

**A NEW METHOD FOR PRODUCTION OF CHIRAL
2-ARYLOXYPROPANOIC ACIDS USING EFFECTIVE KINETIC
RESOLUTION OF RACEMIC 2-ARYLOXYCARBOXYLIC ACIDS**

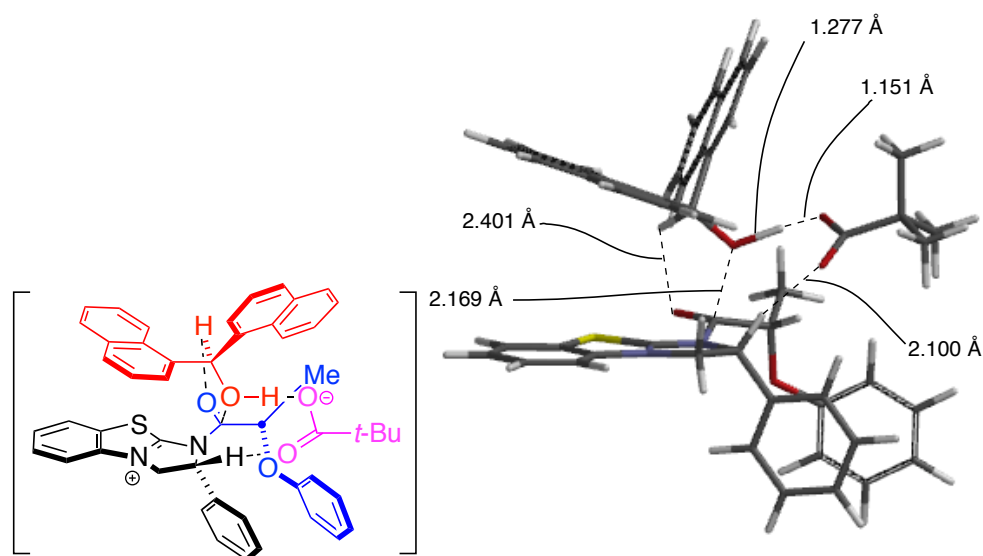
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List of Supplementary Materials

- S2-11 Cartesian Coordinates of (*S*)-**ts1**, (*S*)-**ts2**, (*R*)-**ts1**, and (*R*)-**ts2**
- S12-21 Cartesian Coordinates of (*S*)-*o*-Cl-**ts1**, (*S*)-*o*-Cl-**ts2**, (*R*)-*o*-Cl-**ts1**, (*R*)-*o*-Cl-**ts2**
- S22-99 ¹H and ¹³C NMR Spectroscopic Data of Compounds

All calculations were performed with the program package *Spartan '10 1.1.0* of Wavefunction Inc. All structures were optimized and subjected to frequency analysis with the B3LYP/6-31G* method, followed by single point B3LYP/6-31G* calculation.



Transition Structure (S)-**ts1**

$E(\text{B3LYP}/6\text{-}31\text{G}^*) = -2816.86425 \text{ au}$

$\nu_{\text{ts}} = 400i \text{ cm}^{-1}$

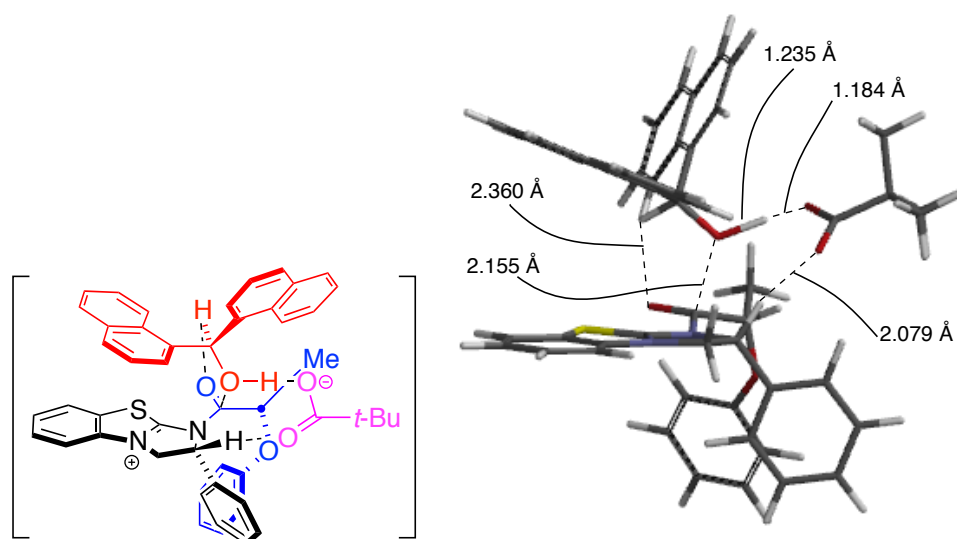
Cartesian Coordinates (Angstroms)

Atomic Number	X	Y	Z
6	0.664805602	0.311366799	1.463042101
6	1.990362053	-0.446997024	1.366842256
8	-0.083817105	0.261298723	2.429827582
7	0.531172002	1.490160463	0.625188258
6	-0.534376850	2.272051412	0.775170361
7	-0.740525627	3.094334710	-0.261327716
6	0.201356581	2.812757056	-1.352616589
6	1.166372657	1.753432999	-0.711179846
6	2.590114227	2.263738157	-0.623170633
6	3.516114046	1.816800563	-1.573137347
6	4.814373153	2.332033960	-1.581770982
6	5.196554845	3.288607683	-0.642306777
6	4.275938431	3.730967832	0.311617061
6	2.977600735	3.225533349	0.318380613
1	2.274147483	3.561598460	1.076563555
1	4.572494710	4.465719027	1.055378518
1	6.210073240	3.680124408	-0.642174924
1	5.528648855	1.974961659	-2.318898052
1	3.210355728	1.067394562	-2.299182441
1	1.125681502	0.825872339	-1.289460026
1	-0.344027959	2.409259803	-2.209446425
1	0.734215147	3.722116720	-1.639423709
8	-0.196325523	-0.955174863	-0.072721480
6	-1.563226539	-1.188622001	0.132287973
6	-2.444479529	-0.423510516	-0.869444022
6	-3.816264851	-0.125988091	-0.565401824
6	-4.598703788	0.623374712	-1.508853211

6	-4.009118230	1.033612431	-2.734517064
6	-2.700504624	0.718345981	-3.012941134
6	-1.917341475	-0.000128928	-2.075356124
1	-0.881560084	-0.227180163	-2.310744686
1	-2.255865428	1.013779245	-3.960898727
1	-4.613955167	1.589253321	-3.447788568
1	-1.807071104	-0.784474596	1.124818990
1	0.461610438	-1.710064298	-0.865598257
8	1.139953871	-2.378370626	-1.512974982
6	1.662426393	-1.775633192	-2.542026681
6	2.510577426	-2.699490590	-3.441465450
8	1.512189163	-0.572219162	-2.808486243
16	-1.699792443	2.428854971	2.042523439
6	-1.848913087	3.927898752	-0.137769233
6	-2.499890918	3.712419134	1.090137823
6	-3.639833951	4.439116405	1.421021652
1	-4.152689449	4.272240789	2.363236464
6	-2.315944038	4.867971944	-1.054302091
1	-1.810309537	5.023291252	-2.001925552
6	-3.456474923	5.593676789	-0.713488761
1	-3.843221649	6.330790870	-1.410484295
6	-4.110330631	5.384166122	0.507693332
1	-4.998563206	5.960110351	0.748168931
6	-1.884342491	-2.694358544	0.144166886
6	-2.405982837	-5.478863459	0.050920302
6	-2.149528579	-3.343234848	-1.046459549
6	-1.863608456	-3.456219667	1.362587147
6	-2.140870125	-4.866911077	1.303940007
6	-2.404748874	-4.731836068	-1.101807715
1	-2.171861614	-2.768491242	-1.967065893
1	-2.607145542	-5.200411141	-2.061506035
1	-2.611195469	-6.546686597	0.022505297
6	1.902998302	-1.806952149	2.044981057
1	1.217219616	-2.450150684	1.492419935
1	1.538705586	-1.686847248	3.067851675
6	1.588996647	-3.807075567	-3.997887259
1	2.166729069	-4.508866796	-4.612287961
1	0.799077372	-3.381347485	-4.628757945
1	1.111278804	-4.361068953	-3.185188466
6	3.621996369	-3.337658254	-2.581763430
1	4.232384363	-4.017275720	-3.189520847
1	3.195404324	-3.902476045	-1.748514299
1	4.290533442	-2.571415936	-2.168086619
6	3.128121592	-1.899891903	-4.597317507
1	3.699048925	-2.568349325	-5.253477728
1	3.804612070	-1.121677218	-4.228408792
1	2.355867924	-1.404441921	-5.193200535
6	-1.587044238	-2.889850594	2.641282902
1	-1.333585118	-1.839390659	2.723847065
6	-2.145030088	-5.629110424	2.503017308
1	-2.359170122	-6.693727218	2.437263754
6	-1.884619474	-5.043769911	3.720148389
1	-1.892040727	-5.639674916	4.629138589
6	-1.599384200	-3.660446321	3.784056185
1	-1.379106775	-3.199140840	4.743491210
6	-4.448563679	-0.542421526	0.641063185
1	-3.893560353	-1.136641176	1.358262260
6	-5.951292787	0.933215263	-1.202300508
1	-6.530322380	1.500333178	-1.928211155

6	-6.524732197	0.521775294	-0.021175206
1	-7.561946462	0.761901914	0.197954684
6	-5.762996748	-0.226111401	0.906767309
1	-6.220904035	-0.561744571	1.833581982
1	2.890131690	-2.275857320	2.071322698
1	2.276670139	-0.540964939	0.316967931
8	2.910434434	0.425816595	2.052179782
6	4.260839916	0.228091726	1.920892051
6	7.055028177	0.017251400	1.816233047
6	4.861389645	-0.644383937	1.005523476
6	5.060343590	0.991201683	2.783881826
6	6.445956460	0.884669662	2.728332092
6	6.255416541	-0.740982809	0.963237315
1	4.264473453	-1.248712689	0.332577194
1	4.570337700	1.656305473	3.488165762
1	7.054027416	1.479963793	3.405024971
1	6.712712651	-1.423970165	0.251794791
1	8.137125203	-0.069688237	1.777331308

Requested basis set is 6-31G(d)
There are 325 shells and 966 basis functions



Transition Structure (S)-ts2

$E(\text{B3LYP}/6\text{-}31\text{G}^*) = -2816.86161 \text{ au}$

$\nu_{\text{ts}} = 575i \text{ cm}^{-1}$

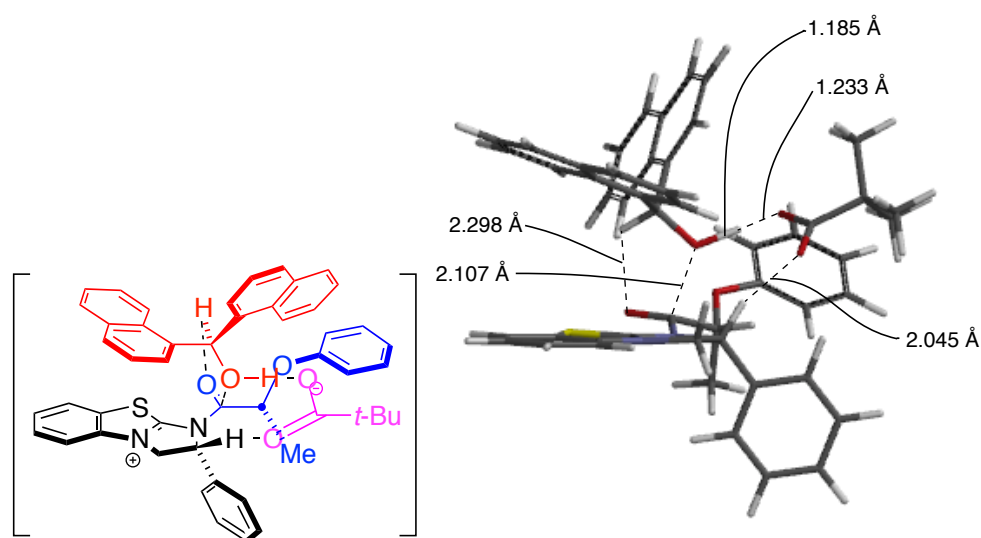
Cartesian Coordinates (Angstroms)

Atomic Number	X	Y	Z
6	-1.119923500	-0.003450965	-1.009142179
6	-2.070784803	-1.188372112	-0.785205969
8	-0.582986788	0.272111308	-2.078386060
7	-1.253645355	1.101383687	-0.076827159
6	-0.570195759	2.220246022	-0.308311549
7	-0.470896121	3.015799320	0.762743121
6	-1.041885537	2.373229438	1.952751478
6	-1.666280470	1.055198243	1.372807690
6	-3.164029968	0.986767537	1.587946189

6	-3.661174632	0.091241237	2.540608402
6	-5.030668431	0.044491103	2.810859162
6	-5.909878274	0.887244834	2.131621278
6	-5.415640521	1.784709403	1.180396998
6	-4.049570507	1.837234503	0.913812843
1	-3.677807193	2.527332080	0.159254263
1	-6.095487223	2.439598664	0.642010402
1	-6.975868853	0.846797696	2.339066334
1	-5.407825372	-0.656507523	3.550716712
1	-2.968799505	-0.559974745	3.068235078
1	-1.174510828	0.192992461	1.834030168
1	-0.247616055	2.167315404	2.675241788
1	-1.800762893	3.016886307	2.404035394
8	0.407378721	-0.941386870	0.187961360
6	1.702430763	-0.720787180	-0.310409470
6	2.486332338	0.292231225	0.538596451
6	3.613985921	0.995460293	-0.004721316
6	4.302470237	1.954371130	0.813767362
6	3.866512723	2.176707649	2.147624943
6	2.792360802	1.481736627	2.649180134
6	2.098090145	0.548654163	1.839978843
1	1.248289686	0.014550771	2.254313776
1	2.470856728	1.636047463	3.677046299
1	4.403337554	2.896033694	2.762326838
1	1.580137286	-0.261113724	-1.300504410
1	0.237123646	-1.847617310	1.010091484
8	0.006883710	-2.734046174	1.759819949
6	-0.365569116	-2.364219523	2.946972863
6	-0.471028759	-3.524845919	3.960919701
8	-0.617945443	-1.192391065	3.280875987
16	0.214305055	2.835809326	-1.720093571
6	0.225653997	4.202733122	0.549952300
6	0.667767986	4.287949750	-0.782549112
6	1.385563274	5.397394511	-1.219067289
1	1.735075482	5.466279972	-2.244586584
6	0.489629707	5.215661247	1.470110486
1	0.150884796	5.139502831	2.498263356
6	1.207005136	6.324627420	1.023765195
1	1.427918242	7.127919486	1.719889659
6	1.648097906	6.417121024	-0.302823945
1	2.204849052	7.291705028	-0.624822030
6	2.467261534	-2.042421216	-0.493808683
6	3.844213398	-4.509126992	-0.715897075
6	3.167035633	-2.580182640	0.569136678
6	2.428146262	-2.761650841	-1.737343828
6	3.141419035	-4.006336387	-1.841804373
6	3.851185317	-3.812130063	0.467941540
1	3.199522953	-2.037538027	1.508784894
1	4.388557861	-4.197373432	1.330538031
1	4.374812881	-5.454014461	-0.809443058
6	-1.702150091	-2.421459501	-1.597734815
1	-0.753627389	-2.810891232	-1.226269270
1	-1.599938220	-2.214296731	-2.663386155
6	0.921149052	-4.182743162	4.082659273
1	0.878981585	-5.032682339	4.775036395
1	1.658863252	-3.470202223	4.472582318
1	1.270775451	-4.536313953	3.108806350
6	-1.482620783	-4.557510713	3.419757971
1	-1.553205042	-5.416185074	4.099482903

1	-1.179040900	-4.917116100	2.432994285
1	-2.485249169	-4.120391058	3.330772777
6	-0.927046055	-3.002203932	5.330440688
1	-0.965648799	-3.826080501	6.053905000
1	-1.922227948	-2.549233755	5.272119636
1	-0.241389540	-2.238811368	5.710932567
6	1.722569326	-2.305742169	-2.889148026
1	1.142390580	-1.391542381	-2.839557531
6	3.130249962	-4.717375144	-3.071993543
1	3.676631757	-5.656337093	-3.131071159
6	2.445443935	-4.239425111	-4.164863846
1	2.445665347	-4.794951335	-5.099113869
6	1.732525282	-3.022602833	-4.066203023
1	1.180826798	-2.650357988	-4.925800103
6	4.091237874	0.786216297	-1.330345526
1	3.609914922	0.049171039	-1.963742058
6	5.413414105	2.658637772	0.276661283
1	5.925585481	3.379550393	0.910440534
6	5.841638279	2.434410729	-1.011611641
1	6.695978379	2.976941679	-1.408205047
6	5.171715991	1.486988120	-1.820297253
1	5.517550783	1.304130356	-2.834469382
1	-2.478517000	-3.179439162	-1.455986967
1	-2.041344474	-1.451201600	0.272361181
8	-3.428449412	-0.738441050	-0.957989134
6	-4.049823798	-0.591906021	-2.176894531
6	-5.579965673	-0.240324338	-4.501483996
6	-3.415850621	-0.308266426	-3.392473834
6	-5.447969299	-0.686675298	-2.125500650
6	-6.204611967	-0.508914461	-3.280044674
6	-4.190265186	-0.142533167	-4.544750599
1	-2.339781183	-0.202979419	-3.444101403
1	-5.914305972	-0.897455443	-1.168162655
1	-7.287703013	-0.586807578	-3.225521611
1	-3.689215915	0.072582887	-5.485462463
1	-6.169827895	-0.108265796	-5.404278109

Requested basis set is 6-31G(d)
There are 325 shells and 966 basis functions



Transition Structure (*R*)-**ts1**

$E(\text{B3LYP}/6\text{-}31\text{G}^*) = -2816.85803 \text{ au}$

$\nu_{\text{ts}} = 575i \text{ cm}^{-1}$

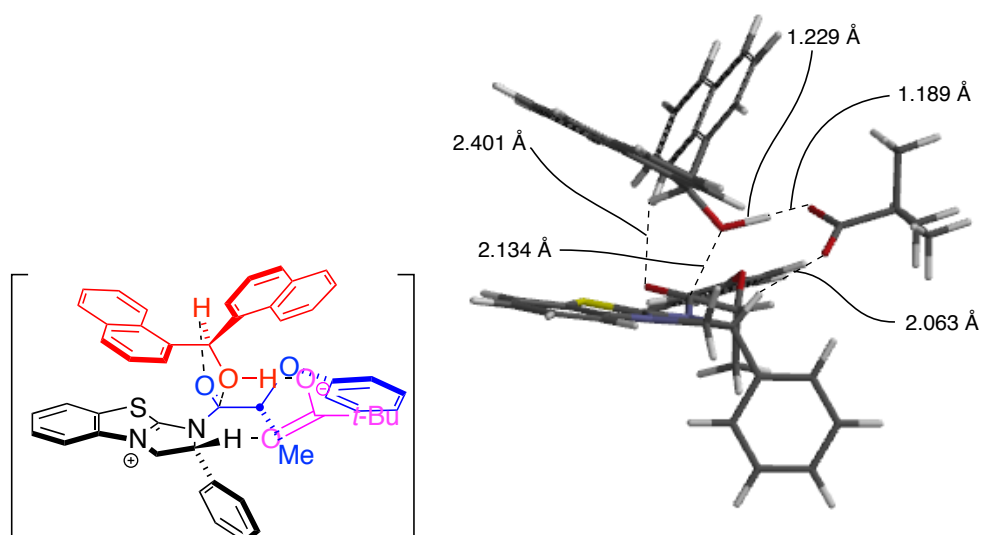
Cartesian Coordinates (Angstroms)

