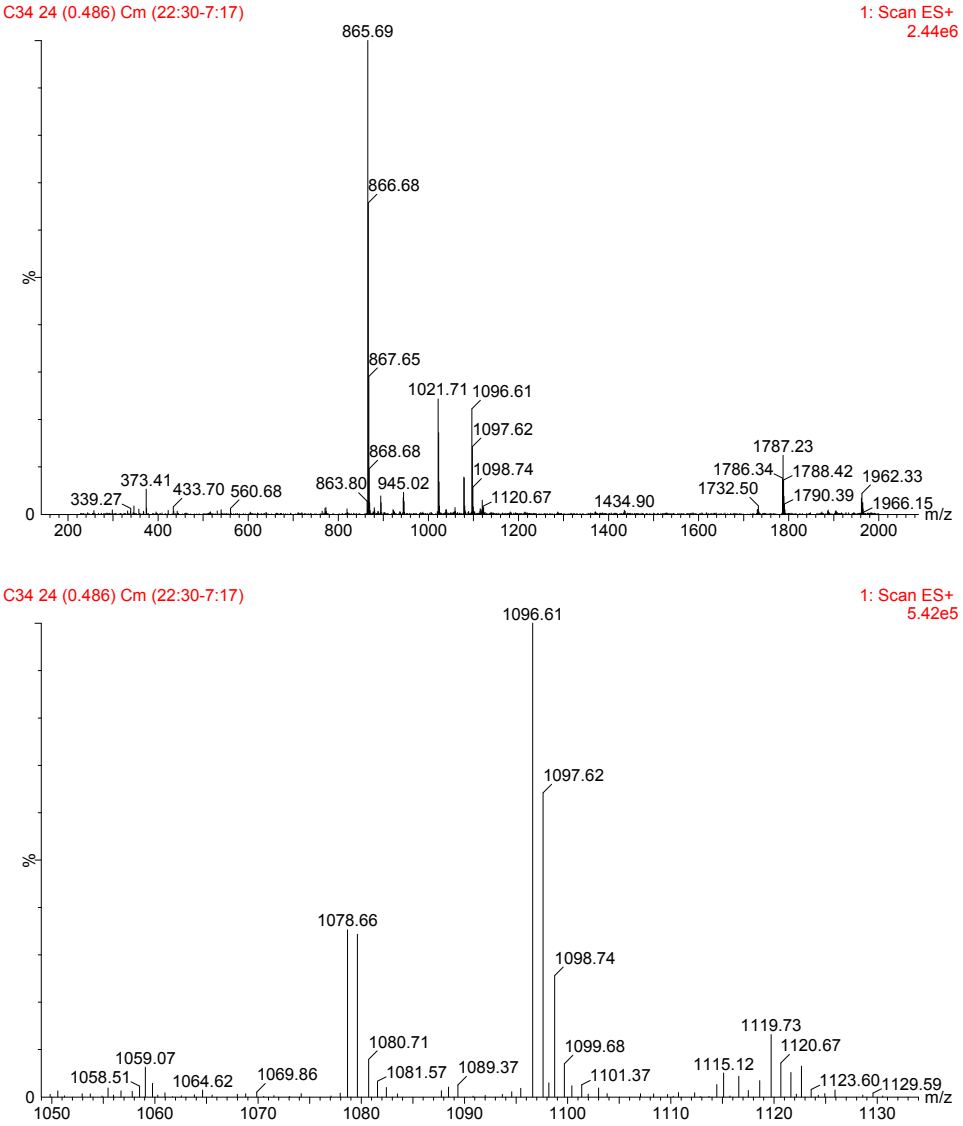


Figure S2.

Calcd. $C_{56}H_{57}Co_2N_4O_7S_2^+$ [$M_{\mathbf{2a}}$ – 3H + Co_2(acac) + H]$^+$: 1079.23, Found: 1079;

Calcd. $C_{56}H_{60}Co_2N_5O_7S_2^+$ [$M_{\mathbf{2a}}$ – 3H + Co_2(acac) + NH_4]$^+$: 1096.26, Found: 1096.61.

1.1.3 ESI-MS of **2a**/Co(acac)$_2$ = 1:2 mixture without the additive of *N*-methyl morpholine

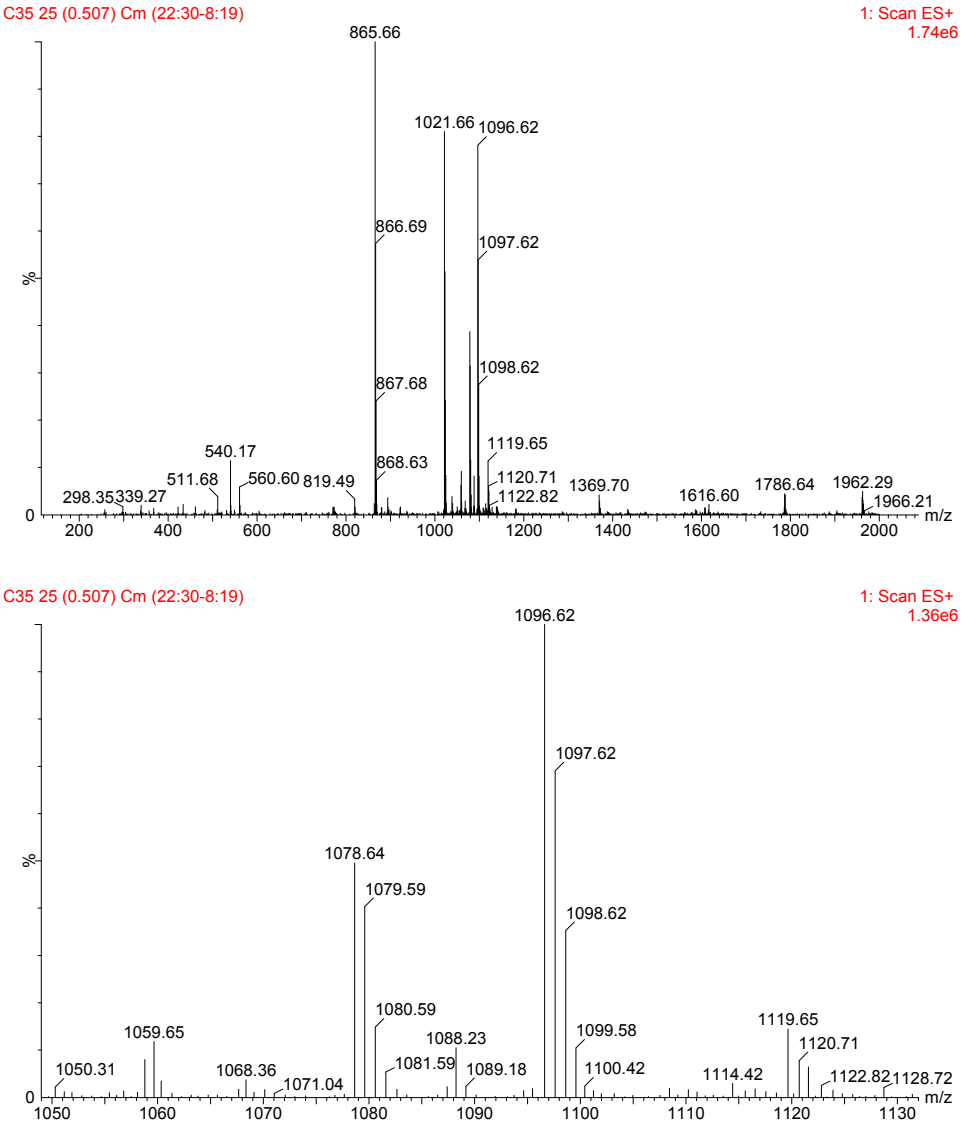


Figure S3.

Calcd. $C_{56}H_{57}Co_2N_4O_7S_2^+$ [$M_{\mathbf{2a}}$ – 3H + Co_2(acac) + H]$^+$: 1079.23, Found: 1079.59;

Calcd. $C_{56}H_{60}Co_2N_5O_7S_2^+$ [$M_{\mathbf{2a}}$ – 3H + Co_2(acac) + NH_4]$^+$: 1096.26, Found: 1096.62.

1.1.4 ESI-MS of **2a**/Co(acac)$_2$ = 1:2 mixture with the additive of *N*-methyl morpholine

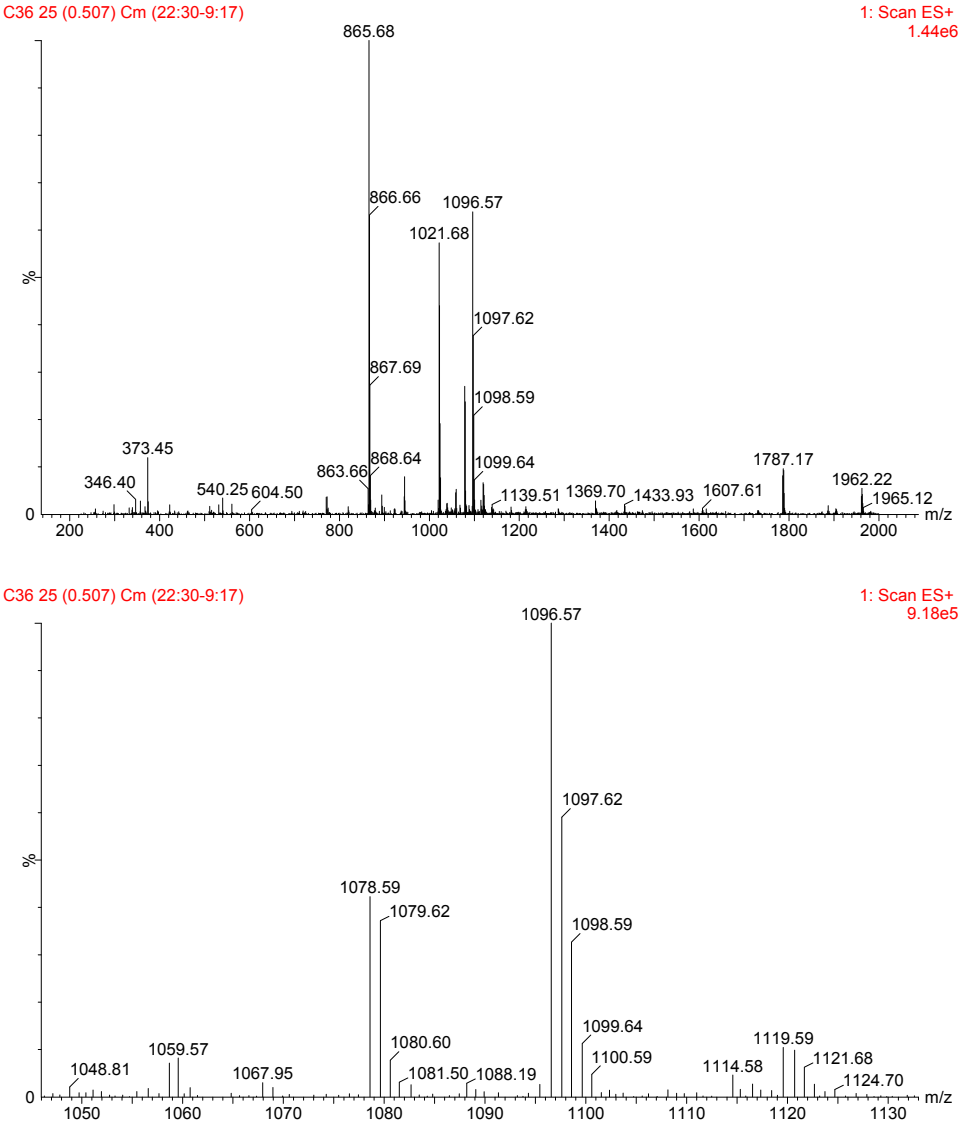


Figure S4.

Calcd. $C_{56}H_{57}Co_2N_4O_7S_2^+$ [$M_{\mathbf{2a}}$ – 3H + Co_2(acac) + H]$^+$: 1079.23, Found: 1079.62;

Calcd. $C_{56}H_{60}Co_2N_5O_7S_2^+$ [$M_{\mathbf{2a}}$ – 3H + Co_2(acac) + NH_4]$^+$: 1096.26, Found: 1096.57.

1.1.5 ESI-MS of **2a**/$Co(acac)_2$ = 1:3 mixture without the additive of *N*-methyl morpholine

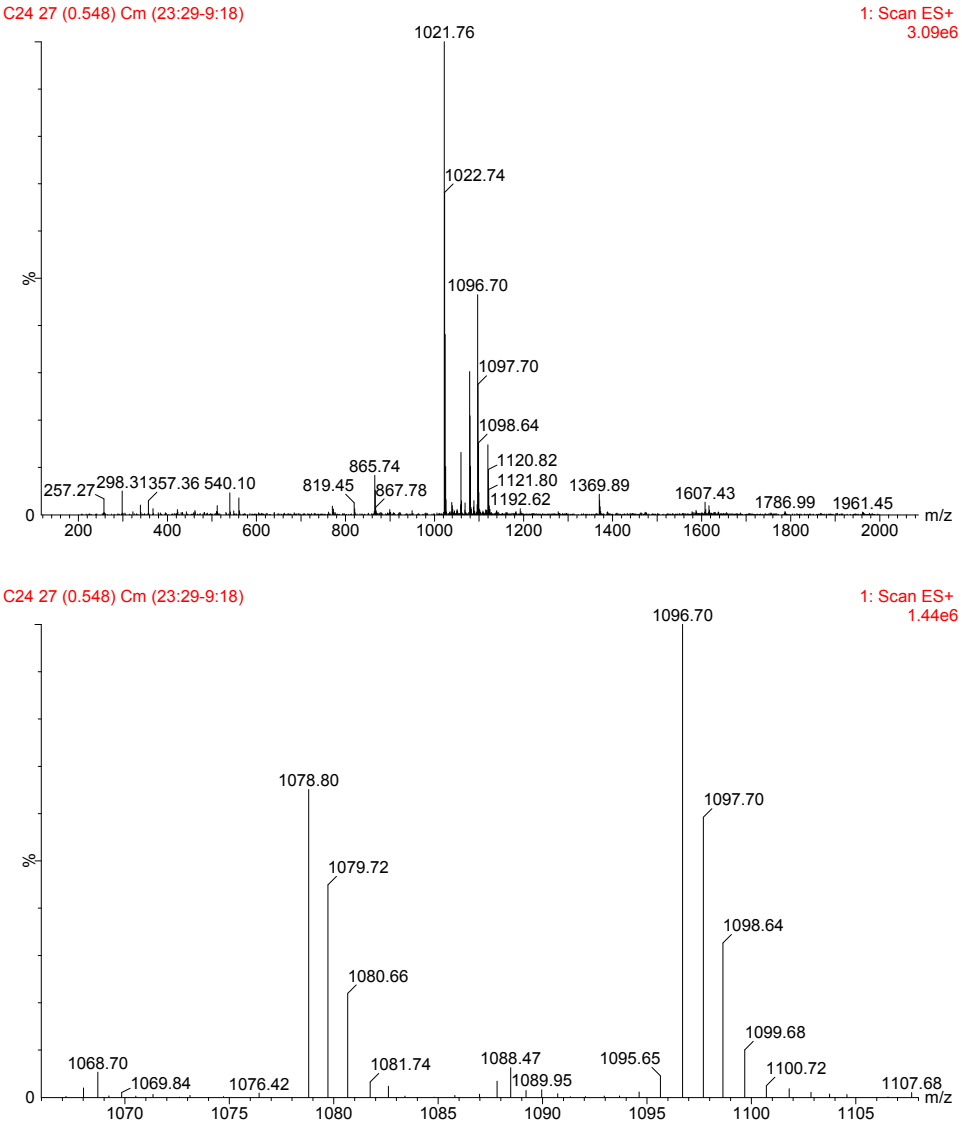


Figure S5.

Calcd. $C_{56}H_{57}Co_2N_4O_7S_2^+$ $[M_{\mathbf{2a}} - 3H + Co_2(acac) + H]^+$: 1079.23, Found: 1079.72;

Calcd. $C_{56}H_{60}Co_2N_5O_7S_2^+$ $[M_{\mathbf{2a}} - 3H + Co_2(acac) + NH_4]^+$: 1096.26, Found: 1096.70.

1.1.6 ESI-MS of **2a**/Co(acac)$_2$ = 1:3 mixture with the additive of *N*-methyl morpholine

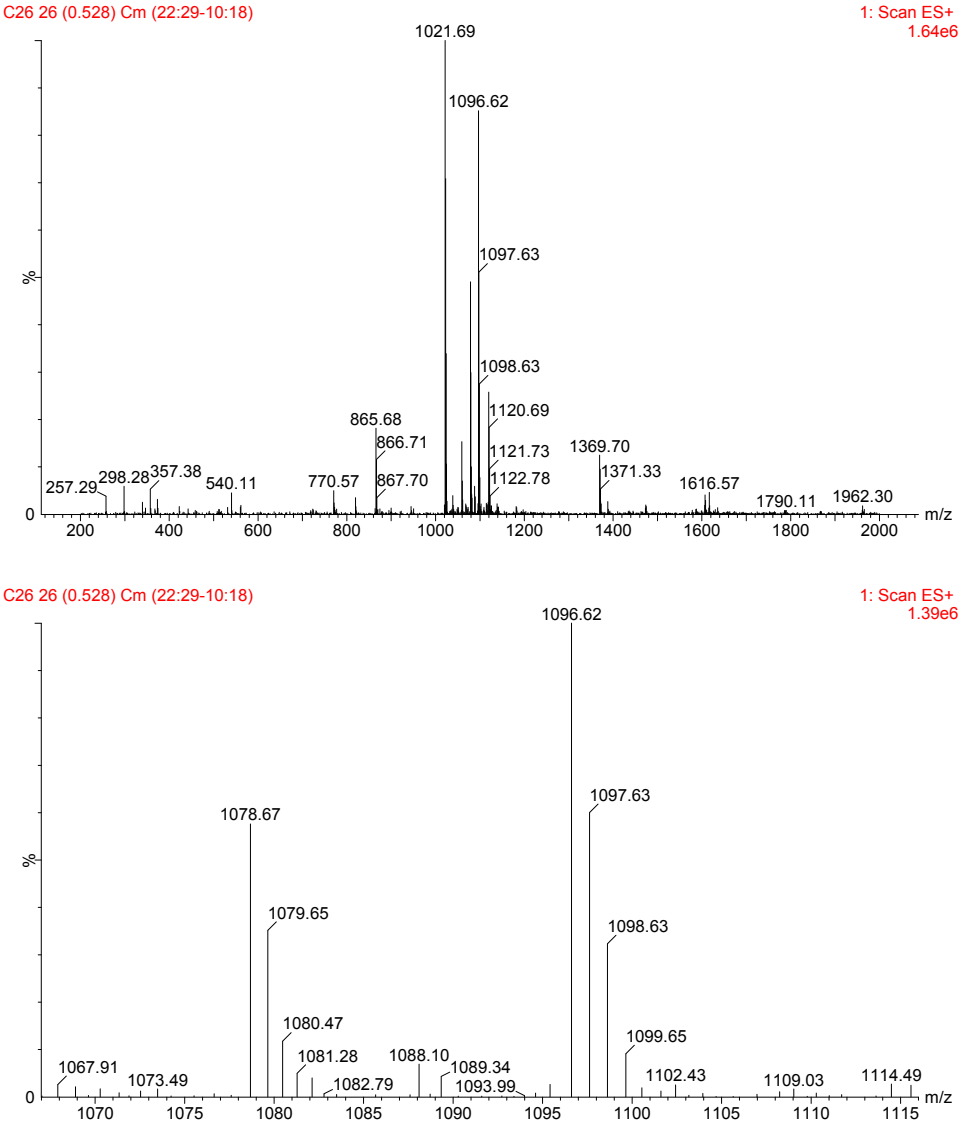


Figure S6.

Calcd. $C_{56}H_{57}Co_2N_4O_7S_2^+$ [$M_{\mathbf{2a}}$ – 3H + Co_2(acac) + H]$^+$: 1079.23, Found: 1079.65;

Calcd. $C_{56}H_{60}Co_2N_5O_7S_2^+$ [$M_{\mathbf{2a}}$ – 3H + Co_2(acac) + NH_4]$^+$: 1096.26, Found: 1096.62.

1.1.7 ESI-MS of **2a**/$Co(acac)_2$ = 1:4 mixture without the additive of *N*-methyl morpholine

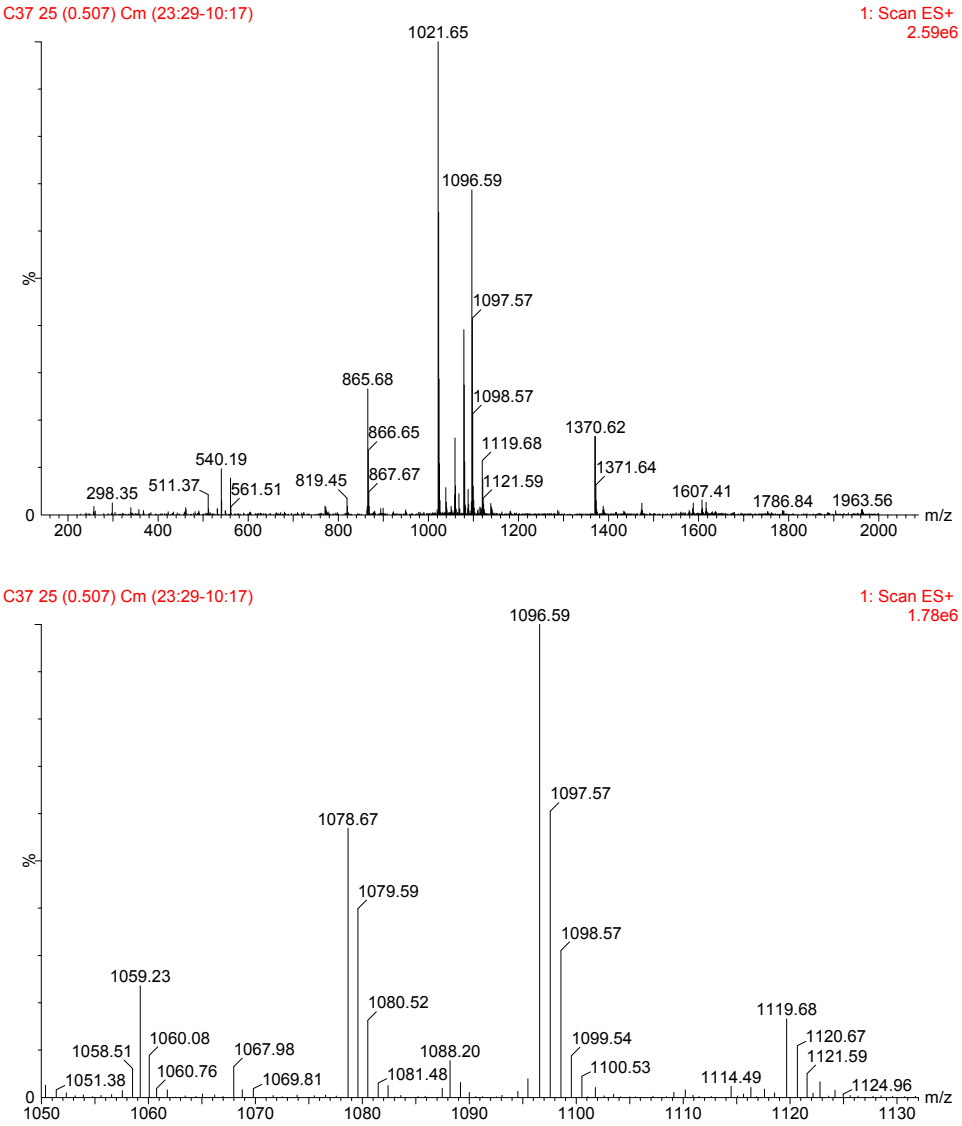


Figure S7.

Calcd. $C_{56}H_{57}Co_2N_4O_7S_2^+$ $[M_{\mathbf{2a}} - 3H + Co_2(acac) + H]^+$: 1079.23, Found: 1079.59;

Calcd. $C_{56}H_{60}Co_2N_5O_7S_2^+$ $[M_{\mathbf{2a}} - 3H + Co_2(acac) + NH_4]^+$: 1096.26, Found: 1096.59.

1.1.8 ESI-MS of **2a**/$Co(acac)_2$ = 1:4 mixture with the additive of *N*-methyl morpholine

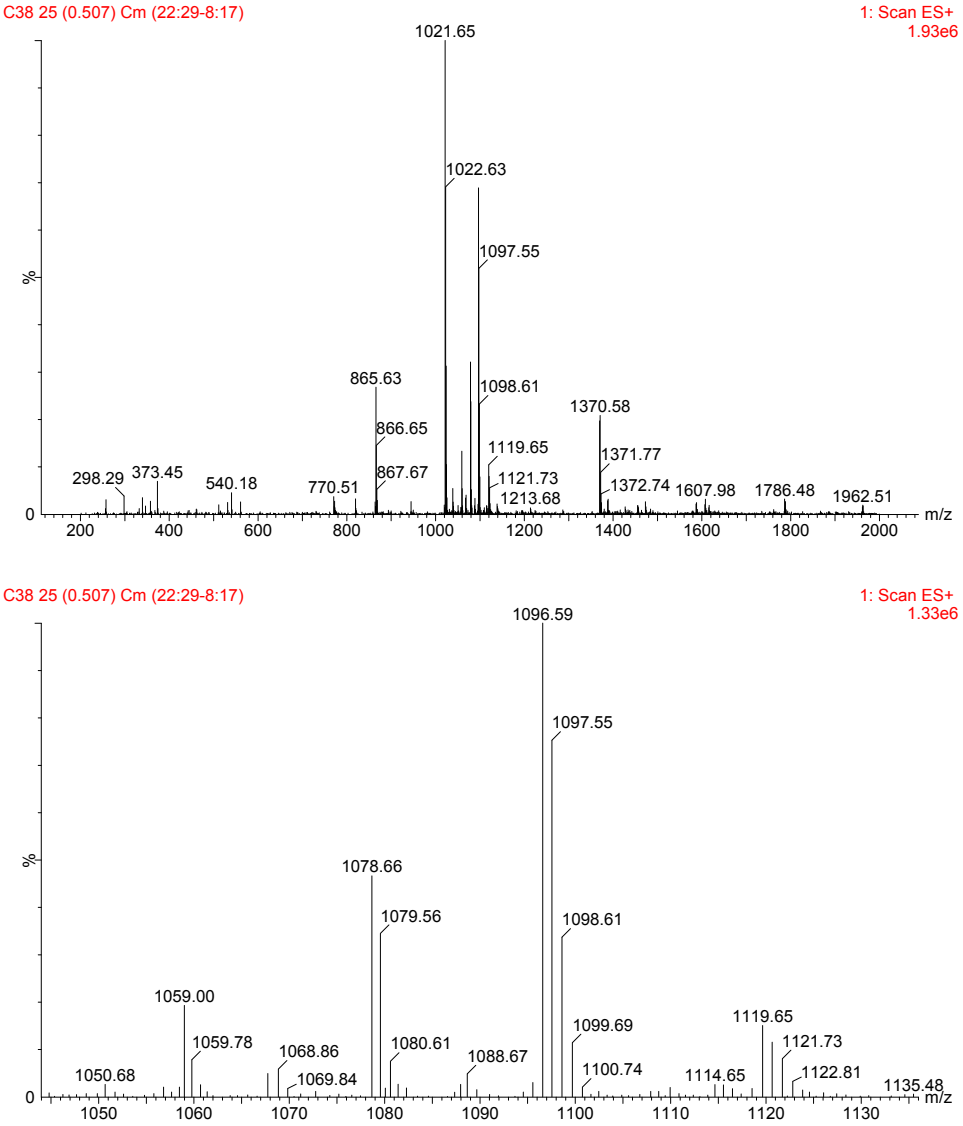


Figure S8.

