

The First 4, 4'-imidazolium-tagged C_2 -symmetric bis(oxazolines): Application in the Asymmetric Henry reaction

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Supplementary data

1. Theoretical calculations results of 9a-Cu-CH₂NO₂

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.471409	2.009239	-3.149307
2	6	0	-0.124228	1.855218	-1.640136
3	6	0	-0.037389	3.259550	-0.976913
4	6	0	-1.263082	1.090499	-0.988749
5	7	0	-1.273815	-0.070111	-0.427355
6	6	0	-2.672769	-0.370579	-0.034904
7	1	0	-2.676659	-0.664012	1.014919
8	6	0	-3.411392	0.970004	-0.248981
9	1	0	-4.314813	0.897145	-0.858642
10	8	0	-2.424875	1.738971	-1.047523
11	6	0	-3.705898	1.733251	1.026922
12	6	0	-3.153674	-1.572583	-0.875789
13	7	0	-4.332795	-2.230507	-0.299462
14	6	0	-5.535980	-2.380170	-0.891436
15	7	0	-6.324131	-3.046770	-0.030206
16	6	0	-5.614275	-3.302317	1.128154
17	6	0	-4.362615	-2.803941	0.962550
18	6	0	-7.749608	-3.334745	-0.222842
19	6	0	-5.900898	-1.949560	-2.268271
20	29	0	0.209995	-1.336262	-0.094203
21	7	0	1.588478	0.139163	-0.901204
22	6	0	1.242032	1.204755	-1.524811
23	8	0	2.199111	1.892603	-2.168749

24	6	0	3.474028	1.197102	-1.943679
25	1	0	4.108069	1.881648	-1.374452
26	6	0	3.046710	-0.029950	-1.085235
27	1	0	3.215348	-0.964749	-1.630546
28	6	0	3.820759	-0.065642	0.242446
29	7	0	3.953101	-1.392850	0.865870
30	6	0	4.836785	-2.340875	0.501359
31	7	0	4.775665	-3.319739	1.424731
32	6	0	3.838635	-2.983708	2.388437
33	6	0	3.325220	-1.778044	2.036827
34	6	0	5.614102	-4.514337	1.424691
35	6	0	5.704717	-2.379686	-0.701288
36	6	0	4.129802	0.878502	-3.271886
37	8	0	0.350255	-1.103146	1.848530
38	6	0	-0.561487	-1.802438	2.439913
39	6	0	-0.518779	-1.777429	3.959923
40	8	0	-1.430463	-2.461092	1.838825
41	8	0	1.402960	-2.946875	-0.261997
42	7	0	0.798127	-3.334586	-1.365777
43	8	0	-0.155619	-2.510007	-1.733842
44	6	0	1.111905	-4.411664	-2.018076
45	1	0	1.901624	-5.029513	-1.621869
46	1	0	0.557792	-4.635908	-2.915429
47	1	0	-1.435480	2.508931	-3.254879
48	1	0	0.299181	2.603248	-3.642255
49	1	0	-0.525841	1.032643	-3.639343
50	1	0	0.189265	3.174266	0.089977
51	1	0	0.752052	3.840700	-1.455561
52	1	0	-0.988908	3.780223	-1.089760
53	1	0	-4.046408	2.744234	0.789467
54	1	0	-4.518401	1.219395	1.547579
55	1	0	-2.822979	1.795017	1.673106
56	1	0	-2.344570	-2.303111	-0.932242
57	1	0	-3.402415	-1.257431	-1.890164
58	1	0	-6.064041	-3.809936	1.965036
59	1	0	-3.484741	-2.812916	1.595156
60	1	0	-8.277422	-2.386257	-0.368705
61	1	0	-7.885427	-3.998407	-1.079988
62	1	0	-8.110465	-3.837802	0.673958
63	1	0	-6.948909	-2.170305	-2.462674
64	1	0	-5.796923	-0.863411	-2.364722
65	1	0	-5.278311	-2.460078	-3.011168
66	1	0	4.835290	0.308967	0.082166
67	1	0	3.326017	0.573371	0.975764

68	1	0	3.618967	-3.632723	3.219661
69	1	0	2.518666	-1.198844	2.458000
70	1	0	6.668256	-4.233350	1.477267
71	1	0	5.357722	-5.115392	2.296518
72	1	0	5.439389	-5.103803	0.521630
73	1	0	5.605751	-1.466372	-1.284786
74	1	0	6.762323	-2.430217	-0.424071
75	1	0	5.446122	-3.242667	-1.325956
76	1	0	3.549855	0.140297	-3.835886
77	1	0	4.224470	1.785670	-3.874882
78	1	0	5.136101	0.498915	-3.075637
79	1	0	-0.523597	-0.744546	4.319741
80	1	0	-1.365990	-2.321143	4.378810
81	1	0	0.411394	-2.236427	4.311000
82	6	0	-8.435575	2.090641	1.712324
83	6	0	-8.113967	2.018436	0.357257
84	6	0	-8.479258	3.052416	-0.506361
85	6	0	-9.174254	4.152646	-0.008784
86	6	0	-9.517058	4.241504	1.347880
87	6	0	-9.131284	3.197256	2.198321
88	6	0	-10.298434	5.423035	1.872608
89	16	0	-7.266662	0.566907	-0.291041
90	8	0	-6.493887	-0.003290	0.855472
91	8	0	-8.332050	-0.352960	-0.790519
92	8	0	-6.386966	1.082230	-1.390295
93	1	0	-8.121804	1.290910	2.374430
94	1	0	-8.199323	2.995676	-1.552727
95	1	0	-9.450949	4.959844	-0.683026
96	1	0	-9.374238	3.253893	3.256863
97	1	0	-11.378670	5.265076	1.761058
98	1	0	-10.103480	5.592837	2.935740
99	1	0	-10.049303	6.341091	1.331415
100	6	0	8.274992	2.470136	1.493336
101	6	0	8.562001	1.729171	0.348267
102	6	0	9.632444	2.091743	-0.471483
103	6	0	10.404590	3.203910	-0.144969
104	6	0	10.126848	3.970697	0.996247
105	6	0	9.056118	3.581695	1.810674
106	6	0	10.952602	5.191973	1.326043
107	16	0	7.531361	0.321424	-0.102771
108	8	0	8.448747	-0.693243	-0.680948
109	8	0	6.854802	-0.113209	1.158916
110	8	0	6.532650	0.849749	-1.100560
111	1	0	7.458339	2.155914	2.134138

112	1	0	9.863960	1.488305	-1.342705
113	1	0	11.242456	3.478556	-0.781746
114	1	0	8.834914	4.152163	2.709887
115	1	0	10.609019	6.068624	0.762212
116	1	0	10.889312	5.443358	2.388852
117	1	0	12.007776	5.042381	1.076014