Atomic Number	X	Y	Z
6	0.035571352	0.782827991	1.687137030
6	1.462221162	1.327257961	1.784729321
1	1.707768076	1.862325067	0.863381873
8	-0.441130647	-0.007132453	2.492834797
7	-0.927099533	1.667361564	1.028385909
6	-2.220325979	1.362865794	1.114790556
7	-2.974483344	1.963038717	0.186123699
6	-2.142790474	2.692759844	-0.779083737
6	-0.702857914	2.553097679	-0.171017277
6	-0.091208339	3.897093506	0.172334000
6	0.954826124	4.383148664	-0.622207129
6	1.498253244	5.644554318	-0.365068881
6	1.004564388	6.424338821	0.681343466
6	-0.042829256	5.944746210	1.472921231
6	-0.590771501	4.688555449	1.216332396
1	-1.402623892	4.315476377	1.837167863
1	-0.430219458	6.547951169	2.289589022
1	1.432773472	7.402740216	0.881792378
1	2.310975714	6.015004339	-0.983917349
1	1.323797968	3.768584979	-1.439813138
1	-0.062291686	2.012933515	-0.877330858
1	-2.220132276	2.220270910	-1.762044073
1	-2.460147607	3.736492924	-0.841872977
8	0.363626746	-0.286199275	-0.098878966
6	-0.263661552	-1.548768805	-0.083545939
6	-1.468664647	-1.580907622	-1.035263849
6	-2.539541508	-2.517210663	-0.842642521
6	-3.673875333	-2.472916663	-1.723581611
6	-3.701242545	-1.526358591	-2.782589150
6	-2.651344662	-0.657435749	-2.961631734
6	-1.542584023	-0.679033441	-2.080401342
1	-0.729590411	0.025294621	-2.229143126
1	-2.661533750	0.052339343	-3.786098362

1	-4.559722293	-1.511182290	-3.450687780
1	-0.665746114	-1.676487948	0.929361190
1	1.298250953	-0.153944962	-0.814829470
8	2.255131036	0.021042899	-1.573025749
6	2.074597761	0.923680425	-2.476523791
6	3.200916631	1.004274849	-3.533873868
8	1.093008661	1.695646390	-2.534419652
16	-3.106795852	0.339168459	2.189636783
6	-4.335855488	1.676556643	0.259877907
6	-4.602848278	0.803777087	1.329668058
6	-5.903798420	0.384868071	1.591442779
1	-6.115495397	-0.295209523	2.410741849
6	-5.354586397	2.148617738	-0.565891462
1	-5.138949961	2.816965154	-1.393268243
6	-6.655626176	1.727345309	-0.294057363
1	-7.468353548	2.078624474	-0.922254238
6	-6.928694122	0.858385265	0.770498581
1	-7.950355284	0.544352494	0.960193590
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6	1.396446881	-3.368650864	0.729128616
6	2.309545336	-4.434930199	0.414160665
6	1.917622253	-4.098187990	-1.953998123
1	0.490683459	-2.562523069	-2.462426099
1	2.105511323	-4.355994145	-2.992902169
1	3.252910218	-5.578307071	-1.161940588
6	3.351706917	-0.384012942	-4.192268010
1	4.177063871	-0.377586696	-4.915644832
1	2.437717716	-0.666623079	-4.730063839
1	3.551467777	-1.147933490	-3.436260291
6	4.514547516	1.371494206	-2.811541324
1	5.345992358	1.404873357	-3.527148027
1	4.749393591	0.640946739	-2.033000817
1	4.442079153	2.358963104	-2.337626034
6	2.868123262	2.060167544	-4.597506493
1	3.663582396	2.101021625	-5.352498455
1	2.766458212	3.055397701	-4.152145116
1	1.923805969	1.830796054	-5.101993142
6	1.550946266	2.244492504	3.015976054
1	1.257218312	1.675587304	3.902702179
1	0.904723827	3.121573405	2.919158039
6	-2.534693665	-3.498967246	0.189457257
1	-1.677220627	-3.580988136	0.848662385
6	-4.745987593	-3.383499790	-1.523312701
1	-5.598271049	-3.336837133	-2.197889551
6	-3.590769506	-4.368779053	0.353677893
1	-3.558472248	-5.111605429	1.146558454
6	-4.711289733	-4.310936132	-0.507657584
1	-5.537179946	-5.003930812	-0.369414172
6	2.956003889	-5.136687770	1.467038502
1	3.639492121	-5.942502399	1.207654467
6	1.203680971	-3.047659174	2.104445861
1	0.574729774	-2.211390325	2.384023709
6	1.846211217	-3.752714831	3.099986911
1	1.681082830	-3.481044200	4.139464041
6	2.727974058	-4.812329387	2.784048537
1	3.227550974	-5.359689625	3.579285832
1	2.579408324	2.590683831	3.147040122

8	2.308785526	0.204959714	1.951443659
6	3.651114855	0.327653220	1.697416745
6	6.419621629	0.334449204	1.247832741
6	4.403004959	-0.835937462	1.911471210
6	4.286568717	1.496282178	1.261563880
6	5.667682087	1.487752456	1.040159069
6	5.774393125	-0.827535735	1.684602441
1	3.888818858	-1.731254194	2.243217454
1	3.729886086	2.409359117	1.083810926
1	6.150465527	2.400634232	0.700347480
1	6.344019006	-1.738839781	1.848212452
1	7.491533998	0.336967896	1.071970353

Requested basis set is 6-31G(d)
There are 325 shells and 966 basis functions



Transition Structure (*R*)-ts2

$E(\text{B3LYP}/6\text{-}31\text{G}^*) = -2816.85262 \text{ au}$

$\nu_{\text{ts}} = 576i \text{ cm}^{-1}$

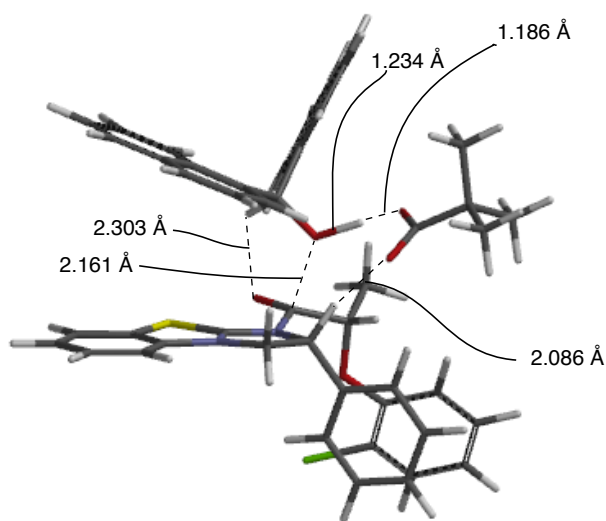
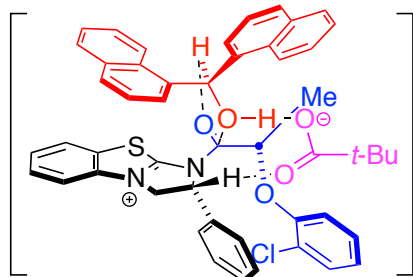
Cartesian Coordinates (Angstroms)

Atomic Number	X	Y	Z
6	0.274428083	0.912465409	1.372393792
6	1.598205626	1.657970778	1.151294523
1	1.607367037	2.044801775	0.129788595
8	0.094617407	0.087220386	2.262770089
7	-0.936849860	1.578782503	0.893240272
6	-2.115268079	1.053760545	1.223048624
7	-3.122830491	1.468745334	0.445247227
6	-2.624707117	2.274492866	-0.675988157
6	-1.108935078	2.460920118	-0.319363732
6	-0.760552057	3.914970718	-0.067622408
6	0.061035888	4.578826537	-0.986271441
6	0.353893044	5.933842710	-0.810701795
6	-0.167992856	6.631400996	0.278461369
6	-0.993549700	5.973695200	1.195279145
6	-1.291337614	4.623243911	1.020737781

1	-1.926412447	4.115726624	1.743991396
1	-1.401870408	6.512382660	2.046203332
1	0.065138170	7.683858281	0.415692821
1	0.993721435	6.441737746	-1.527141882
1	0.454364105	4.026236263	-1.835882408
1	-0.487332130	2.053582327	-1.123114352
1	-2.764748253	1.723748482	-1.609481937
1	-3.150775349	3.230829803	-0.722894085
8	0.451674565	-0.161845945	-0.463098473
6	0.048128081	-1.504507980	-0.374214544
6	-1.302353666	-1.730964076	-1.071799160
6	-2.154740476	-2.825757919	-0.704194080
6	-3.419720050	-2.982503220	-1.367270167
6	-3.791037810	-2.069861235	-2.390484821
6	-2.946383675	-1.043920505	-2.742879410
6	-1.709260548	-0.870600481	-2.075050484
1	-1.053228334	-0.054654505	-2.365484462
1	-3.219741934	-0.360121527	-3.543888868
1	-4.744853120	-2.206828950	-2.895470447
1	-0.110587589	-1.717601112	0.692507766
1	1.277686850	0.127414919	-1.326404331
8	2.067001385	0.457357224	-2.151870679
6	1.642498277	1.353837443	-2.982288057
6	2.624235330	1.652789503	-4.137968044
8	0.544187621	1.938893883	-2.905523661
16	-2.590476417	-0.064951058	2.452556515
6	-4.370885910	0.940570423	0.767544555
6	-4.276310250	0.082759964	1.877731661
6	-5.407672619	-0.557559545	2.374218935
1	-5.339255003	-1.228968470	3.224535068
6	-5.589099968	1.178272932	0.133610384
1	-5.652596640	1.836387649	-0.726852715
6	-6.718318444	0.535849799	0.639715401
1	-7.679874819	0.701398357	0.163673469
6	-6.631286724	-0.319239774	1.746108474
1	-7.525485433	-0.808271500	2.119809114
6	1.128581467	-2.468343798	-0.896345361
6	3.098573474	-4.210518976	-1.950562480
6	1.157647599	-2.803499680	-2.236423509
6	2.134551087	-3.003894850	-0.023083007
6	3.118862544	-3.901288910	-0.565666103
6	2.142330090	-3.664133263	-2.771242367
1	0.398790965	-2.401327521	-2.899820643
1	2.127775752	-3.898236015	-3.832596190
1	3.852701119	-4.886901463	-2.346986802
6	2.743874650	0.369611450	-4.990210598
1	3.471362263	0.514422008	-5.798698575
1	1.780933325	0.109957424	-5.447372043
1	3.068348374	-0.473819402	-4.373953461
6	4.003225810	2.004233778	-3.543453876
1	4.729001507	2.185108460	-4.346396839
1	4.371180111	1.191683159	-2.911905293
1	3.949119761	2.913326935	-2.931087212
6	2.104103437	2.812250249	-4.999315614
1	2.779922019	2.993212279	-5.844861717
1	2.033320740	3.738606152	-4.418234358
1	1.106428160	2.594735452	-5.392063894
6	1.744366744	2.826601328	2.135435460
1	1.639340270	2.506791175	3.174270796

1	0.996867623	3.594690185	1.927617659
6	-1.802018141	-3.779470215	0.293400357
1	-0.838804071	-3.708057321	0.786702503
6	-4.271944859	-4.057068508	-0.995387858
1	-5.226167253	-4.163267485	-1.507257312
6	-2.651565146	-4.811233843	0.628128032
1	-2.354531728	-5.528734953	1.388672619
6	-3.901519964	-4.952667200	-0.018907364
1	-4.561544148	-5.772865038	0.251699381
6	4.100302368	-4.464323922	0.293325556
1	4.832854094	-5.145189740	-0.135150319
6	2.213544641	-2.695786727	1.364623695
1	1.526380051	-1.977477179	1.794582635
6	3.181185618	-3.257950065	2.168462051
1	3.226183358	-2.989235666	3.220117390
6	4.131820541	-4.157213326	1.633461922
1	4.890185298	-4.592495384	2.279194761
1	2.736080419	3.272292716	2.011636533
8	2.678976246	0.729864920	1.188756800
6	3.490610990	0.585376237	2.294051423
6	5.298512266	0.186853378	4.393648443
6	4.865363102	0.713694734	2.070733316
6	3.016334045	0.242765339	3.565994292
6	3.925442611	0.054868945	4.609234025
6	5.764024023	0.509026076	3.116880836
1	5.206206171	0.962184176	1.070410240
1	1.952111192	0.105400460	3.718647332
1	3.553017069	-0.208016873	5.596581425
1	6.830942073	0.607251768	2.933069558
1	5.998882595	0.033041083	5.210028688

Requested basis set is 6-31G(d)
There are 325 shells and 966 basis functions



Transition Structure (*S*)-*o*-Cl-**ts1**

$E(\text{B3LYP}/6\text{-}31\text{G}^*) = -3276.45681 \text{ au}$

$\nu_{\text{ts}} = 607i \text{ cm}^{-1}$

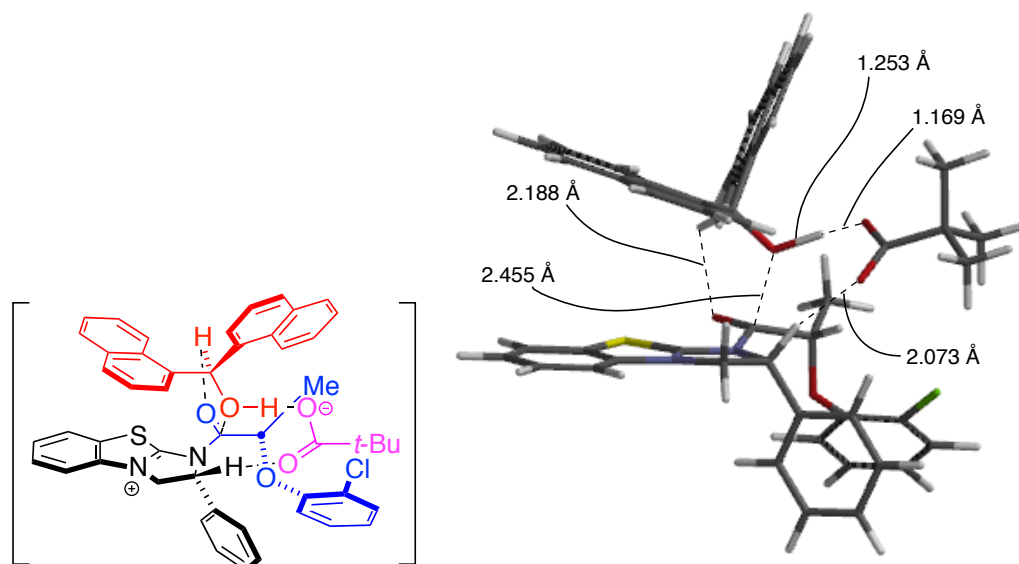
Cartesian Coordinates (Angstroms)

Atomic Number	X	Y	Z
6	-0.763871246	-0.372505244	1.084371376
6	-2.044512998	0.457269235	0.951522817
8	-0.152341332	-0.499310107	2.136431079
7	-0.584165466	-1.431597228	0.112213238
6	0.358358020	-2.347555546	0.321882372
7	0.664901278	-3.054415095	-0.772237864
6	-0.043170016	-2.537822968	-1.950457469
6	-0.986746350	-1.441699852	-1.336425402
6	-2.450879997	-1.750937106	-1.575662600
6	-3.103034621	-1.083587719	-2.620696585
6	-4.424432526	-1.404556930	-2.938838334
6	-5.103739374	-2.383704900	-2.213817044
6	-4.458161971	-3.043864956	-1.165063604
6	-3.136323142	-2.733043750	-0.849757634
1	-2.649332133	-3.237097903	-0.019093386
1	-4.986031585	-3.797148830	-0.586833457
1	-6.134318509	-2.627380910	-2.457430598
1	-4.922760699	-0.881925259	-3.751125743
1	-2.565694590	-0.320185640	-3.178469171
1	-0.730295078	-0.467638698	-1.763511125
1	0.676381932	-2.109314219	-2.652949922
1	-0.609979127	-3.336930573	-2.433486275
8	0.376119258	1.029004162	-0.102260077
6	1.682934946	1.160606828	0.400905560
6	2.717860821	0.422443066	-0.461025904
6	3.977779117	0.012122836	0.092730893
6	4.899427595	-0.720839921	-0.730181734
6	4.559290458	-1.004316243	-2.080192349
6	3.356868811	-0.581496670	-2.593817618
6	2.434506292	0.121806617	-1.779991720
1	1.485452460	0.434852631	-2.204468313
1	3.104900096	-0.777819005	-3.633773447
1	5.270603066	-1.549490408	-2.696812136

1	1.688966195	0.656413144	1.376163054
1	-0.018086254	1.854292831	-0.930810787
8	-0.456274207	2.653420699	-1.689848558
6	-0.679989942	2.207419475	-2.886858070
6	-1.044567461	3.304975969	-3.911381341
8	-0.598775747	1.012895633	-3.227387756
16	1.251425590	-2.798991679	1.730025741
6	1.624380724	-4.045170185	-0.579588123
6	2.055437494	-4.066026519	0.759431803
6	3.015126073	-4.982585128	1.178277052
1	3.356237839	-4.999766918	2.208790118
6	2.137591339	-4.933680361	-1.522669424
1	1.804006953	-4.907177180	-2.555046766
6	3.095955054	-5.850997760	-1.093596117
1	3.513430340	-6.554172320	-1.807664554
6	3.528677545	-5.878012829	0.238650606
1	4.275809377	-6.602682658	0.547157579
6	2.049844398	2.636805319	0.625260972
6	2.655909068	5.390671791	0.909166331
6	2.581509094	3.373094773	-0.415854052
6	1.797472654	3.288137631	1.881410971
6	2.115032509	4.684688501	2.015285279
6	2.882095762	4.746955648	-0.283166826
1	2.779718159	2.883015620	-1.363708270
1	3.299618393	5.286658575	-1.129228762
1	2.888833218	6.446825290	1.025154050
6	-1.974857190	1.737646312	1.767108562
1	-1.208244025	2.388838103	1.346457308
1	-1.720727303	1.505040931	2.803594206
6	0.176784712	4.241390814	-4.048052943
1	-0.043261058	5.051556684	-4.754144401
1	1.049854683	3.695264777	-4.426669827
1	0.440066784	4.678512466	-3.080719175
6	-2.249504305	4.107226106	-3.378752818
1	-2.497753955	4.926268941	-4.065712878
1	-2.029015766	4.530738991	-2.395392331
1	-3.138318299	3.470160839	-3.286079772
6	-1.381044229	2.679558322	-5.272255563
1	-1.593519990	3.466578703	-6.006423469
1	-2.259798927	2.029144548	-5.205294905
1	-0.550565717	2.072326095	-5.644173224
6	1.252141814	2.623801132	3.018686591
1	0.970708647	1.579256572	2.951476092
6	1.883072916	5.339753335	3.254732694
1	2.129891919	6.396319311	3.334200819
6	1.358501711	4.662957903	4.331000764
1	1.185023728	5.177408107	5.272597671
6	1.040212474	3.291279524	4.205893986
1	0.617877955	2.756698795	5.053045543
6	4.363345345	0.297332576	1.434043382
1	3.701484070	0.873996629	2.070681665
6	6.139705589	-1.142698274	-0.180221836
1	6.827220497	-1.696288365	-0.816245387
6	6.474326717	-0.854951773	1.123000364
1	7.428989953	-1.179774441	1.528712850
6	5.575343128	-0.125063301	1.935195716
1	5.845786207	0.110649698	2.961196793
1	-2.935499999	2.257526188	1.743590525
1	-2.249938733	0.663907493	-0.103098655

8	-3.021487079	-0.473337108	1.476715344
6	-4.338112330	-0.143363552	1.551058685
6	-7.088250444	0.379384653	1.846764732
6	-5.112404947	-0.844316442	2.494788585
6	-4.972593150	0.809943532	0.745183085
6	-6.335277386	1.069970663	0.898009006
6	-6.471526470	-0.586450496	2.642961862
1	-4.400226757	1.347278536	-0.002994966
1	-6.804707309	1.820195349	0.267888538
1	-7.033176278	-1.138792401	3.389593310
1	-8.146295266	0.587303072	1.973173960
17	-4.351210861	-2.059356296	3.509125939