Calcd. $C_{56}H_{57}Co_2N_4O_7S_2^+$ [$M_{\mathbf{2a}}$ – 3H + Co_2(acac) + H]$^+$: 1079.23, Found: 1079.56;

Calcd. $C_{56}H_{60}Co_2N_5O_7S_2^+$ [$M_{\mathbf{2a}}$ – 3H + Co_2(acac) + NH_4]$^+$: 1096.26, Found: 1096.59.

1.2 ESI-MS analysis of the mixture of **2a**/$Co(acac)_2$ and **4a**

1.2.1 ESI-MS of **2a**/$Co(acac)_2$ = 1:2 and **4a** mixture without the additive of *N*-methyl morpholine

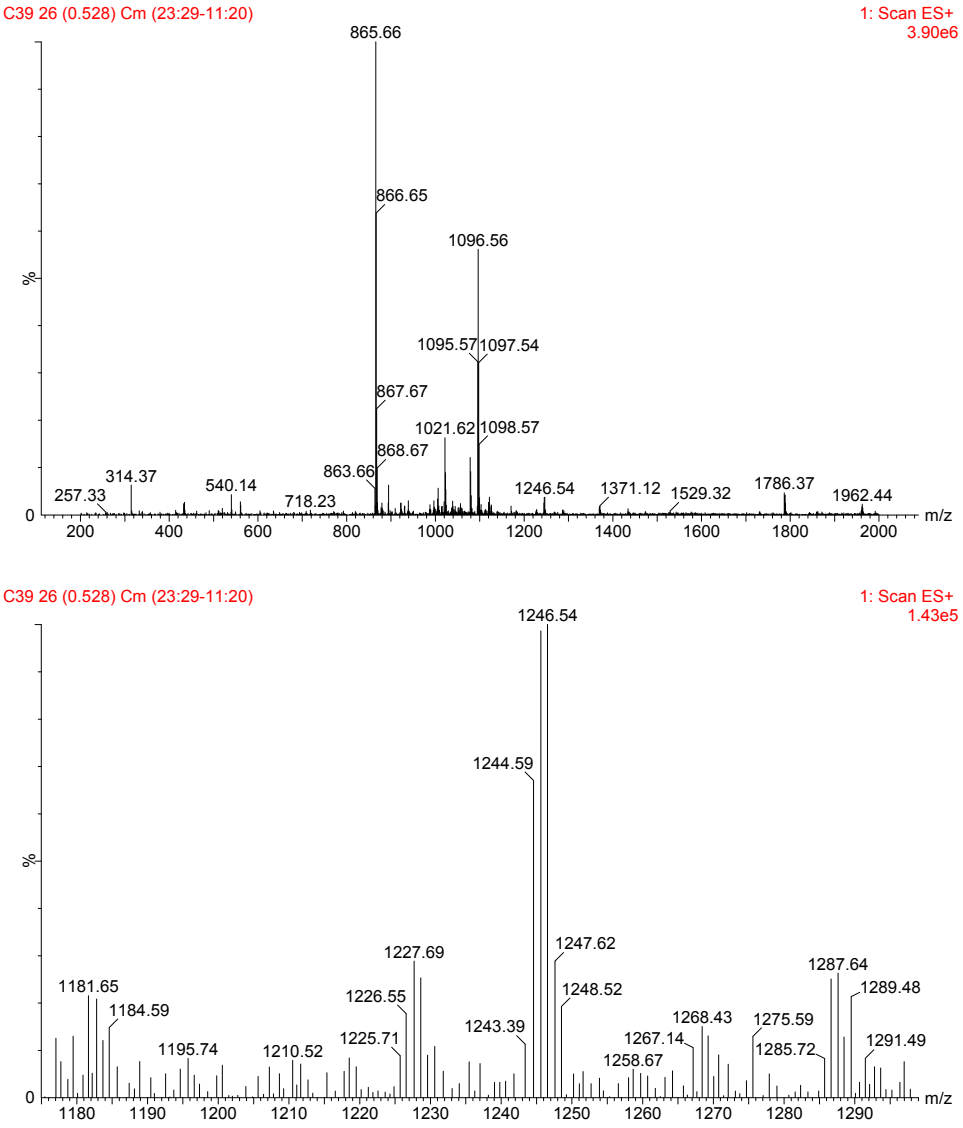


Figure S9.

Calcd. $C_{64}H_{63}Co_2N_5O_9S_2^+$ [$M_{\mathbf{2a}}$ – 3H + $Co_2(acac)$ + $M_{\mathbf{4a}}$]$^+$: 1227.27, Found: 1227.69;

Calcd. $C_{64}H_{64}Co_2N_5O_9S_2^+$ [$M_{\mathbf{2a}}$ – 3H + $Co_2(acac)$ + $M_{\mathbf{4a}}$ + H]$^+$: 1228.28, Found: 1228;

Calcd. $C_{64}H_{67}Co_2N_6O_9S_2^+$ [$M_{\mathbf{2a}}$ – 3H + $Co_2(acac)$ + $M_{\mathbf{4a}}$ + NH_4]$^+$: 1245.31, Found: 1245.

1.2.2 ESI-MS of **2a**/Co(acac)$_2$ = 1:2 and **4a** mixture with the additive of *N*-methyl morpholine

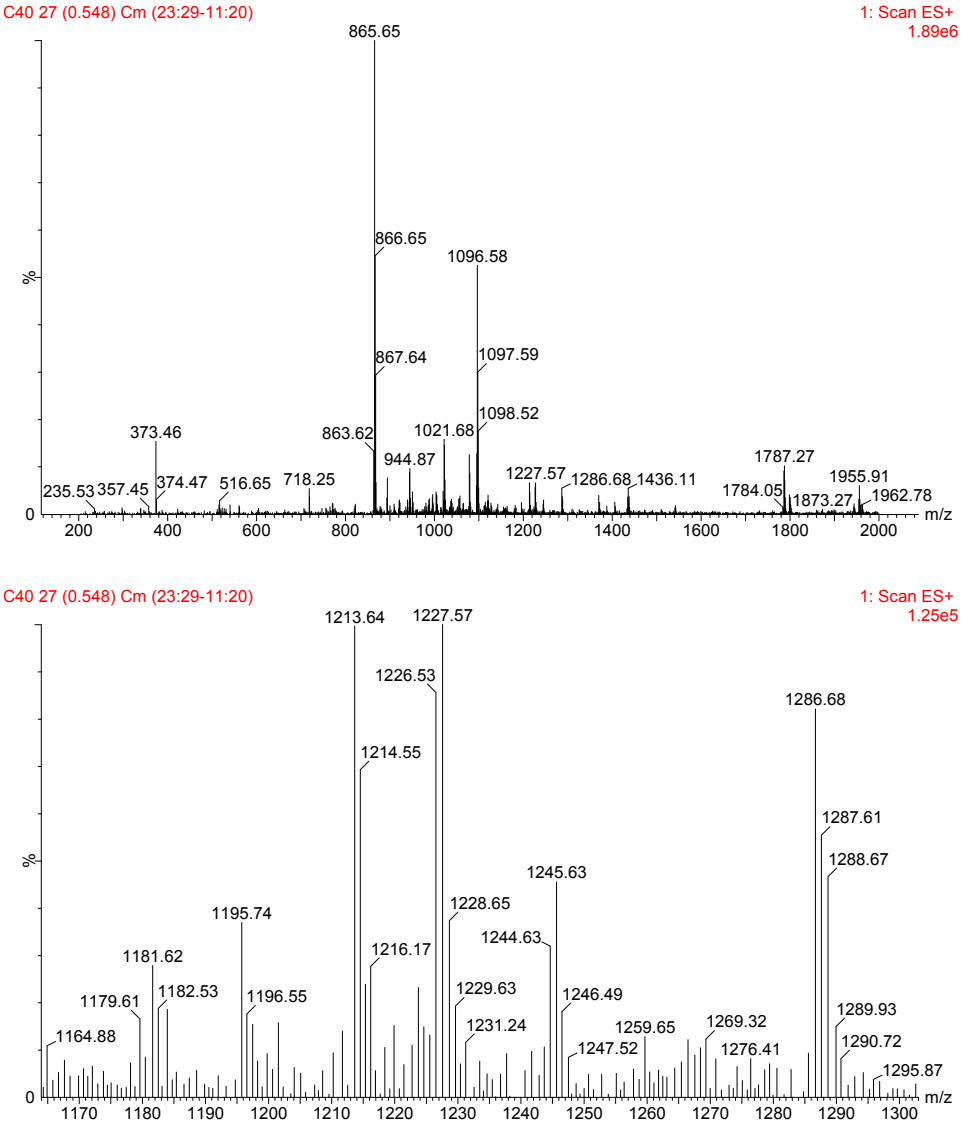


Figure S10.

Calcd. $C_{64}H_{63}Co_2N_5O_9S_2^+$ [$M_{\mathbf{2a}}$ – 3H + Co_2(acac) + $M_{\mathbf{4a}}$]$^+$: 1227.27, Found: 1227.57;

Calcd. $C_{64}H_{64}Co_2N_5O_9S_2^+$ [$M_{\mathbf{2a}}$ – 3H + Co_2(acac) + $M_{\mathbf{4a}}$ + H]$^+$: 1228.28, Found: 1228.65;

Calcd. $C_{64}H_{67}Co_2N_6O_9S_2^+$ [$M_{\mathbf{2a}}$ – 3H + Co_2(acac) + $M_{\mathbf{4a}}$ + NH_4]$^+$: 1245.31, Found: 1245.63.

1.2.3 ESI-MS of **2a**/Co(acac)$_2$ = 1:3 and **4a** mixture without the additive of *N*-methyl morpholine

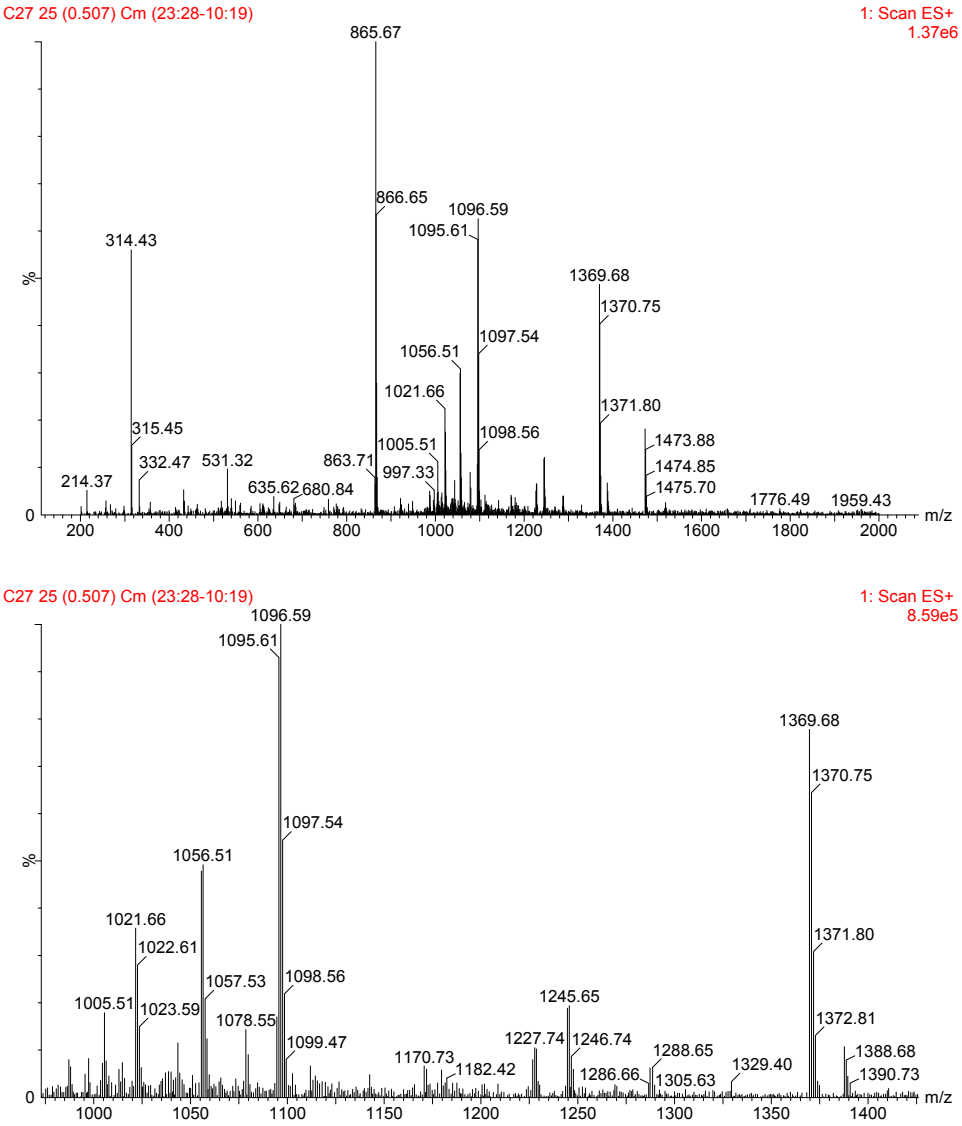


Figure S11.

Calcd. $C_{64}H_{63}Co_2N_5O_9S_2^+$ [$M_{\mathbf{2a}}$ – 3H + Co_2(acac) + $M_{\mathbf{4a}}$]$^+$: 1227.27, Found: 1227.74;

Calcd. $C_{64}H_{67}Co_2N_6O_9S_2^+$ [$M_{\mathbf{2a}}$ – 3H + Co_2(acac) + $M_{\mathbf{4a}}$ + NH_4]$^+$: 1245.31, Found: 1245.65.

1.2.4 ESI-MS of **2a**/Co(acac)$_2$ = 1:3 and **4a** mixture with the additive of *N*-methyl morpholine

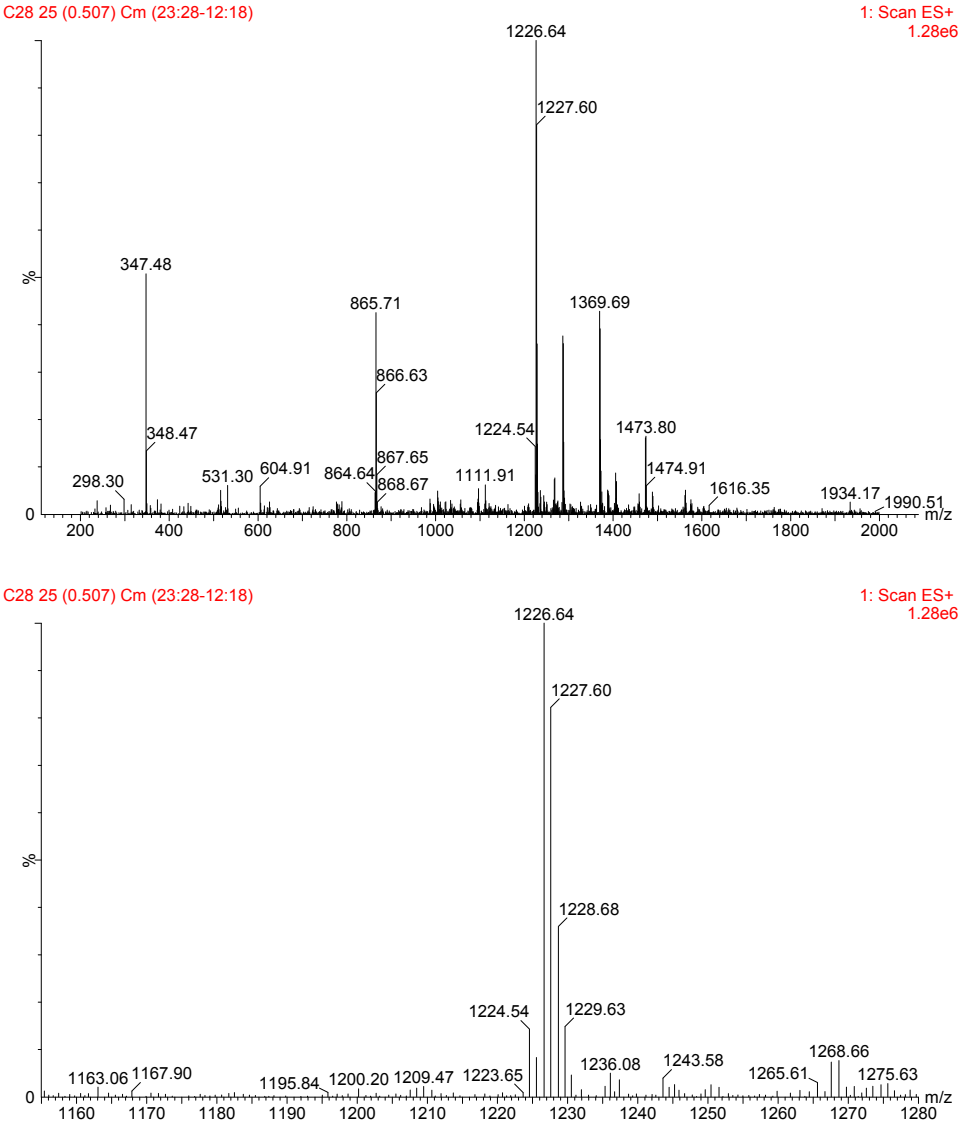


Figure S12.

Calcd. $C_{64}H_{63}Co_2N_5O_9S_2^+$ [$M_{\mathbf{2a}}$ – 3H + Co_2(acac) + $M_{\mathbf{4a}}$]$^+$: 1227.27, Found: 1227.60;

Calcd. $C_{64}H_{64}Co_2N_5O_9S_2^+$ [$M_{\mathbf{2a}}$ – 3H + Co_2(acac) + $M_{\mathbf{4a}}$ + H]$^+$: 1228.28, Found: 1228.68;

1.2.5 ESI-MS of **2a**/Co(acac)$_2$ = 1:4 and **4a** mixture without the additive of *N*-methyl morpholine

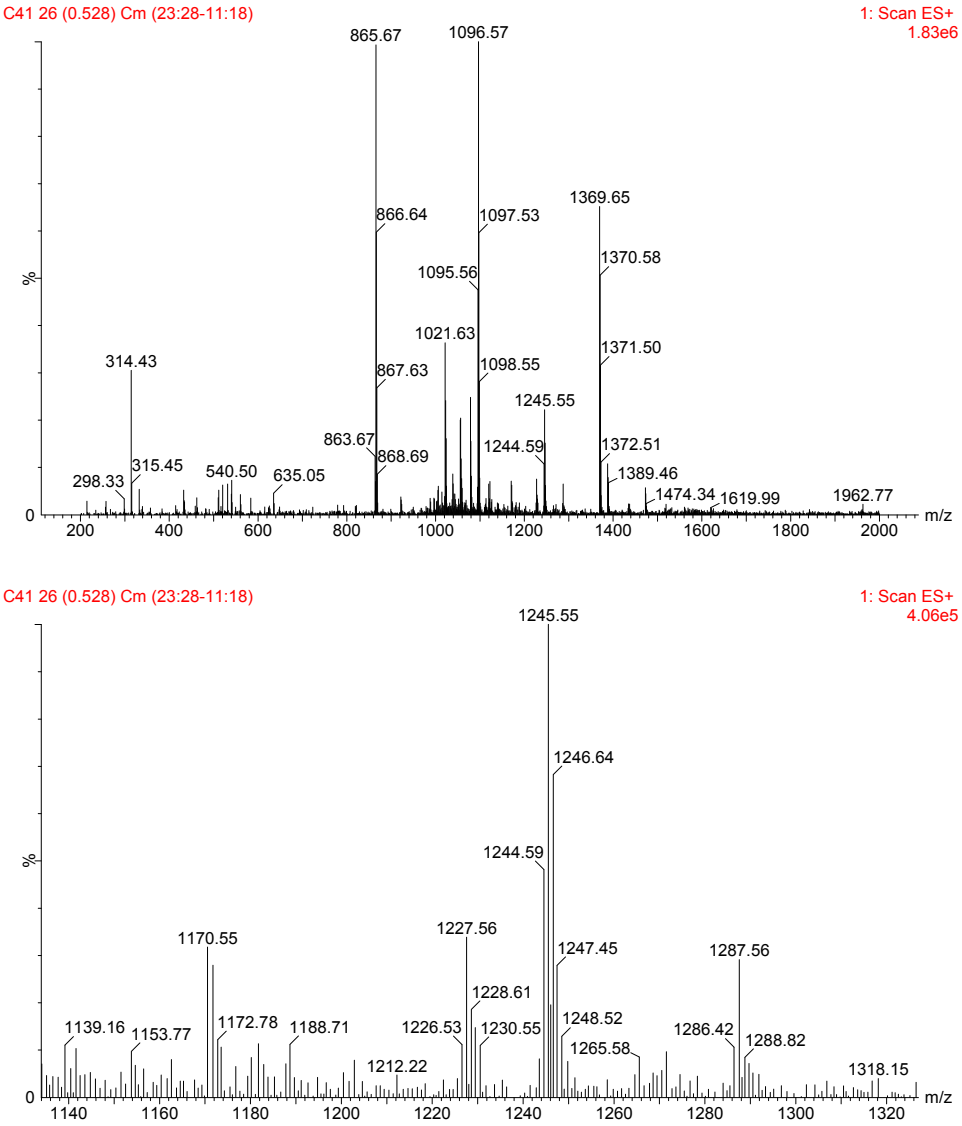


Figure S13.

Calcd. $C_{64}H_{63}Co_2N_5O_9S_2^+$ [$M_{\mathbf{2a}}$ – 3H + Co_2(acac) + $M_{\mathbf{4a}}$]$^+$: 1227.27, Found: 1227.56;

Calcd. $C_{64}H_{64}Co_2N_5O_9S_2^+$ [$M_{\mathbf{2a}}$ – 3H + Co_2(acac) + $M_{\mathbf{4a}}$ + H]$^+$: 1228.28, Found: 1228.61;

Calcd. $C_{64}H_{67}Co_2N_6O_9S_2^+$ [$M_{\mathbf{2a}}$ – 3H + Co_2(acac) + $M_{\mathbf{4a}}$ + NH_4]$^+$: 1245.31, Found: 1245.55.

1.2.6 ESI-MS of **2a**/Co(acac)$_2$ = 1:4 and **4a** mixture with the additive of *N*-methyl morpholine

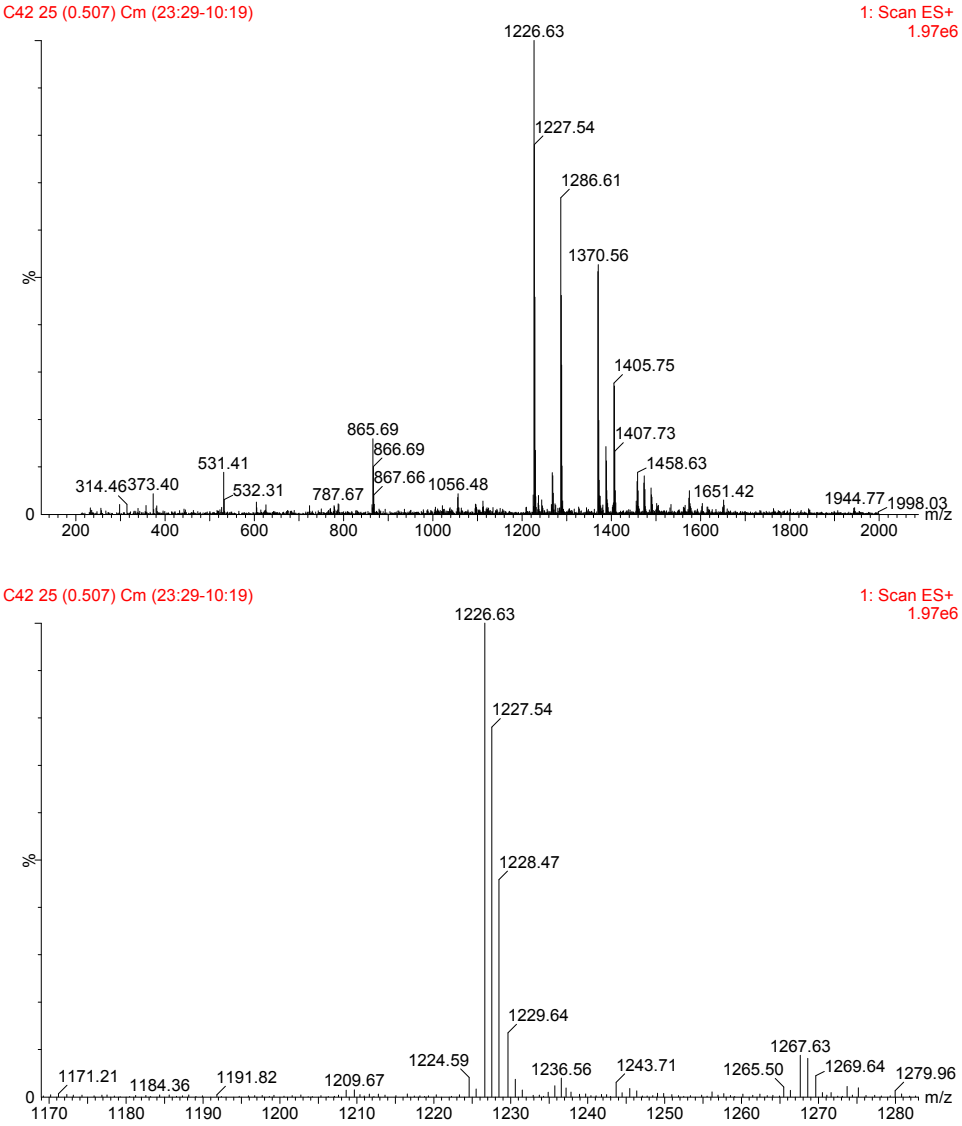


Figure S14.