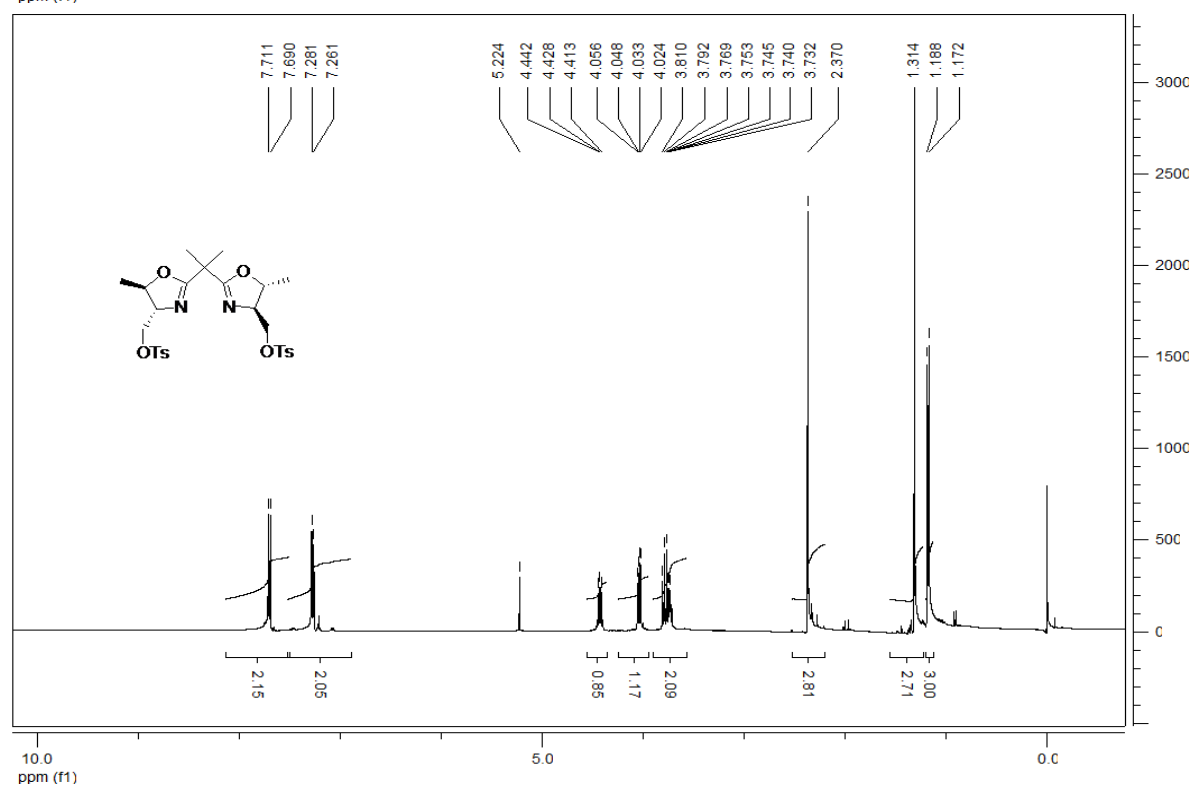
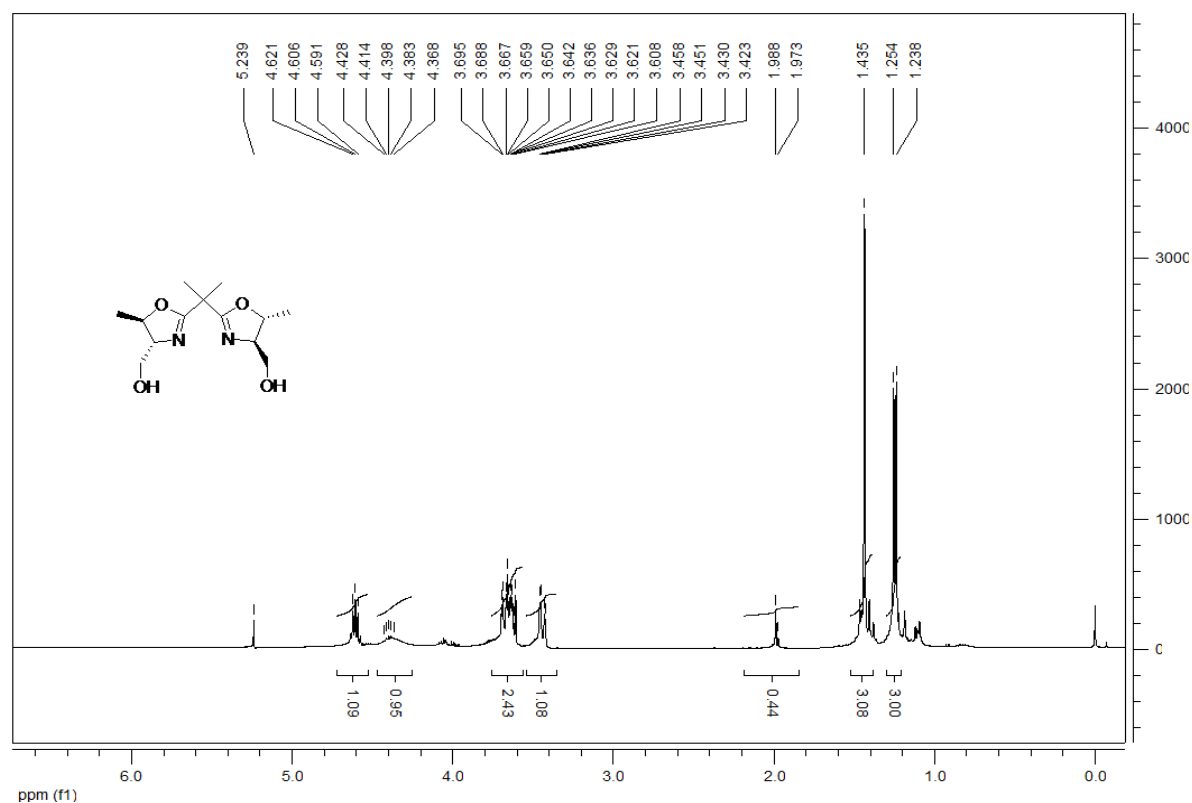
2. Theoretical calculations results of 9b-Cu-CH₂NO₂