Requested basis set is 6-31G(d)
There are 328 shells and 983 basis functions



Transition Structure (*S*)-*o*-Cl-**ts2**

$E(\text{B3LYP}/6\text{-}31\text{G}^*) = -3276.45154 \text{ au}$

$\nu_{\text{ts}} = 492i \text{ cm}^{-1}$

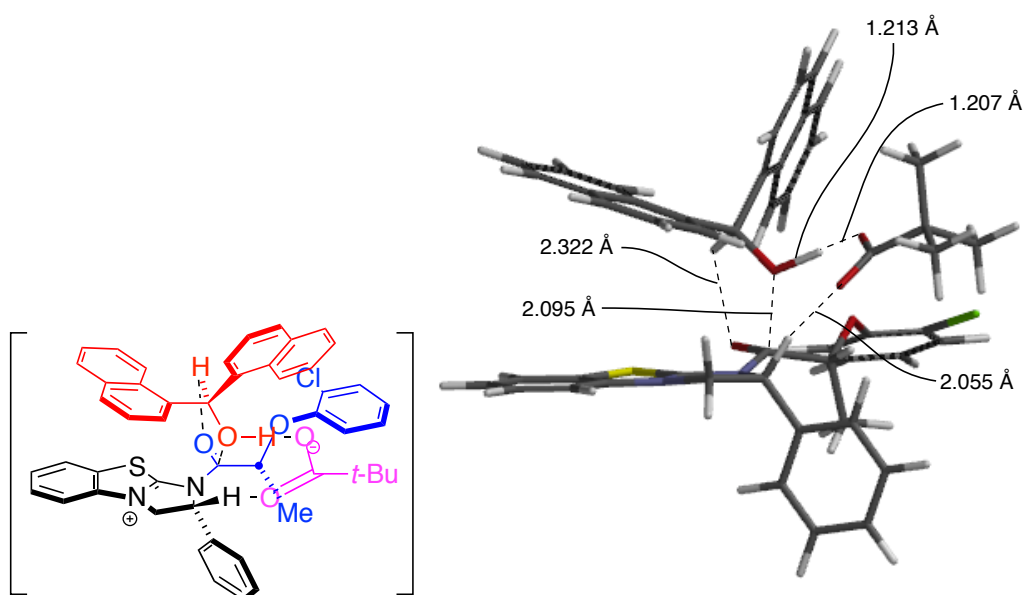
Cartesian Coordinates (Angstroms)

Atomic Number	X	Y	Z
6	0.649413933	0.414431135	1.225921899
6	2.033524436	-0.175287987	0.944351289
8	0.048648656	0.272829507	2.283563994
7	0.256153112	1.556125256	0.427768206
6	-0.852983561	2.217572850	0.747239164
7	-1.297350636	3.015264243	-0.231225653
6	-0.512606570	2.824274386	-1.458597910
6	0.673769086	1.916865622	-0.971754882
6	1.999931525	2.645817068	-1.054726284
6	2.830719568	2.377000507	-2.148532208
6	4.009131341	3.105146241	-2.325490750
6	4.367088250	4.096641523	-1.412140415
6	3.543770772	4.359494868	-0.314214215

6	2.363587993	3.640000701	-0.138361140
1	1.737727195	3.838016591	0.728482331
1	3.824267791	5.121230811	0.408509089
1	5.287981551	4.657557299	-1.547993090
1	4.652209059	2.887681067	-3.174012160
1	2.549101694	1.592766784	-2.846882938
1	0.704468484	0.998109947	-1.565282863
1	-1.133776834	2.330201261	-2.210405290
1	-0.153568618	3.784172498	-1.835269979
8	-0.246578159	-0.982439666	-0.200137265
6	-1.555054673	-1.354058843	0.140060516
6	-2.603828598	-0.677332082	-0.756497274
6	-3.952086735	-0.482306569	-0.302741631
6	-4.889639591	0.194466148	-1.156029590
6	-4.475950944	0.627108574	-2.444140157
6	-3.187011853	0.405397827	-2.867350710
6	-2.250259474	-0.233908018	-2.017538723
1	-1.231062048	-0.374457747	-2.365232535
1	-2.874989021	0.716042133	-3.862233283
1	-5.198043069	1.123530221	-3.088680437
1	-1.735912822	-0.984007038	1.159069367
1	0.339968041	-1.625109219	-1.101805587
8	0.968030046	-2.227380496	-1.882934036
6	1.368373428	-1.540373803	-2.909836877
6	2.184081806	-2.361373634	-3.932111700
8	1.123855046	-0.335512593	-3.096456462
16	-1.832523213	2.234052698	2.172194428
6	-2.461300544	3.718847681	0.069059089
6	-2.896311081	3.427622140	1.374640726
6	-4.047282094	4.019783807	1.885180434
1	-4.392230218	3.791659574	2.888948203
6	-3.161173996	4.604189505	-0.748919184
1	-2.822972040	4.818572229	-1.757559088
6	-4.311932654	5.195063965	-0.228773844
1	-4.877735711	5.885833452	-0.846290847
6	-4.750002291	4.909601614	1.071075986
1	-5.650226648	5.381938877	1.451693817
6	-1.719796819	-2.884960493	0.166223638
6	-1.975574795	-5.707840658	0.111519310
6	-2.098556587	-3.556818049	-0.979556647
6	-1.433923162	-3.642230619	1.354080073
6	-1.580592327	-5.072530038	1.318145347
6	-2.221287959	-4.964146969	-1.016672010
1	-2.317799117	-2.988834900	-1.877705401
1	-2.520187001	-5.449518327	-1.942112332
1	-2.078331497	-6.790592418	0.099117479
6	2.207205359	-1.518156906	1.630478739
1	1.482948333	-2.213866887	1.205619896
1	2.032519172	-1.434830584	2.706038604
6	1.254671215	-3.447981291	-4.516111684
1	1.806424097	-4.080286168	-5.222997044
1	0.412297539	-2.999118140	-5.057036826
1	0.850373636	-4.080366085	-3.720819452
6	3.365994393	-3.033032609	-3.202400394
1	3.956822395	-3.630842982	-3.907540793
1	3.009641892	-3.683979859	-2.400075735
1	4.033582389	-2.284916503	-2.756903721
6	2.702976618	-1.454773463	-5.057455323
1	3.261569407	-2.049531559	-5.790859173

1	3.369401589	-0.677620595	-4.668246907
1	1.879401201	-0.951388398	-5.572789643
6	-1.011673243	-3.050683909	2.580120456
1	-0.844690070	-1.981171742	2.633558486
6	-1.326109506	-5.830761092	2.492377340
1	-1.446176931	-6.911047365	2.446005906
6	-0.933773787	-5.222160194	3.661937207
1	-0.741540808	-5.815740254	4.552080597
6	-0.771188273	-3.818239308	3.699629906
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6	-4.412795571	-0.928872306	0.969504228
1	-3.739025593	-1.472206654	1.622939705
6	-6.217535944	0.410942140	-0.699113070
1	-6.914269949	0.925900718	-1.357124770
6	-6.622049284	-0.023855777	0.541869289
1	-7.642285591	0.144894576	0.876771522
6	-5.708431982	-0.703927189	1.380801134
1	-6.033974369	-1.059575471	2.355042684
1	3.212018597	-1.909096288	1.454987910
1	2.199822715	-0.269711473	-0.129329270
8	2.910644857	0.877099375	1.453265894
6	4.099714482	0.585451270	2.060797989
6	6.552326468	0.210628421	3.383262352
6	5.222272084	0.101513579	1.369169252
6	4.233462396	0.884095805	3.421977420
6	5.448329270	0.705337614	4.080061659
6	6.437060684	-0.092877425	2.027106934
1	3.357403327	1.262276119	3.940171160
1	5.529666671	0.946151862	5.136390580
1	7.284981092	-0.472216307	1.465869466
1	7.502827596	0.062457039	3.887731455
17	5.120492952	-0.249102613	-0.347493258

Requested basis set is 6-31G(d)
There are 328 shells and 983 basis functions



Transition Structure (*R*)-*o*-Cl-ts1

$E(\text{B3LYP}/6\text{-}31\text{G}^*) = -3276.44736 \text{ au}$

$\nu_{ts} = 661i \text{ cm}^{-1}$

Cartesian Coordinates (Angstroms)

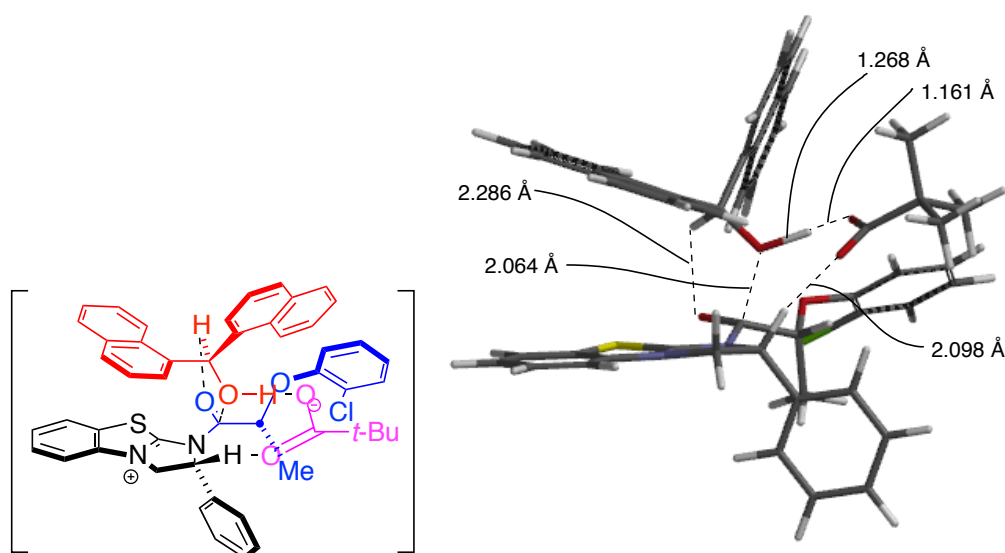
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7	-0.936779777	1.642562845	1.010286269
6	-2.207291715	1.313502345	1.224573251
7	-3.062671868	1.913040796	0.385652082
6	-2.341003595	2.655852266	-0.656629585
6	-0.856860884	2.598074931	-0.153410005
6	-0.330581699	3.967992908	0.233894352
6	0.685480767	4.545073256	-0.537871529
6	1.151040318	5.827259904	-0.233307744
6	0.610000811	6.537844898	0.838264483
6	-0.406197120	5.966277187	1.609194583
6	-0.876298714	4.689616907	1.305816957
1	-1.663809877	4.250183983	1.914822465
1	-0.830601947	6.514234436	2.446209059
1	0.976744131	7.532998292	1.074772376
1	1.940660396	6.268237069	-0.835711129
1	1.096106089	3.983142189	-1.373268882
1	-0.210676205	2.146629654	-0.914027868
1	-2.475014744	2.152583905	-1.617823998
1	-2.708194888	3.682852089	-0.716600702
8	0.337674085	-0.234059292	-0.265008070
6	-0.400101409	-1.432555678	-0.288698361
6	-1.605445974	-1.337450524	-1.239409262
6	-2.740271152	-2.205558278	-1.087053902
6	-3.850027359	-2.072827465	-1.990806966
6	-3.797034796	-1.103052615	-3.027499581
6	-2.694265971	-0.293948394	-3.162268435
6	-1.606374011	-0.406485822	-2.261488725
1	-0.751096164	0.251553220	-2.379336818

1	-2.644436325	0.435414064	-3.968067409
1	-4.637100650	-1.021548590	-3.713905489
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1	1.265623988	-0.119334270	-1.037970756
8	2.153367004	0.030166028	-1.842341727
6	2.009347653	1.066306395	-2.601930731
6	3.011603281	1.143364842	-3.776733295
8	1.136975851	1.945640405	-2.452197399
16	-2.964850337	0.264646790	2.372913704
6	-4.404029569	1.595902228	0.588565881
6	-4.547060046	0.708693882	1.670513801
6	-5.807073327	0.261361962	2.055364244
1	-5.923485984	-0.428800856	2.885208719
6	-5.508862516	2.052697254	-0.127738518
1	-5.389410662	2.732369801	-0.965313296
6	-6.768010061	1.601159546	0.265821546
1	-7.645436849	1.939650201	-0.276477787
6	-6.917498891	0.719565891	1.344216890
1	-7.908856790	0.382539784	1.630655042
6	0.466109631	-2.663903035	-0.605044044
6	2.002549804	-4.934341180	-1.315503999
6	0.776524687	-2.946056779	-1.921420007
6	0.955523973	-3.532289483	0.429434083
6	1.712497810	-4.696465830	0.053185556
6	1.554194899	-4.067737065	-2.282783125
1	0.403595264	-2.293475162	-2.703862838
1	1.778806957	-4.247272596	-3.331021012
1	2.584150676	-5.814231244	-1.581760705
6	2.792986286	-0.099953818	-4.667903003
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1	4.645447875	1.999182057	-2.590351368
6	2.782937633	2.423062028	-4.595023615
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1	2.919133731	3.318325067	-3.978755089
1	1.767378619	2.457001443	-5.001828397
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1	1.483230740	1.781649700	3.650264944
1	0.987567674	3.185328042	2.666240851
6	-2.824455678	-3.204505260	-0.074775483
1	-1.993883946	-3.355418710	0.605467590
6	-4.980353056	-2.919827730	-1.837062814
1	-5.811081666	-2.805688821	-2.530282618
6	-3.935917791	-4.010424576	0.045125638
1	-3.968481231	-4.768935490	0.823036397
6	-5.028135739	-3.868431104	-0.841818487
1	-5.897706139	-4.512409981	-0.738866486
6	2.160261243	-5.595136905	1.058303273
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6	0.724793193	-3.315274113	1.818825516
1	0.232332386	-2.408659459	2.149802097
6	1.172480309	-4.210307166	2.766378600
1	0.987384602	-4.011792401	3.819040063
6	1.889669460	-5.368207379	2.387425144
1	2.236763184	-6.065260936	3.145810554

1	2.695046025	2.726753102	2.754967213
8	2.427588238	0.302070103	1.656880906
6	3.751162948	0.517415108	1.418679999
6	6.527391315	0.761414362	0.987326157
6	4.648315967	-0.458266334	1.894269536
6	4.276909634	1.619943443	0.732406600
6	5.651439446	1.738405837	0.521484892
6	6.017310959	-0.340493309	1.674431145
1	3.616633811	2.386983333	0.345226596
1	6.030081150	2.602854705	-0.016763785
1	6.674932515	-1.117318243	2.050618719
1	7.596799917	0.849432598	0.821281411
17	4.038113900	-1.842966930	2.773140712

Requested basis set is 6-31G(d)

There are 328 shells and 983 basis functions



Transition Structure (*R*)-*o*-Cl-ts2

$E(\text{B3LYP}/6\text{-}31\text{G}^*) = -3276.45042 \text{ au}$

$\nu_{\text{ts}} = 528i \text{ cm}^{-1}$

Cartesian Coordinates (Angstroms)

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7	0.256153112	1.556125256	0.427768206
6	-0.852983561	2.217572850	0.747239164
7	-1.297350636	3.015264243	-0.231225653
6	-0.512606570	2.824274386	-1.458597910
6	0.673769086	1.916865622	-0.971754882
6	1.999931525	2.645817068	-1.054726284
6	2.830719568	2.377000507	-2.148532208
6	4.009131341	3.105146241	-2.325490750

6	4.367088250	4.096641523	-1.412140415
6	3.543770772	4.359494868	-0.314214215
6	2.363587993	3.640000701	-0.138361140
1	1.737727195	3.838016591	0.728482331
1	3.824267791	5.121230811	0.408509089
1	5.287981551	4.657557299	-1.547993090
1	4.652209059	2.887681067	-3.174012160
1	2.549101694	1.592766784	-2.846882938
1	0.704468484	0.998109947	-1.565282863
1	-1.133776834	2.330201261	-2.210405290
1	-0.153568618	3.784172498	-1.835269979
8	-0.246578159	-0.982439666	-0.200137265
6	-1.555054673	-1.354058843	0.140060516
6	-2.603828598	-0.677332082	-0.756497274
6	-3.952086735	-0.482306569	-0.302741631
6	-4.889639591	0.194466148	-1.156029590
6	-4.475950944	0.627108574	-2.444140157
6	-3.187011853	0.405397827	-2.867350710
6	-2.250259474	-0.233908018	-2.017538723
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1	-2.874989021	0.716042133	-3.862233283
1	-5.198043069	1.123530221	-3.088680437
1	-1.735912822	-0.984007038	1.159069367
1	0.339968041	-1.625109219	-1.101805587
8	0.968030046	-2.227380496	-1.882934036
6	1.368373428	-1.540373803	-2.909836877
6	2.184081806	-2.361373634	-3.932111700
8	1.123855046	-0.335512593	-3.096456462
16	-1.832523213	2.234052698	2.172194428
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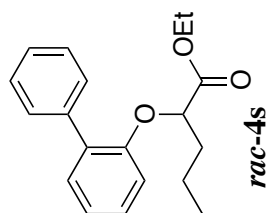
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Requested basis set is 6-31G(d)
There are 328 shells and 983 basis functions