Calcd. $C_{64}H_{63}Co_2N_5O_9S_2^+$ [$M_{\mathbf{2a}}$ – 3H + Co_2(acac) + $M_{\mathbf{4a}}$]$^+$: 1227.27, Found: 1227.54;

Calcd. $C_{64}H_{64}Co_2N_5O_9S_2^+$ [$M_{\mathbf{2a}}$ – 3H + Co_2(acac) + $M_{\mathbf{4a}}$ + H]$^+$: 1228.28, Found: 1228.47;

2. The structure of the dinuclear Co-aminophenol sulfonamide complex optimized by DFT

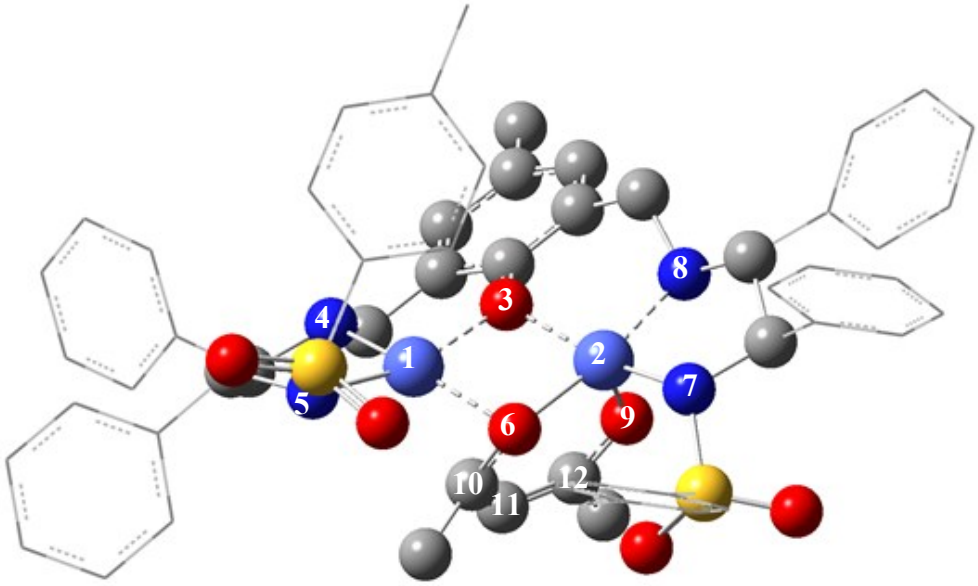


Figure S15. Topview

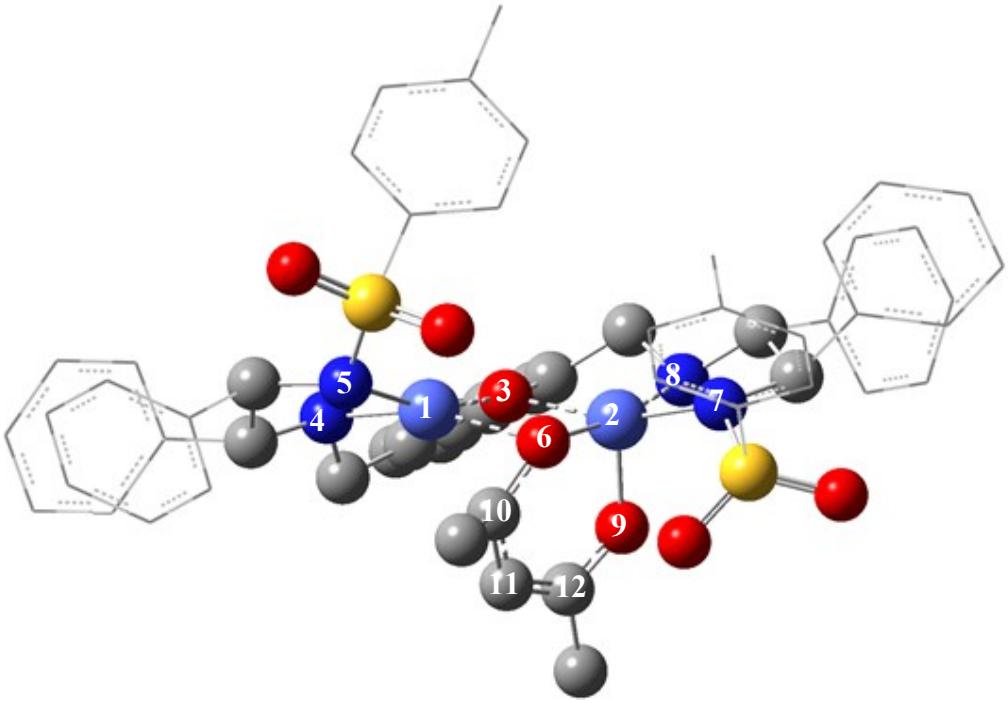


Figure S16. Sideview

2.1 Computational Methods: DFT calculations were carried out using the Gaussian 09 software package[1]. Considering both the desired precision of structures and available computer resources,

the geometry optimizations were performed using the Becke's three-parameter nonlocal exchange functional[2] and the Lee, Yang, and Parr nonlocal correlation function (LYP)[3] at a mixed basis set level. The Lan2DZ basis set[4] with the associated effective core potential was used for Ni, while the 6-31G(d) basis set[5] was used for all other atoms (C, H, O, N, S).

2.1 Selectedbond length (Å)

$Co^1–O^3$	$Co^1–O^6$	$Co^1–N^4$	$Co^1–N^5$	$Co^2–O^3$	$Co^2–O^6$	$Co^2–N^7$
1.9368	1.9948	1.9591	1.9545	1.9318	1.9144	1.8709
$Co^2–N^8$	$Co^2–O^9$	$C^{10}–O^6$	$C^{10}–C^{11}$	$C^{11}–C^{12}$	$C^{12}–O^9$	
1.9646	1.8347	1.3504	1.4486	1.3663	1.3185	

2.2 Selected dihedral angles (°)

$\angle O^6–C^{10}–C^{11}–C^1$ 2	0.19179
$\angle C^{10}–C^{11}–C^{12}–O$ 9	-6.05704

2.3 Cartesian coordinates for the calculated structure

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.738689	1.476483	0.383613
2	6	0	4.108305	0.285330	-0.532425
3	6	0	-1.020537	7.123667	0.132326
4	6	0	1.830407	2.999564	0.870895
5	6	0	0.564692	3.649599	0.375924

[1] M. J. Frisch, G. W. , 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, Jr., 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, J. M. 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, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox. Gaussian 09, revision D.01; Gaussian, Inc.: Wallingform, CT, 2009.

[2]A. D. Becke, *J. Phys. Chem.* **1993**, *98*, 5648-5652.

[3] (a) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* **1988**, *37*, 785-789. (b) B. Miehlich, A. Savin, H. Stoll, and H. Preuss, *Chem. Phys. Lett.* **1989**, *157*, 200-206.

[4] (a) P. J. Hay, W. R. Wadt, *J. Chem. Phys.* **1985**, *82*, 270-283. (b) W. R. Wadt, P. J. Hay, *J. Chem. Phys.* **1985**, *82*, 284-298. (c) P. J. Hay, W. R. Wadt, *J. Chem. Phys.* **1985**, *82*, 299-310.

[5] P. C. Hariharan, J. A. Pople, *Theoretica. Chimica. Acta.* **1973**, *28*, 213-222.

6	6	0	-0.494287	2.822275	-0.051654
7	6	0	-1.741824	3.388649	-0.381708
8	6	0	0.382586	5.030711	0.429049
9	6	0	-1.888572	4.777658	-0.290217
10	6	0	-2.896143	2.536934	-0.863511
11	6	0	-0.841724	5.623382	0.092555
12	6	0	-1.648304	-0.603257	4.683128
13	6	0	-4.344278	0.551666	-0.366850
14	6	0	-5.602147	1.342685	-0.042809
15	6	0	-4.256044	-0.822581	0.352376
16	6	0	-5.371691	-1.736437	-0.151631
17	6	0	-0.270066	-0.347552	4.648446
18	6	0	-5.844380	1.824647	1.252900
19	6	0	-6.544965	1.613270	-1.042020
20	6	0	-6.994739	2.559796	1.539046
21	6	0	-7.927502	2.821406	0.532572
22	6	0	-7.700682	2.343643	-0.758566
23	6	0	-5.251111	-2.403094	-1.376778
24	6	0	-6.555944	-1.879850	0.578886
25	6	0	-6.295362	-3.190524	-1.862784
26	6	0	-7.476637	-3.322949	-1.129559
27	6	0	-7.602573	-2.666404	0.095774
28	6	0	0.455833	-0.784202	3.530595
29	6	0	-1.546189	-1.680168	2.523658
30	6	0	-0.168919	-1.445576	2.472754
31	6	0	-2.285824	-1.272195	3.637508
32	1	0	-0.445084	7.575909	0.947903
33	1	0	0.403970	-1.804534	1.623904
34	1	0	1.531684	-0.621032	3.496883
35	1	0	-2.227286	-0.292663	5.550442
36	1	0	-3.342798	-1.511633	3.693766
37	1	0	-0.683351	7.595352	-0.800752
38	1	0	3.487700	1.072900	1.370064
39	1	0	-2.071705	7.397561	0.271945
40	1	0	-8.512067	-2.773171	0.681602
41	1	0	-8.287653	-3.941752	-1.504924
42	1	0	-6.181606	-3.710340	-2.810913
43	1	0	-6.656866	-1.379643	1.538975
44	1	0	-4.320039	-2.328159	-1.929105
45	1	0	-8.422188	2.538019	-1.547456
46	1	0	-8.825450	3.391206	0.755321
47	1	0	-7.165153	2.923405	2.548848
48	1	0	-6.377431	1.237846	-2.048534
49	1	0	-5.137741	1.618134	2.054685

50	1	0	-4.437308	-0.641124	1.424684
51	1	0	-4.307672	0.363326	-1.444288
52	1	0	-2.722938	2.199826	-1.892145
53	1	0	-3.815283	3.134882	-0.852619
54	1	0	-2.855041	5.214361	-0.536886
55	1	0	1.207316	5.659500	0.761075
56	1	0	1.614002	2.377376	1.748953
57	1	0	2.556645	3.762836	1.171969
58	7	0	-2.890218	-1.327404	0.107425
59	8	0	-3.547591	-3.184249	1.743532
60	8	0	-1.342389	-3.291778	0.464572
61	8	0	1.919152	-1.437418	-3.064970
62	8	0	4.419526	-1.428275	-2.664546
63	16	0	-2.388157	-2.501953	1.141057
64	16	0	3.048877	-1.557845	-2.137258
65	1	0	4.592992	0.671081	-1.437096
66	6	0	4.857955	2.493750	0.536810
67	6	0	5.311935	3.236103	-0.564307
68	6	0	5.455342	2.708672	1.784461
69	6	0	6.333054	4.174750	-0.417056
70	6	0	6.481948	3.643343	1.933383
71	1	0	5.121644	2.131956	2.643640
72	6	0	6.921198	4.380765	0.833326
73	1	0	6.673271	4.740085	-1.280262
74	1	0	6.936645	3.793530	2.908673
75	1	0	7.719030	5.109397	0.947146
76	6	0	5.112883	-0.606513	0.195628
77	6	0	4.711533	-1.404578	1.274837
78	6	0	6.462180	-0.597380	-0.173935
79	6	0	5.643072	-2.171027	1.976052
80	1	0	3.659612	-1.451216	1.543916
81	6	0	7.396629	-1.359796	0.528393
82	1	0	6.778767	0.001938	-1.023007
83	6	0	6.989851	-2.147333	1.607254
84	1	0	5.314486	-2.794341	2.803531
85	1	0	8.440652	-1.344036	0.226803
86	1	0	7.715714	-2.746037	2.151252
87	6	0	2.928783	-3.141866	-1.303331
88	6	0	4.056038	-3.959648	-1.240472
89	6	0	1.707999	-3.547619	-0.754276
90	6	0	3.953296	-5.203861	-0.615730
91	1	0	4.991995	-3.621923	-1.671078
92	6	0	1.629115	-4.787563	-0.127050
93	1	0	0.831991	-2.911276	-0.805249

94	6	0	2.746094	-5.636075	-0.052098
95	1	0	4.828675	-5.847277	-0.565413
96	1	0	0.678321	-5.087004	0.305857
97	7	0	2.470429	2.084583	-0.123463
98	1	0	2.643745	2.604027	-0.987931
99	8	0	-0.294697	1.496319	-0.081496
100	7	0	2.841305	-0.398561	-0.885129
101	1	0	4.877539	3.076941	-1.549352
102	6	0	0.420993	0.331675	5.808320
103	1	0	-0.238127	1.053901	6.302097
104	1	0	1.323325	0.861899	5.484822
105	1	0	0.728761	-0.398727	6.568647
106	6	0	2.635710	-6.988904	0.611293
107	1	0	3.618426	-7.451666	0.748222
108	1	0	2.025837	-7.674949	0.009344
109	1	0	2.154507	-6.913512	1.593466
110	27	0	-1.585470	0.069206	-0.301723
111	27	0	1.296711	0.651717	-0.778507
112	8	0	1.197487	1.627692	-2.328915
113	6	0	0.218867	1.430825	-3.190237
114	6	0	0.297043	2.382821	-4.361499
115	1	0	-0.540670	2.240499	-5.048762
116	1	0	1.232937	2.218060	-4.908404
117	1	0	0.299668	3.421558	-4.009630
118	6	0	-1.496695	-1.865080	-2.617889
119	1	0	-0.785261	-2.323773	-3.318024
120	1	0	-2.426336	-1.662661	-3.159572
121	1	0	-1.692108	-2.554351	-1.798615
122	6	0	-0.874496	-0.576550	-2.123172
123	8	0	0.034040	-0.741619	-1.137783
124	7	0	-3.088318	1.300871	-0.051495
125	1	0	-3.110819	1.570373	0.936474
126	6	0	-0.762705	0.484407	-3.103167
127	1	0	-1.479672	0.439790	-3.916164

The energies for the structure(a.u.):

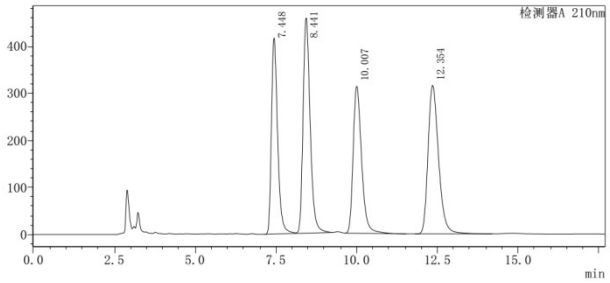
Sum of electronic and zero-point Energies= -3998.699612 Sum of electronic and thermal Energies= -3998.633957

Sum of electronic and thermal Enthalpies= -3998.633013

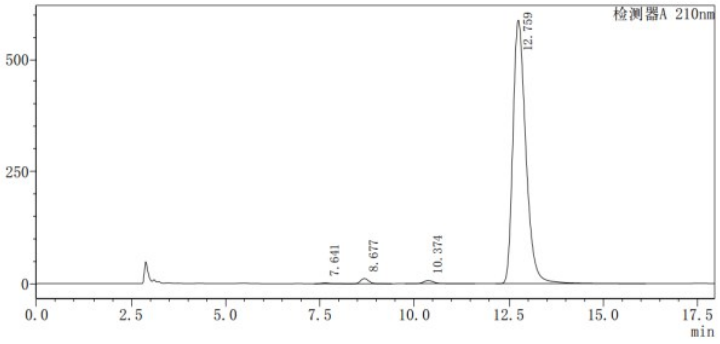
Sum of electronic and thermal Free Energies= -3998.807529

3. Copies of HPLC charts

(1) **5aa**

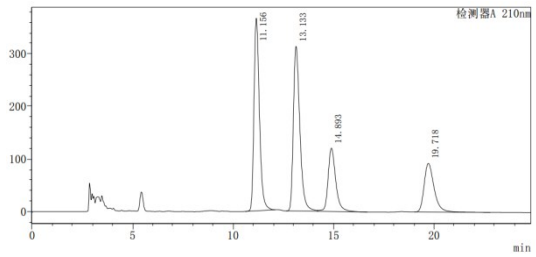


Peak	Retention Time	Area Percent
1	7.448	21.846
2	8.441	27.458
3	10.007	22.366
4	12.354	28.331
Total		100.000

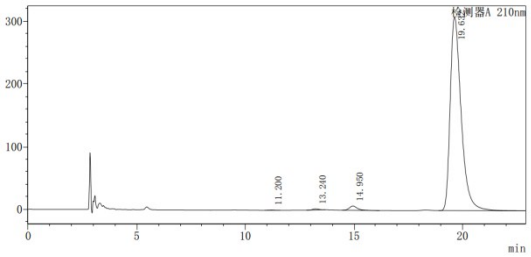


Peak	Retention Time	Area Percent
1	7.641	0.205
2	8.677	1.238
3	10.374	0.992
4	12.759	97.565
Total		100.000

(2) **5ab**

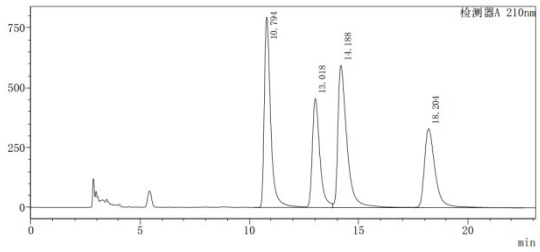


Peak	Retention Time	Area Percent
1	11.156	33.912
2	13.133	34.643
3	14.893	15.730
4	19.718	15.715
Total		100.000

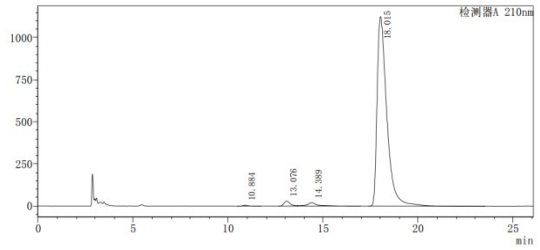


Peak	Retention Time	Area Percent
1	11.200	0.059
2	13.240	0.323
3	14.950	1.581
4	19.632	98.037
Total		100.000

(3) **5ac**

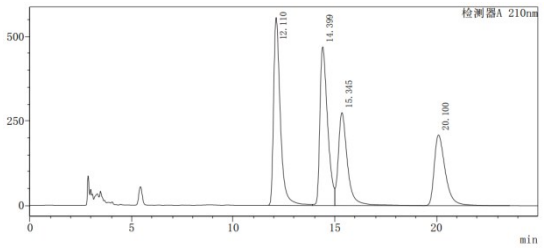


Peak	Retention Time	Area Percent
1	10.794	29.304
2	13.018	19.581
3	14.188	30.869
4	18.204	20.245
Total		100.000

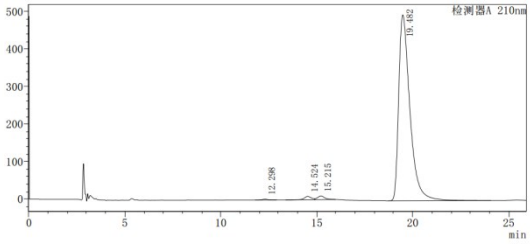


Peak	Retention Time	Area Percent
1	10.884	0.268
2	13.076	1.638
3	14.389	2.045
4	18.015	96.049
Total		100.000

(4) **5ad**

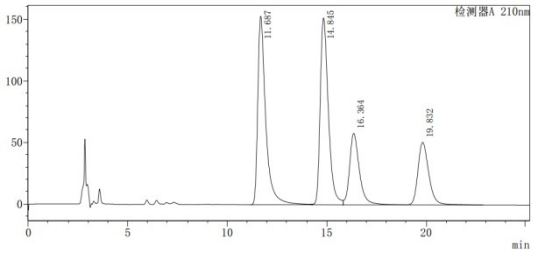


Peak	Retention Time	Area Percent
1	12.110	30.793
2	14.399	29.662
3	15.345	20.687
4	20.100	18.858
Total		100.000

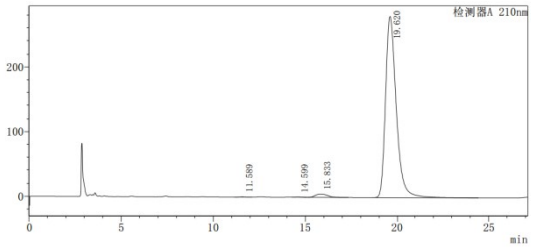


Peak	Retention Time	Area Percent
1	12.298	0.194
2	14.524	1.107
3	15.215	1.210
4	19.482	97.489
Total		100.000

(5) **5ae**

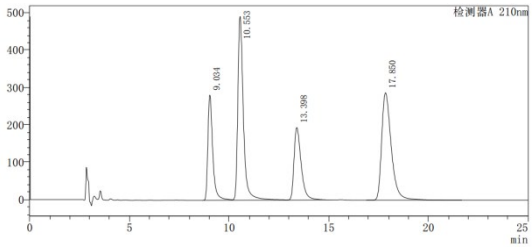


Peak	Retention Time	Area Percent
1	11.687	34.241
2	14.845	34.362
3	16.364	16.015
4	19.832	15.383
Total		100.000

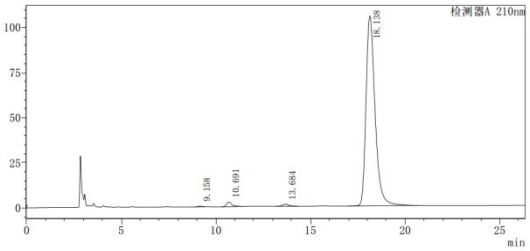


Peak	Retention Time	Area Percent
1	11.589	0.067
2	14.599	0.065
3	15.833	1.993
4	19.620	97.876
Total		100.000

(6) **5af**

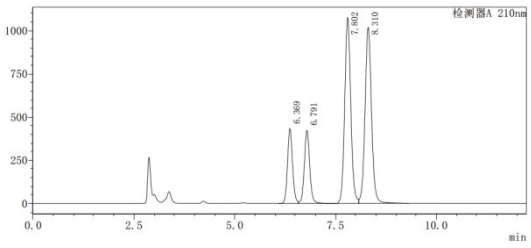


Peak	Retention Time	Area Percent
1	9.034	16.610
2	10.553	33.126
3	13.398	16.798
4	17.850	33.465
Total		100.000

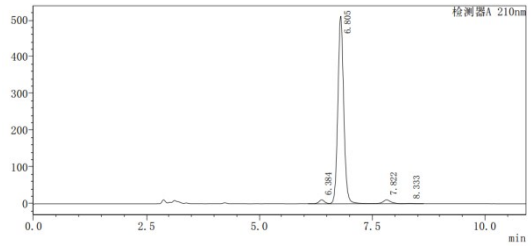


Peak	Retention Time	Area Percent
1	9.158	0.147
2	10.691	1.425
3	13.684	0.740
4	18.138	97.687
Total		100.000

(7) **5ag**

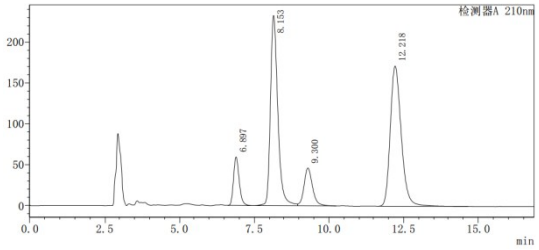


Peak	Retention Time	Area Percent
1	6.369	12.389
2	6.791	12.930
3	7.802	36.983
4	8.310	37.698
Total		100.000

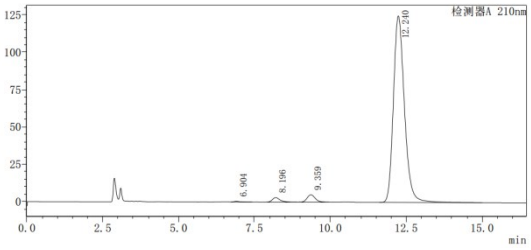


Peak	Retention Time	Area Percent
1	6.384	1.855
2	6.805	95.293
3	7.822	2.633
4	8.333	0.219
Total		100.000

(8) **5ah**

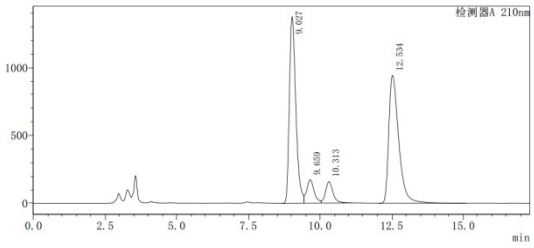


Peak	Retention Time	Area Percent
1	6.897	7.778
2	8.153	39.694
3	9.300	9.099
4	12.218	43.428
Total		100.000

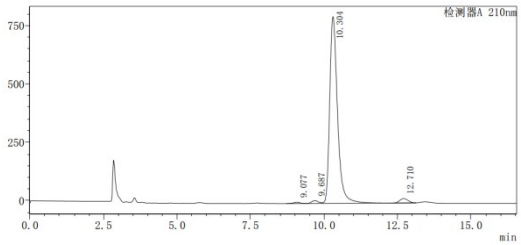


Peak	Retention Time	Area Percent
1	6.904	0.185
2	8.196	1.718
3	9.359	2.870
4	12.240	95.227
Total		100.000

(9) **5ai**

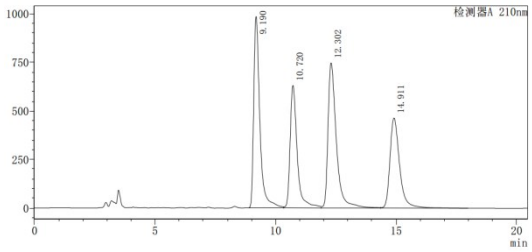


Peak	Retention Time	Area Percent
1	9.027	42.931
2	9.659	6.139
3	10.313	5.687
4	12.534	45.242
Total		100.000

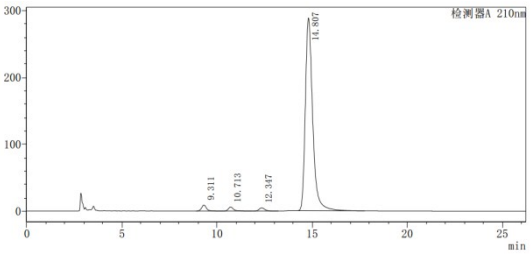


Peak	Retention Time	Area Percent
1	9.077	0.489
2	9.687	1.228
3	10.304	95.807
4	12.710	2.476
Total		100.000

(10) **5aj**

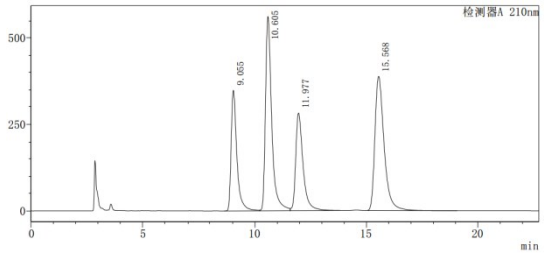


Peak	Retention Time	Area Percent
1	9.190	28.455
2	10.720	21.077
3	12.302	29.396
4	14.911	21.072
Total		100.000

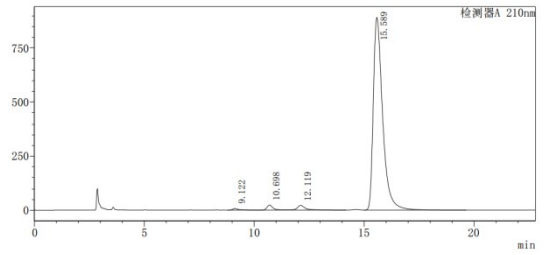


Peak	Retention Time	Area Percent
1	9.311	1.920
2	10.713	1.436
3	12.347	1.247
4	14.807	95.396
Total		100.000

(11) **5ak**

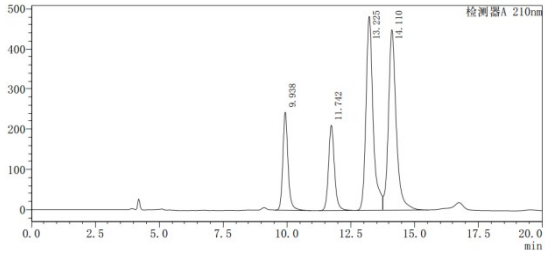


Peak	Retention Time	Area Percent
1	9.055	17.893
2	10.605	31.394
3	11.977	18.602
4	15.568	32.111
Total		100.000