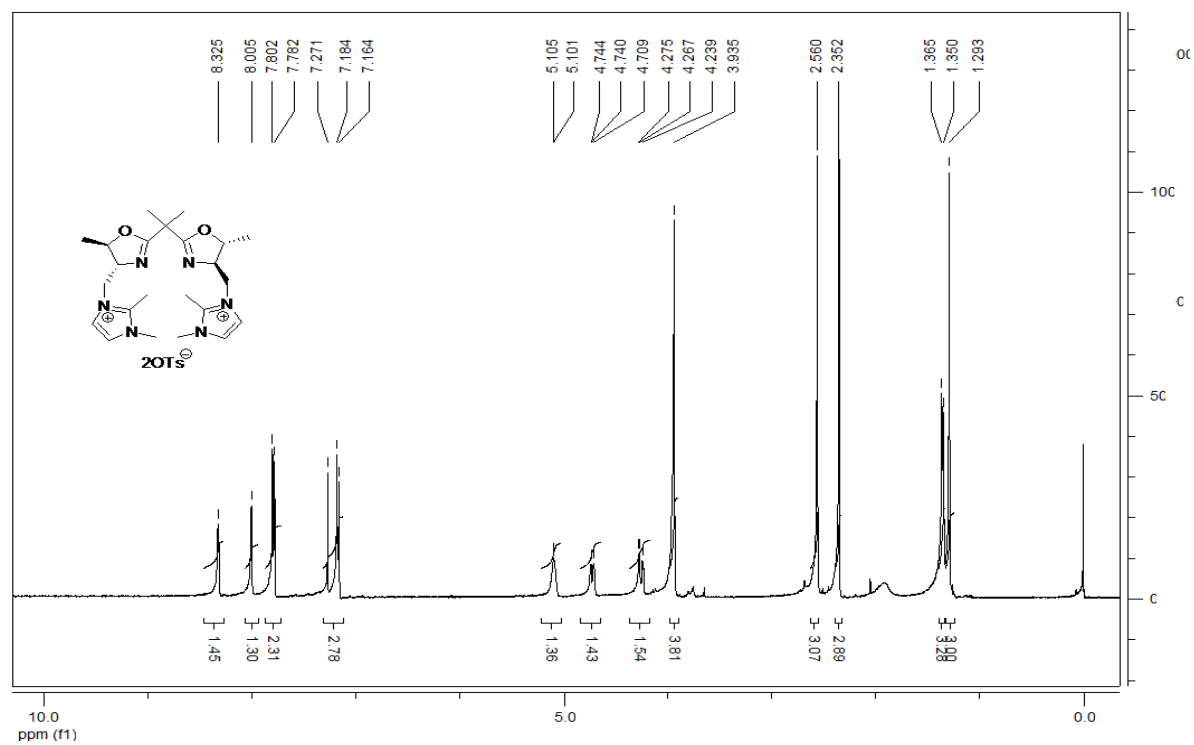
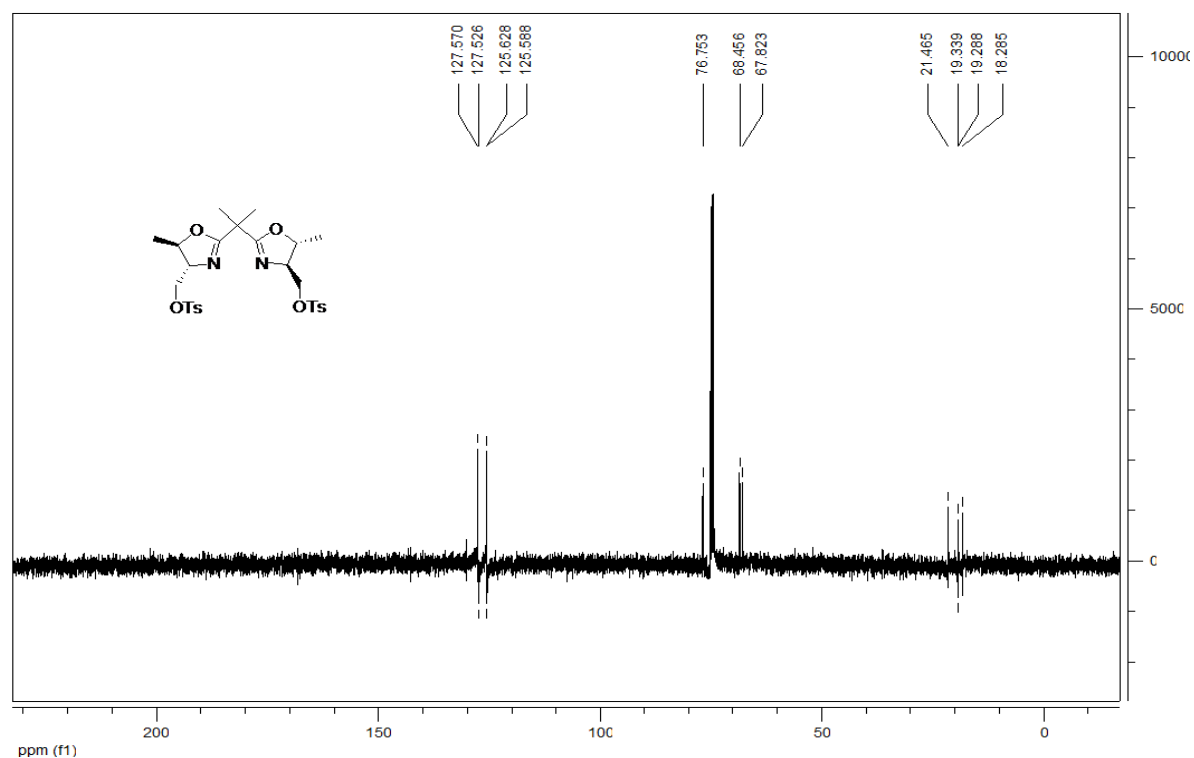
Standard orientation:

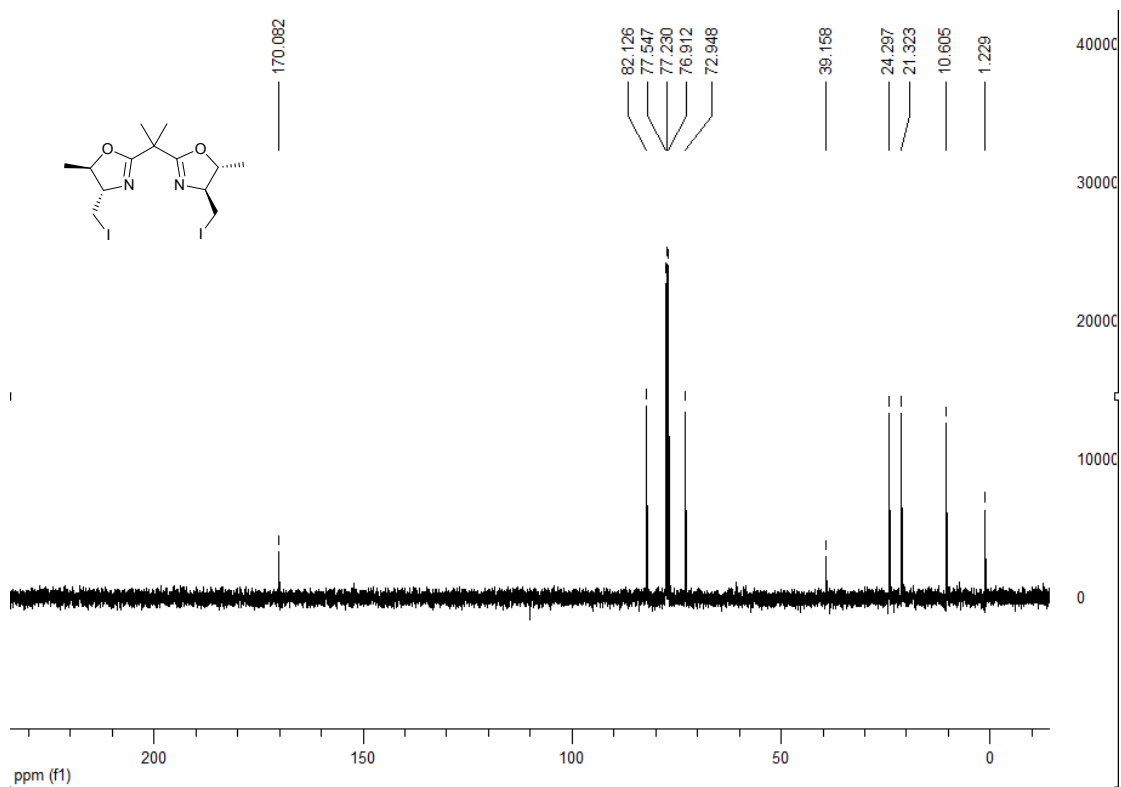
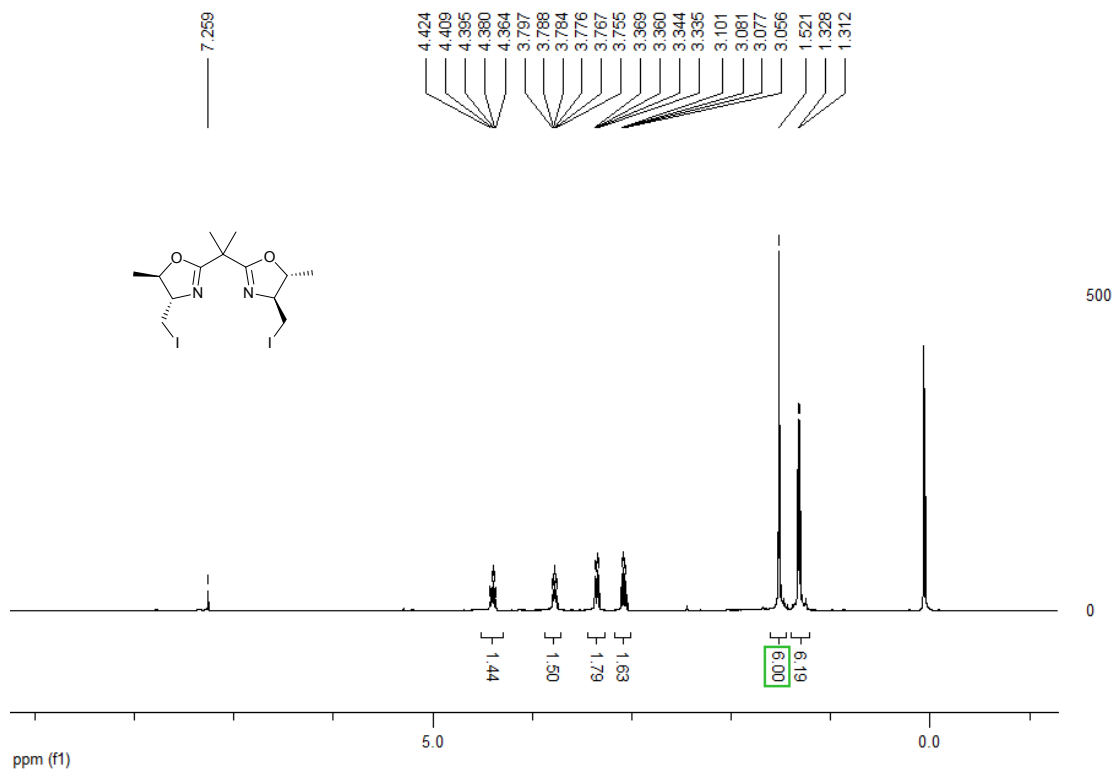
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.067348	3.621571	1.520185
2	6	0	-0.468414	3.269738	0.053997
3	6	0	-0.992195	4.533323	-0.667575
4	6	0	0.772050	2.738257	-0.646227
5	7	0	1.189319	1.531194	-0.659021
6	6	0	2.443707	1.482091	-1.427554
7	1	0	2.255746	0.865229	-2.311956
8	6	0	2.705405	2.967357	-1.806256
9	1	0	3.568915	3.377497	-1.270228
10	8	0	1.533519	3.666850	-1.265042
11	6	0	2.810757	3.252466	-3.293061
12	6	0	3.521803	0.787926	-0.581776
13	7	0	4.618378	0.234637	-1.388104
14	6	0	5.915992	0.583719	-1.313961
15	7	0	6.612116	-0.308014	-2.041167
16	6	0	5.737964	-1.246154	-2.564915
17	6	0	4.488137	-0.911816	-2.157056
18	6	0	8.071947	-0.419372	-2.071172
19	6	0	6.469862	1.753840	-0.580400
20	29	0	0.156370	-0.169699	0.227913
21	7	0	-1.475263	0.945763	0.084808
22	6	0	-1.578049	2.230143	0.123998
23	8	0	-2.806660	2.721234	0.304702
24	6	0	-3.664841	1.568553	0.688904
25	1	0	-4.628268	1.712817	0.202550
26	6	0	-2.842779	0.385148	0.135965
27	1	0	-2.869678	-0.456799	0.830406