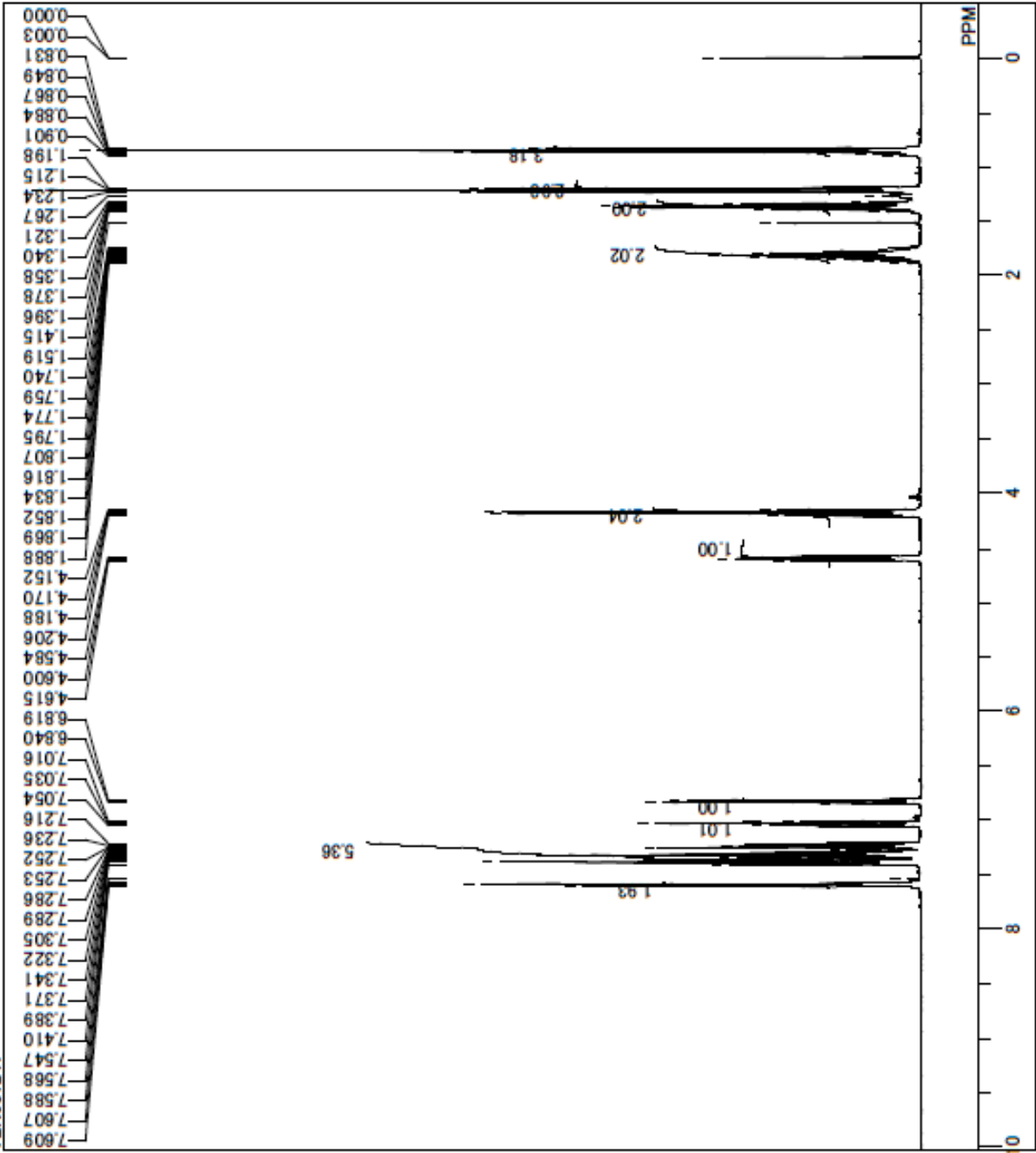
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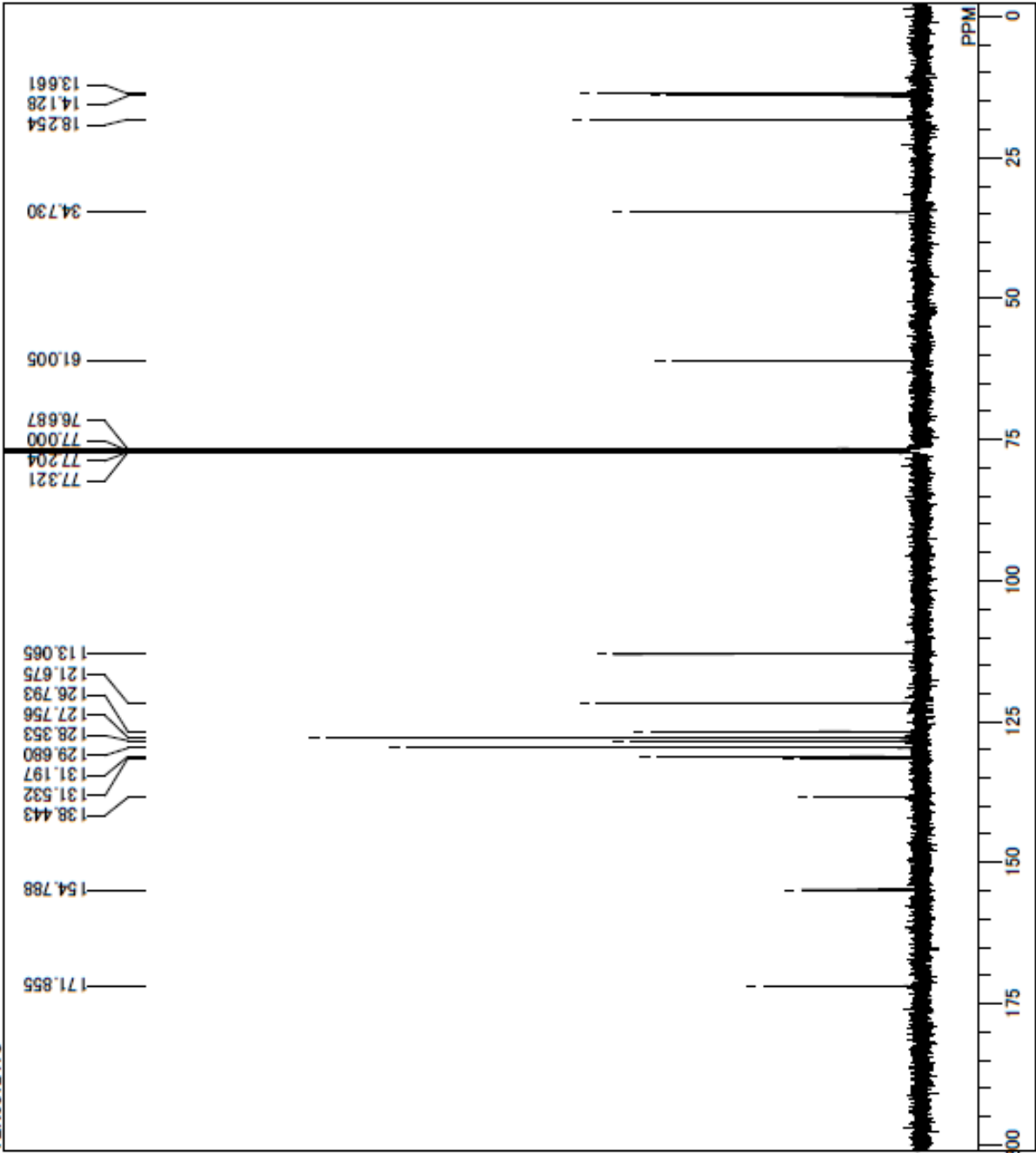


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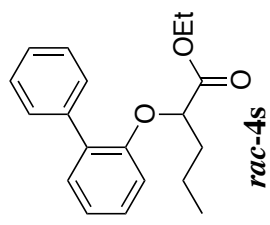
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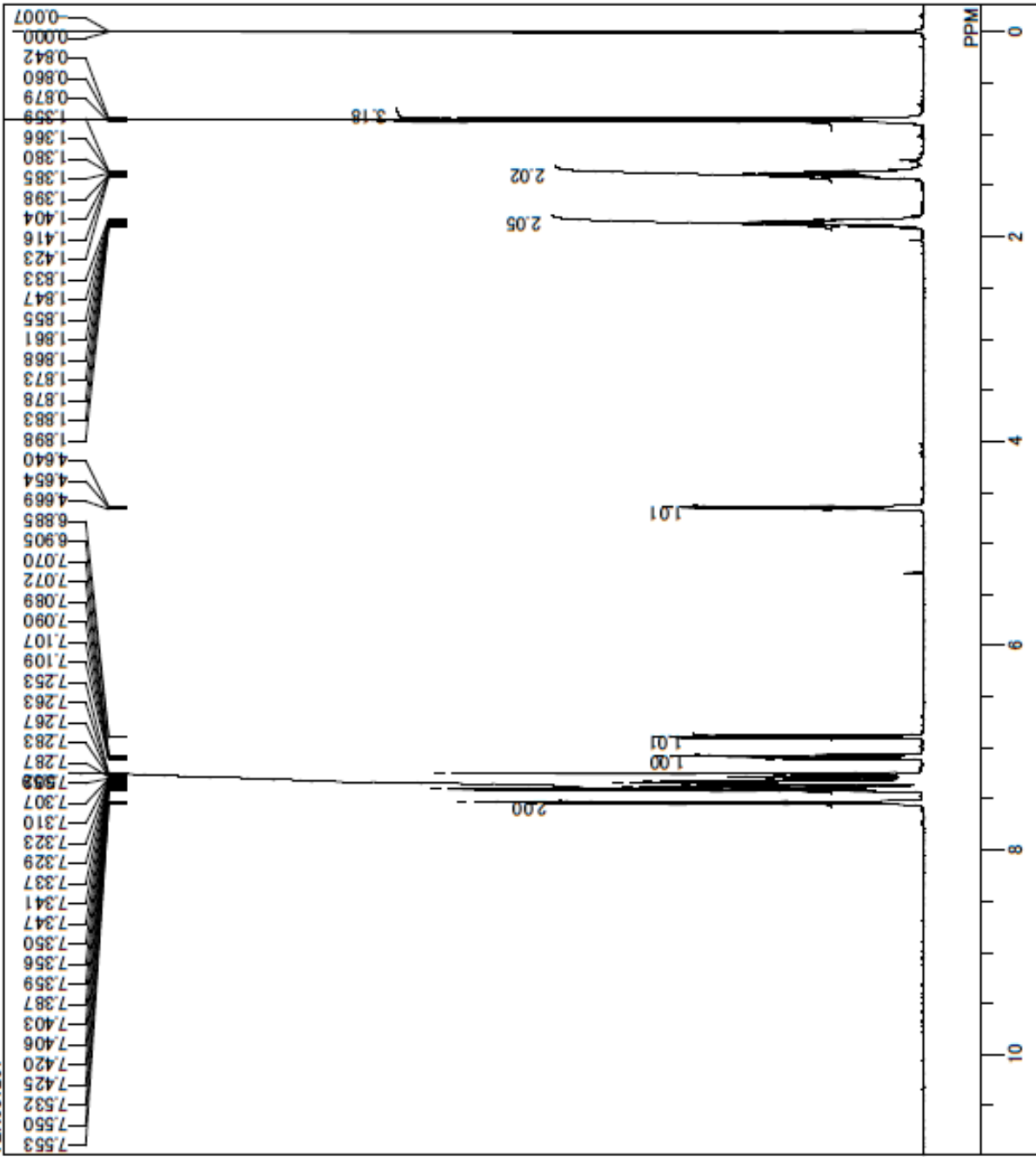


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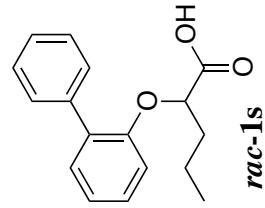


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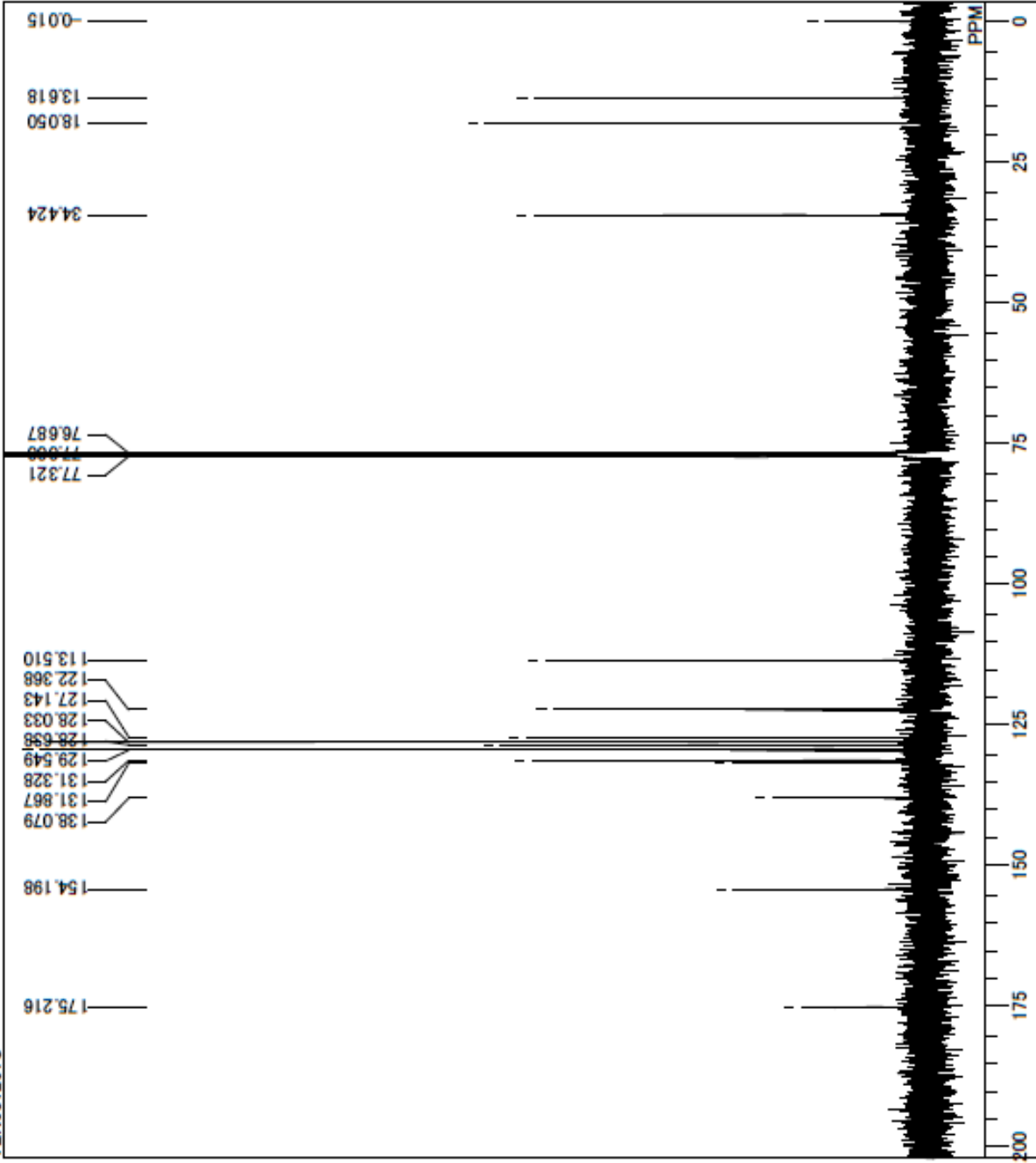


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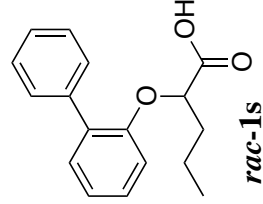


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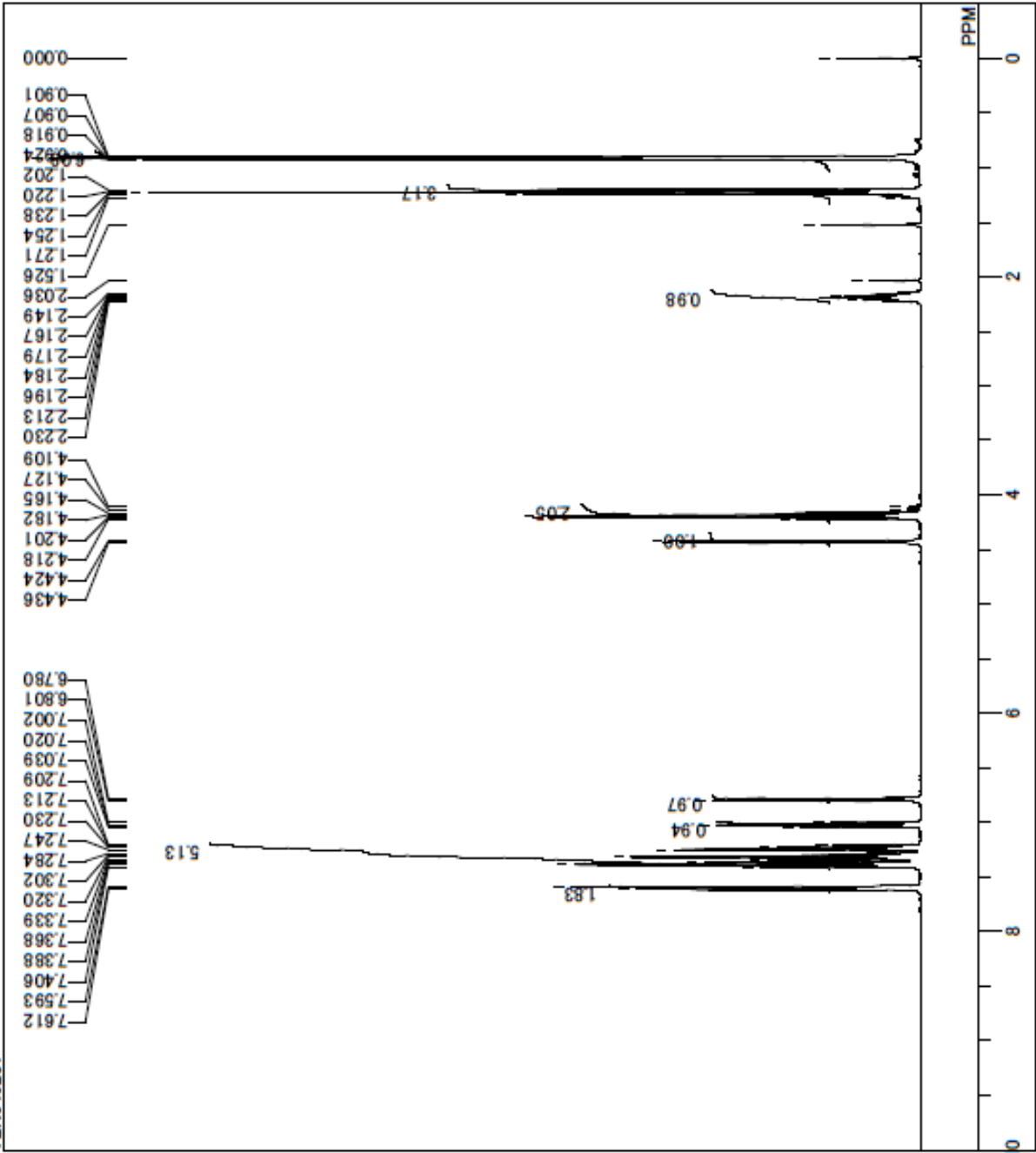


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IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator\予
TEN031261C
2011/Dec/10 01:53:33
13C
ZGPG30
100.63 MHz
0.00 KHz
10060.25 Hz
32768
24038.46 Hz
512
0.0000 sec
0.0000 sec
7.10 usec
OFF
30.9 c
CDCL3
77.00 ppm
0.25 Hz
57

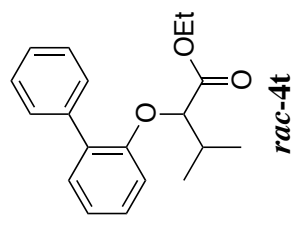


TEN040231

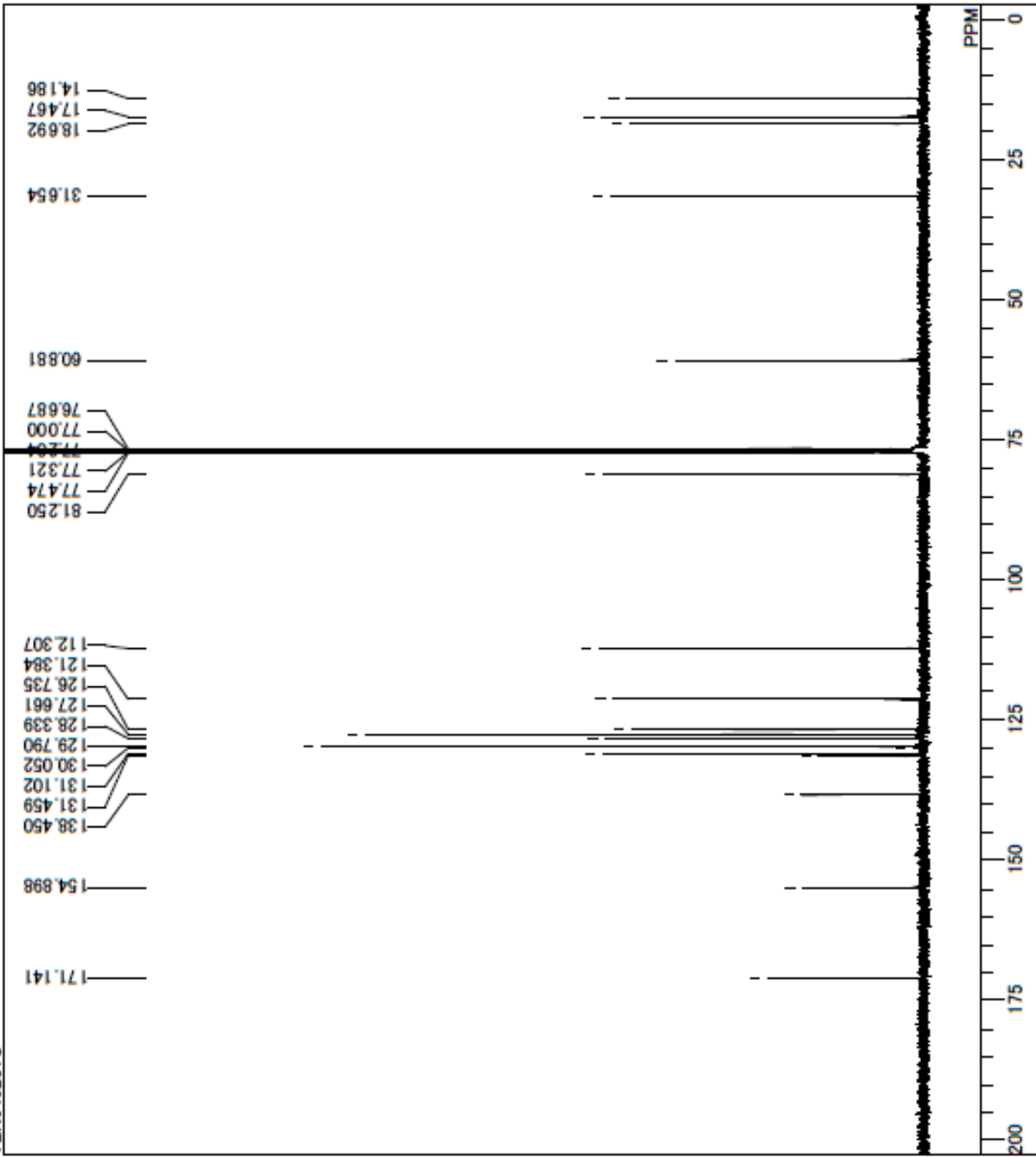


DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFREQ
OBSSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator\予
TEN040231
2012/Jan/23 00:57:00
IH
ZG30
400.18 MHz
0.00 KHz
2478.60 Hz
32768
8223.68 Hz
16
0.0000 sec
0.0000 sec
13.00 usec
OFF
29.9 c
CDCL3
0.00 ppm
0.25 Hz
228