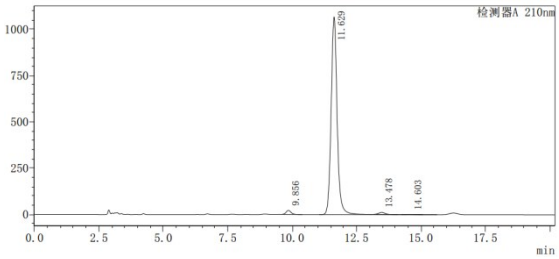


Peak	Retention Time	Area Percent
1	9.122	0.522
2	10.698	1.598
3	12.119	2.174
4	15.589	95.707
Total		100.000

(12) **5al**

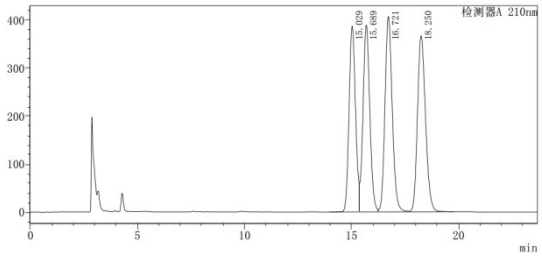


Peak	Retention Time	Area Percent
1	9.938	13.222
2	11.742	13.362
3	13.225	36.638
4	14.110	36.778
Total		100.000

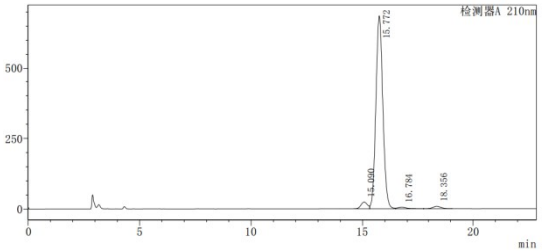


Peak	Retention Time	Area Percent
1	9.856	1.574
2	11.629	97.244
3	13.478	1.051
4	14.603	0.132
Total		100.000

(13) **5am**

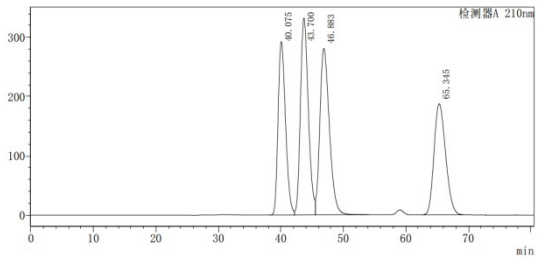


Peak	Retention Time	Area Percent
1	15.029	22.585
2	15.689	23.923
3	16.721	26.823
4	18.250	26.669
Total		100.000

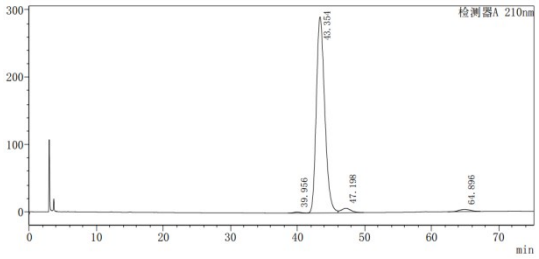


Peak	Retention Time	Area Percent
1	15.090	3.091
2	15.772	94.516
3	16.784	1.015
4	18.356	1.378
Total		100.000

(14) **5an**

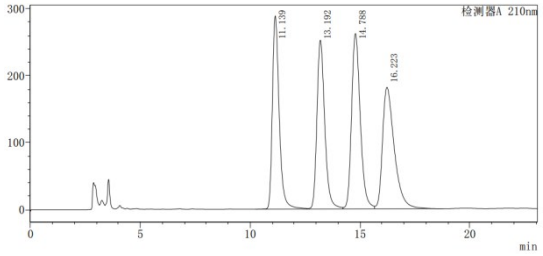


Peak	Retention Time	Area Percent
1	40.075	22.541
2	43.700	27.117
3	46.883	27.784
4	65.345	22.557
Total		100.000

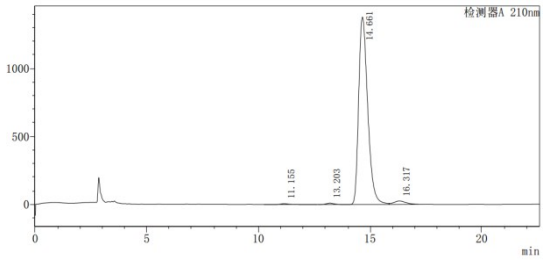


Peak	Retention Time	Area Percent
1	39.956	0.408
2	43.354	95.745
3	47.198	2.457
4	64.896	1.390
Total		100.000

(15) **5ao**

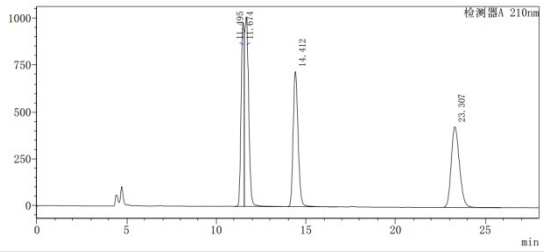


Peak	Retention Time	Area Percent
1	11.139	23.553
2	13.192	23.555
3	14.788	27.239
4	16.223	25.654
Total		100.000

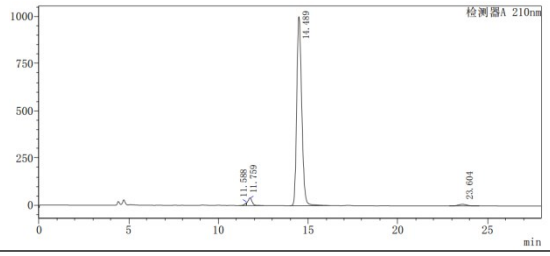


Peak	Retention Time	Area Percent
1	11.155	0.442
2	13.203	0.625
3	14.661	96.440
4	16.317	2.493
Total		100.000

(16) **5ap**

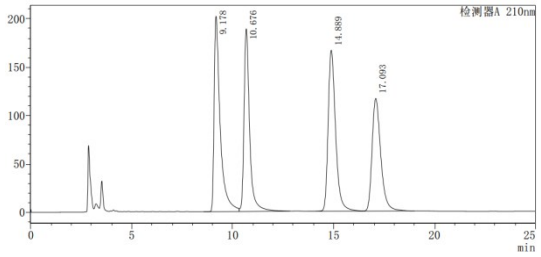


Peak	Retention Time	Area Percent
1	11.495	22.123
2	11.674	27.660
3	14.412	25.225
4	23.307	24.992
Total		100.000

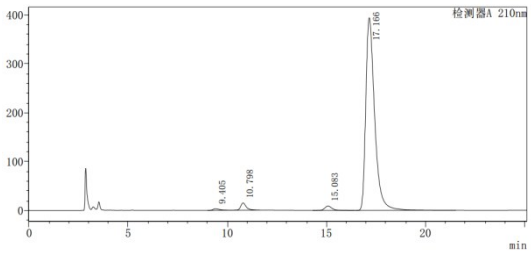


Peak	Retention Time	Area Percent
1	11.588	0.602
2	11.759	3.018
3	14.489	95.099
4	23.604	1.280
Total		100.000

(17) **5aq**

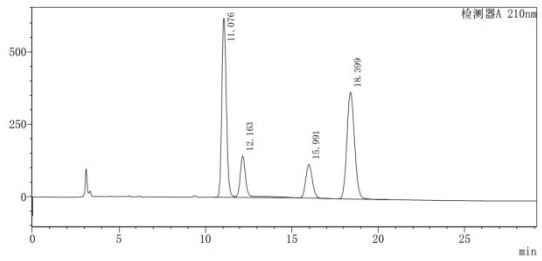


Peak	Retention Time	Area Percent
1	9.178	27.075
2	10.676	23.309
3	14.889	27.327
4	17.093	22.289
Total		100.000

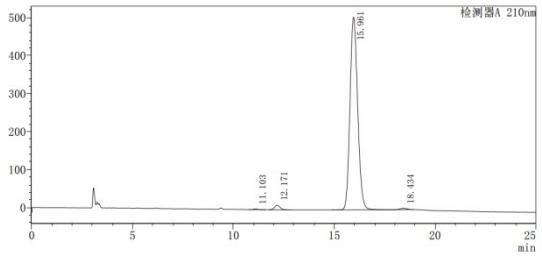


Peak	Retention Time	Area Percent
1	9.405	0.715
2	10.798	2.451
3	15.083	1.785
4	17.166	95.049
Total		100.000

(18) **5ar**

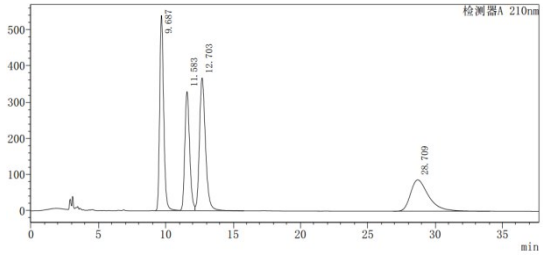


Peak	Retention Time	Area Percent
1	11.076	38.758
2	12.163	11.642
3	15.991	10.534
4	18.399	39.067
Total		100.000

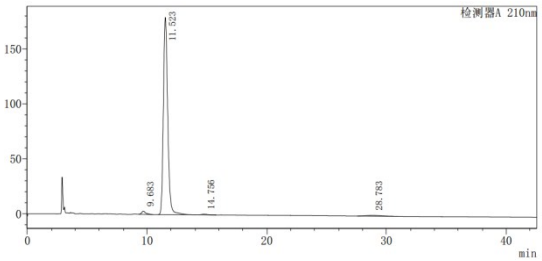


Peak	Retention Time	Area Percent
1	11.103	0.247
2	12.171	1.681
3	15.961	97.365
4	18.434	0.707
Total		100.000

(19) **5as**

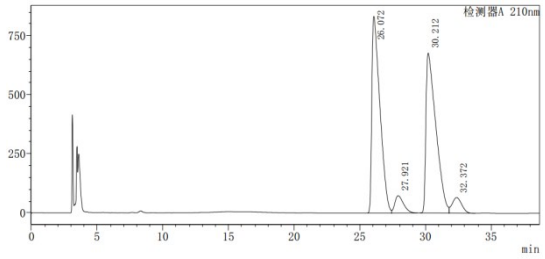


Peak	Retention Time	Area Percent
1	9.687	28.680
2	11.583	21.076
3	12.703	29.412
4	28.709	20.833
Total		100.000

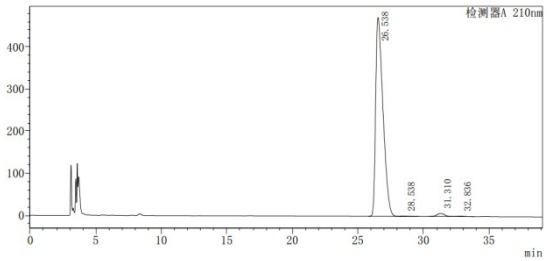


Peak	Retention Time	Area Percent
1	9.683	1.491
2	11.523	96.855
3	14.756	0.430
4	28.783	1.224
Total		100.000

(20) **5at**

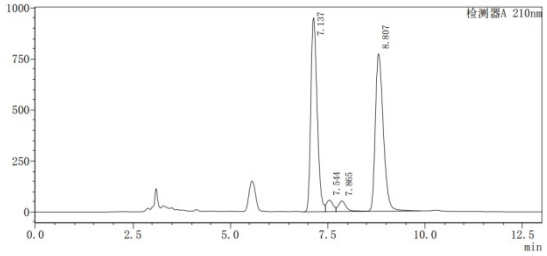


Peak	Retention Time	Area Percent
1	26.072	45.612
2	27.921	4.327
3	30.212	45.747
4	32.372	4.314
Total		100.000

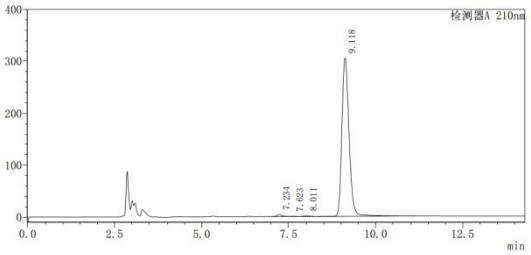


Peak	Retention Time	Area Percent
1	26.538	98.275
2	28.538	0.008
3	31.310	1.524
4	32.836	0.193
Total		100.000

(21) **5au**

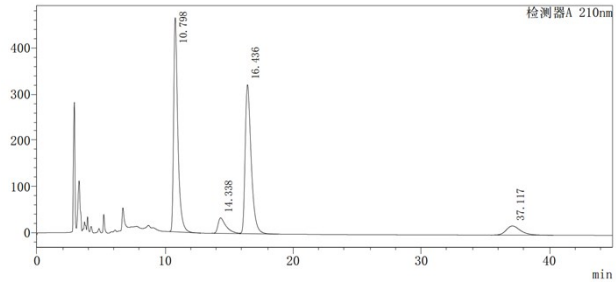


Peak	Retention Time	Area Percent
1	7.137	46.310
2	7.544	2.991
3	7.865	3.097
4	8.807	47.602
Total		100.000

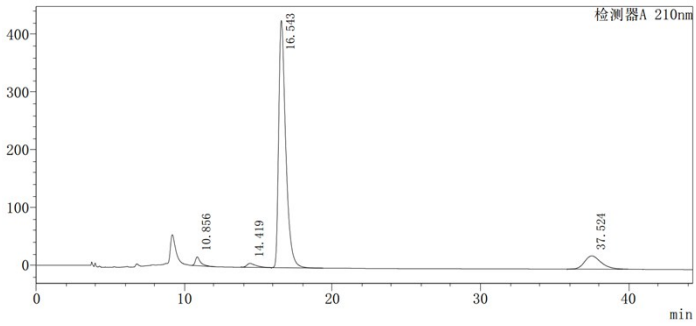


Peak	Retention Time	Area Percent
1	7.234	0.848
2	7.623	0.117
3	8.011	0.319
4	9.118	98.715
Total		100.000

(22) **5ba**

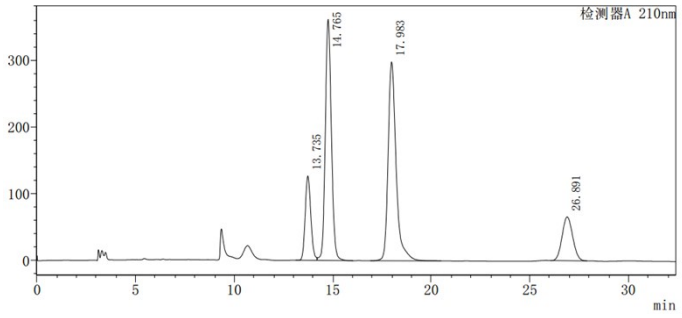


Peak	Retention Time	Area Percent
1	10.798	43.656
2	14.338	6.102
3	16.436	43.918
4	37.117	6.325
Total		100.000

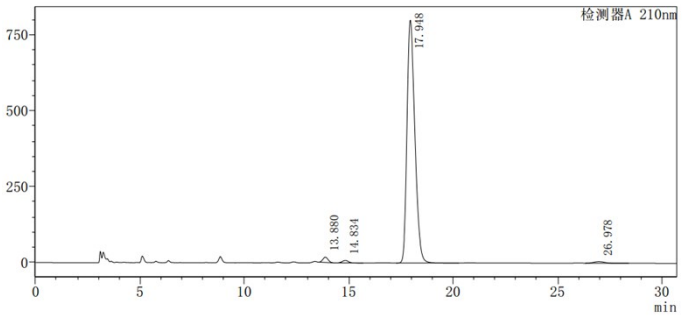


Peak	Retention Time	Area Percent
1	10.856	2.207
2	14.419	1.674
3	16.543	85.347
4	37.524	10.773
Total		100.000

(23) **5ca**

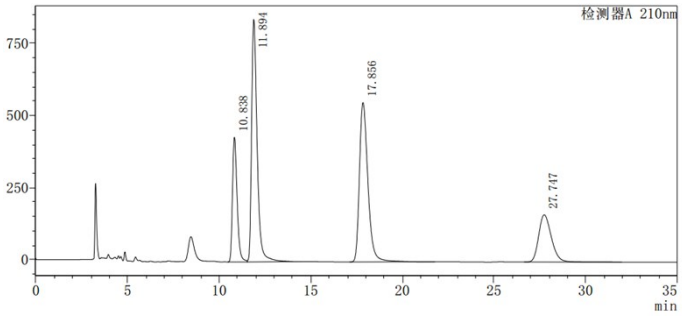


Peak	Retention Time	Area Percent
1	13.735	11.883
2	14.765	36.625
3	17.983	39.900
4	26.891	11.592
Total		100.000

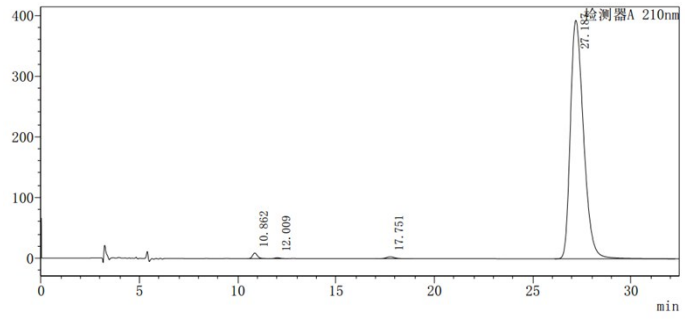


Peak	Retention Time	Area Percent
1	13.880	1.414
2	14.834	0.781
3	17.948	96.966
4	26.978	0.839
Total		100.000

(24) **5da**

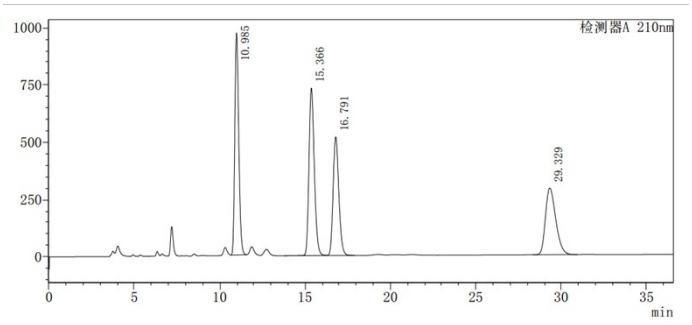


Peak	Retention Time	Area Percent
1	10.838	14.874
2	11.894	34.687
3	17.856	34.958
4	27.747	15.480
Total		100.000

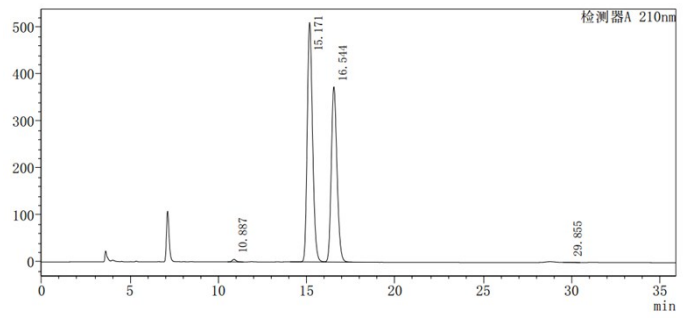


Peak	Retention Time	Area Percent
1	10.862	0.873
2	12.009	0.146
3	17.751	0.502
4	27.187	98.480
Total		100.000

(25) **5ea**



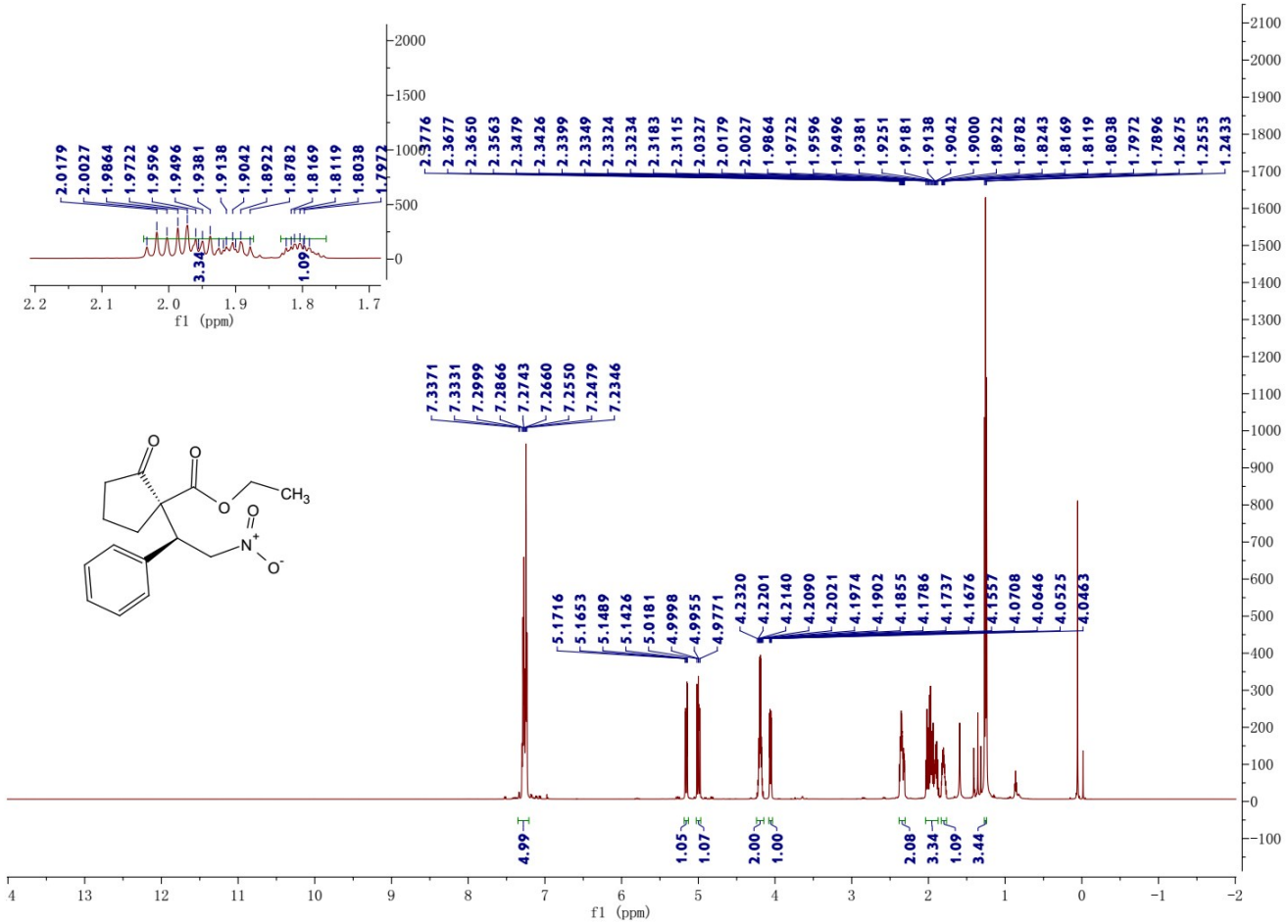
Peak	Retention Time	Area Percent
1	10.985	27.815
2	15.366	28.613
3	16.791	21.634
4	29.329	21.938
Total		100.000



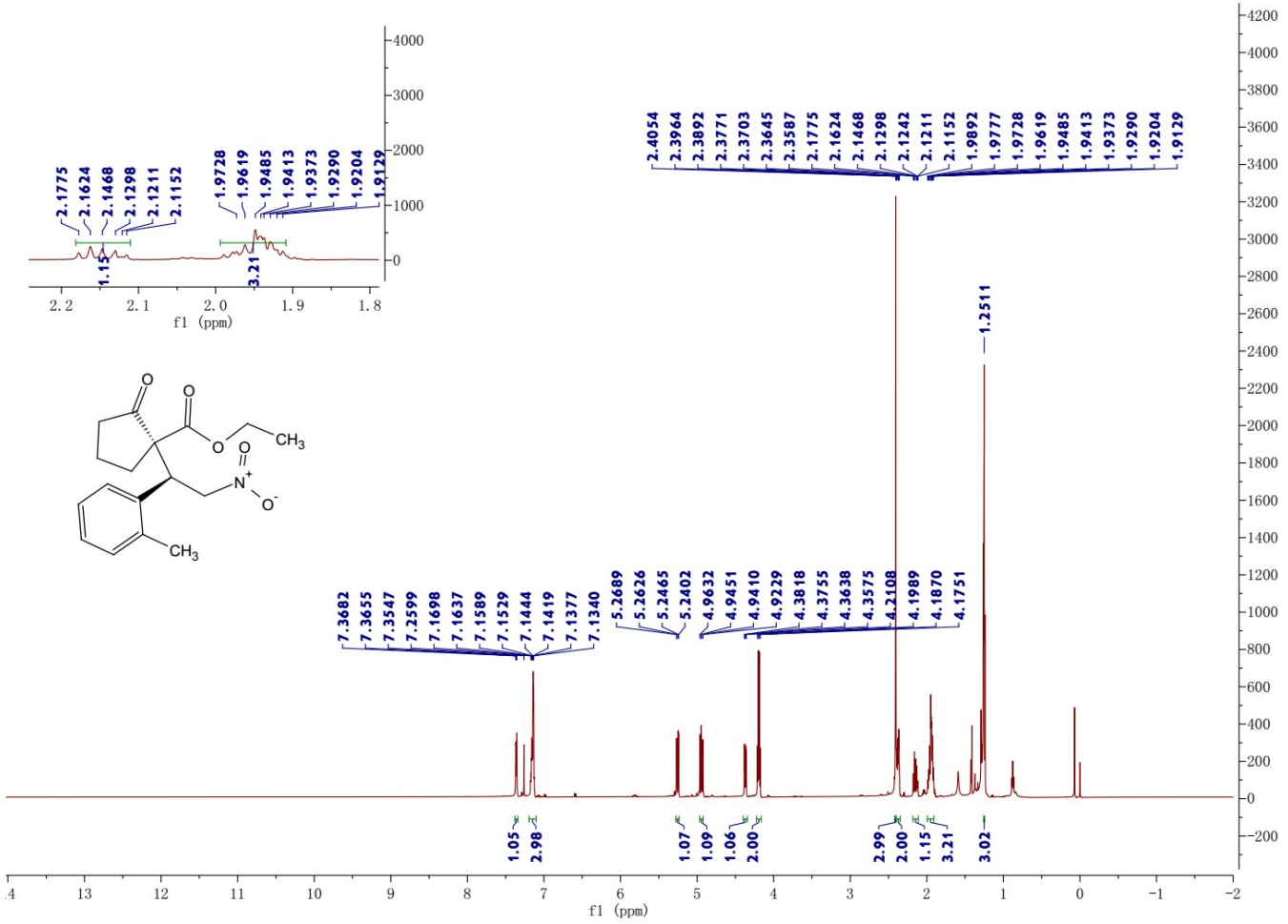
Peak	Retention Time	Area Percent
1	10.887	0.417
2	15.171	55.750
3	16.544	43.812
4	29.855	0.021
Total		100.000