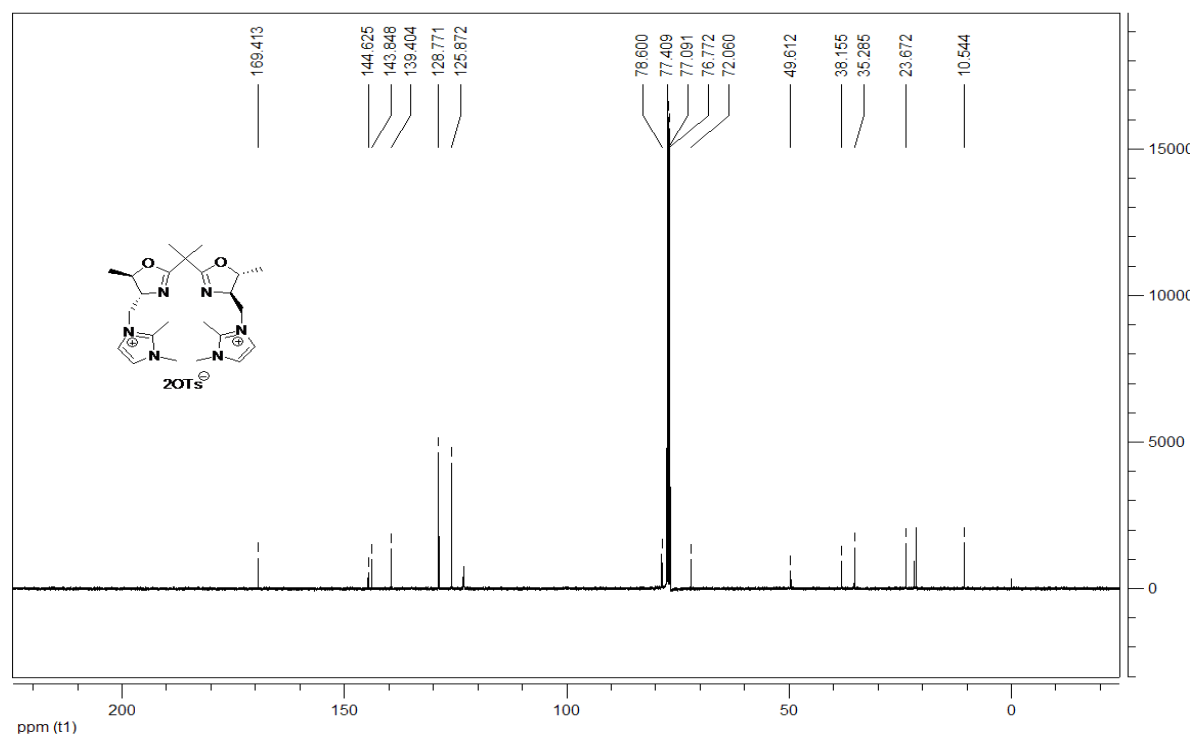
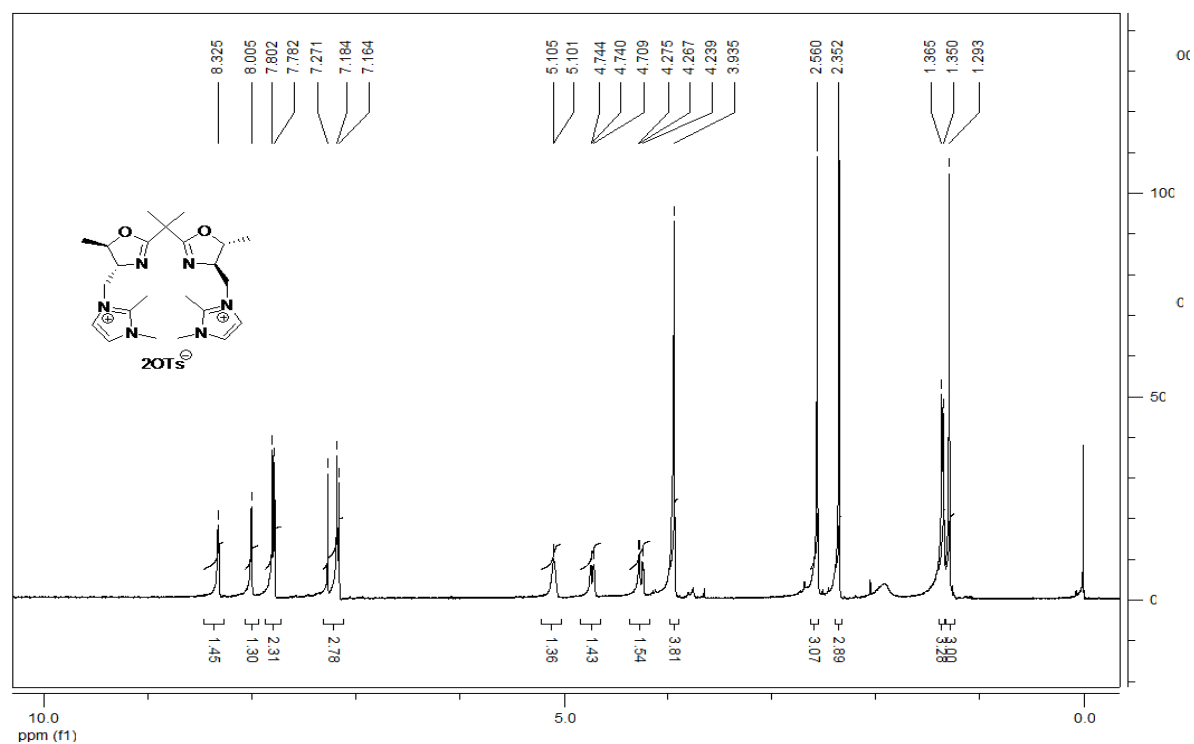
28	6	0	-3.186945	-0.111655	-1.294664
29	7	0	-3.996178	-1.334089	-1.300708
30	6	0	-5.261184	-1.467740	-1.741062
31	7	0	-5.636733	-2.735580	-1.492154
32	6	0	-4.592984	-3.406916	-0.875915
33	6	0	-3.559393	-2.534531	-0.763305
34	6	0	-6.974478	-3.294136	-1.714857
35	6	0	-6.057253	-0.421777	-2.435434
36	6	0	-3.804730	1.564728	2.199148
37	8	0	-0.487215	-1.606178	-0.932479
38	6	0	0.389575	-2.008591	-1.804208
39	6	0	0.114800	-3.374355	-2.415890
40	8	0	1.399150	-1.367062	-2.129970
41	8	0	1.648314	-1.176659	1.010273
42	7	0	1.569732	-0.520235	2.165920
43	8	0	0.515313	0.277965	2.194702
44	6	0	2.435183	-0.645180	3.115697
45	1	0	3.289642	-1.288623	2.958303
46	1	0	2.269826	-0.059996	4.007797
47	1	0	0.713276	4.387114	1.505843
48	1	0	-0.936571	4.021629	2.048289
49	1	0	0.300014	2.736264	2.044803
50	1	0	-1.277020	4.317986	-1.701236
51	1	0	-1.865537	4.921228	-0.143413
52	1	0	-0.213842	5.296677	-0.680018
53	1	0	1.933808	2.868131	-3.822333
54	1	0	2.893666	4.325552	-3.484095
55	1	0	3.698794	2.759453	-3.701914
56	1	0	3.067656	-0.054284	-0.054338
57	1	0	3.949613	1.452266	0.168230
58	1	0	6.088386	-2.076751	-3.154605
59	1	0	3.519958	-1.372003	-2.311703
60	1	0	8.335117	-1.234795	-2.744052
61	1	0	8.518806	0.503959	-2.445215
62	1	0	8.422694	-0.637447	-1.061058
63	1	0	6.002692	2.682771	-0.922097
64	1	0	6.298569	1.617729	0.489326
65	1	0	7.544675	1.829685	-0.737285
66	1	0	-3.718422	0.656405	-1.857829
67	1	0	-2.247986	-0.350202	-1.795306
68	1	0	-4.680940	-4.438560	-0.578125
69	1	0	-2.544323	-2.642919	-0.409071
70	1	0	-7.690377	-2.751992	-1.096732
71	1	0	-7.243247	-3.218877	-2.770494