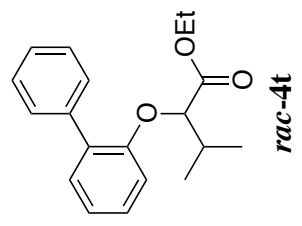


TEN040231C

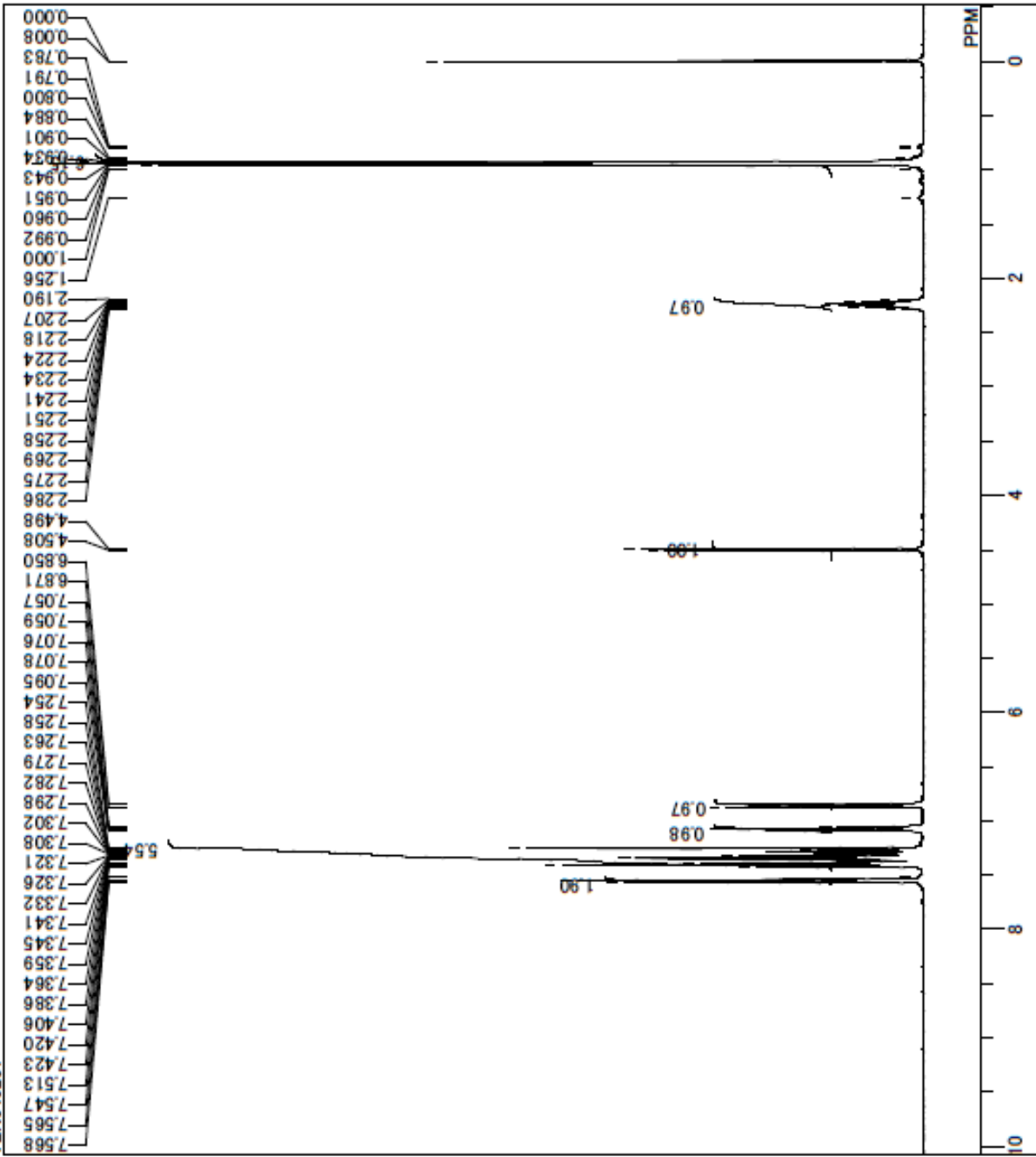


DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREOU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator\予
TEN040231C
2012/Jan/24 00:27:34
13C
ZGPG30
100.63 MHz
0.00 KHz
10060.25 Hz
32768
24038.46 Hz
1024
0.0000 sec
0.0000 sec
7.10 usec
OFF
30.9 c
CDCL3
77.00 ppm
0.25 Hz
64

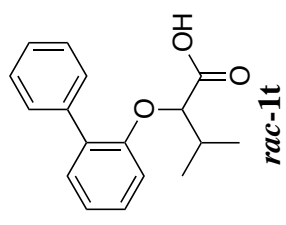


TEN040251



DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFREQ
OBSSET
OBFIN
POINT
FREOU
SCANS
ACQTM
PD
PWI
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator\...
TEN040251
2012/Jan/23 11:31:17
IH
ZG30
400.18 MHz
0.00 KHz
2478.60 Hz
32768
8223.68 Hz
16
0.0000 sec
0.0000 sec
13.00 usec
OFF
30.9 c
CDCL3
0.00 ppm
0.25 Hz
512

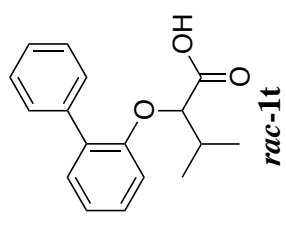


C:\Documents and Settings\Administrator\...

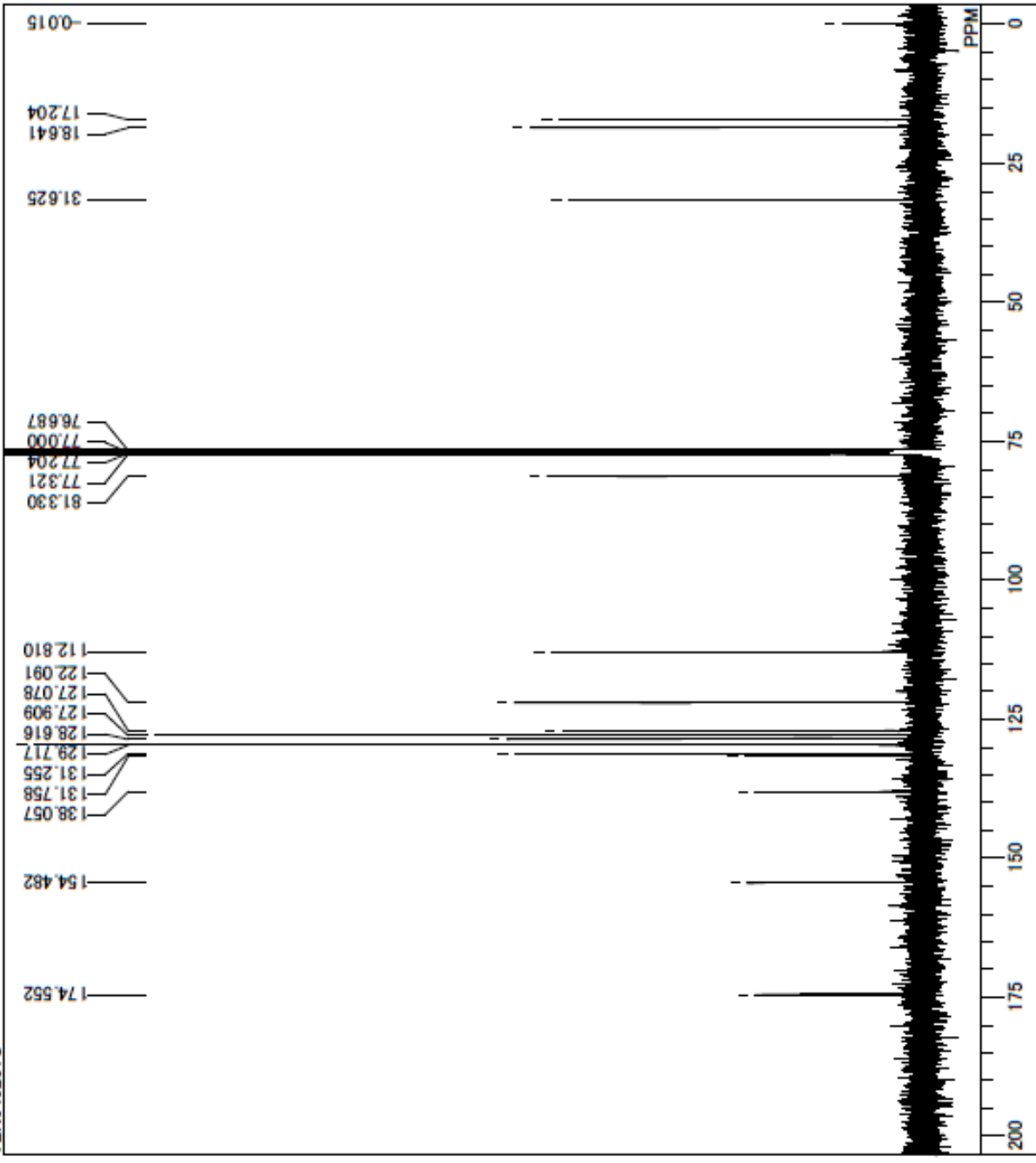
TEN040251C
2012/Jan/23 23:22:15

13C
ZGPG30
100.63 MHz
0.00 KHz
10060.25 Hz
32768
24038.46 Hz
1024
0.0000 sec
0.0000 sec
7.10 usec
OFF
29.9 c
CDCL3
77.00 ppm
0.25 Hz
64

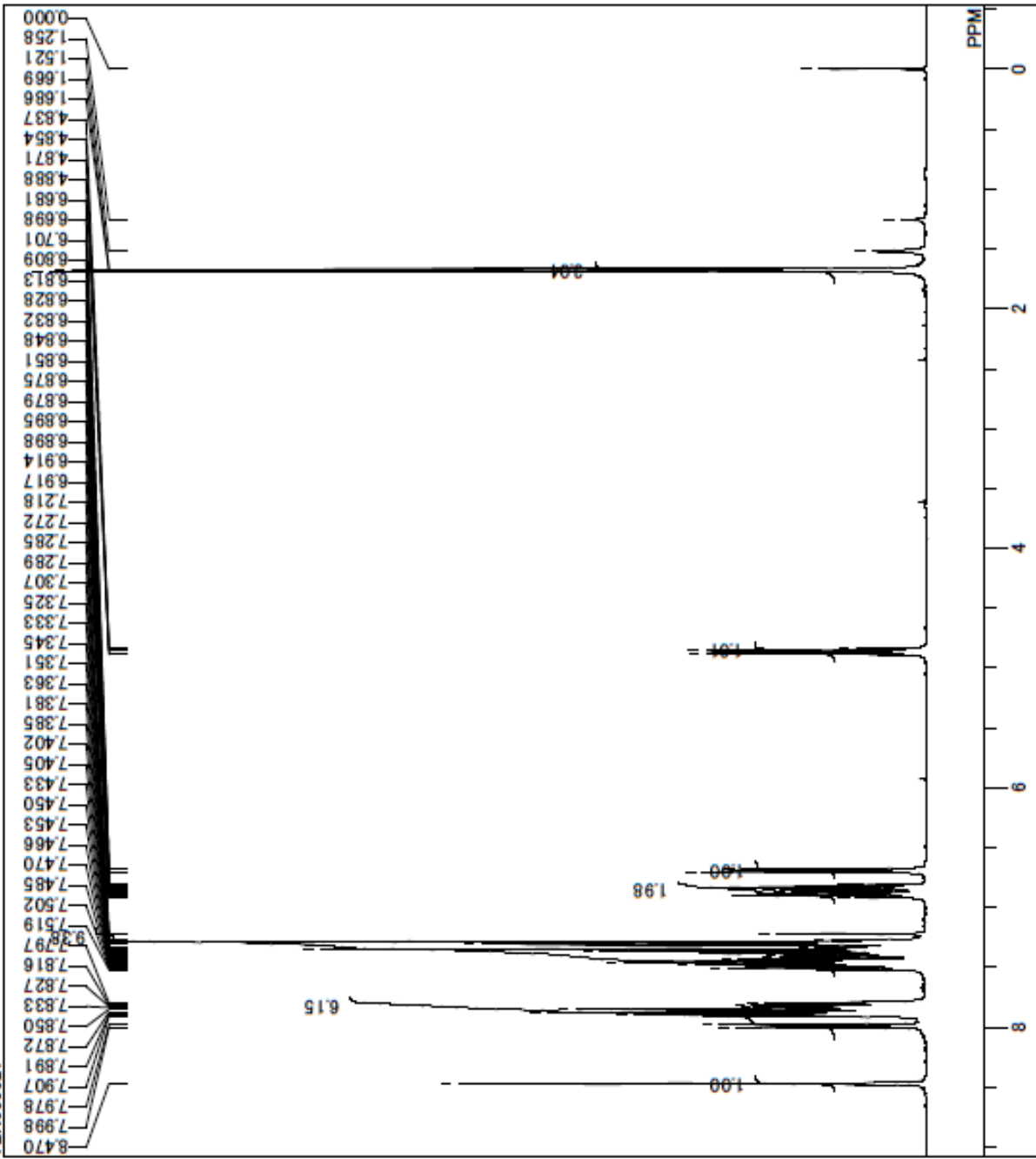
DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFREQ
OBSET
OBFIN
POINT
FREOU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN



TEN040251C

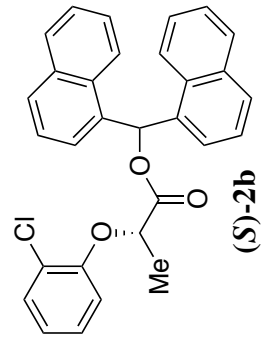


TEN050621

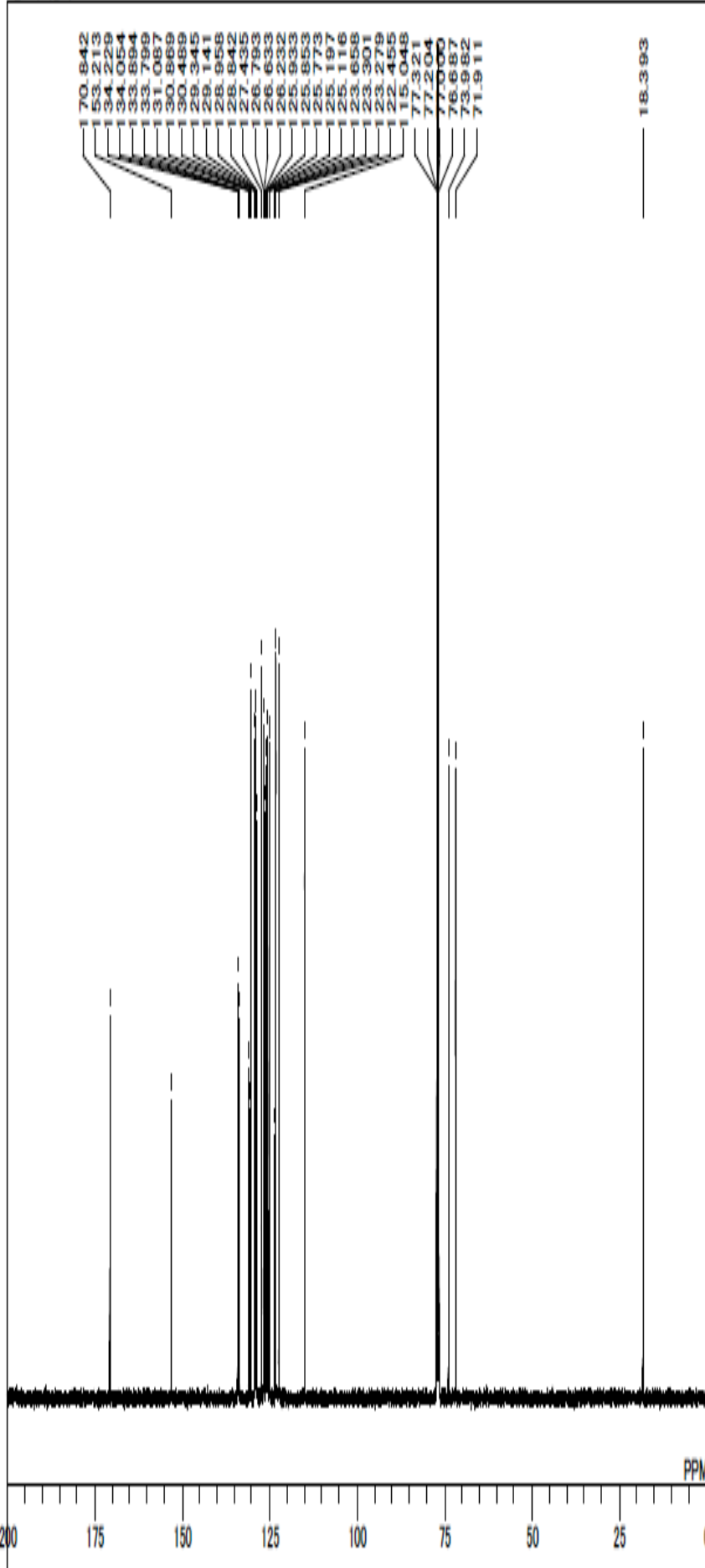


DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFREQ
OBSETE
OBFIN
POINT
FREOU
SCANS
ACQTM
PD
PWI
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator\...
TEN050621
2012/May/28 21:13:13
IH
ZG30
400.18 MHz
0.00 KHz
2478.60 Hz
32768
8223.68 Hz
16
0.0000 sec
0.0000 sec
13.00 usec
OFF
29.9 c
CDCL3
0.00 ppm
0.25 Hz
101



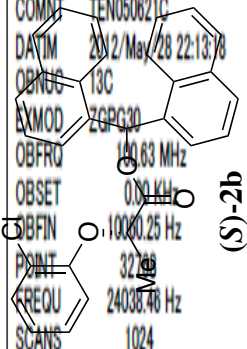
TEN050821C



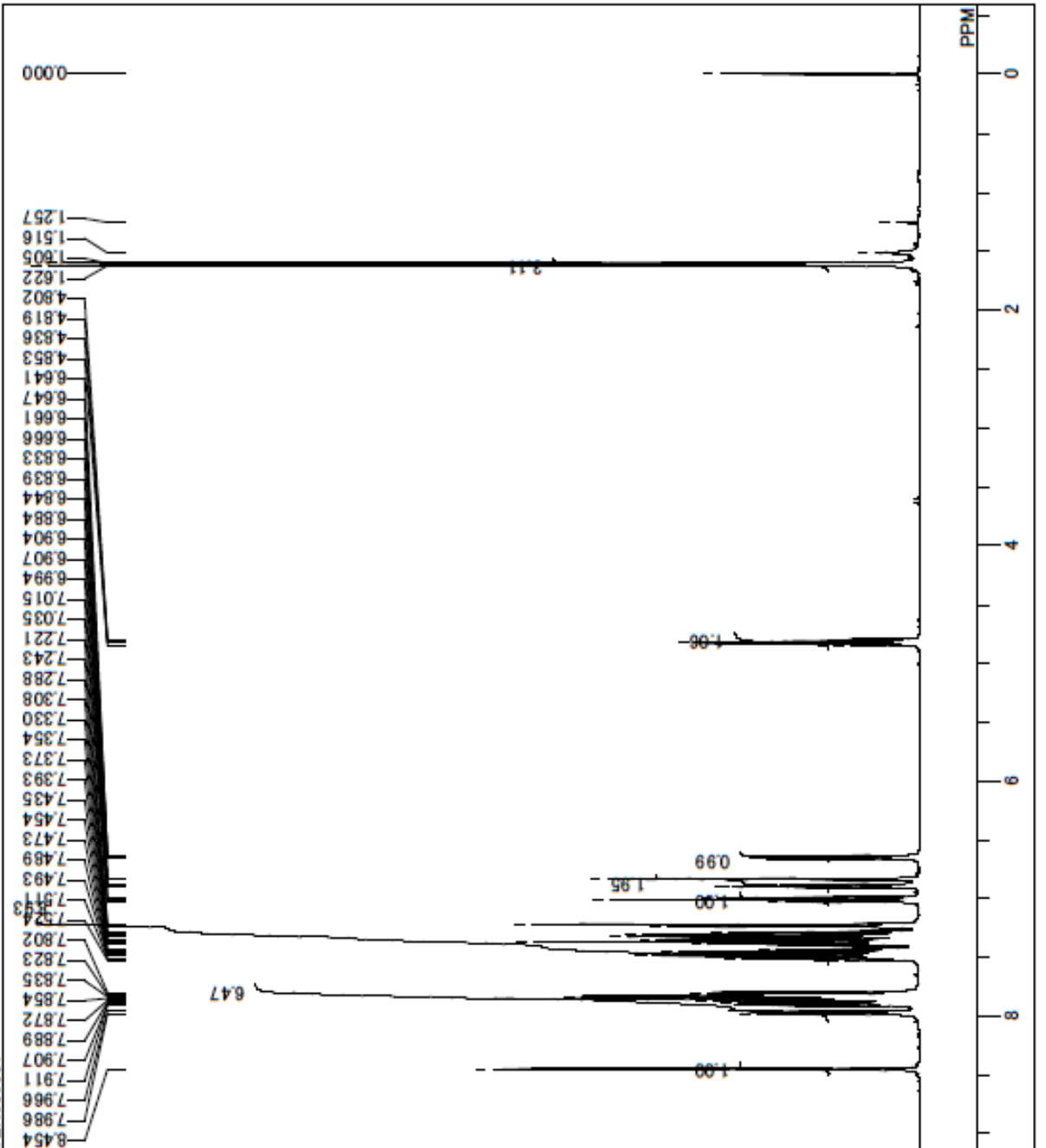
70.842
53.213
34.229
34.054
33.894
33.799
31.087
30.869
29.489
29.345
28.958
28.842
27.435
26.793
26.633
26.232
25.933
25.853
25.773
25.197
25.116
23.859
23.591
23.279
22.455
15.048
77.321
77.204
77.000
76.687
73.982
71.911