4. Copies of NMR spectra

5aa



5ab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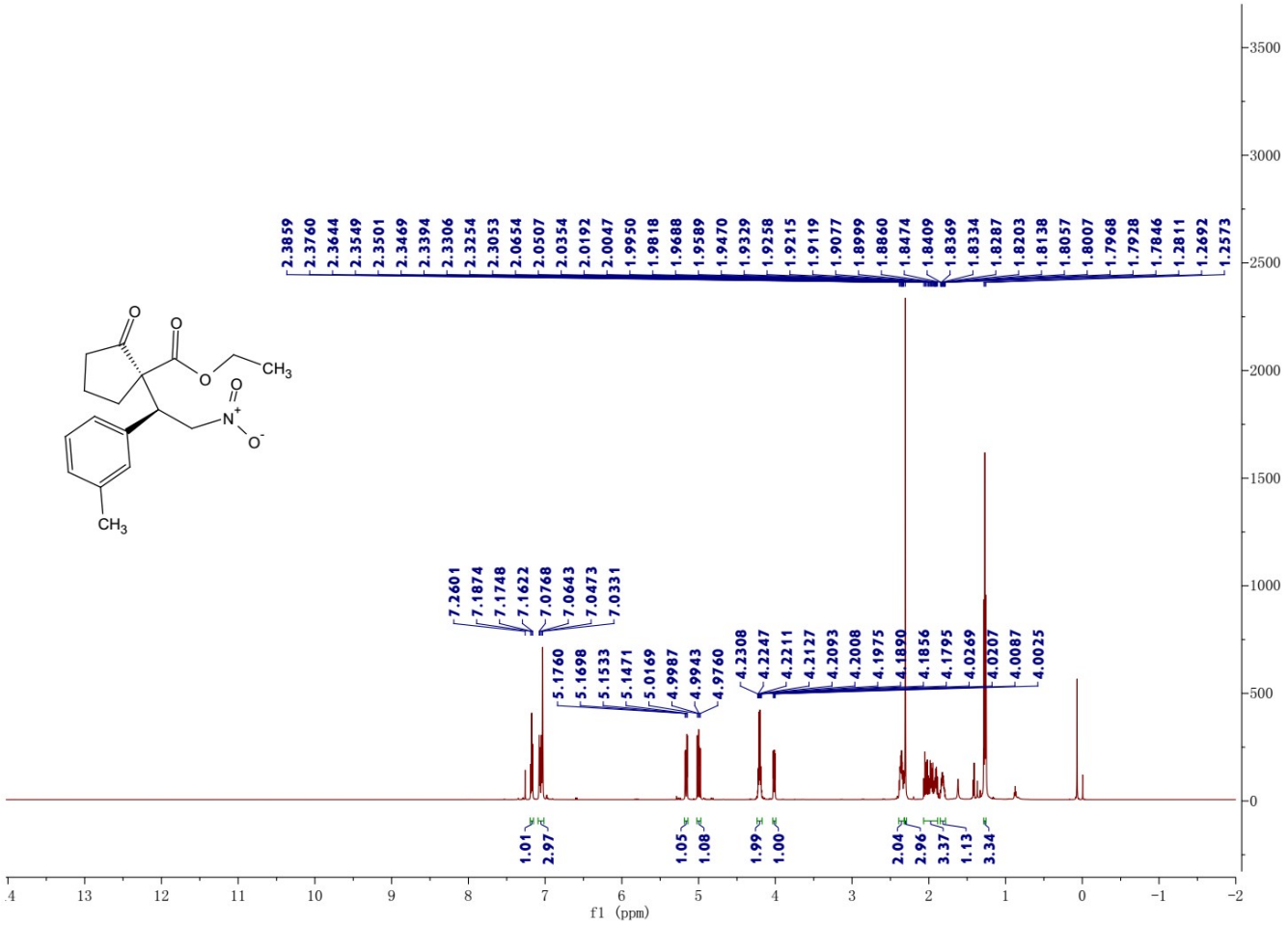
2.3771
2.3703
2.3645
2.3587
2.1775
2.1624
2.1468
2.1298
2.1242
2.1211
2.1152
1.9892
1.9777
1.9728
1.9619
1.9485
1.9413
1.9373
1.9290
1.9204
1.9129
1.2511
7.3682
7.3655
7.3547
7.2599
7.1698
7.1637
7.1589
7.1529
7.1444
7.1419
7.1377
7.1340
5.2689
5.2626
5.2465
5.2402
4.9632
4.9451
4.9410
4.9229
4.3818
4.3755
4.3638
4.3575
4.2108
4.1989
4.1870
4.1751
1.05
2.98
1.07
1.09
1.06
2.00
2.99
2.00
1.15
3.21
3.02
f1 (ppm)
O
O
O
CH3
O
N+
O-
CH3

5ac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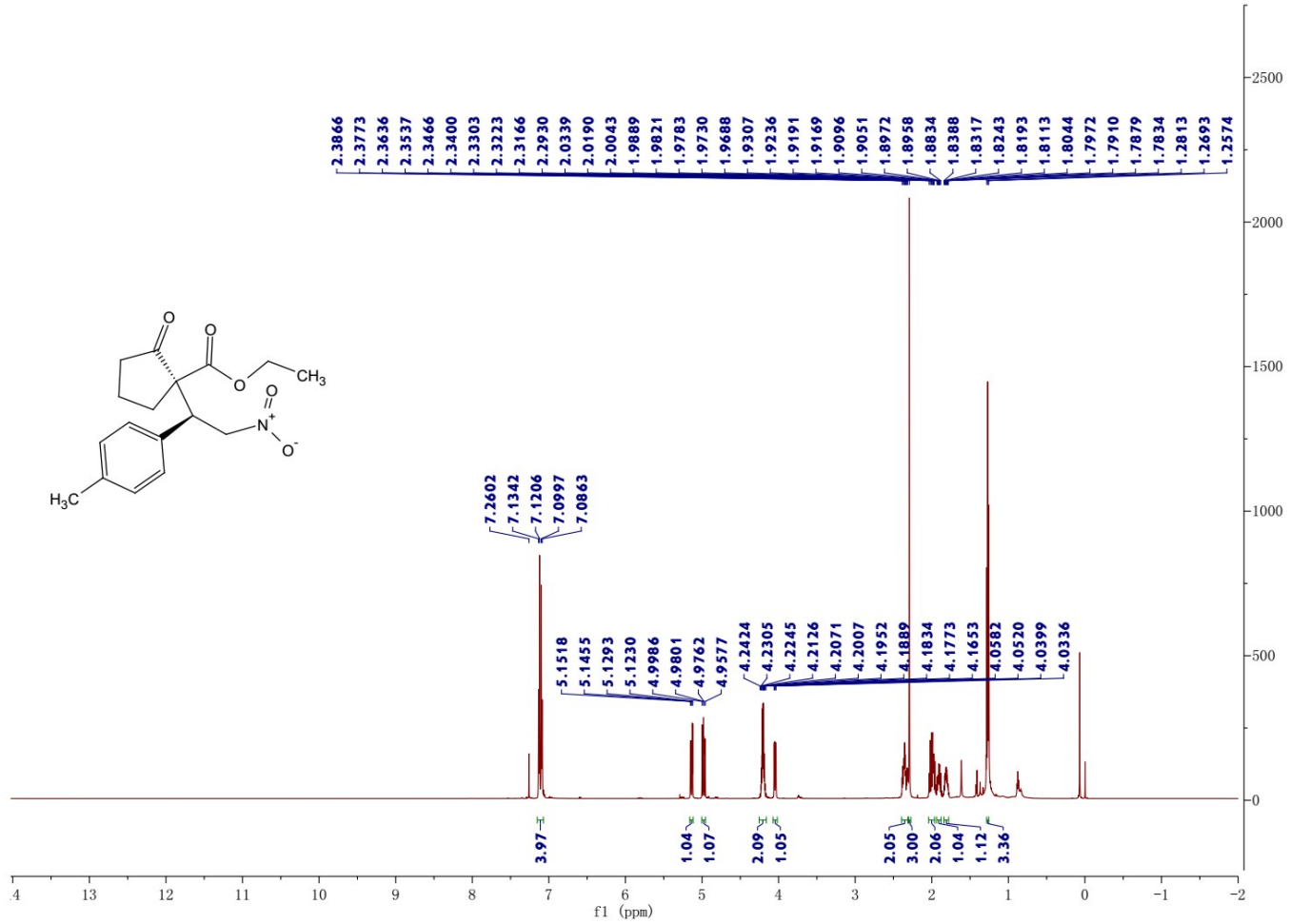
2.3760
2.3644
2.3549
2.3501
2.3469
2.3394
2.3306
2.3254
2.3053
2.0654
2.0507
2.0354
2.0192
2.0047
1.9950
1.9818
1.9688
1.9589
1.9470
1.9329
1.9258
1.9215
1.9119
1.9077
1.8999
1.8860
1.8474
1.8409
1.8369
1.8334
1.8287
1.8203
1.8138
1.8057
1.8007
1.7968
1.7928
1.7846
1.2811
1.2692
1.2573
7.2601
7.1874
7.1748
7.1622
7.0768
7.0643
7.0473
7.0331
5.1760
5.1698
5.1533
5.1471
5.0169
4.9987
4.9943
4.9760
4.2308
4.2247
4.2211
4.2127
4.2093
4.2008
4.1975
4.1890
4.1856
4.1795
4.0269
4.0207
4.0087
4.0025
1.01
2.97
1.05
1.08
1.99
1.00
2.04
2.96
3.37
1.13
3.34
f1 (ppm)

5ad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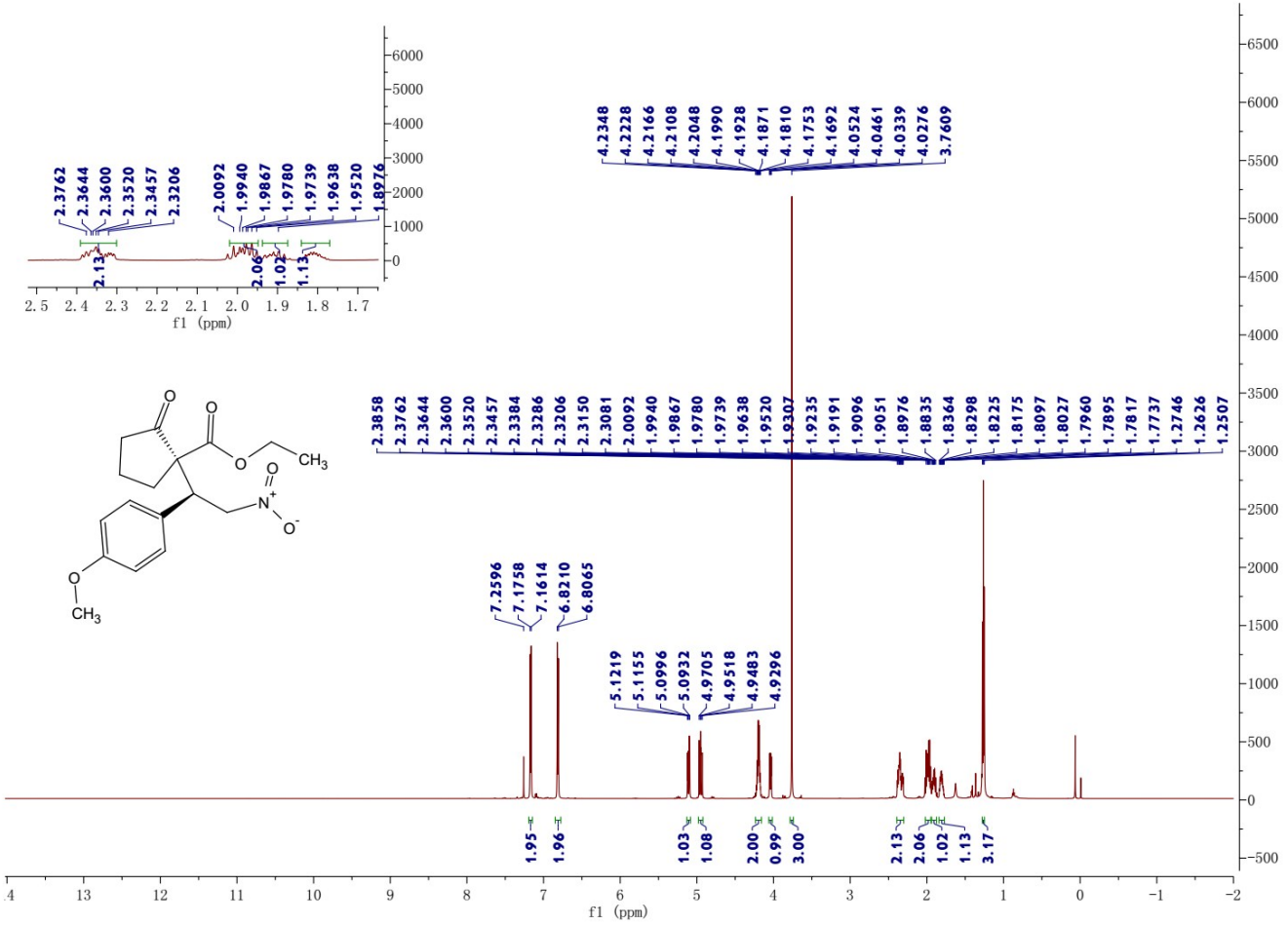
2.3773
2.3636
2.3537
2.3466
2.3400
2.3303
2.3223
2.3166
2.2930
2.0339
2.0190
2.0043
1.9889
1.9821
1.9783
1.9730
1.9688
1.9307
1.9236
1.9191
1.9169
1.9096
1.9051
1.8972
1.8958
1.8834
1.8388
1.8317
1.8243
1.8193
1.8113
1.8044
1.7972
1.7910
1.7879
1.7834
1.2813
1.2693
1.2574
7.2602
7.1342
7.1206
7.0997
7.0863
5.1518
5.1455
5.1293
5.1230
4.9986
4.9801
4.9762
4.9577
4.2424
4.2305
4.2245
4.2126
4.2071
4.2007
4.1952
4.1889
4.1834
4.1773
4.1653
4.0582
4.0520
4.0399
4.0336
3.97
1.04
1.07
2.09
1.05
2.05
3.00
2.06
1.04
1.12
3.36
f1 (ppm)

5ae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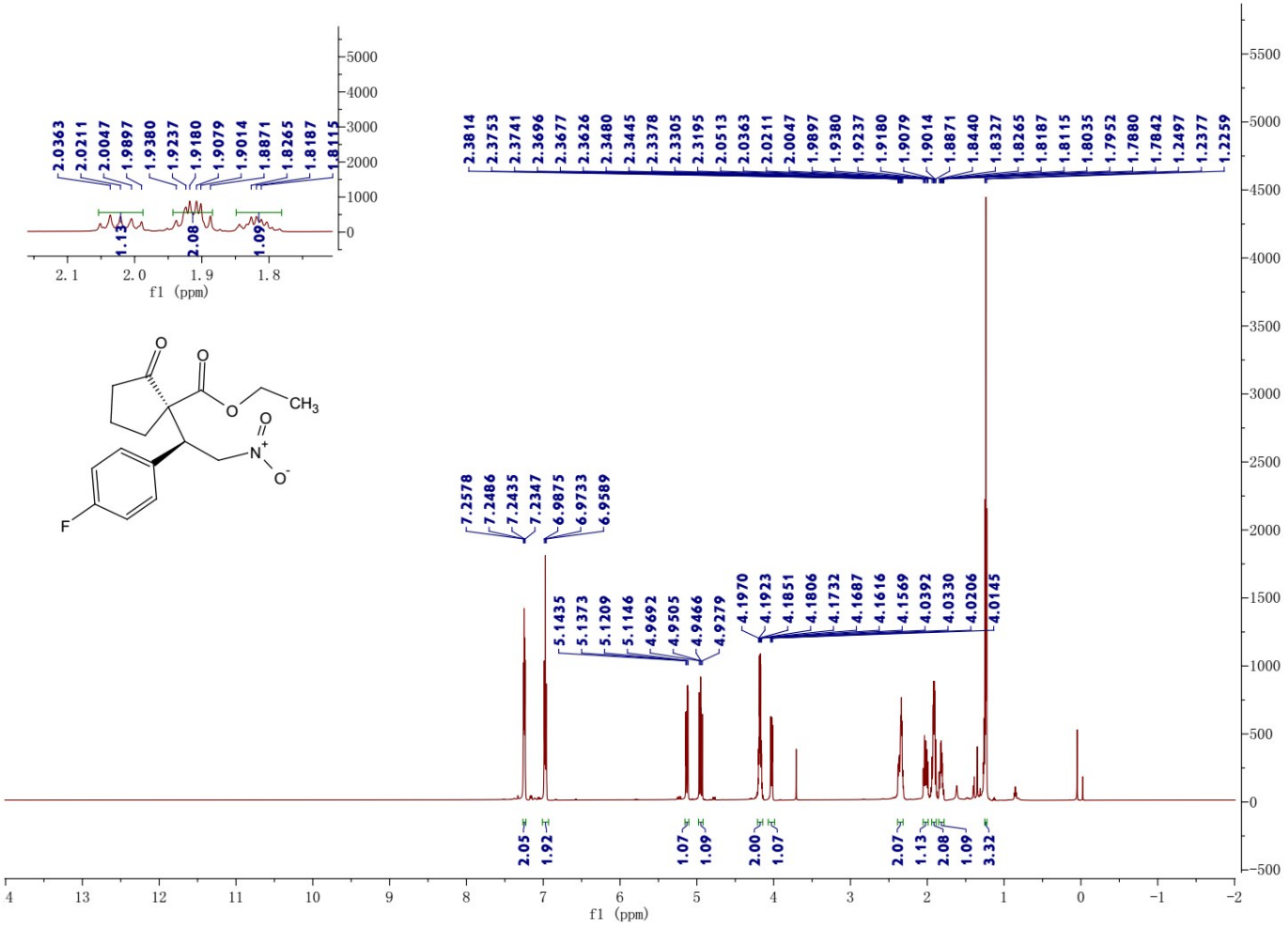
2.3600
2.3520
2.3457
2.3206
2.0092
1.9940
1.9867
1.9780
1.9739
1.9638
1.9520
1.8976
2.13
2.06
1.02
1.13
f1 (ppm)
4.2348
4.2228
4.2166
4.2108
4.2048
4.1990
4.1928
4.1871
4.1810
4.1753
4.1692
4.0524
4.0461
4.0339
4.0276
3.7609
2.3858
2.3762
2.3644
2.3600
2.3520
2.3457
2.3384
2.3286
2.3206
2.3150
2.3081
2.0092
1.9940
1.9867
1.9780
1.9739
1.9638
1.9520
1.9307
1.9235
1.9191
1.9096
1.9051
1.8976
1.8835
1.8364
1.8298
1.8225
1.8175
1.8097
1.8027
1.7960
1.7895
1.7817
1.7737
1.2746
1.2626
1.2507
7.2596
7.1758
7.1614
6.8210
6.8065
5.1219
5.1155
5.0996
5.0932
4.9705
4.9518
4.9483
4.9296
1.95
1.96
1.03
1.08
2.00
0.99
3.00
2.13
2.06
1.02
1.13
3.17
f1 (ppm)

5af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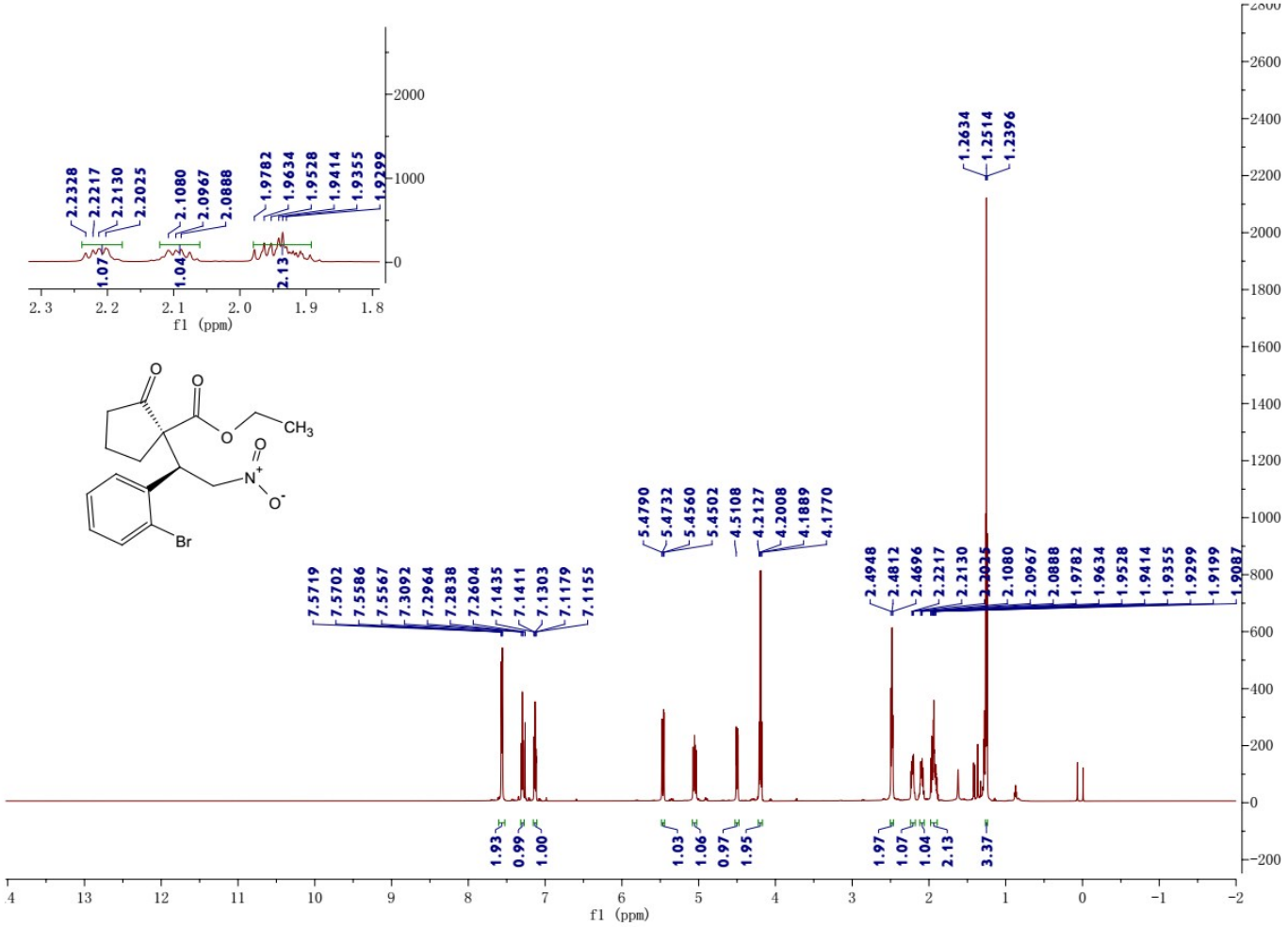
2.0211
2.0047
1.9897
1.9380
1.9237
1.9180
1.9079
1.9014
1.8871
1.8265
1.8187
1.8115
1.13
2.08
1.09
f1 (ppm)
O
O
O
CH3
O
N+
O-
F
7.2578
7.2486
7.2435
7.2347
6.9875
6.9733
6.9589
5.1435
5.1373
5.1209
5.1146
4.9692
4.9505
4.9466
4.9279
4.1970
4.1923
4.1851
4.1806
4.1732
4.1687
4.1616
4.1569
4.0392
4.0330
4.0206
4.0145
2.05
1.92
1.07
1.09
2.00
1.07
2.07
1.13
2.08
1.09
3.32
f1 (ppm)

5ag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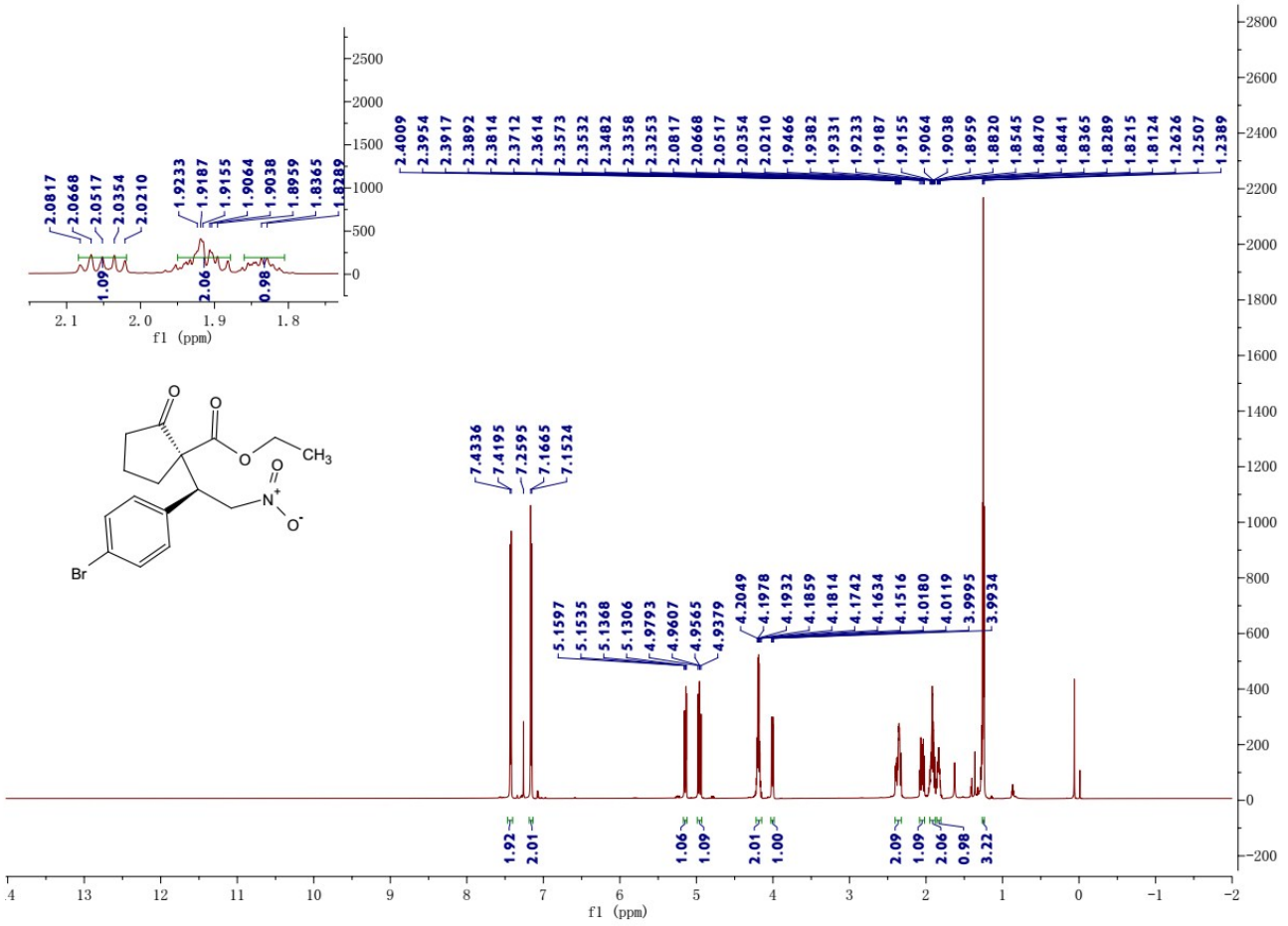
2.2130
2.2025
2.1080
2.0967
2.0888
1.9782
1.9634
1.9528
1.9414
1.9355
1.9299
1.07
1.04
2.13
f1 (ppm)
O
O
O
CH3
N+
O-
Br
7.5719
7.5702
7.5586
7.5567
7.3092
7.2964
7.2838
7.2604
7.1435
7.1411
7.1303
7.1179
7.1155
5.4790
5.4732
5.4560
5.4502
4.5108
4.2127
4.2008
4.1889
4.1770
2.4948
2.4812
2.4696
2.2217
2.2130
2.1080
2.0967
2.0888
1.9782
1.9634
1.9528
1.9414
1.9355
1.9299
1.9199
1.9087
1.2634
1.2514
1.2396
1.93
0.99
1.00
1.03
1.06
0.97
1.95
1.97
1.07
1.04
2.13
3.37
f1 (ppm)