72	1	0	-6.950035	-4.345991	-1.432279
73	1	0	-5.498756	-0.025040	-3.289103
74	1	0	-6.996738	-0.836678	-2.796423
75	1	0	-6.308319	0.383077	-1.740276
76	1	0	-4.500353	0.776577	2.486406
77	1	0	-2.835954	1.401430	2.682783
78	1	0	-4.221227	2.515450	2.539320
79	1	0	-0.955989	-3.534811	-2.565190
80	1	0	0.648519	-3.483244	-3.361220
81	1	0	0.472067	-4.145707	-1.724755
82	15	0	6.439124	-1.263486	1.847928
83	9	0	7.013531	-0.644996	3.225949
84	9	0	5.845055	-1.816617	0.419313
85	9	0	5.278927	-2.080275	2.652479
86	9	0	7.571292	-0.398447	0.990848
87	9	0	5.407674	0.038896	1.711837
88	9	0	7.448478	-2.520715	1.929382
89	15	0	-7.349364	0.030801	1.103904
90	9	0	-6.876355	1.266535	0.092520
91	9	0	-7.745678	-1.224432	2.038676
92	9	0	-8.809515	0.692719	1.245711
93	9	0	-5.829984	-0.620861	0.881576
94	9	0	-7.851567	-0.808409	-0.234335
95	9	0	-6.789466	0.866889	2.376179







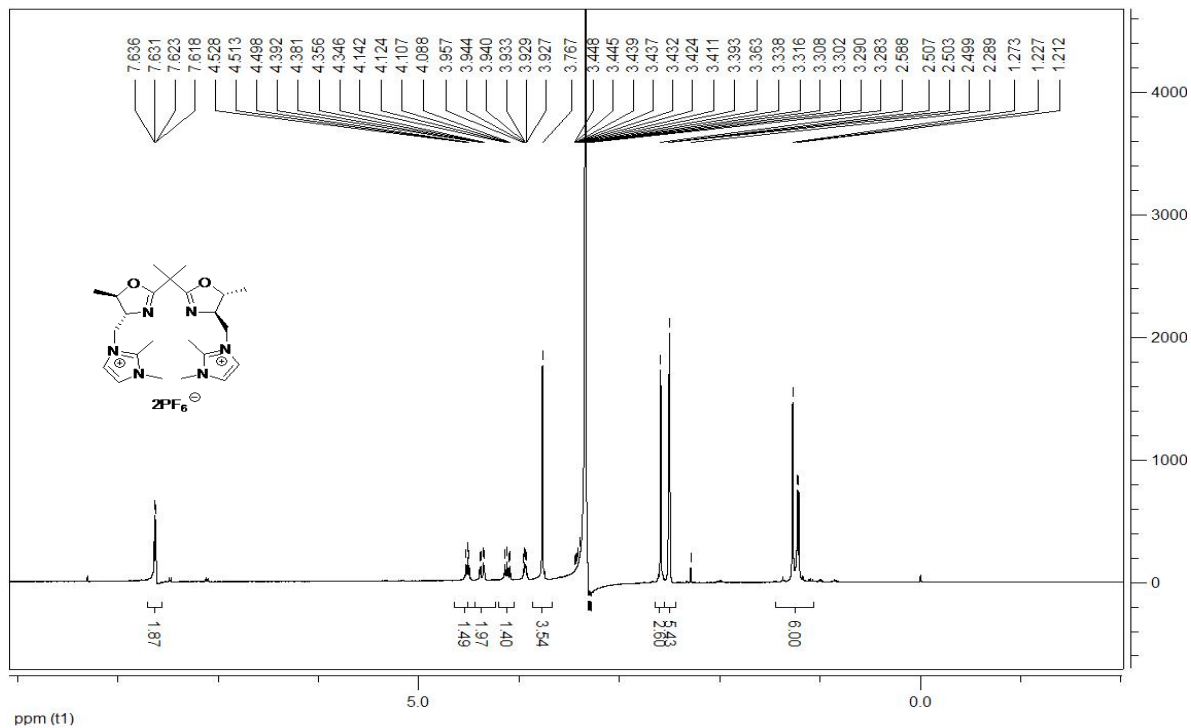
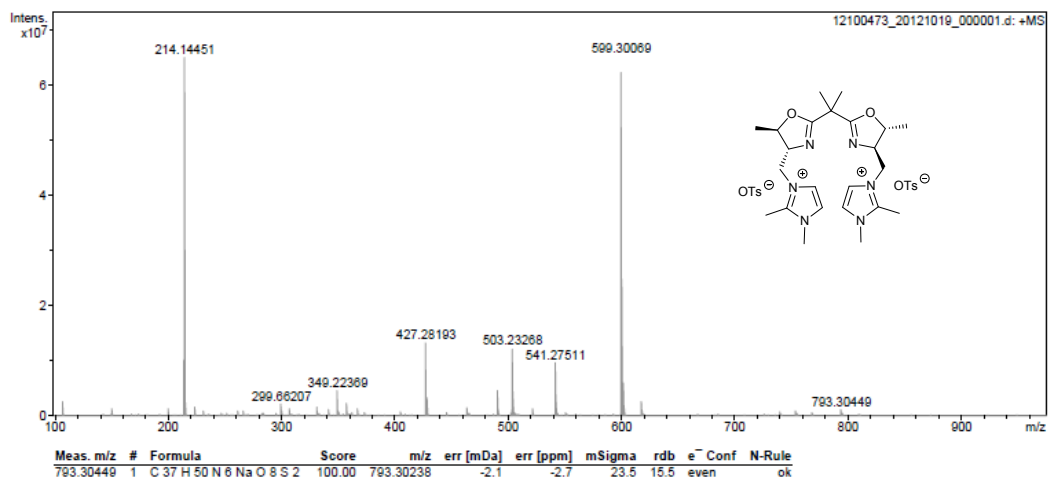