18.393

DFILE C:\Documents and Settings\Administrator\T
COMNT TEN050821C
DAYM 29/2/May/28 22:13:78
OBNUC 13C
EXMOD ZGPG30
OBFRQ 100.63 MHz
OBSET 0.000 MHz
SFBIN 10000.25 Hz
POINT 327
FREQU 24038.48 Hz
SCANS 1024
ACOTM 0.0000 sec
PD 0.0000 sec
PW1 7.10 usec
IRNUC OFF
CTEMP 29.9 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.25 Hz
RGAIN 382

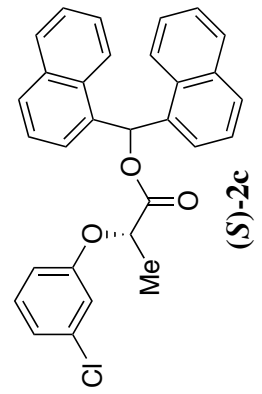


TEN050631

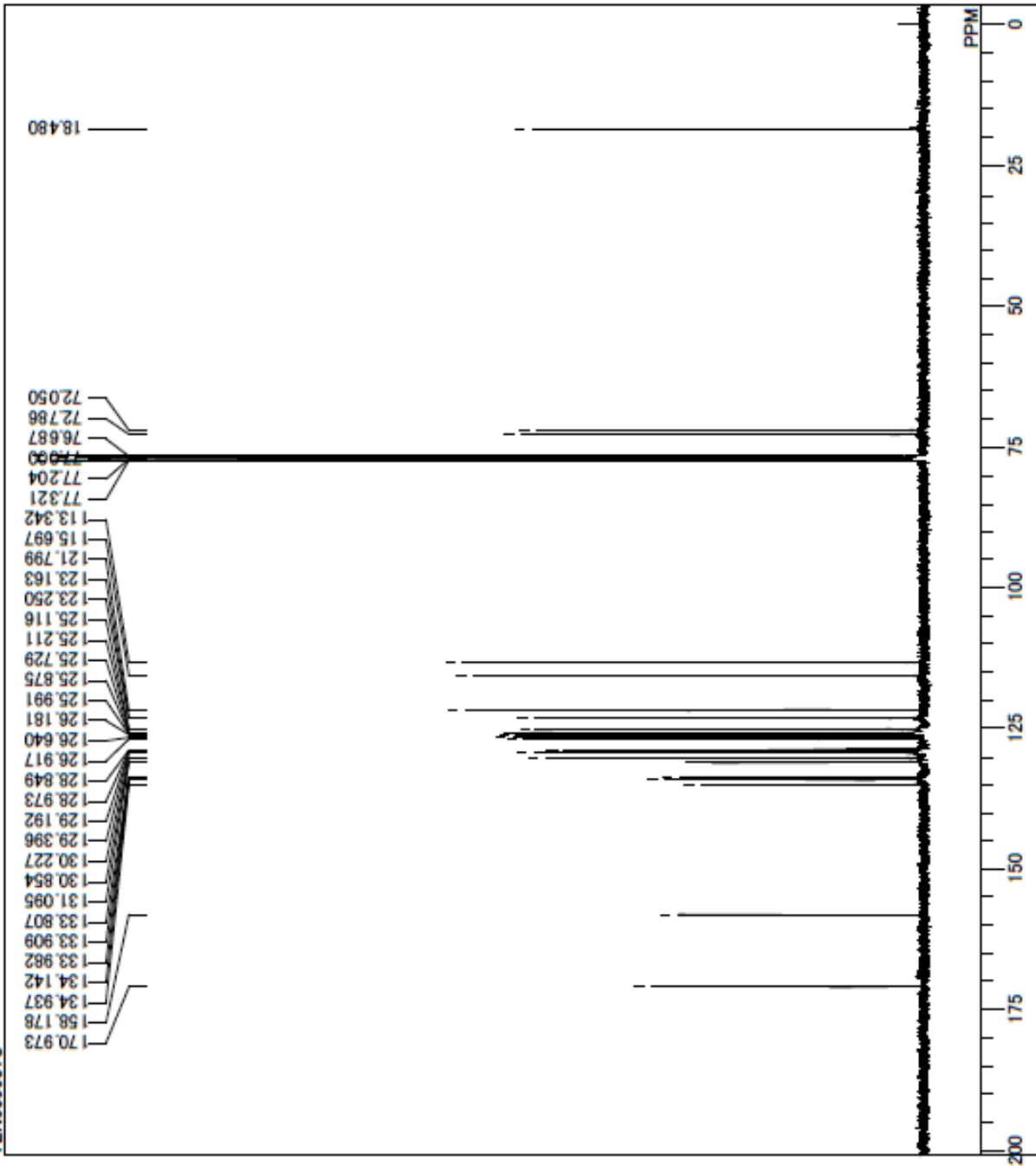


DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREOU
SCANS
ACQTM
PD
PWI
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator\7;
TEN050631
2012/May/28 22:20:53
IH
ZG30
400.18 MHz
0.00 KHz
2478.60 Hz
32768
8223.68 Hz
16
0.0000 sec
0.0000 sec
13.00 usec
OFF
29.9 c
CDCL3
0.00 ppm
0.25 Hz
181

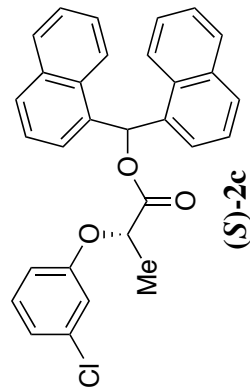


TEN050631C



DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREOU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

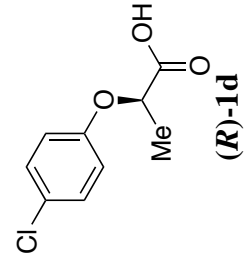
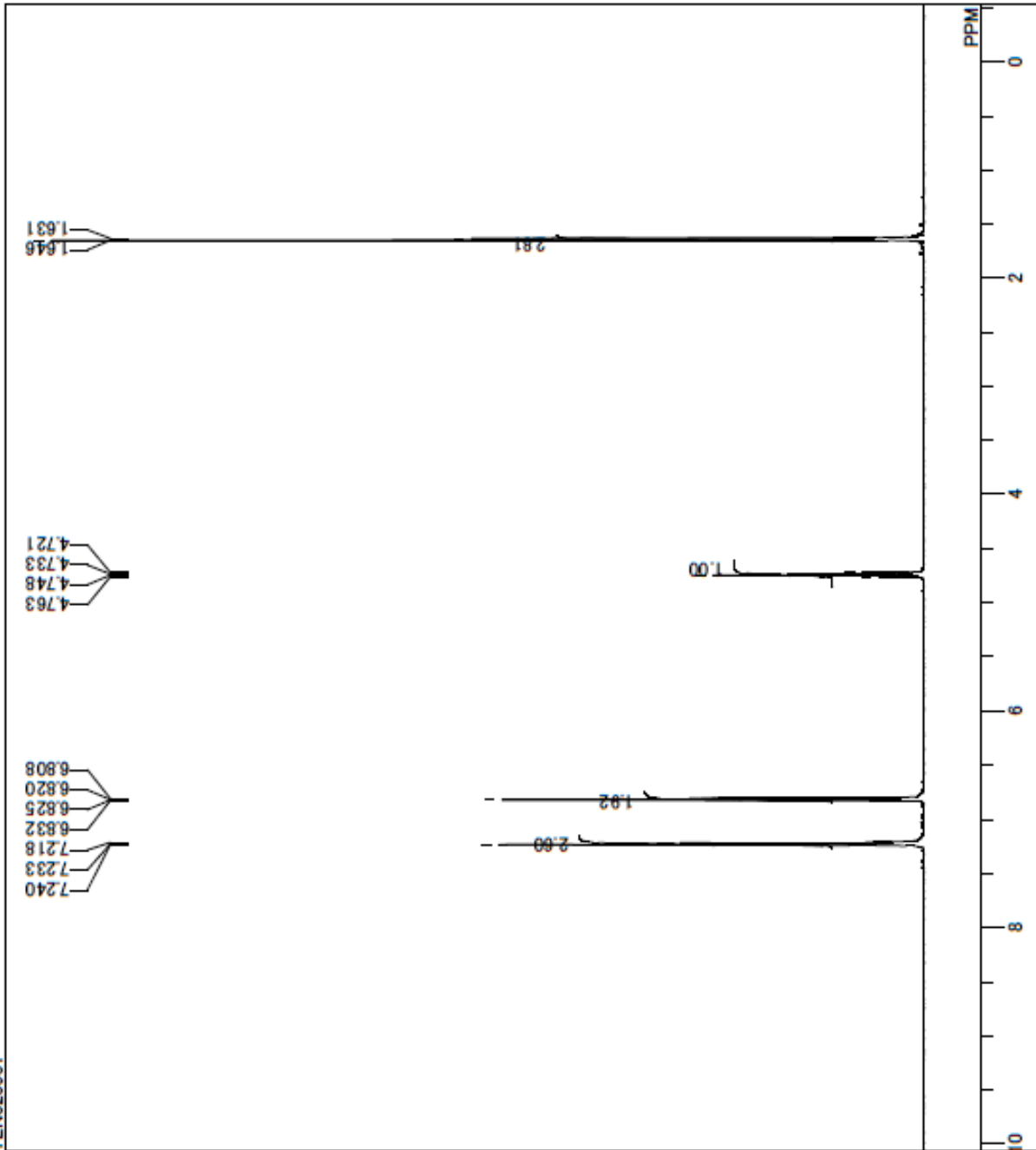
C:\Documents and Settings\Administrator\予;
TEN050631C
2012/May/28 23:21:34
13C
ZGPG30
100.63 MHz
0.00 KHz
10060.25 Hz
32768
24038.46 Hz
1024
0.0000 sec
0.0000 sec
7.10 usec
OFF
29.9 c
CDCL3
77.00 ppm
0.25 Hz
64



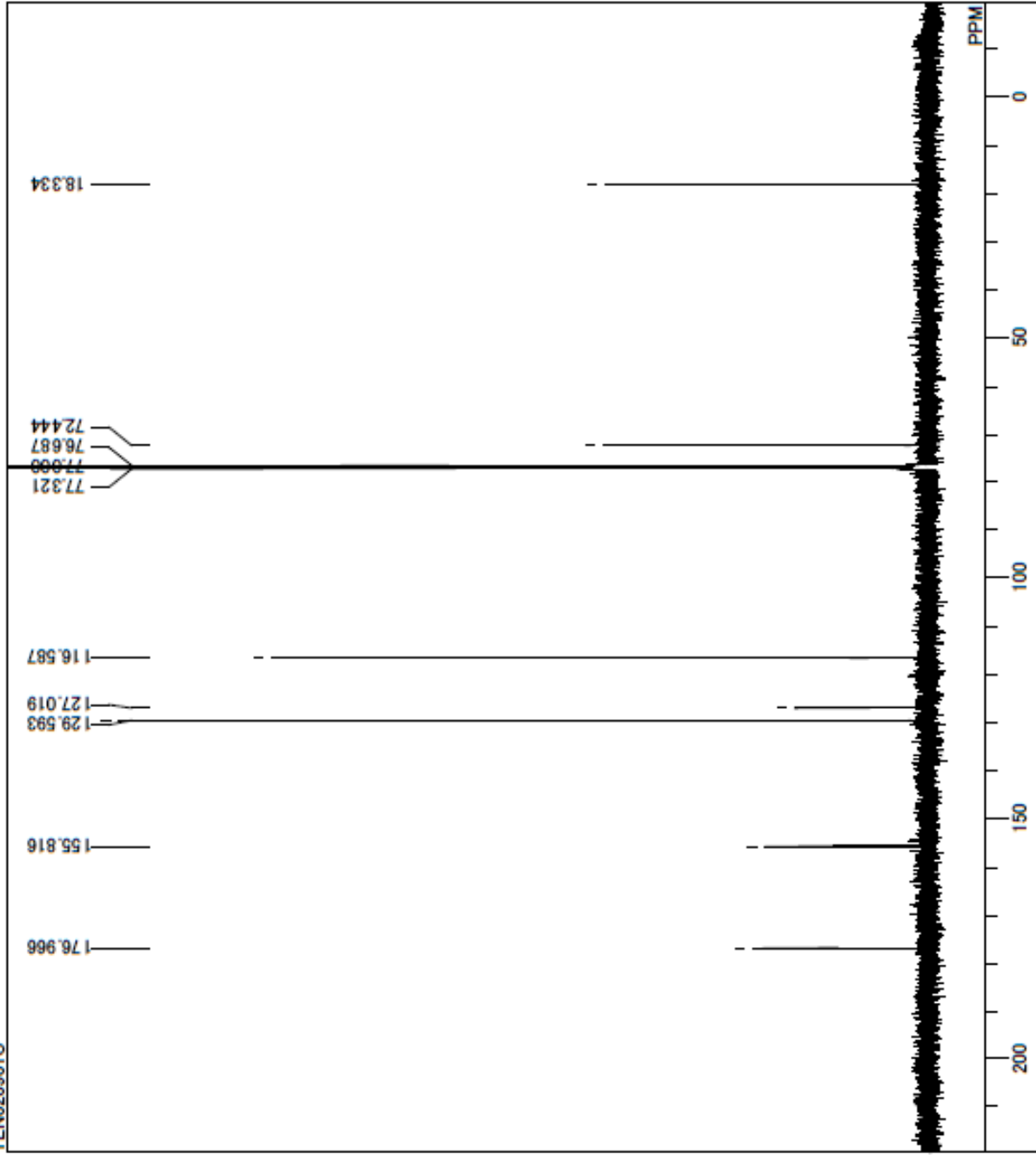
TEN020901

DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREOU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator\予
TEN020901
Fri Sep 16 14:21:49 2011
IH
non
500.00 MHz
0.00 KHz
162160.00 Hz
8192
10000.00 Hz
16
0.8192 sec
6.1808 sec
6.20 usec
IH
27.0 c
CDCL3
7.24 ppm
0.12 Hz
25



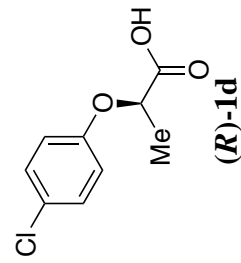
TEN020901C



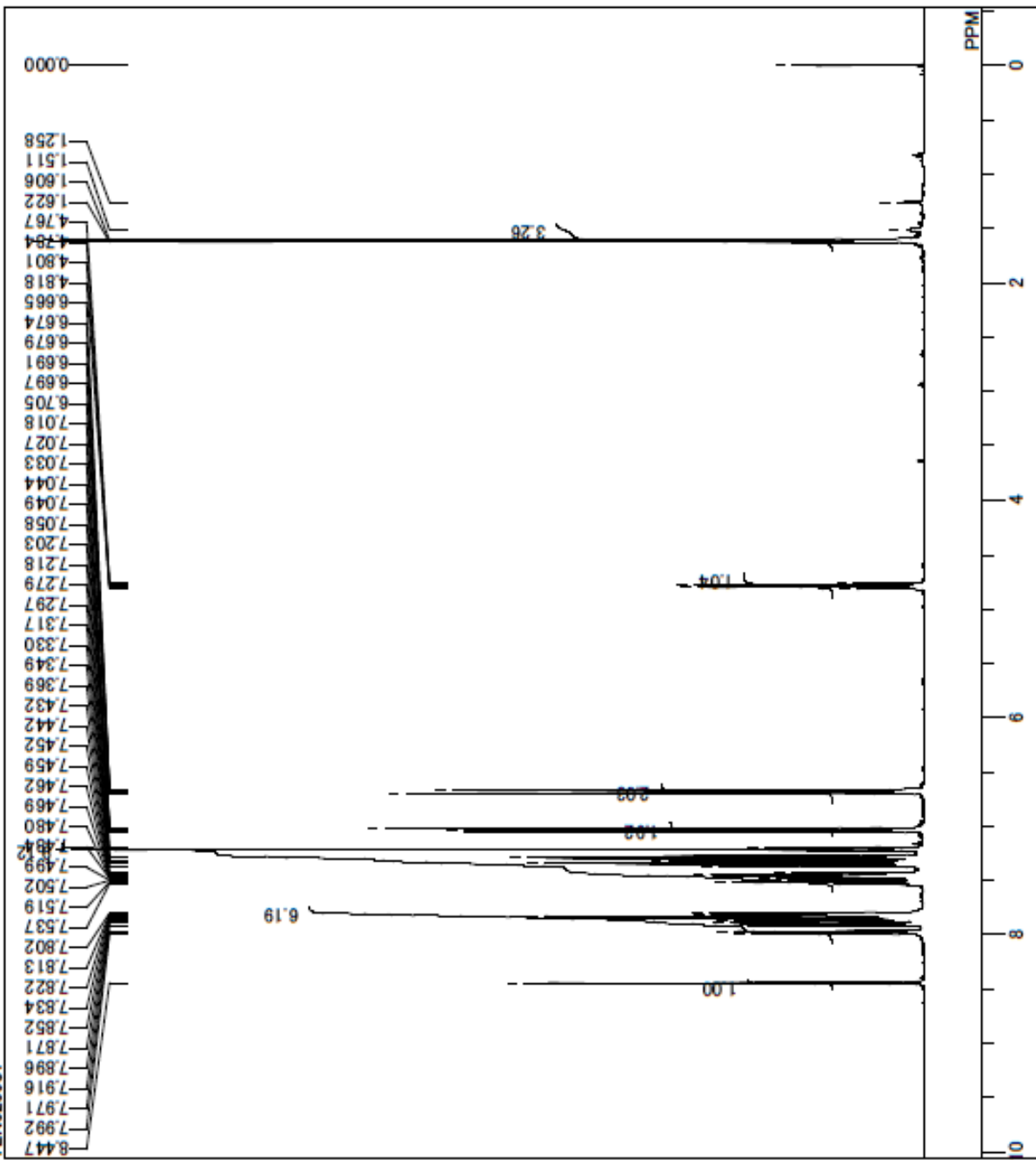
DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREOU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator\予,
TEN020901C
2011/Dec/17 02:24:01
13C
ZGPG30

100.63 MHz
0.00 KHz
10060.25 Hz
32768
24038.46 Hz
512
0.0000 sec
0.0000 sec
7.10 usec
OFF
29.9 c
CDCL3
77.00 ppm
0.25 Hz
64