5ah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2.0517
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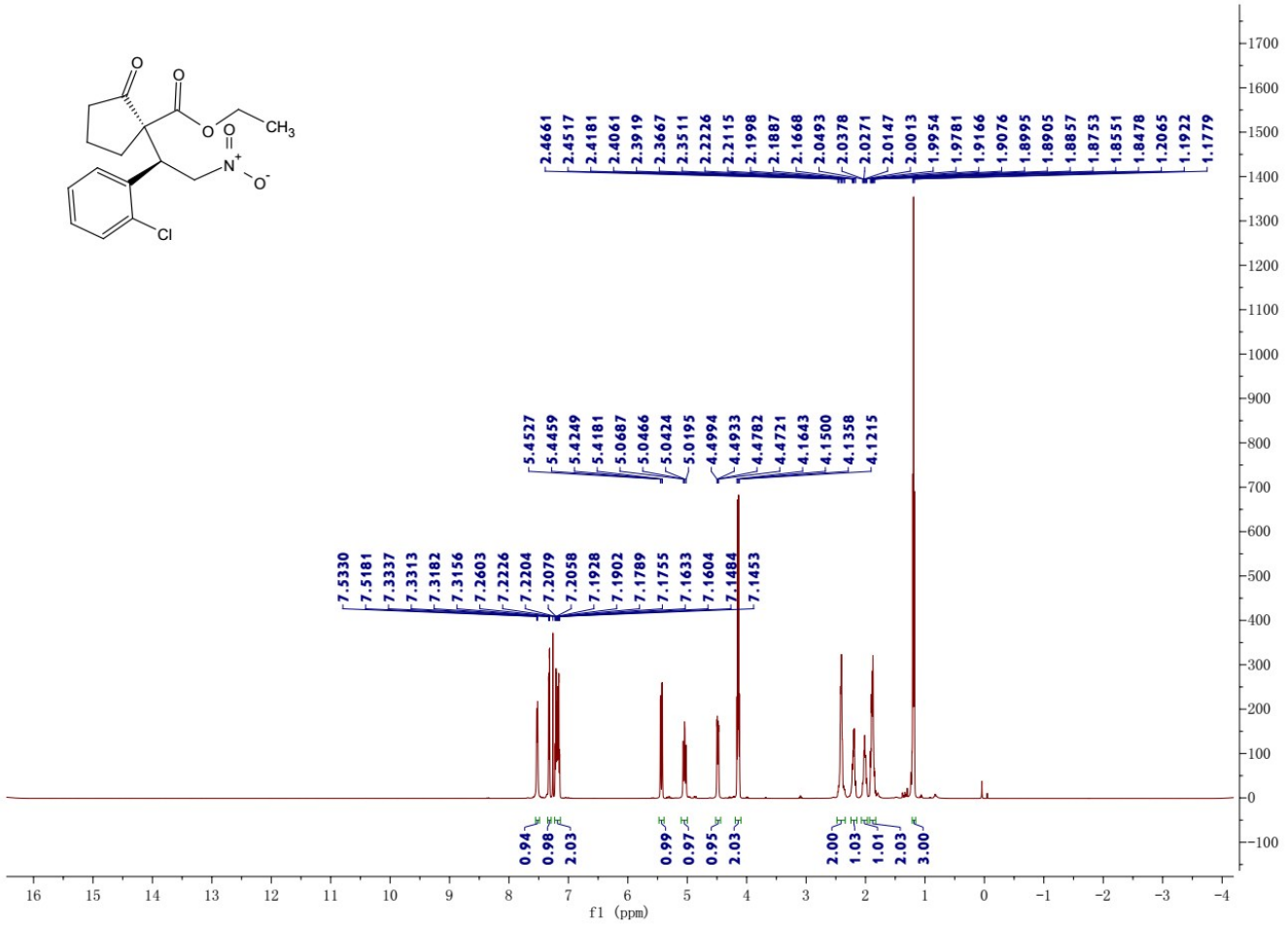
2.0210
1.9233
1.9187
1.9155
1.9064
1.9038
1.8959
1.8365
1.8289
1.09
2.06
0.98
f1 (ppm)
O
O
O
CH3
N+
O-
Br
7.4336
7.4195
7.2595
7.1665
7.1524
5.1597
5.1535
5.1368
5.1306
4.9793
4.9607
4.9565
4.9379
4.2049
4.1978
4.1932
4.1859
4.1814
4.1742
4.1634
4.1516
4.0180
4.0119
3.9995
3.9934
1.92
2.01
1.06
1.09
2.01
1.00
2.09
1.09
2.06
0.98
3.22
f1 (ppm)

5ai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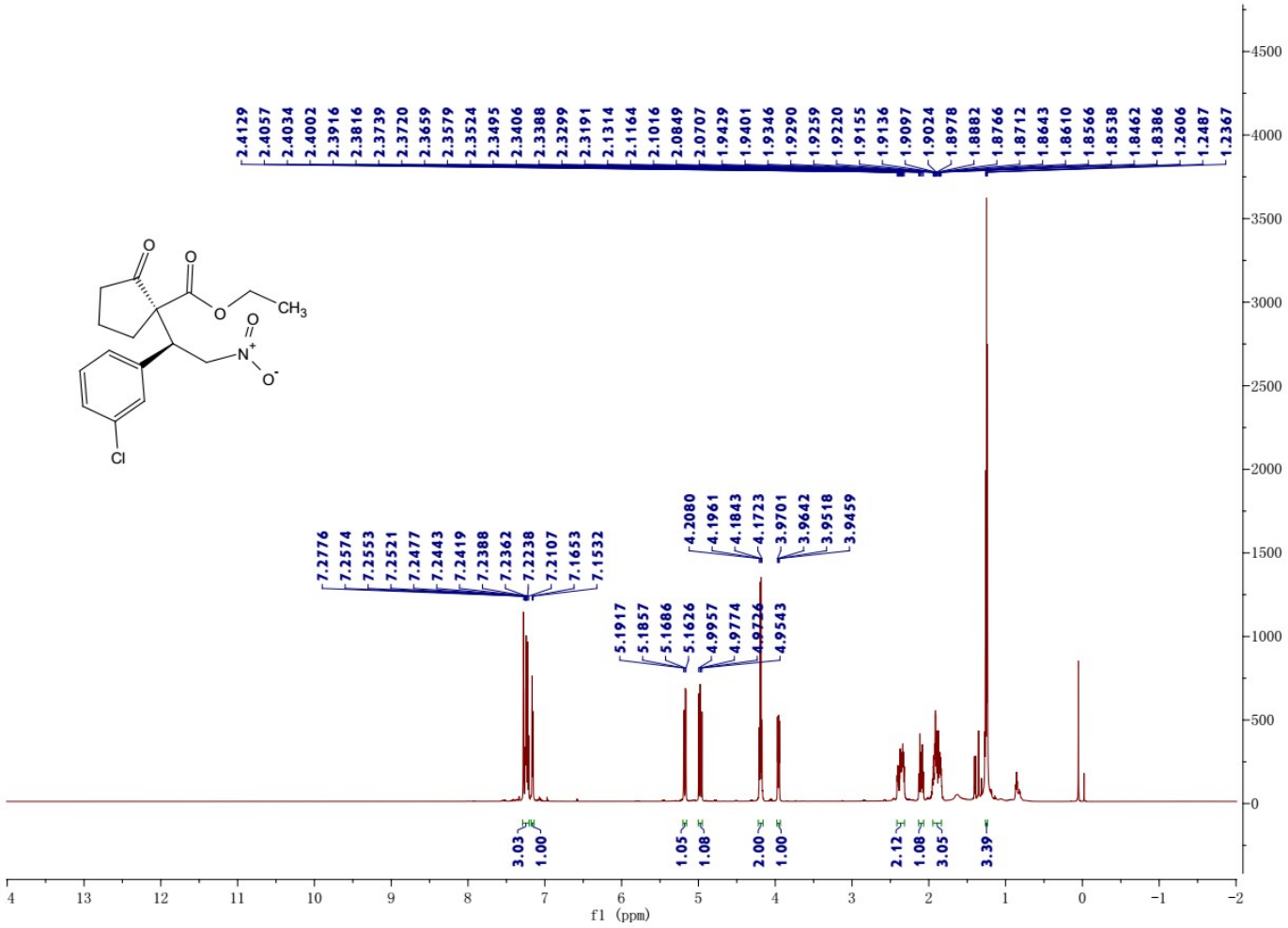
2.4517
2.4181
2.4061
2.3919
2.3667
2.3511
2.2226
2.2115
2.1998
2.1887
2.1668
2.0493
2.0378
2.0271
2.0147
2.0013
1.9954
1.9781
1.9166
1.9076
1.8995
1.8905
1.8857
1.8753
1.8551
1.8478
1.2065
1.1922
1.1779
5.4527
5.4459
5.4249
5.4181
5.0687
5.0466
5.0424
5.0195
4.4994
4.4933
4.4782
4.4721
4.1643
4.1500
4.1358
4.1215
7.5330
7.5181
7.3337
7.3313
7.3182
7.3156
7.2603
7.2226
7.2204
7.2079
7.2058
7.1928
7.1902
7.1789
7.1755
7.1633
7.1604
7.1484
7.1453
0.94
0.98
2.03
0.99
0.97
0.95
2.03
2.00
1.03
1.01
2.03
3.00
f1 (ppm)

5aj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1.9024
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1.8566
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7.2477
7.2443
7.2419
7.2388
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7.2238
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7.1532
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5.1626
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4.9736
4.9543
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2.00
1.00
2.12
1.08
3.05
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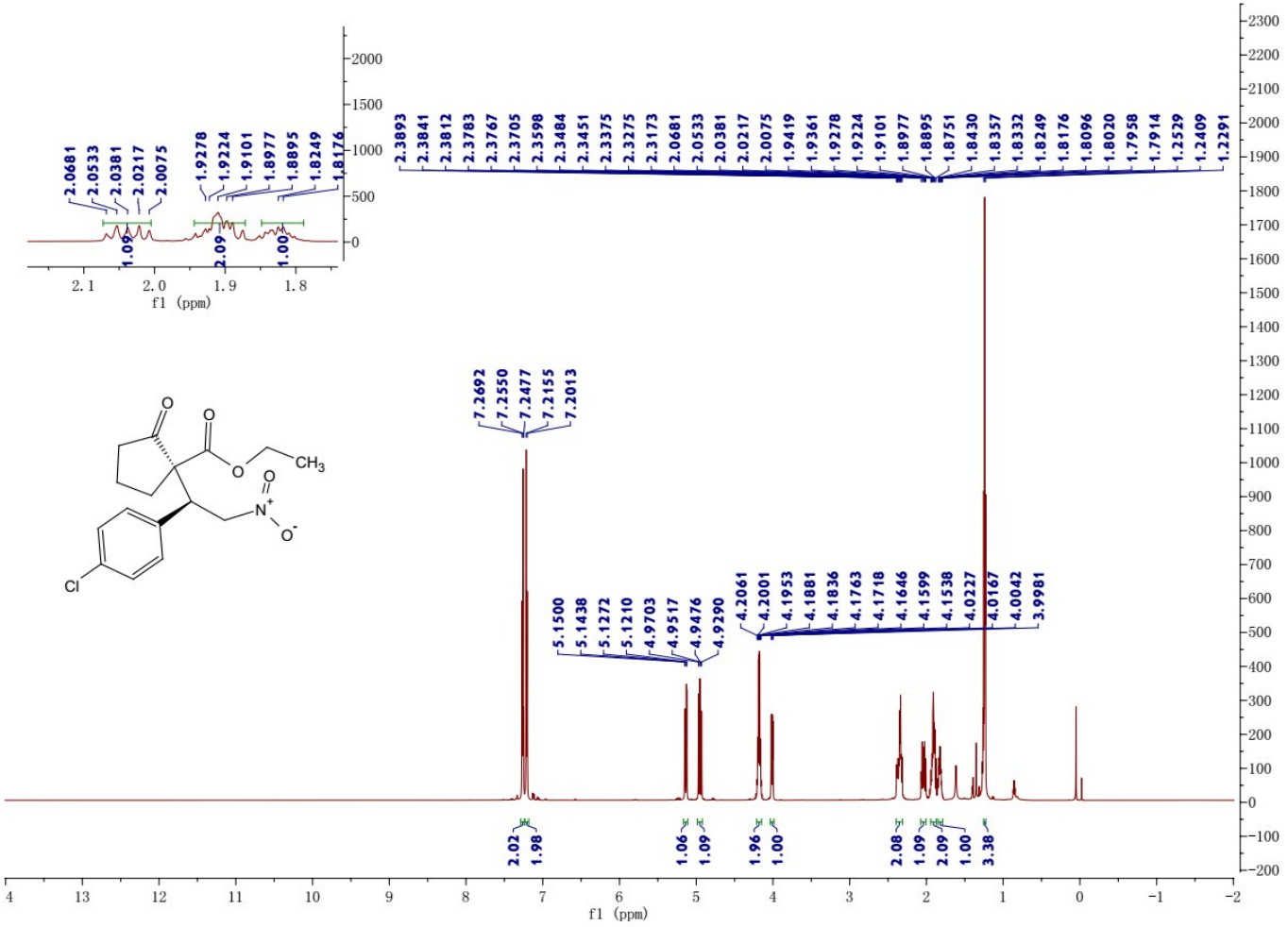
f1 (ppm)

5ak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1.00
f1 (ppm)
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3.9981
O
O
O
CH3
O
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O-
Cl
2.02
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1.09
2.09
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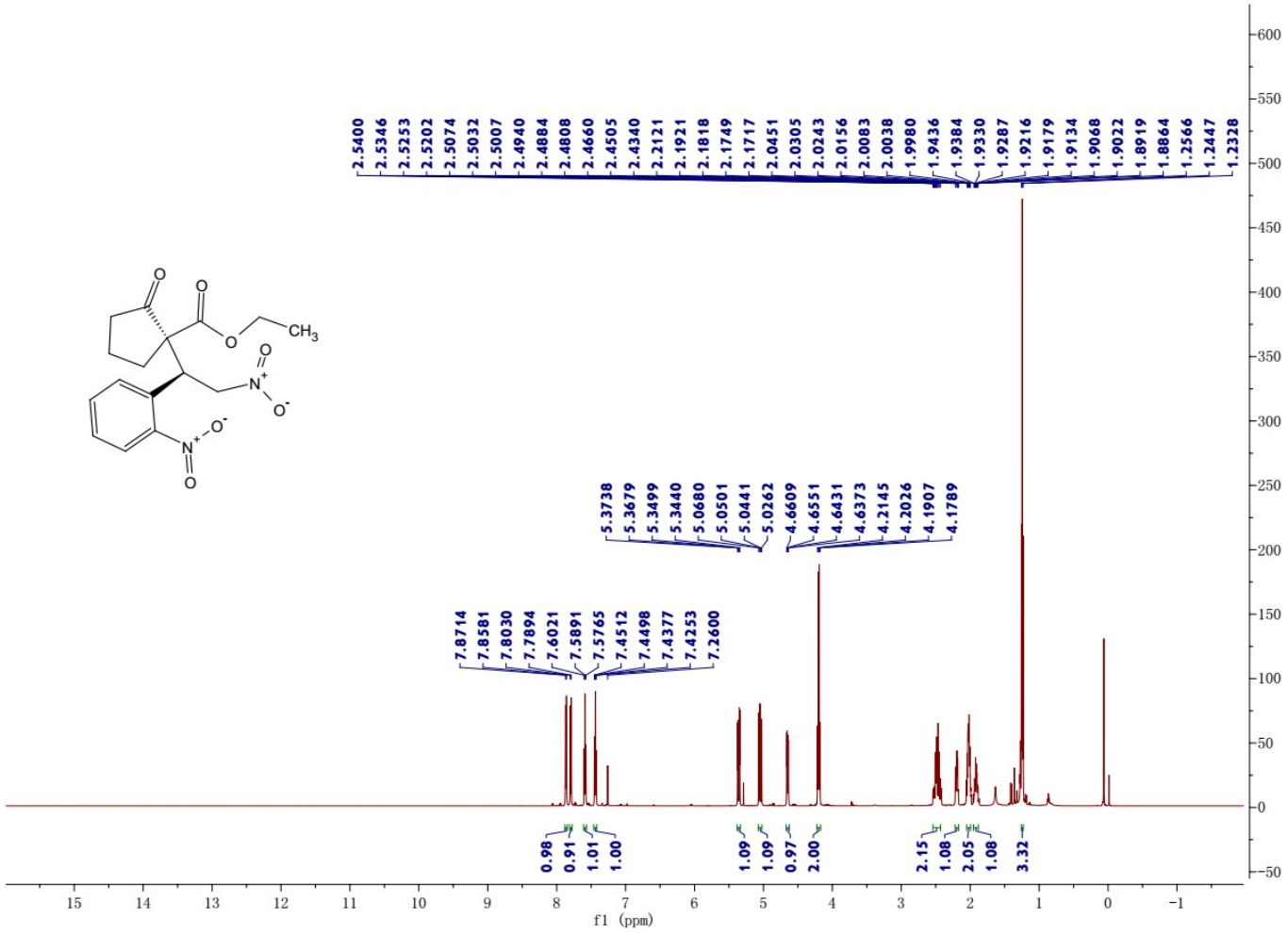
f1 (ppm)

5al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1.9330
1.9287
1.9216
1.9179
1.9134
1.9068
1.9022
1.8919
1.8864
1.2566
1.2447
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4.6609
4.6551
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7.4253
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2.05
1.08
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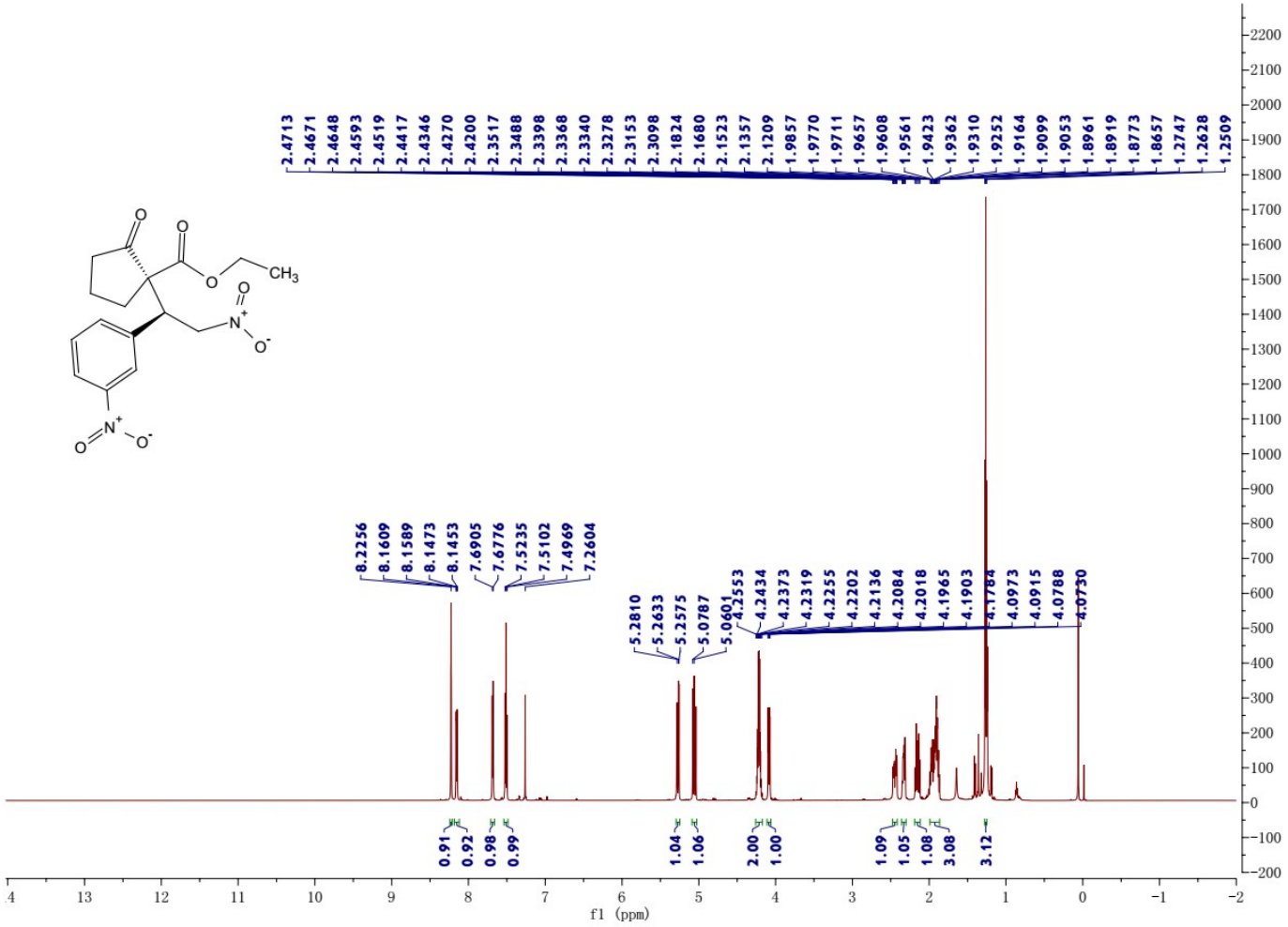
f1 (ppm)

5am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2.3340
2.3278
2.3153
2.3098
2.1824
2.1680
2.1523
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1.9423
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1.9310
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1.9099
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1.8961
1.8919
1.8773
1.8657
1.2747
1.2628
1.2509
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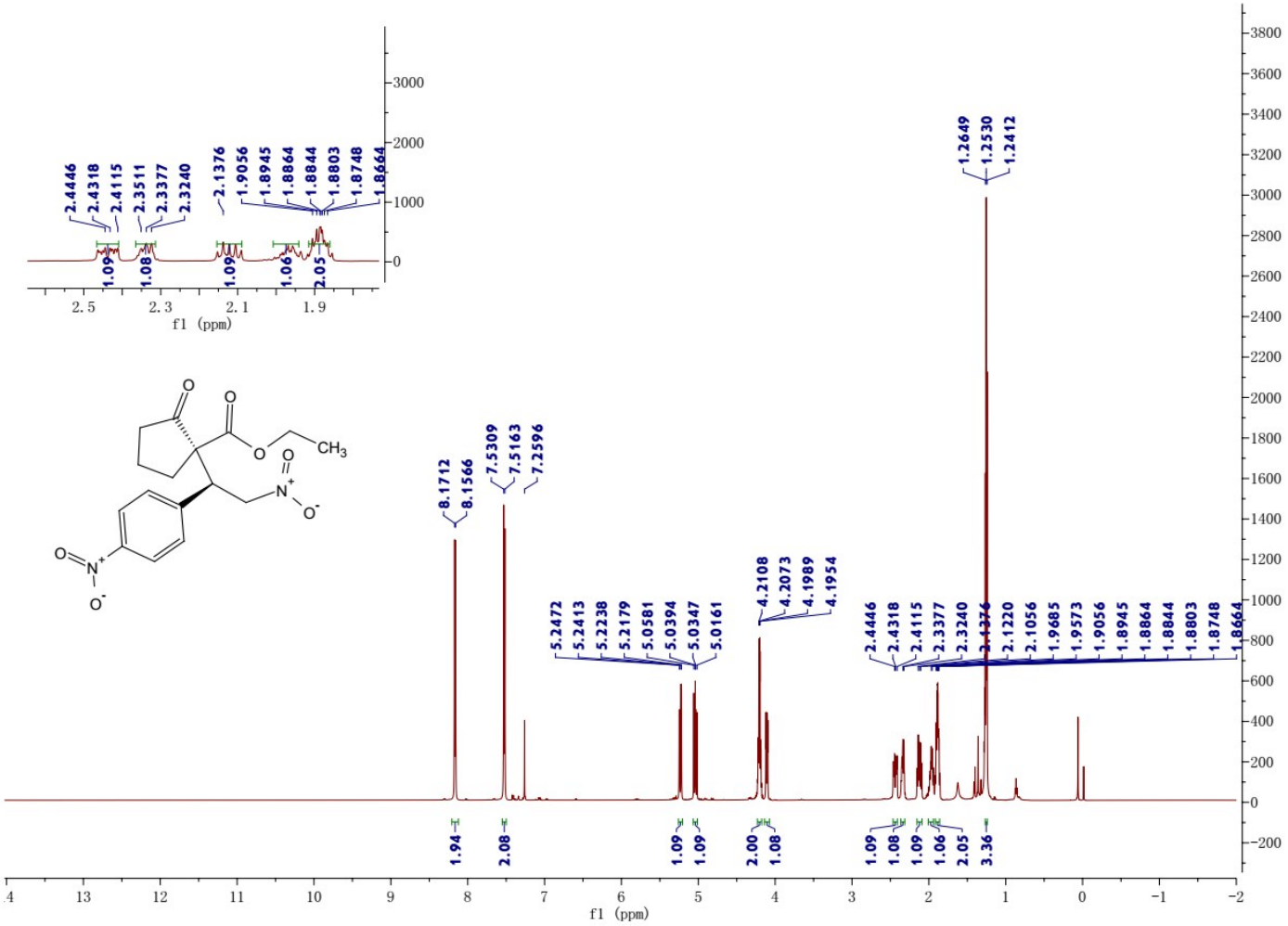
8.1589
8.1473
8.1453
7.6905
7.6776
7.5235
7.5102
7.4969
7.2604
5.2810
5.2633
5.2575
5.0787
5.0601
4.2553
4.2434
4.2373
4.2319
4.2255
4.2202
4.2136
4.2084
4.2018
4.1965
4.1903
4.1784
4.0973
4.0915
4.0788
4.0730
0.91
0.92
0.98
0.99
1.04
1.06
2.00
1.00
1.09
1.05
1.08
3.08
3.12
f1 (ppm)