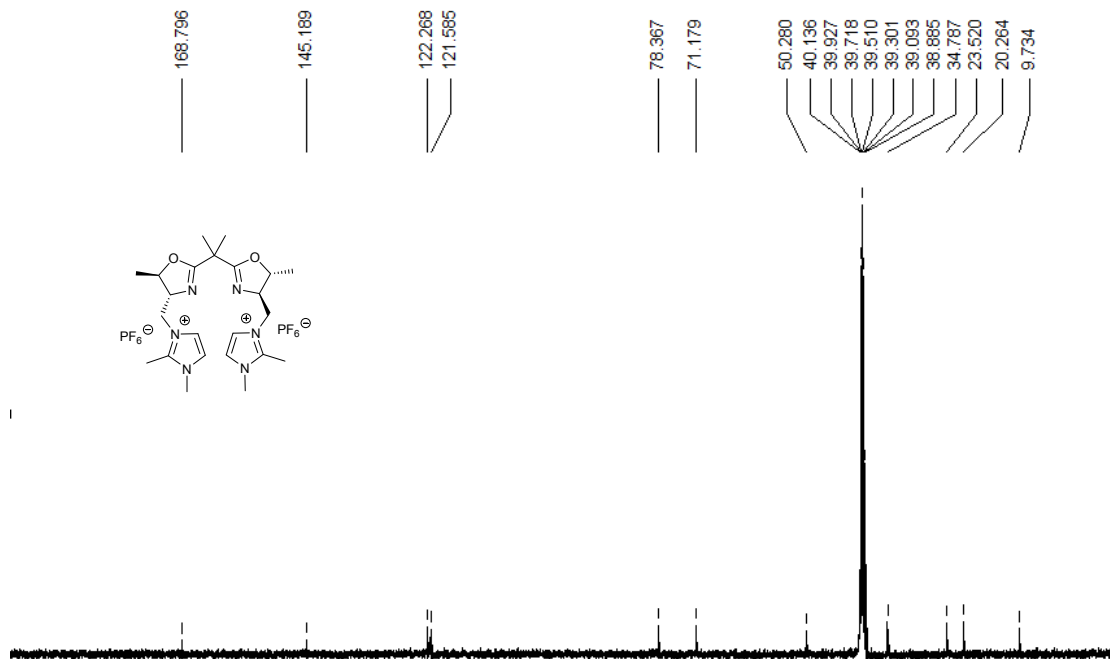
Peking University Mass Spectrometry Sample Analysis Report

Analysis Info

Analysis Name 12100473_20121019_000001.d
 Sample BITLYQ-1
 Comment ESI Positive

Acquisition Date 10/19/2012 10:07:41 AM
 Instrument Bruker Apex IV FTMS
 Operator Peking University



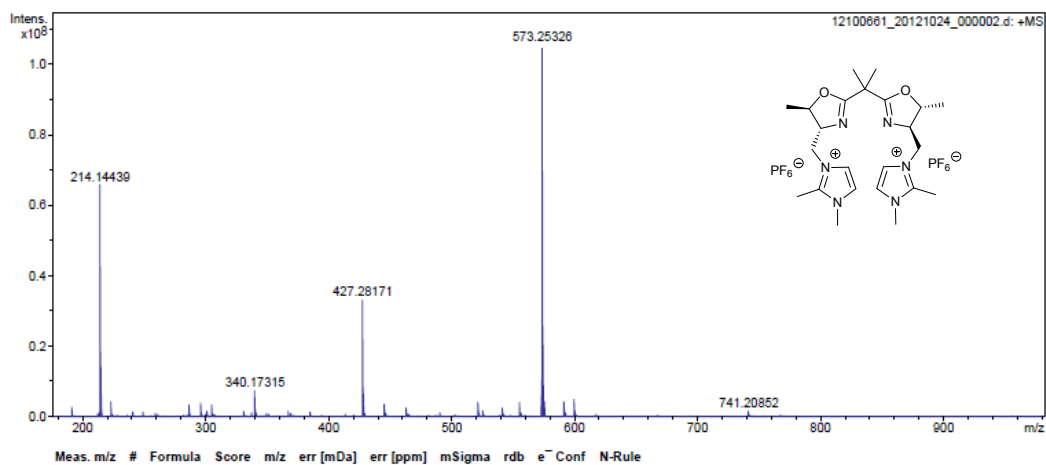


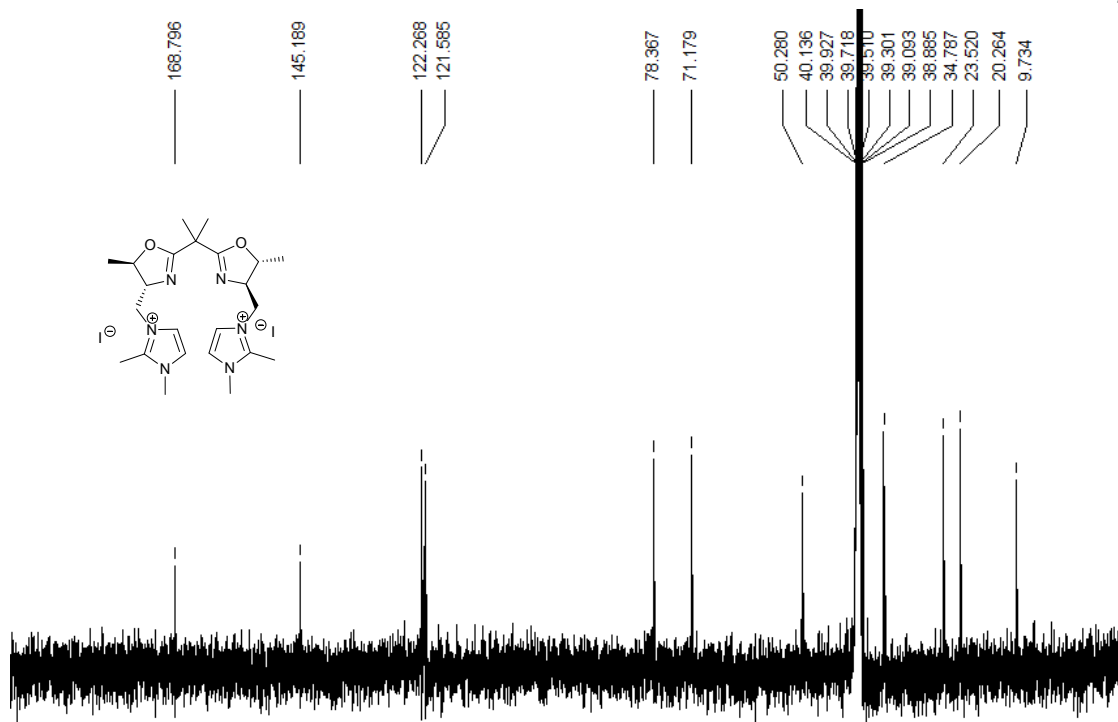
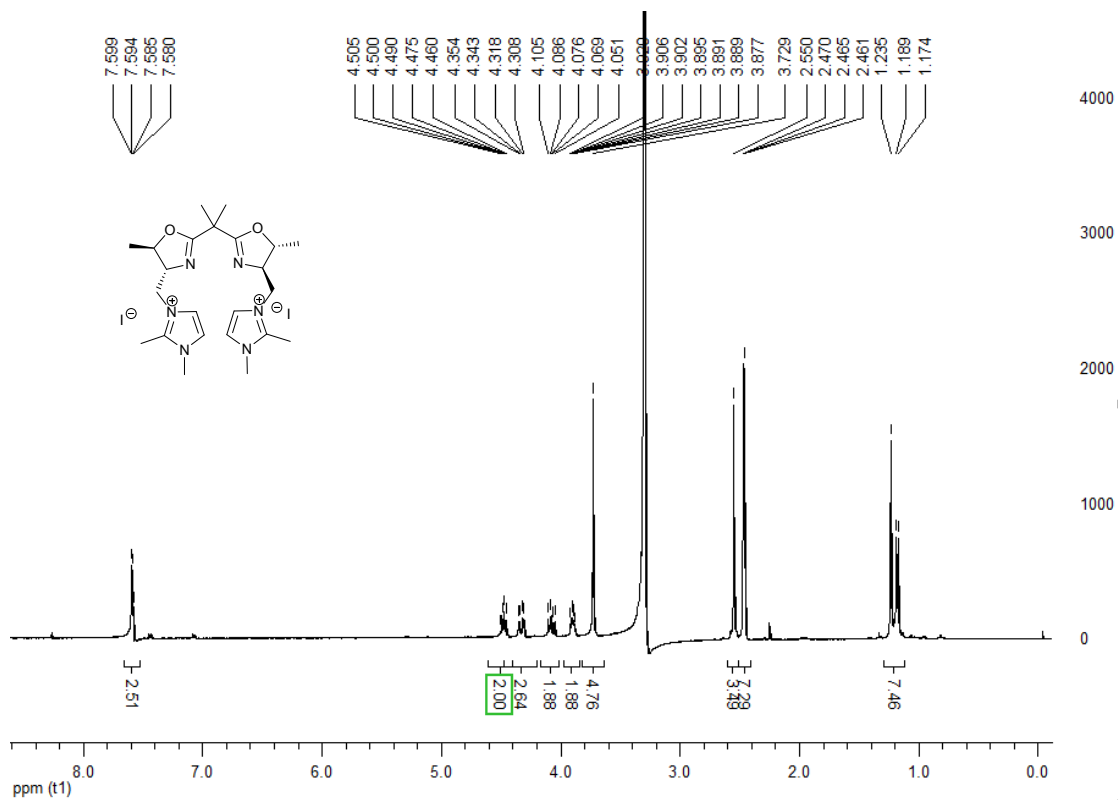
Peking University Mass Spectrometry Sample Analysis Report