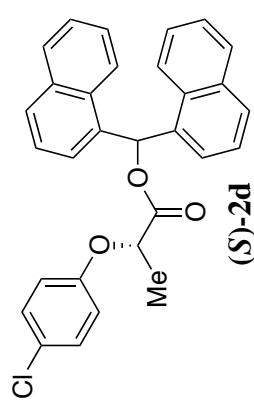
TEN020981



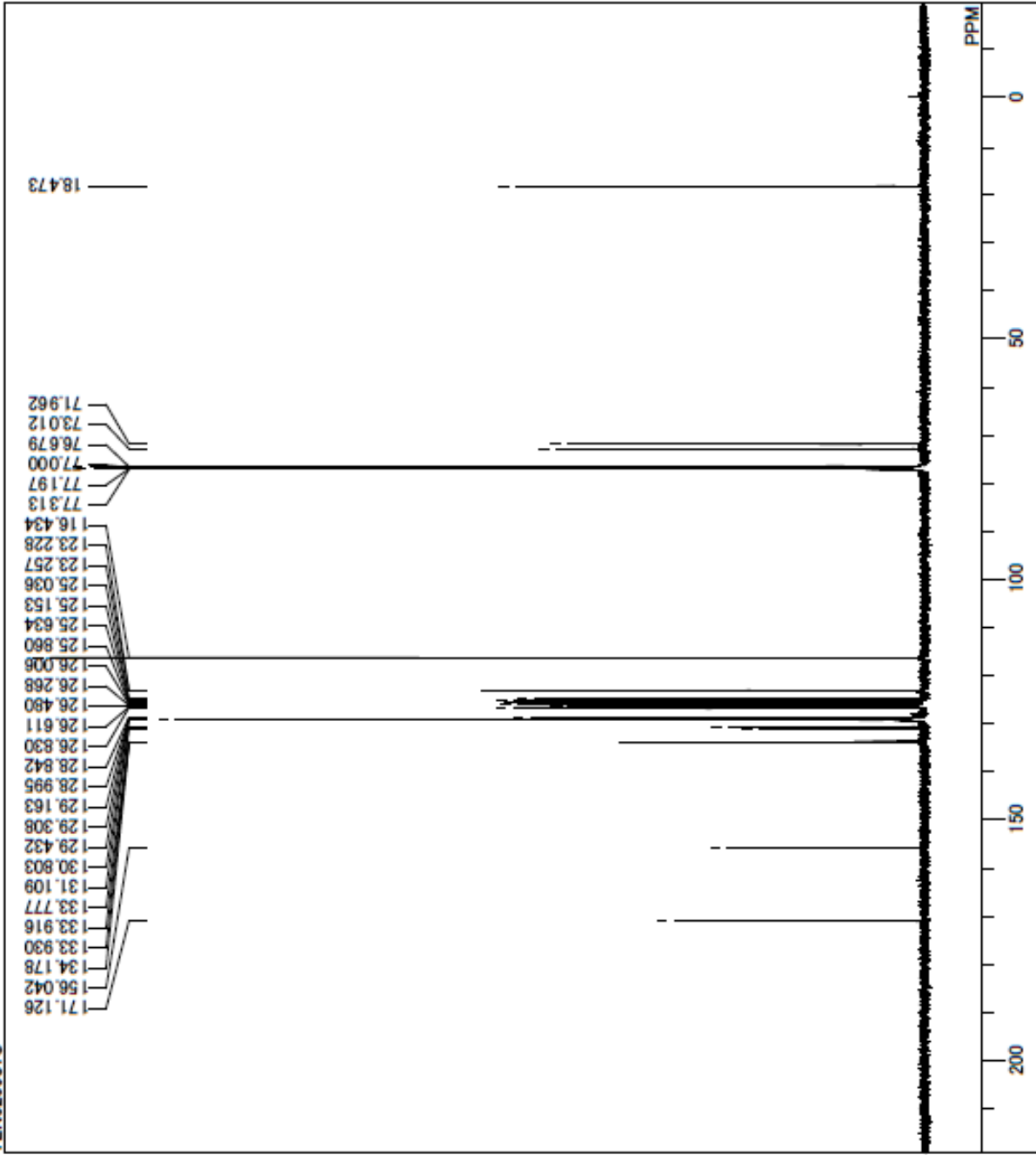
DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREOU
SCANS
ACQTM
PD
PWI
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator\予
TEN020981
2012/May/26 04:38:23
1H
ZG30

400.18 MHz
0.00 KHz
2478.60 Hz
32768
8223.68 Hz
16
0.0000 sec
0.0000 sec
13.00 usec
OFF
29.9 c
CDCL3
0.00 ppm
0.25 Hz
101



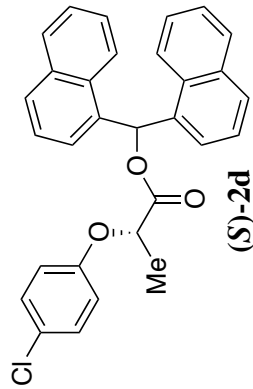
TEN020981C



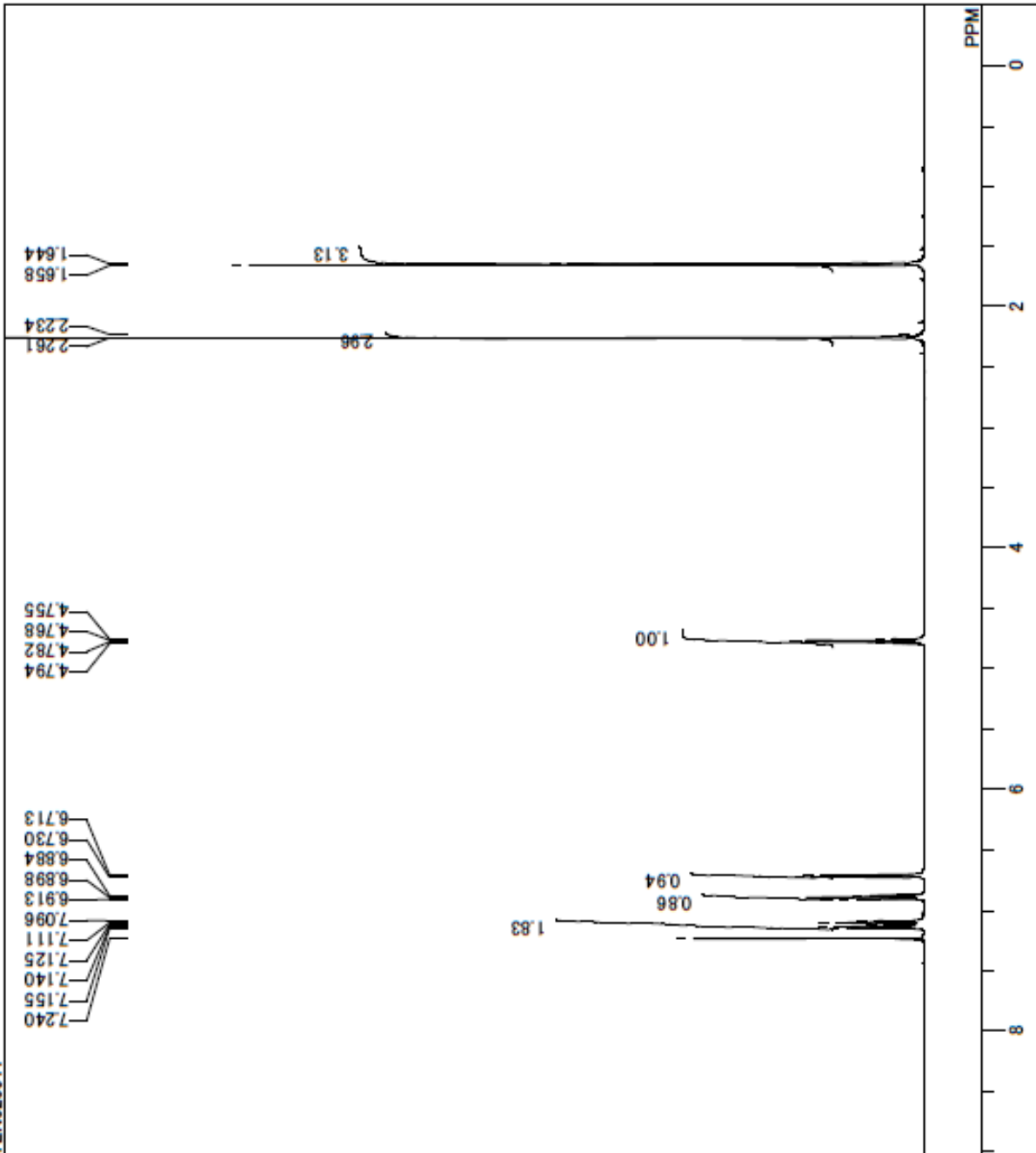
DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREOU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator\予
TEN020981C
2012/May/27 22:28:50
13C

ZGPG30
100.63 MHz
0.00 KHz
10060.25 Hz
32768
24038.46 Hz
1024
0.0000 sec
0.0000 sec
7.10 usec
OFF
29.9 c
CDCL3
77.00 ppm
0.25 Hz
406

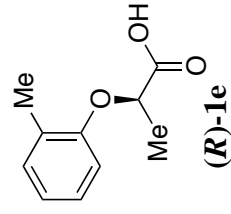


TEN020911

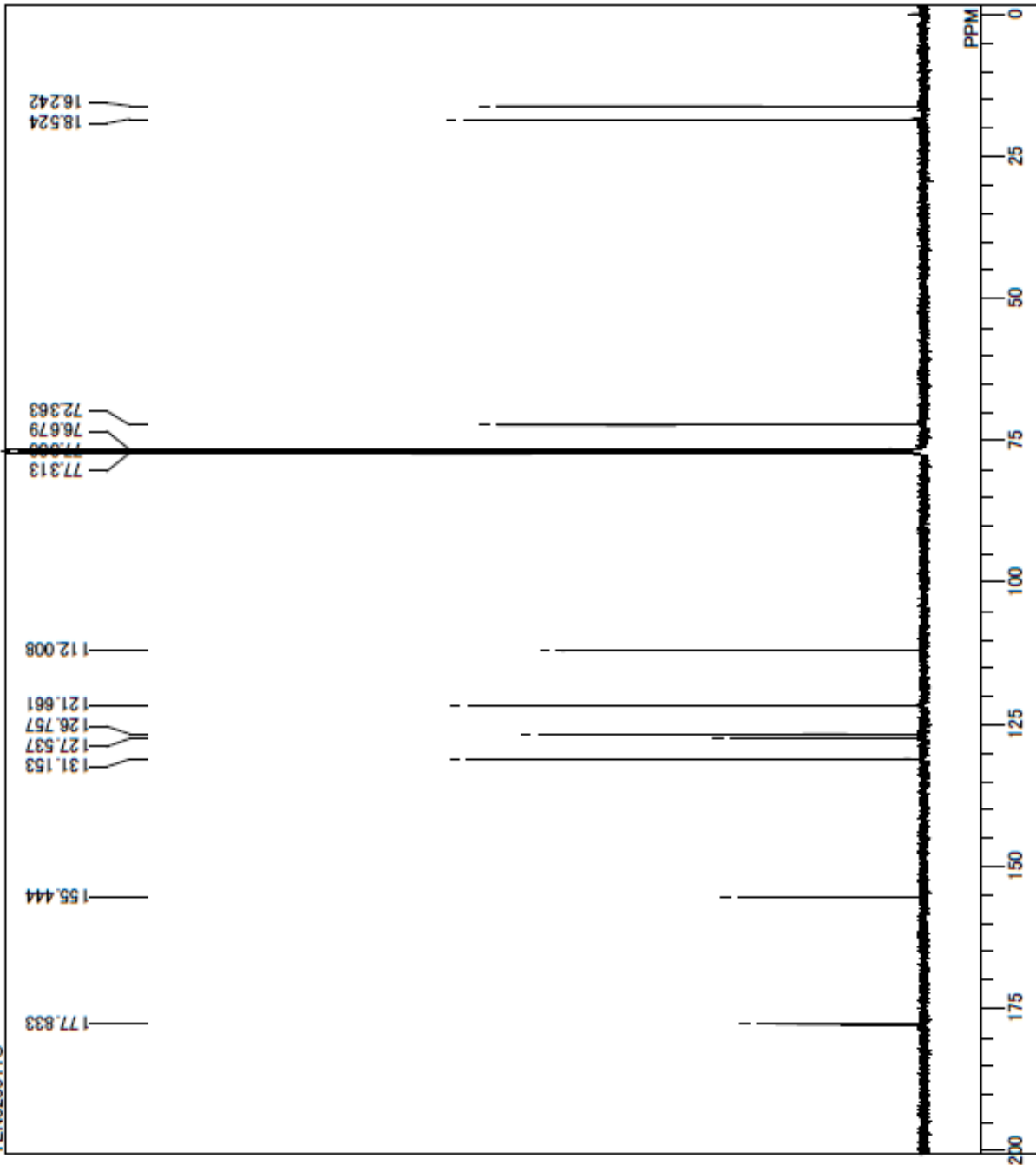


DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREOU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator*子*
TEN020911
Fri Sep 16 14:29:03 2011
1H
non
500.00 MHz
0.00 KHz
162160.00 Hz
8192
10000.00 Hz
16
0.8192 sec
6.1808 sec
6.20 usec
1H
27.1 c
CDCL3
7.24 ppm
0.12 Hz
23

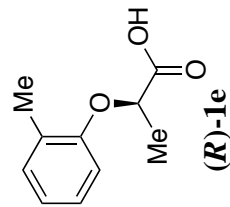


TEN020911C

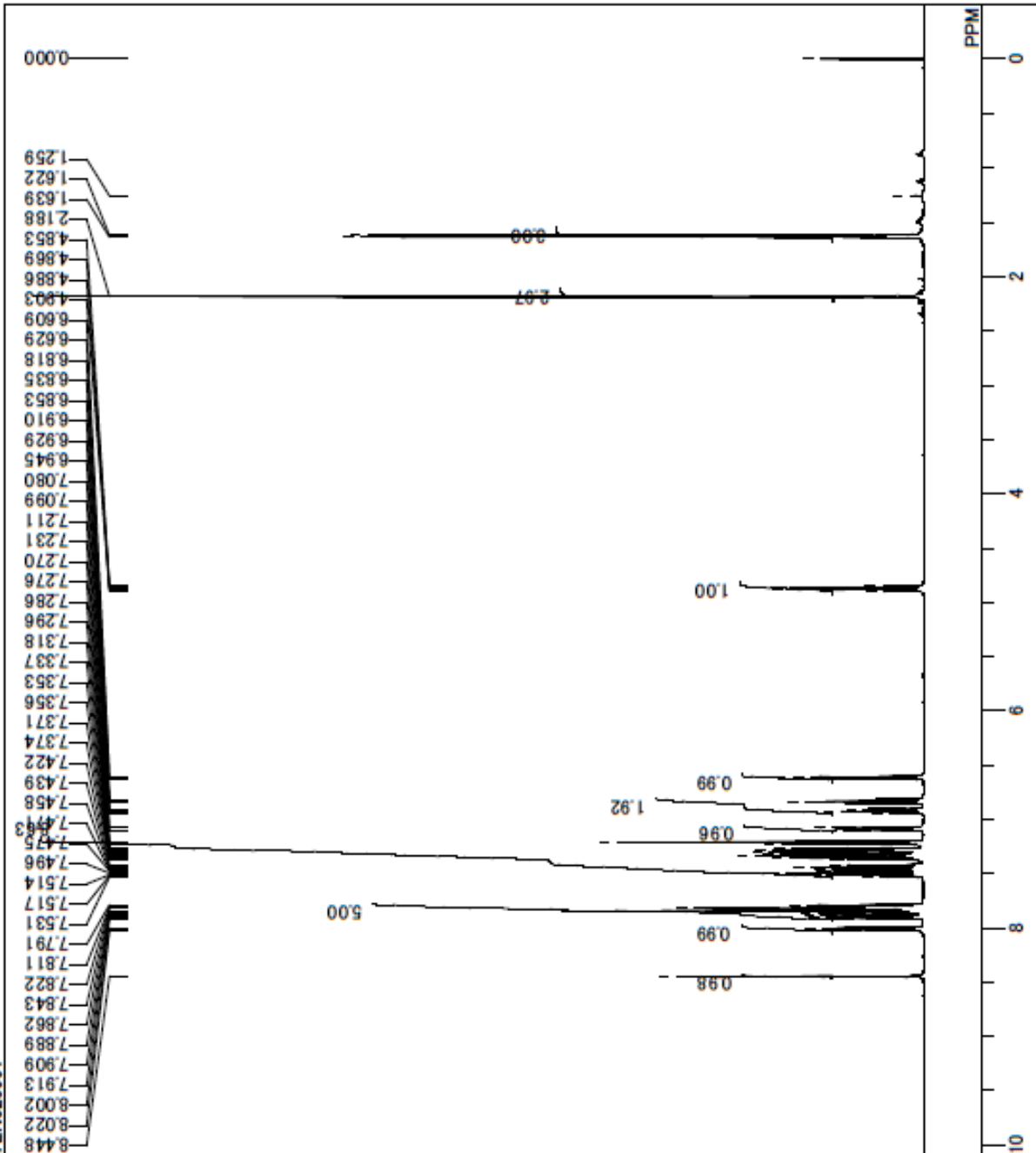


DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREOU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator\予
TEN020911C
2012/May/07 21:11:56
13C
ZGPG30
100.63 MHz
0.00 KHz
10060.25 Hz
32768
24038.46 Hz
1024
0.0000 sec
0.0000 sec
7.10 usec
OFF
26.9 c
CDCL3
77.00 ppm
0.25 Hz
362

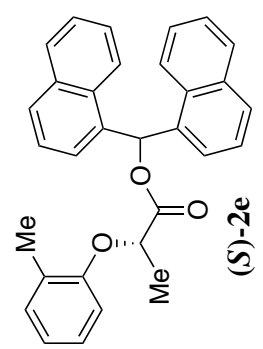


TEN020991

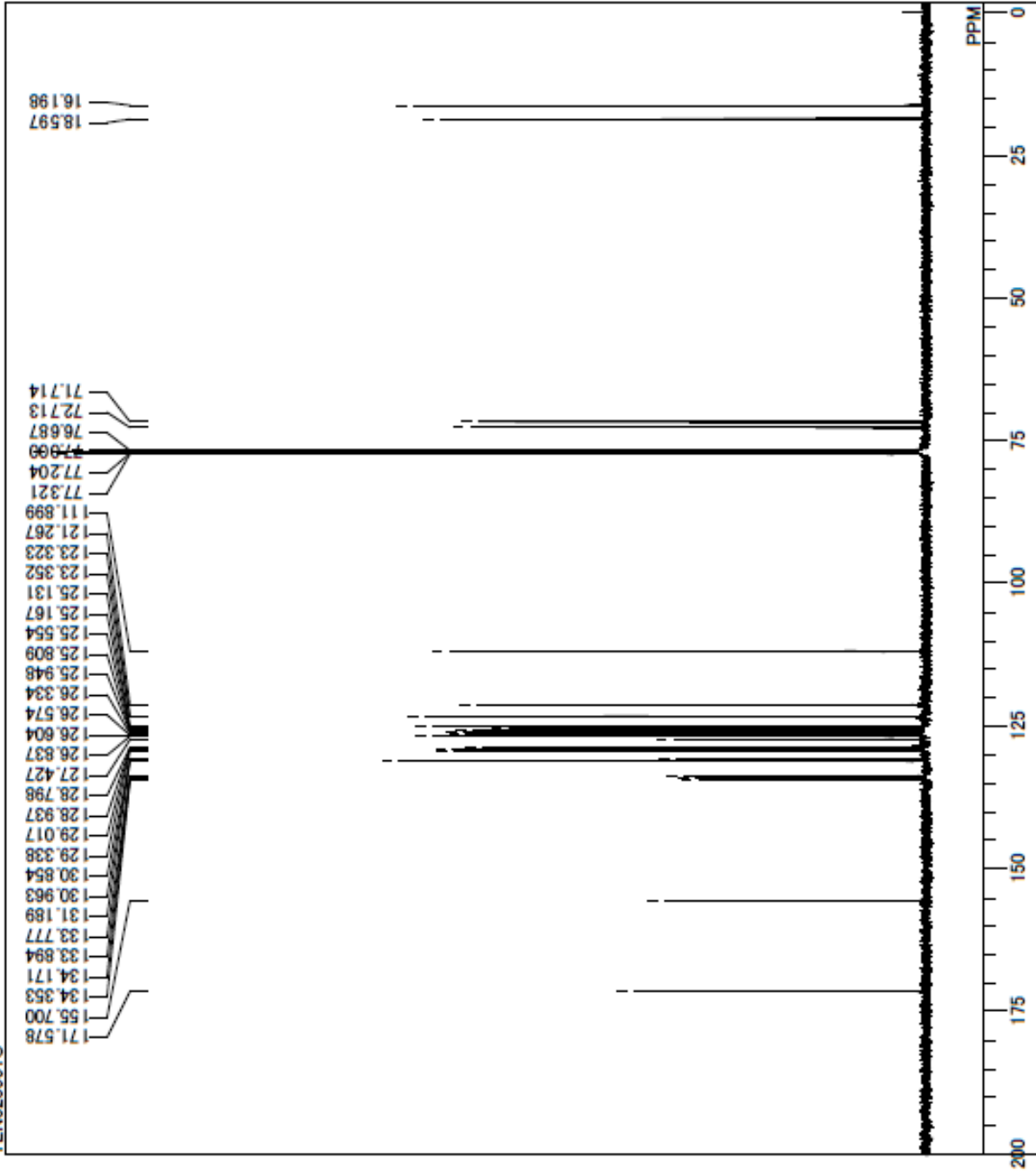


DFILE
 COMNT
 DATIM
 OBNUC
 EXMOD
 OBFREQ
 OBSET
 OBFIN
 POINT
 FREOU
 SCANS
 ACQTM
 PD
 PW1
 IRNUC
 CTEMP
 SLVNT
 EXREF
 BF
 RGAIN