5an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5.2179
5.0581
5.0394
5.0347
5.0161
4.2108
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4.1954
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2.4318
2.4115
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2.3240
2.1376
2.1220
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1.8844
1.8803
1.8748
1.8664
1.2649
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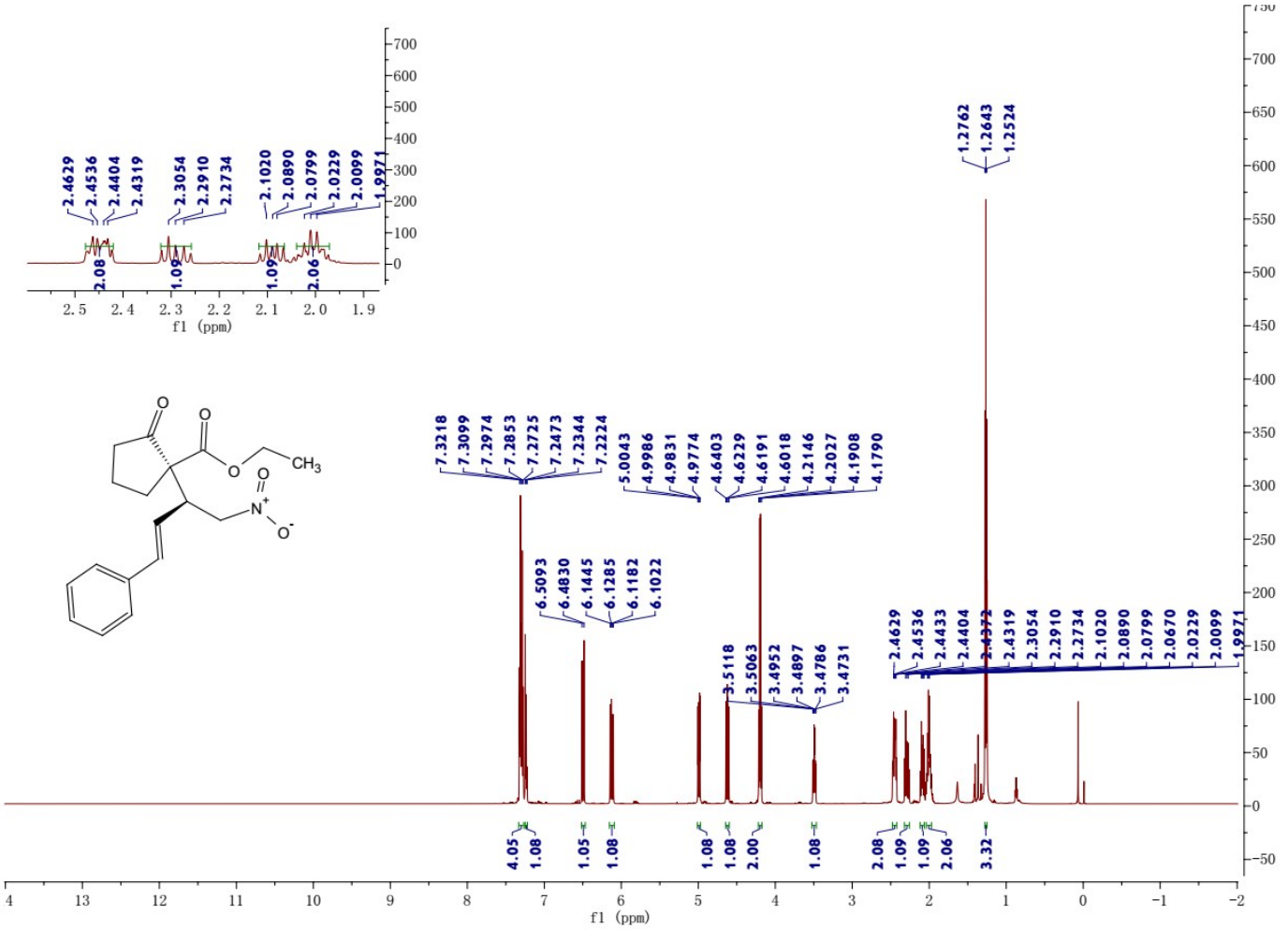
1.2412
1.94
2.08
1.09
1.09
2.00
1.08
1.09
1.08
1.09
1.06
2.05
3.36
f1 (ppm)

5ao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2.2734
2.1020
2.0890
2.0799
2.0229
2.0099
1.9971
2.08
1.05
1.09
2.06
f1 (ppm)
7.3218
7.3099
7.2974
7.2853
7.2725
7.2473
7.2344
7.2224
5.0043
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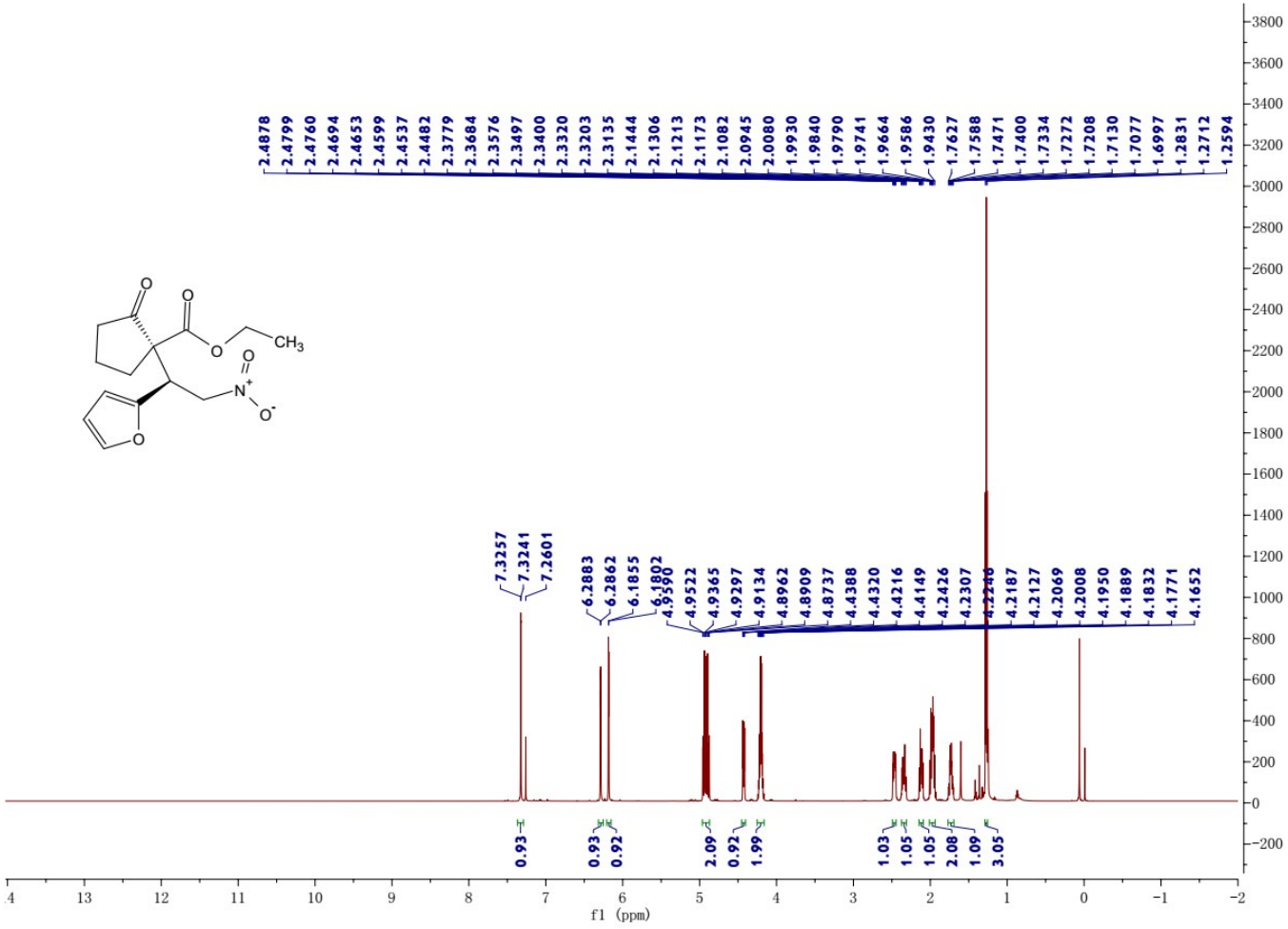
4.9831
4.9774
4.6403
4.6229
4.6191
4.6018
4.2146
4.2027
4.1908
4.1790
6.5093
6.4830
6.1445
6.1285
6.1182
6.1022
3.5118
3.5063
3.4952
3.4897
3.4786
3.4731
1.2762
1.2643
1.2524
4.05
1.08
1.05
1.08
1.08
1.08
2.00
1.08
2.08
1.09
1.09
2.06
3.32
f1 (ppm)

5ap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2.3400
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2.1306
2.1213
2.1173
2.1082
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1.9840
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1.7208
1.7130
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7.2601
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6.2862
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4.9522
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4.9134
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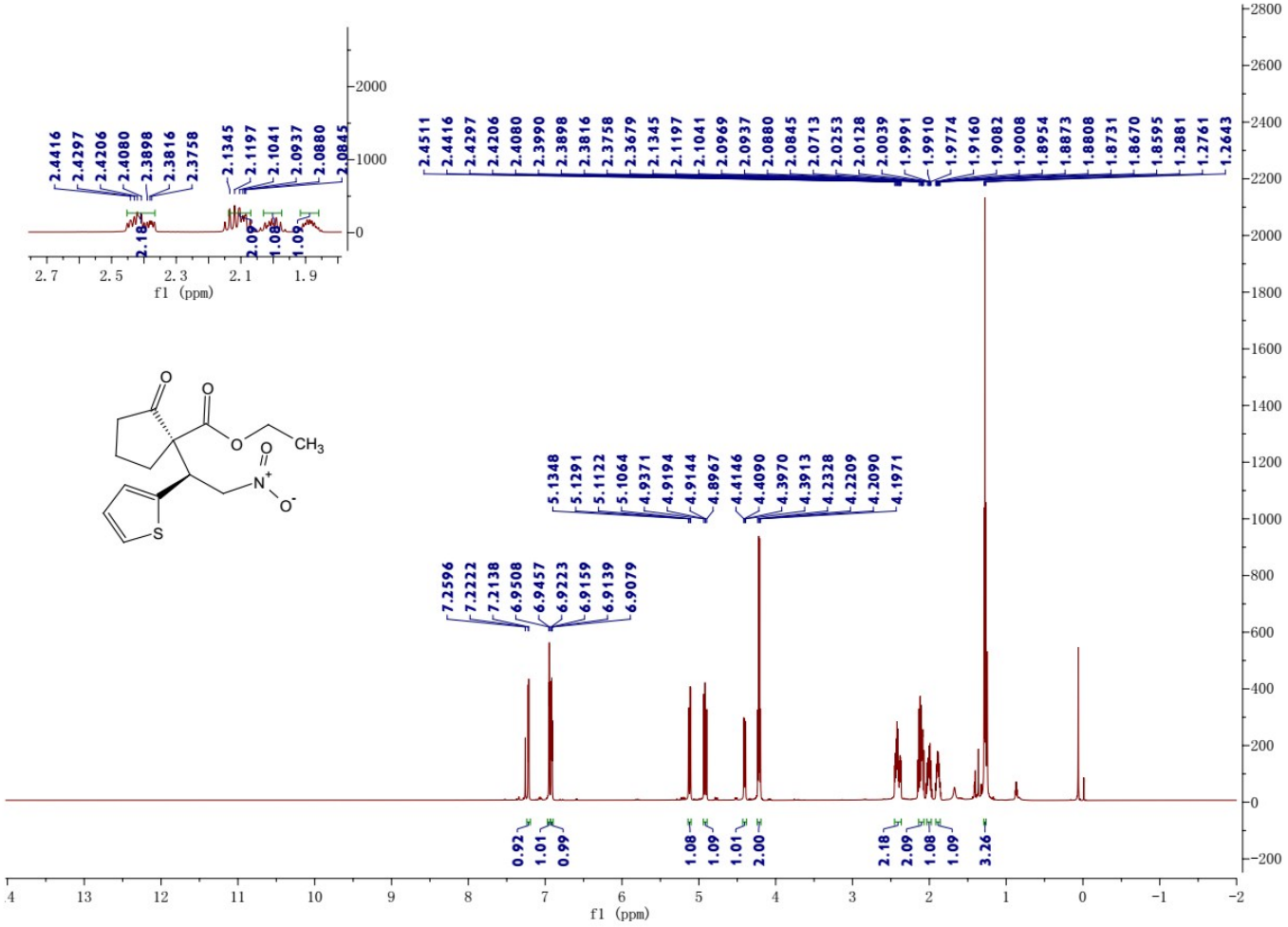
4.2307
4.2240
4.2187
4.2127
4.2069
4.2008
4.1950
4.1889
4.1832
4.1771
4.1652
0.93
0.93
0.92
2.09
0.92
1.99
1.03
1.05
1.05
2.08
1.09
3.05
f1 (ppm)

5aq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2.1197
2.1041
2.0937
2.0880
2.0845
2.18
2.09
1.08
1.00
f1 (ppm)
2.4511
2.4416
2.4297
2.4206
2.4080
2.3990
2.3898
2.3816
2.3758
2.3679
2.1345
2.1197
2.1041
2.0969
2.0937
2.0880
2.0845
2.0713
2.0253
2.0128
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1.9910
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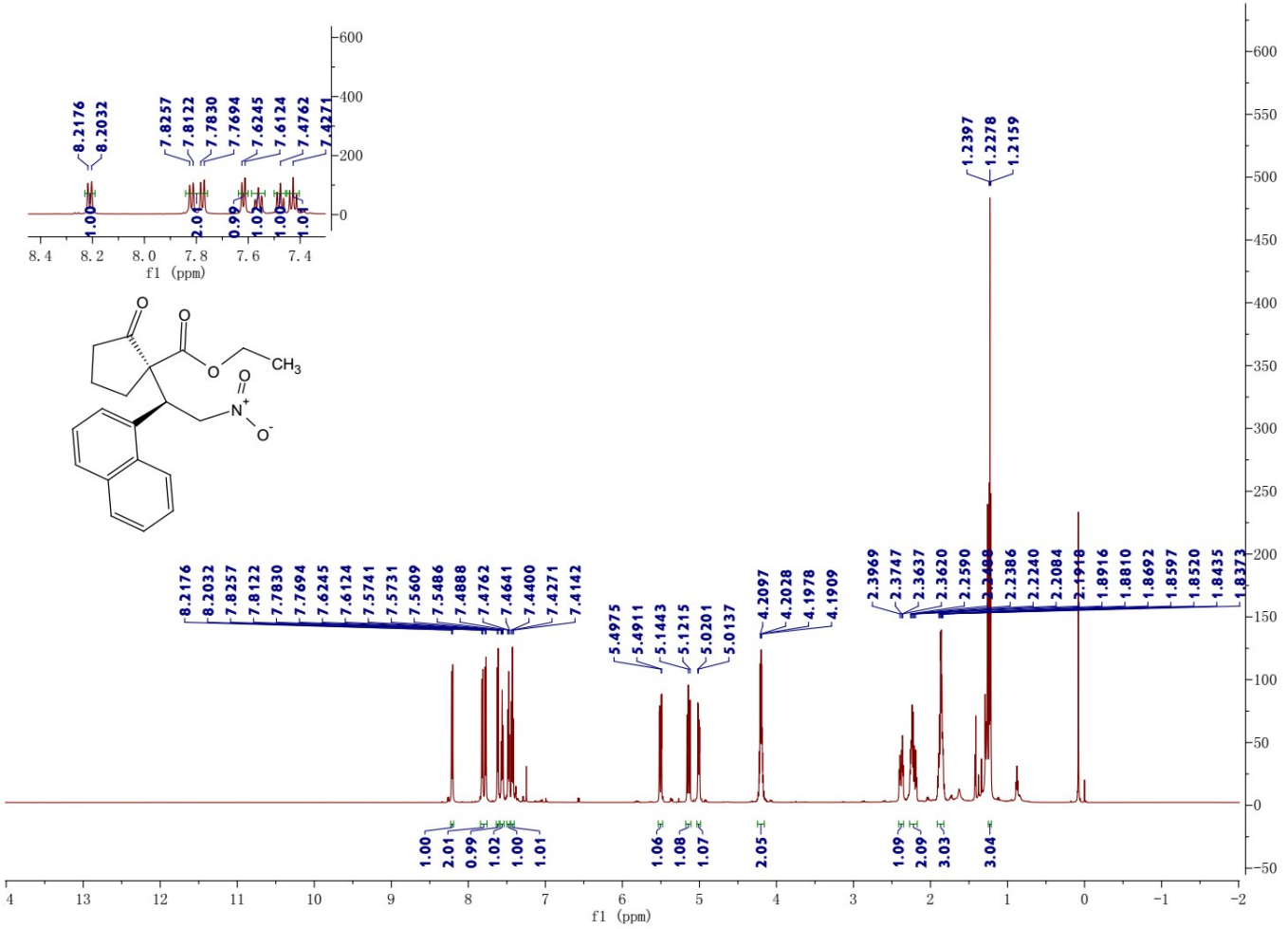
3.26
f1 (ppm)

5ar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2.01
0.99
1.02
1.00
1.01
f1 (ppm)
O
O
O
CH3
O
N+
O-
8.2176
8.2032
7.8257
7.8122
7.7830
7.7694
7.6245
7.6124
7.5741
7.5731
7.5609
7.5486
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7.4400
7.4271
7.4142
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5.4911
5.1443
5.1215
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4.2028
4.1978
4.1909
2.3969
2.3747
2.3637
2.3620
2.2386
2.2240
2.2084
1.8916
1.8810
1.8692
1.8597
1.8520
1.8435
1.2397
1.2278
1.2159
1.00
2.01
0.99
1.02
1.00
1.01
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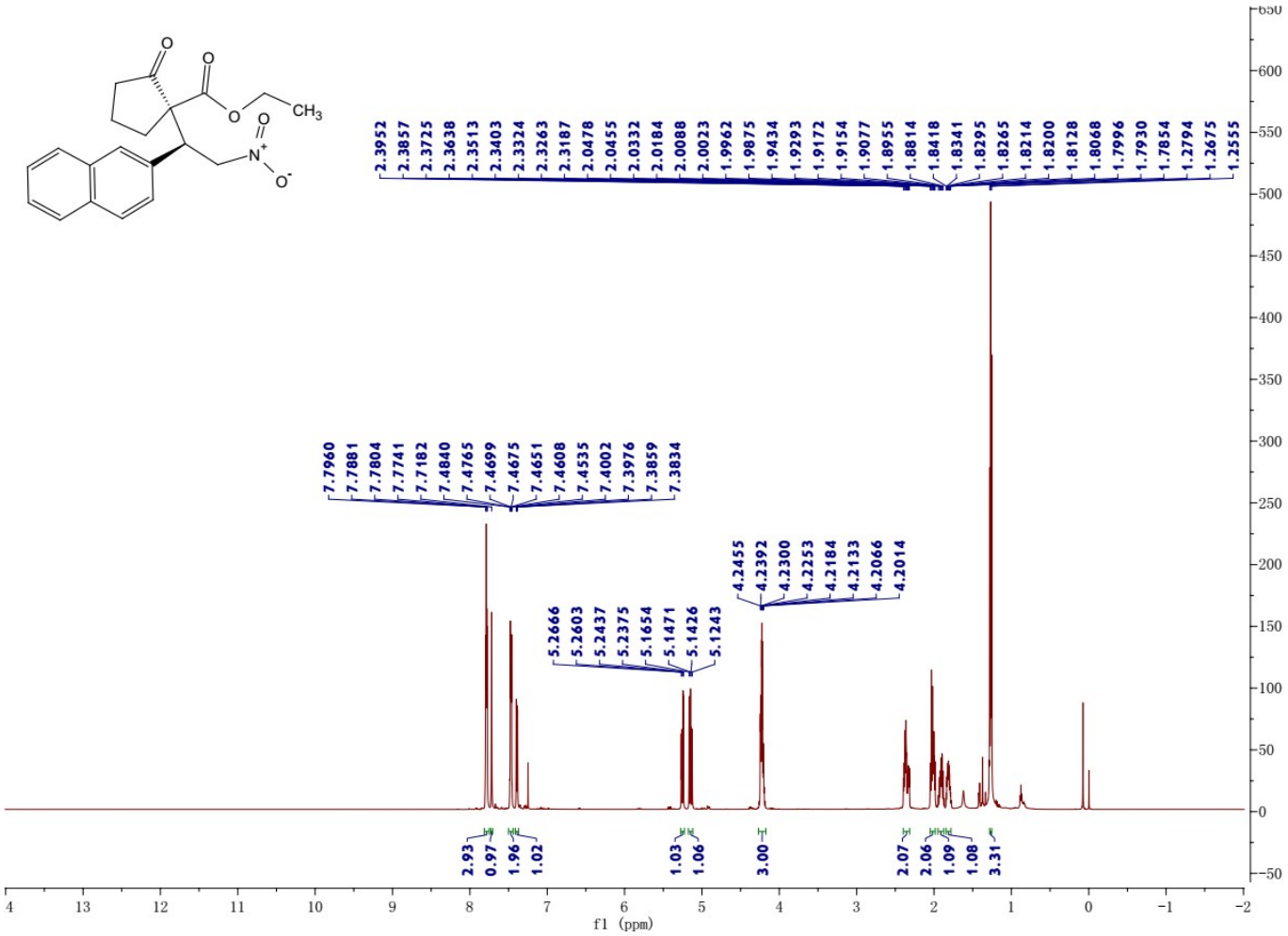
1.08
1.07
2.05
1.09
2.09
3.03
3.04
f1 (ppm)

5as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2.0455
2.0332
2.0184
2.0088
2.0023
1.9962
1.9875
1.9434
1.9293
1.9172
1.9154
1.9077
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1.8814
1.8418
1.8341
1.8295
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1.8214
1.8200
1.8128
1.8068
1.7996
1.7930
1.7854
1.2794
1.2675
1.2555
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7.7881
7.7804
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7.7182
7.4840
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7.4675
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7.4608
7.4535
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7.3976
7.3859
7.3834
5.2666
5.2603
5.2437
5.2375
5.1654
5.1471
5.1426
5.1243
4.2455
4.2392
4.2300
4.2253
4.2184
4.2133
4.2066
4.2014
2.93
0.97
1.96
1.02
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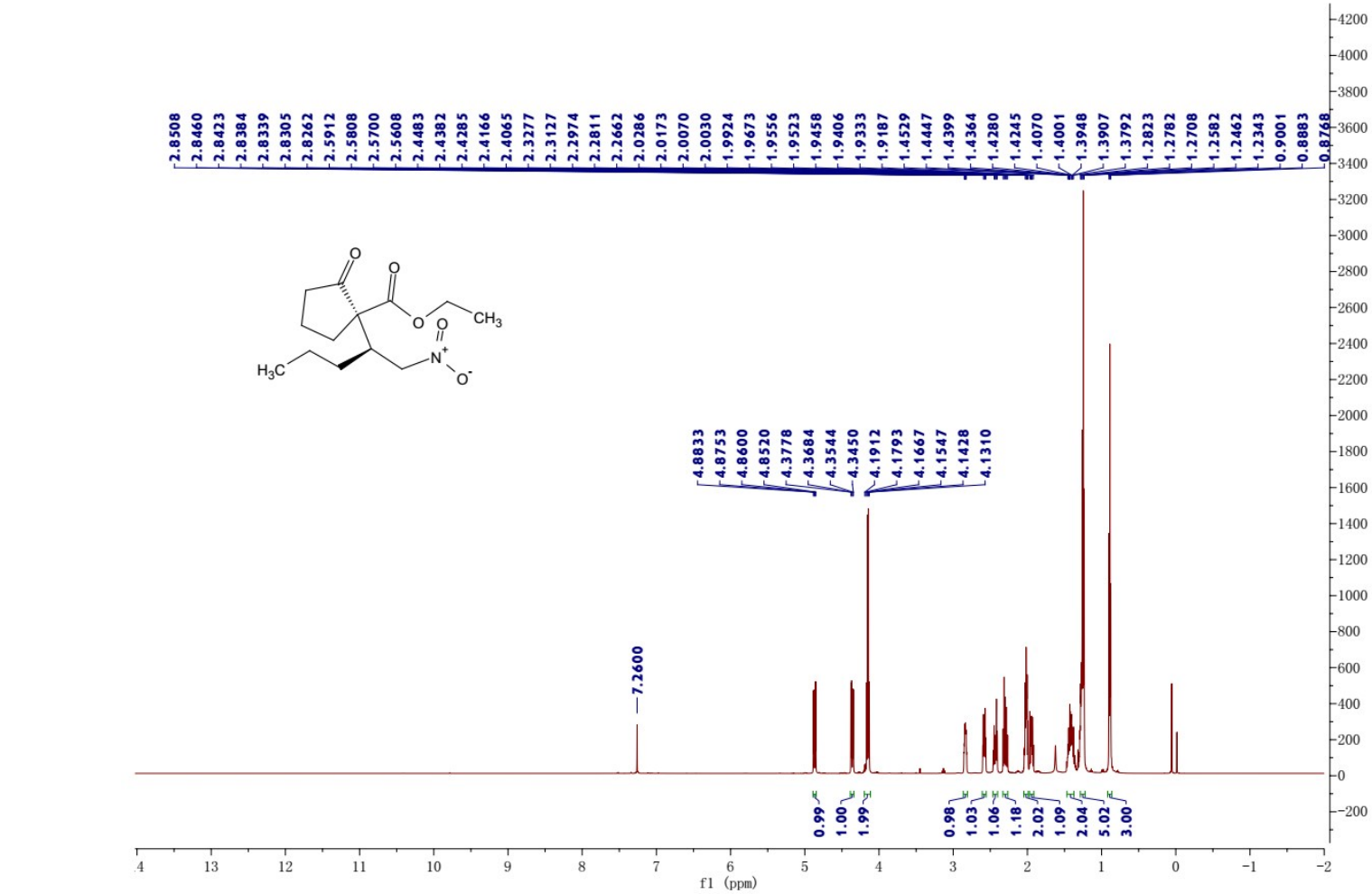
1.06
3.00
2.07
2.06
1.09
1.08
3.31
f1 (ppm)

5at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2.4285
2.4166
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1.3907
1.3792
1.2823
1.2782
1.2708
1.2582
1.2462
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4.3544
4.3450
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4.1793
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4.1547
4.1428
4.1310
7.2600
0.99
1.00
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0.98
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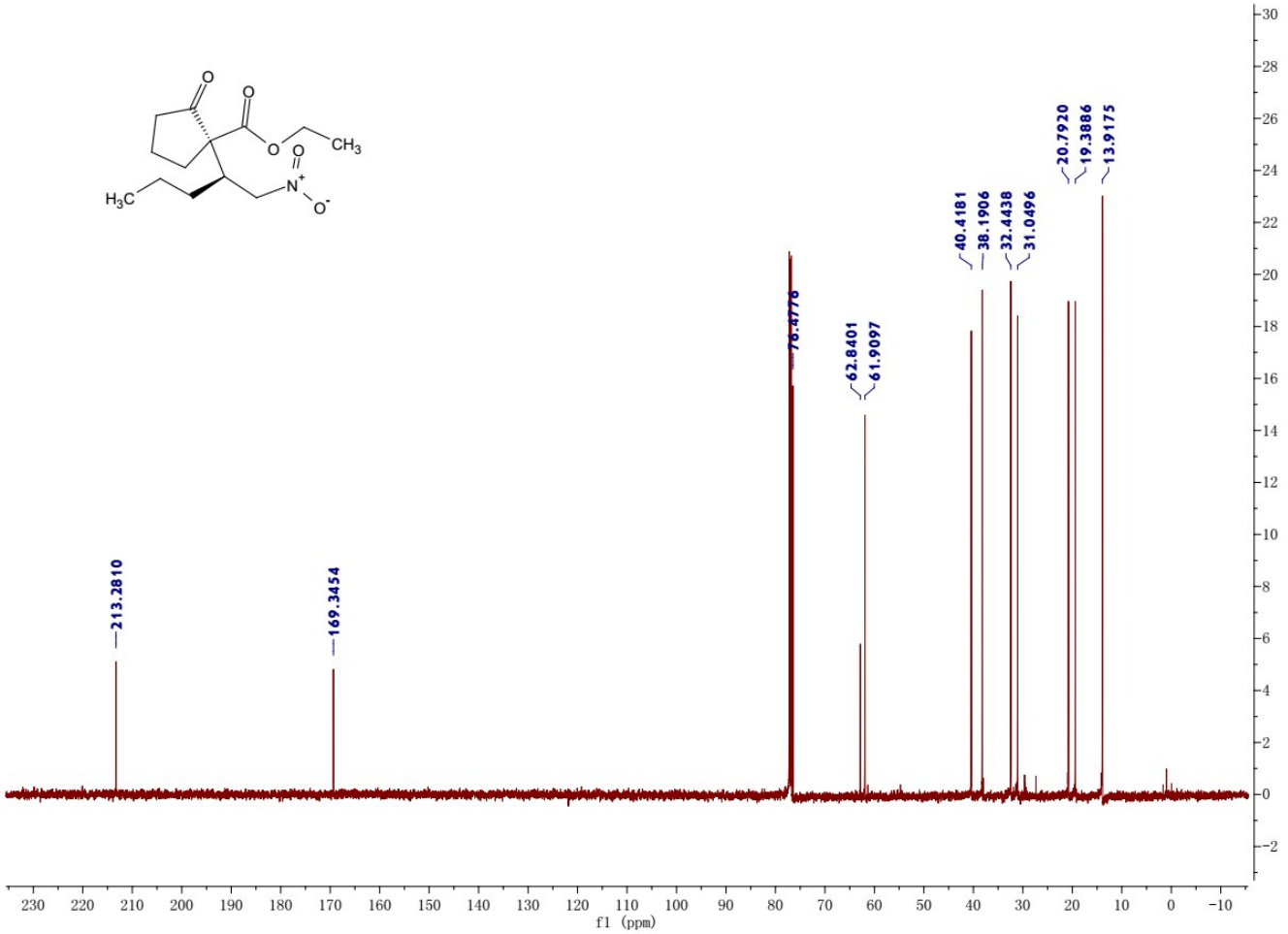
1.06
1.18
2.02
1.09
2.04
5.02
3.00
f1 (ppm)