Analysis Info

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 Sample L-PF6
 Comment ESI Positive

Acquisition Date 10/24/2012 10:49:10 AM
 Instrument Bruker Apex IV FTMS
 Operator Peking University



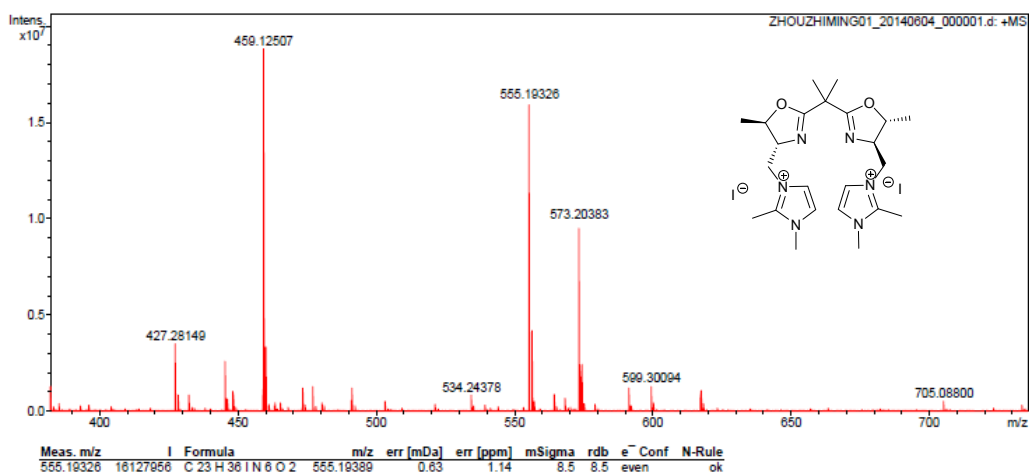


Peking University Mass Spectrometry Sample Analysis Report

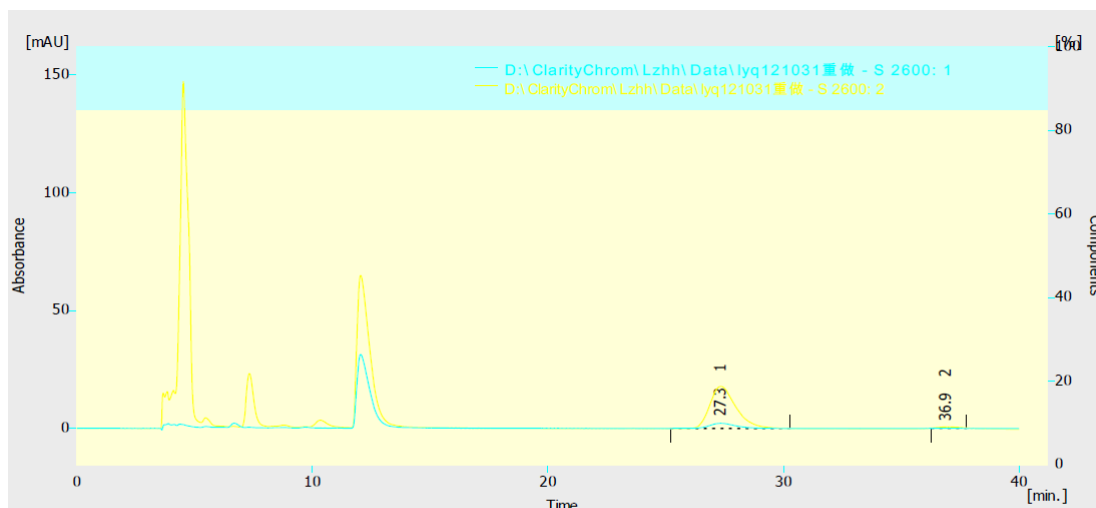
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Analysis Name ZHOZHIMING01_20140604_000001.d
 Sample TP-30
 Comment ESI Positive

Acquisition Date 6/4/2014 12:05:56 PM
 Instrument Bruker Apex IV FTMS
 Operator Peking University



Ee value of 11k



Result Table (Uncal - D:\ClarityChrom\Lzh\h\Data\lyq121031重微 - S 2600: 1)

	Reten. Time [min]	Start Time [min]	End Time [min]	Start Value [mAU]	End Value [mAU]	Area [mAU.s]	Height [mAU]	Area [%]	Height [%]	W05 [min]
1	27.333	25.217	30.283	-0.111	-0.134	185.876	2.220	97.3	95.6	1.22
2	36.883	36.283	37.767	-0.052	-0.092	5.088	0.103	2.7	4.4	0.65
	Total	Total	Total	Total	Total	190.964	2.323	100.0	100.0	