5at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31.0496
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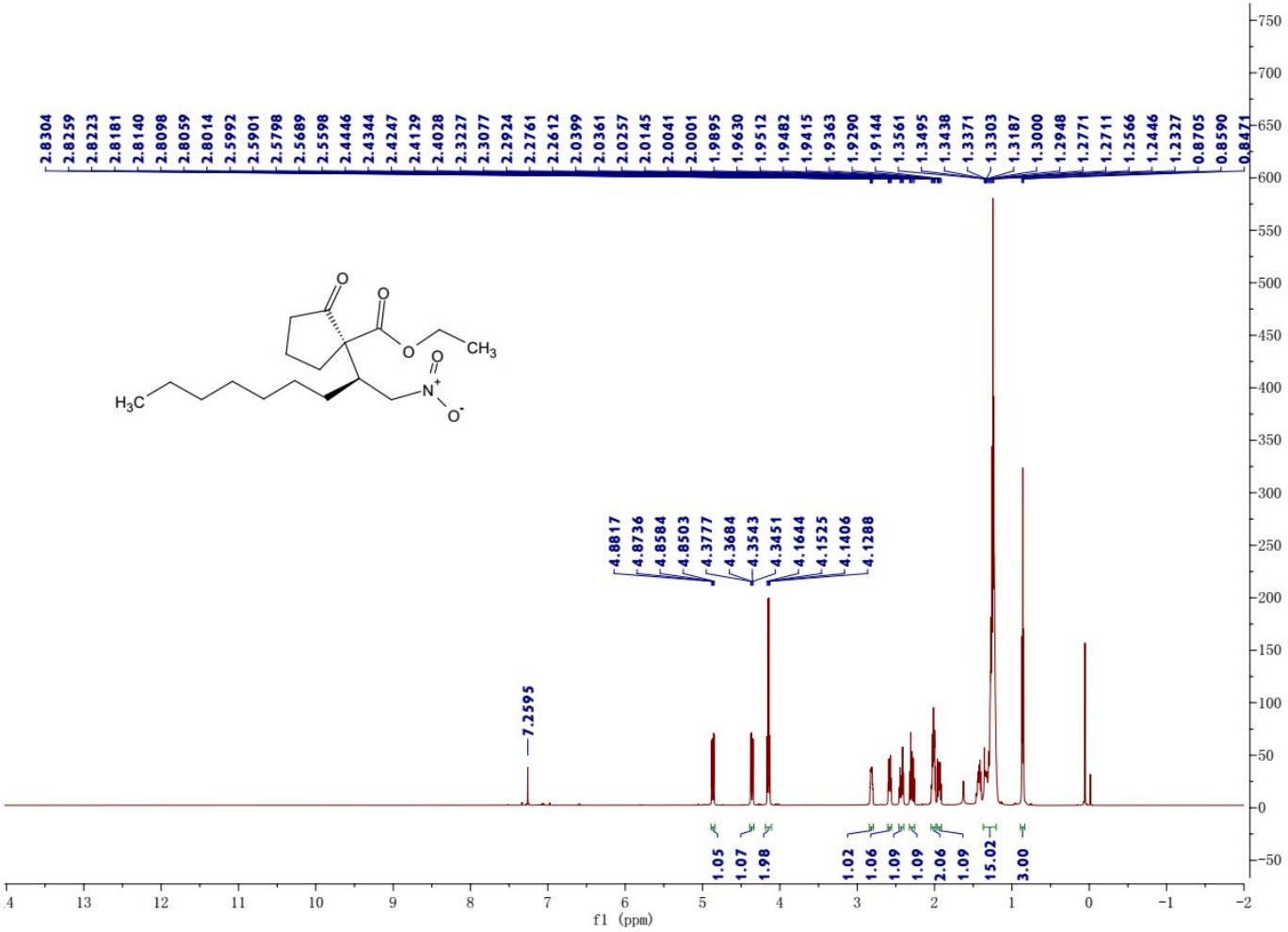
19.3886
13.9175
f1 (ppm)

5au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2.5798
2.5689
2.5598
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2.4344
2.4247
2.4129
2.4028
2.3227
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2.2924
2.2761
2.2612
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2.0257
2.0145
2.0041
2.0001
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1.9512
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1.9290
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1.3561
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1.3438
1.3371
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1.3187
1.3000
1.2948
1.2771
1.2711
1.2566
1.2446
1.2327
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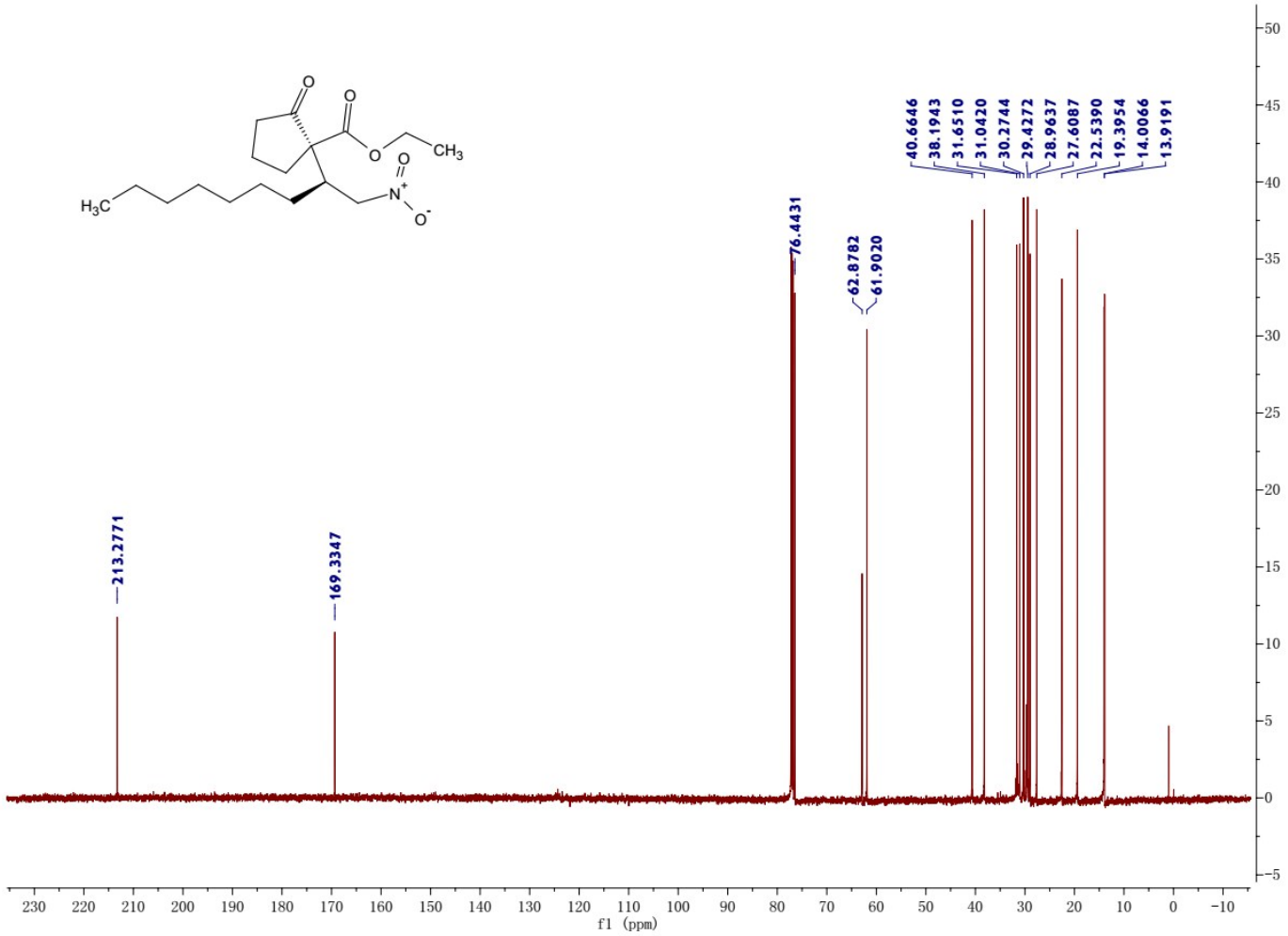
0.8590
0.8471
4.8817
4.8736
4.8584
4.8503
4.3777
4.3684
4.3543
4.3451
4.1644
4.1525
4.1406
4.1288
7.2595
1.05
1.07
1.98
1.02
1.06
1.09
1.09
2.06
1.09
15.02
3.00
f1 (ppm)

5au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38.1943
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31.0420
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28.9637
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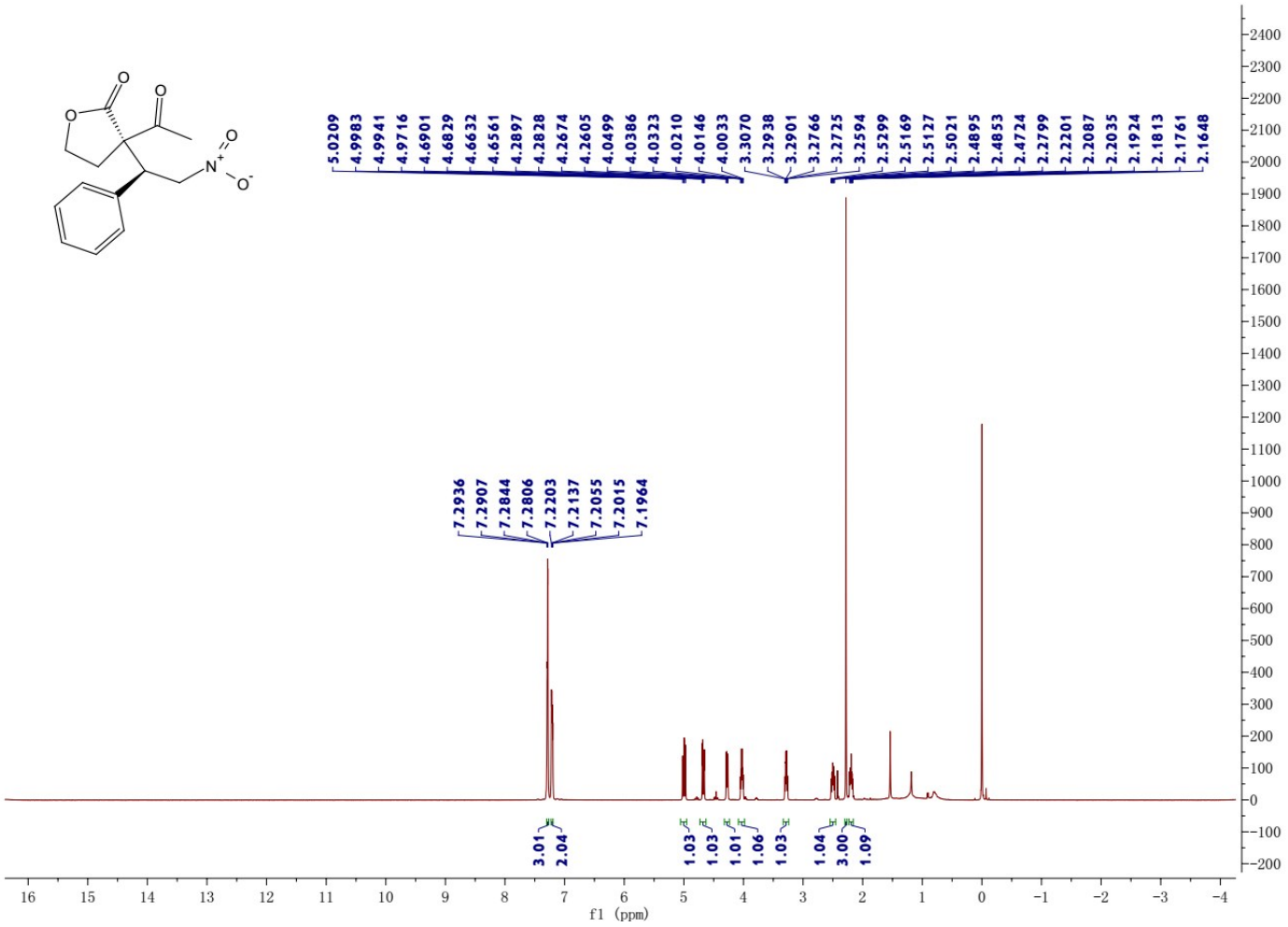
22.5390
19.3954
14.0066
13.9191
f1 (ppm)

5ba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4.2605
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4.0386
4.0323
4.0210
4.0146
4.0033
3.3070
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3.2901
3.2766
3.2725
3.2594
2.5299
2.5169
2.5127
2.5021
2.4895
2.4853
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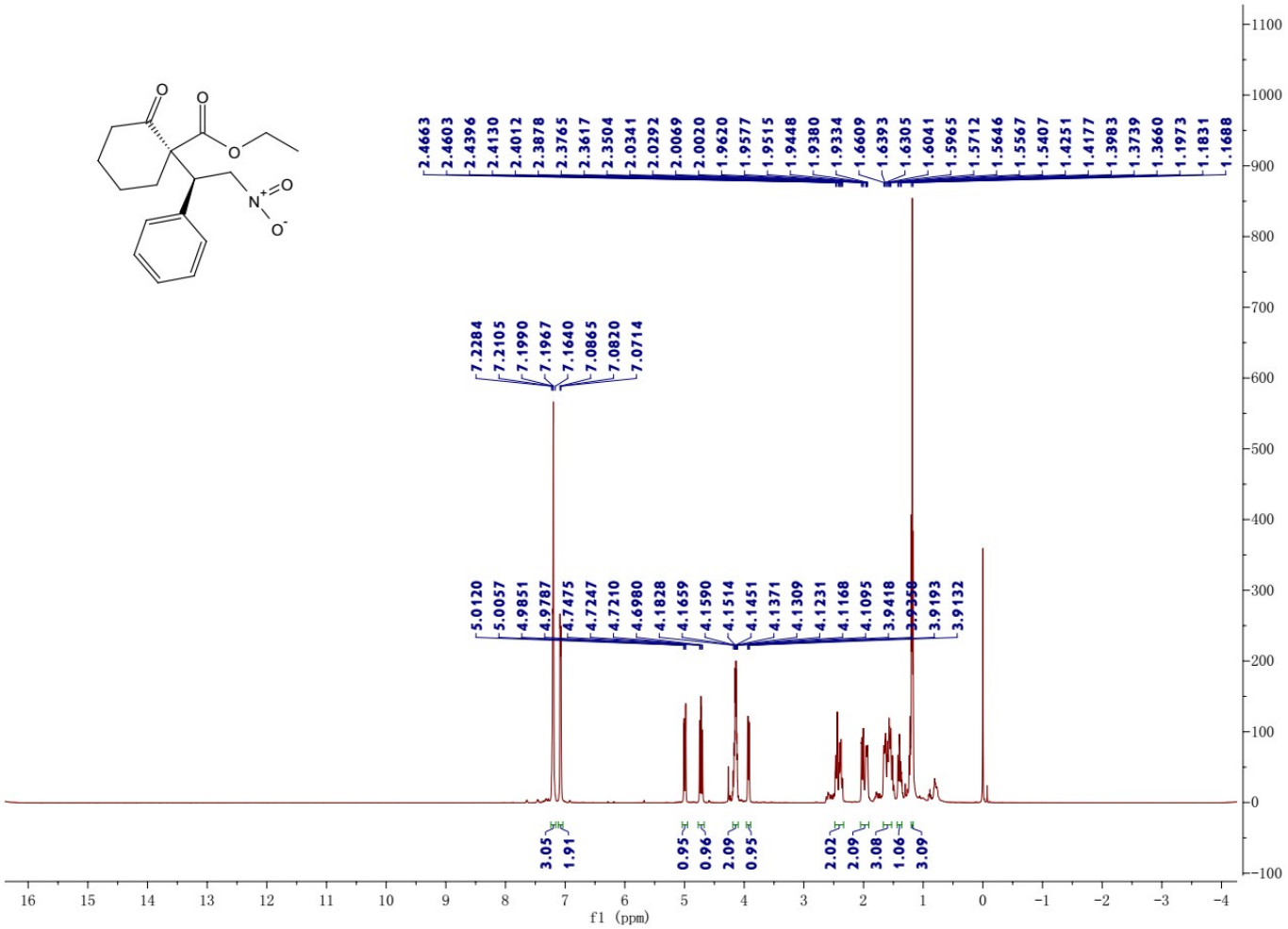
3.00
1.09
f1 (ppm)

5ca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2.0020
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1.3739
1.3660
1.1973
1.1831
1.1688
7.2284
7.2105
7.1990
7.1967
7.1640
7.0865
7.0820
7.0714
5.0120
5.0057
4.9851
4.9787
4.7475
4.7247
4.7210
4.6980
4.1828
4.1659
4.1590
4.1514
4.1451
4.1371
4.1309
4.1231
4.1168
4.1095
3.9418
3.9350
3.9193
3.9132
3.05
1.91
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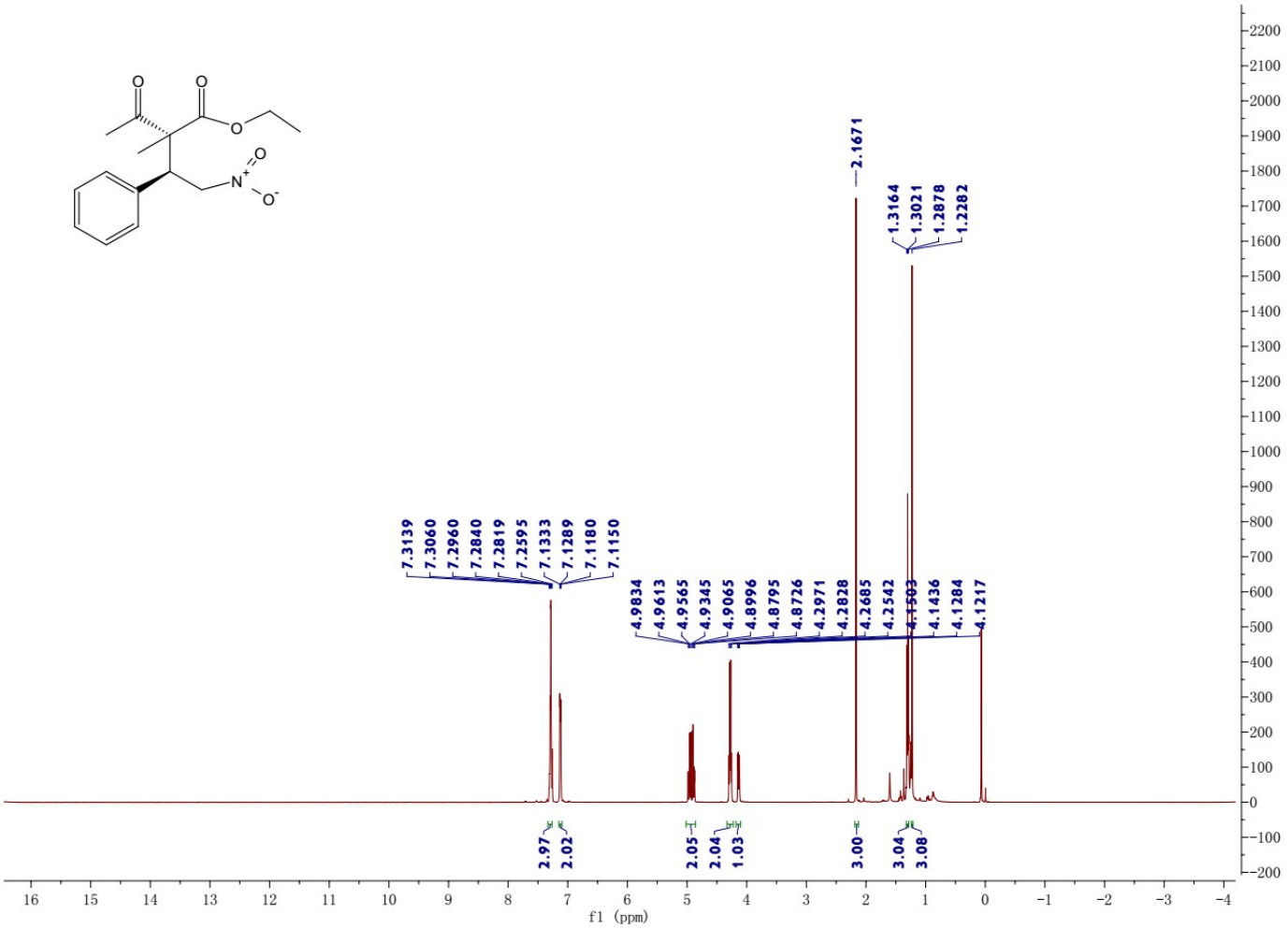
0.96
2.09
0.95
2.02
2.09
3.08
1.06
3.09
f1 (ppm)

5da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4.9613
4.9565
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4.9065
4.8996
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4.8726
4.2971
4.2828
4.2685
4.2542
4.1503
4.1436
4.1284
4.1217
2.1671
1.3164
1.3021
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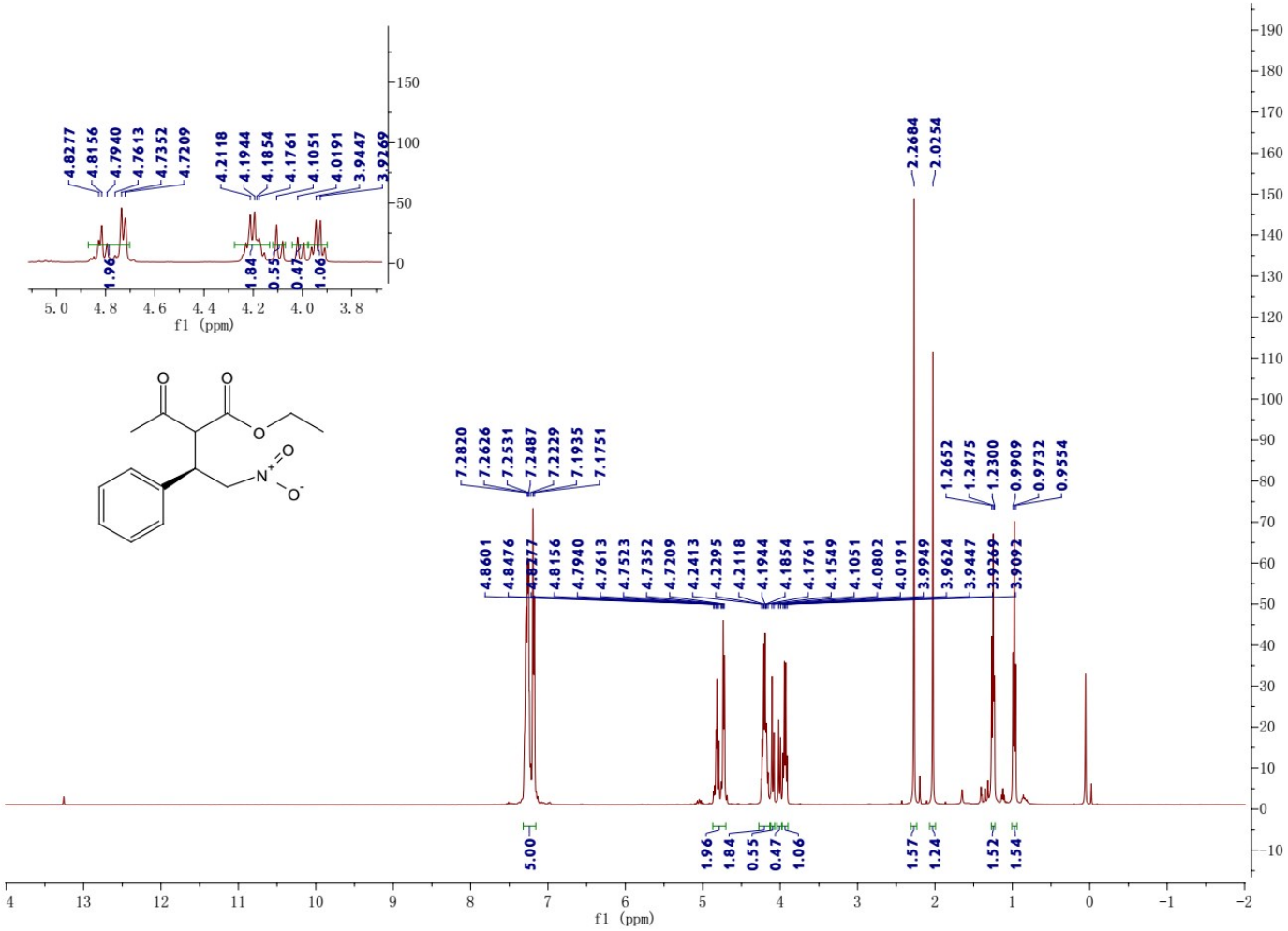
2.02
2.05
2.04
1.03
3.00
3.04
3.08
f1 (ppm)

5ea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4.1854
4.1761
4.1051
4.0191
3.9447
3.9269
1.96
1.84
0.55
0.47
1.06
f1 (ppm)
O
O
O
N+
O-
7.2820
7.2626
7.2531
7.2487
7.2229
7.1935
7.1751
4.8601
4.8476
4.8277
4.8156
4.7940
4.7613
4.7523
4.7352
4.7209
4.2413
4.2295
4.2118
4.1944
4.1854
4.1761
4.1549
4.1051
4.0802
4.0191
3.9949
3.9624
3.9447
3.9269
3.9092
2.2684
2.0254
1.2652
1.2475
1.2300
0.9909
0.9732
0.9554
5.00
1.96
1.84
0.55
0.47
1.06
1.57
1.24
1.52
1.54
f1 (ppm)