C:\Documents and Settings\Administrator*
 TEN020991
 2012/May/26 04:45:40
 1H
 ZG30
 400.18 MHz
 0.00 KHz
 2478.60 Hz
 32768
 8223.68 Hz
 16
 0.0000 sec
 0.0000 sec
 13.00 usec
 OFF
 29.9 c
 CDCL3
 0.00 ppm
 0.25 Hz
 101

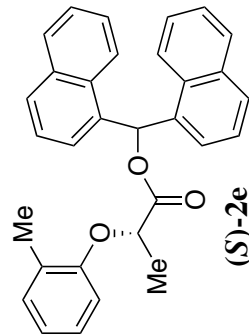


TEN020991C

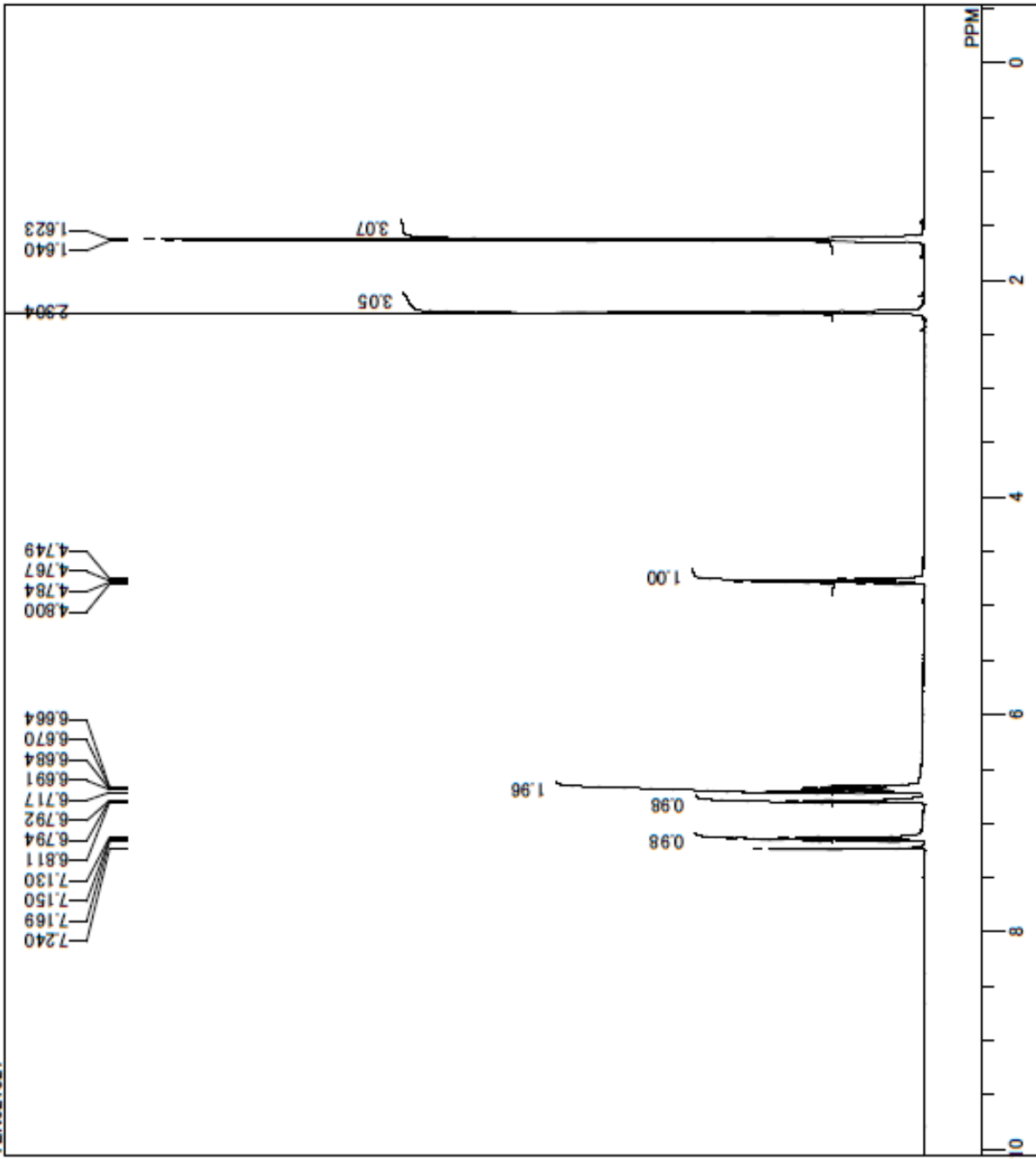


DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREOU
SCANS
ACQTM
PD
PWI
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator\予
TEN020991C
2012/May/27 23:34:23
13C
ZGPG30
100.63 MHz
0.00 KHz
10060.25 Hz
32768
24038.46 Hz
1024
0.0000 sec
0.0000 sec
7.10 usec
OFF
29.9 c
CDCL3
77.00 ppm
0.25 Hz
645

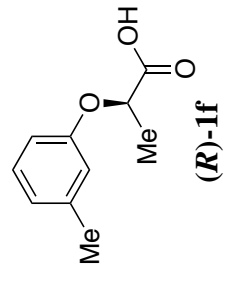


TEN021321

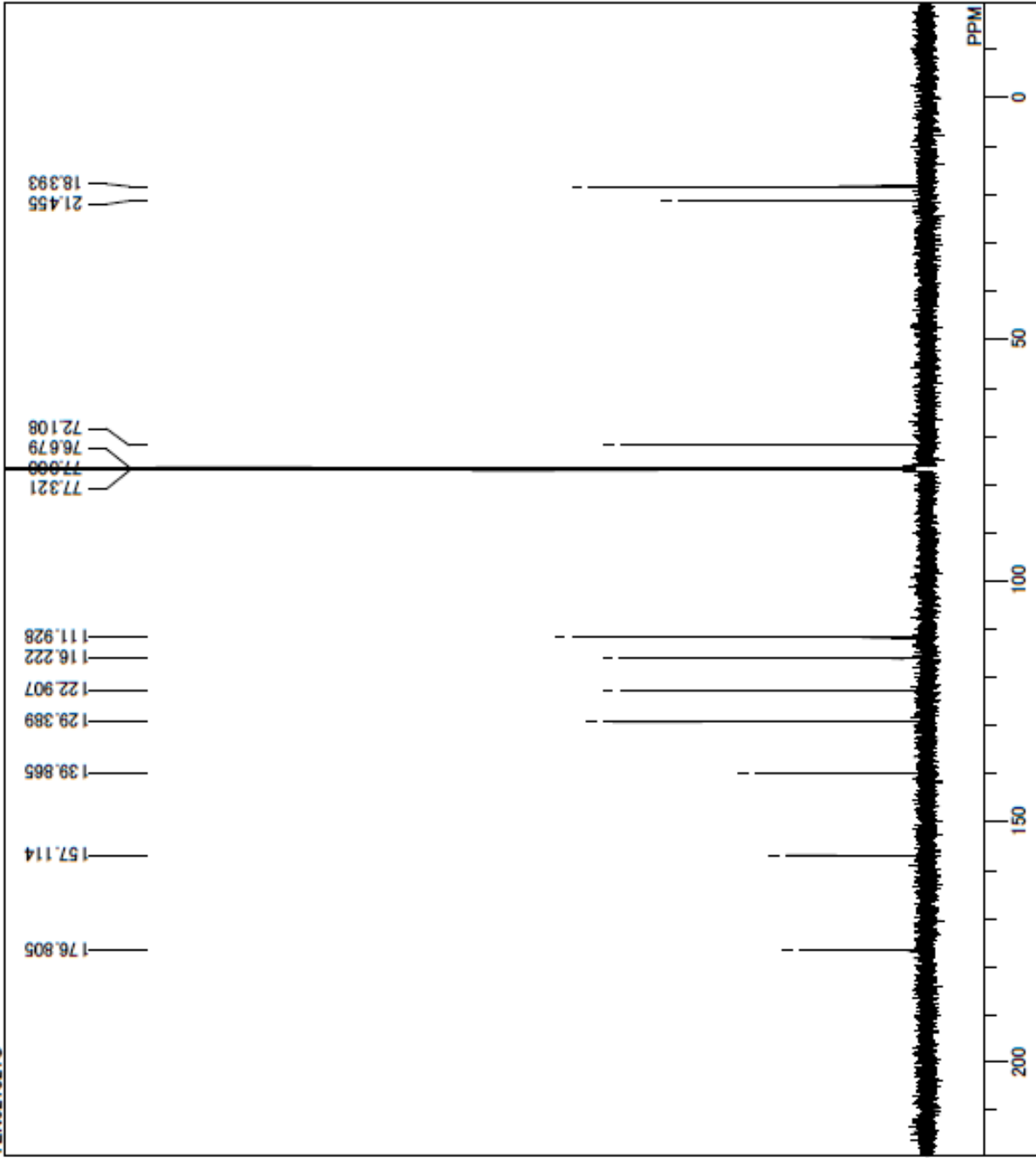


DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFREQ
OBSET
OBFIN
POINT
FREOU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator*
TEN021321
2011/Sep/30 06:05:26
1H
ZG30
400.18 MHz
0.00 KHz
2478.60 Hz
32768
8223.68 Hz
16
0.0000 sec
0.0000 sec
13.00 usec
OFF
30.9 c
CDCL3
7.24 ppm
0.25 Hz
406

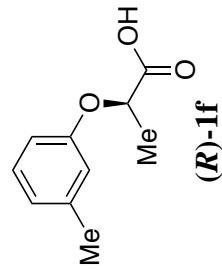


TEN021321C

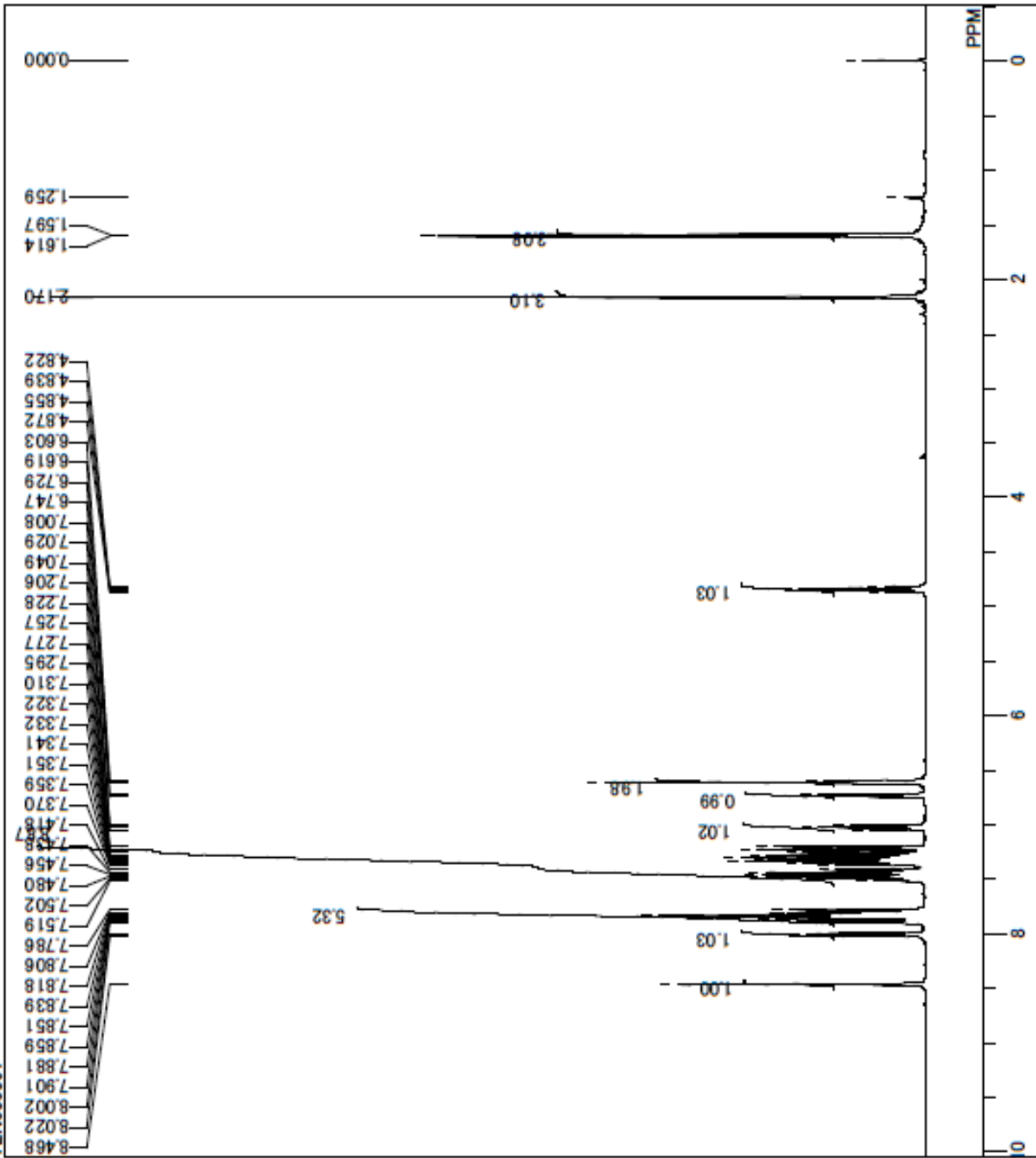


DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREOU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator*子*
TEN021321C
2011/Sep/30 23:59:13
13C
ZGPG30
100.63 MHz
0.00 KHz
10060.25 Hz
32768
24038.46 Hz
512
0.0000 sec
0.0000 sec
7.10 usec
OFF
29.9 c
CDCL3
77.00 ppm
0.25 Hz
57



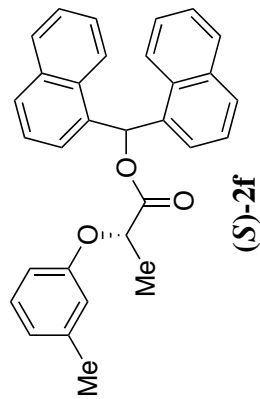
TEN050591



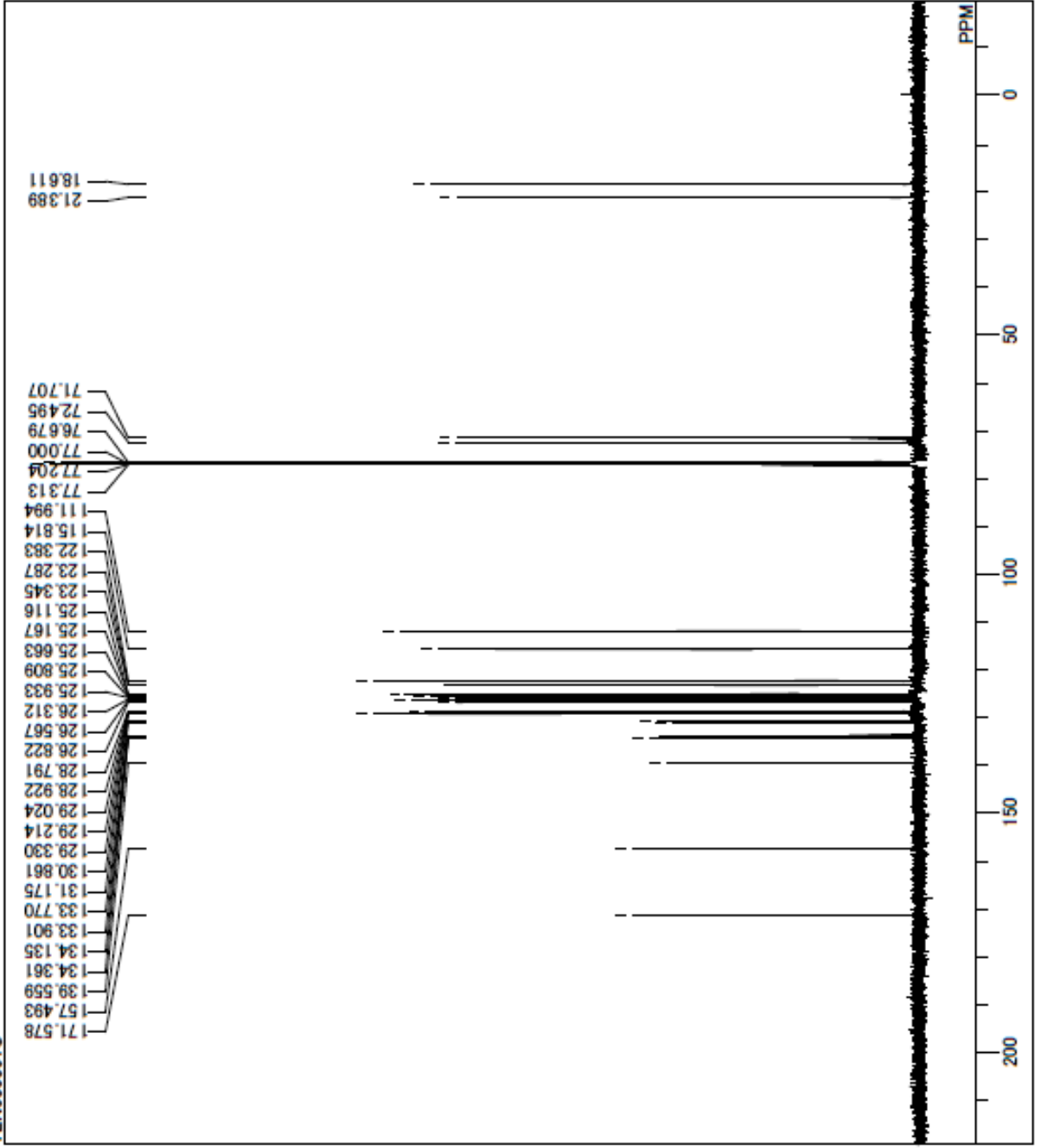
DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRO
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PWI
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator\予;
TEN050591
2012/May/24 04:19:47
1H
ZG30

400.18 MHz
0.00 KHz
2478.60 Hz
32768
8223.68 Hz
16
0.0000 sec
0.0000 sec
13.00 usec
OFF
29.9 c
CDCL3
0.00 ppm
0.25 Hz
90

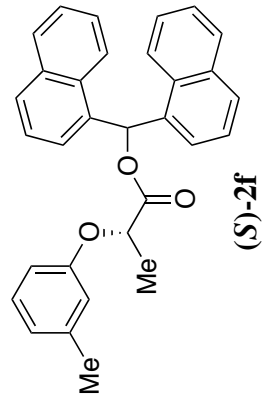


TEN050591C

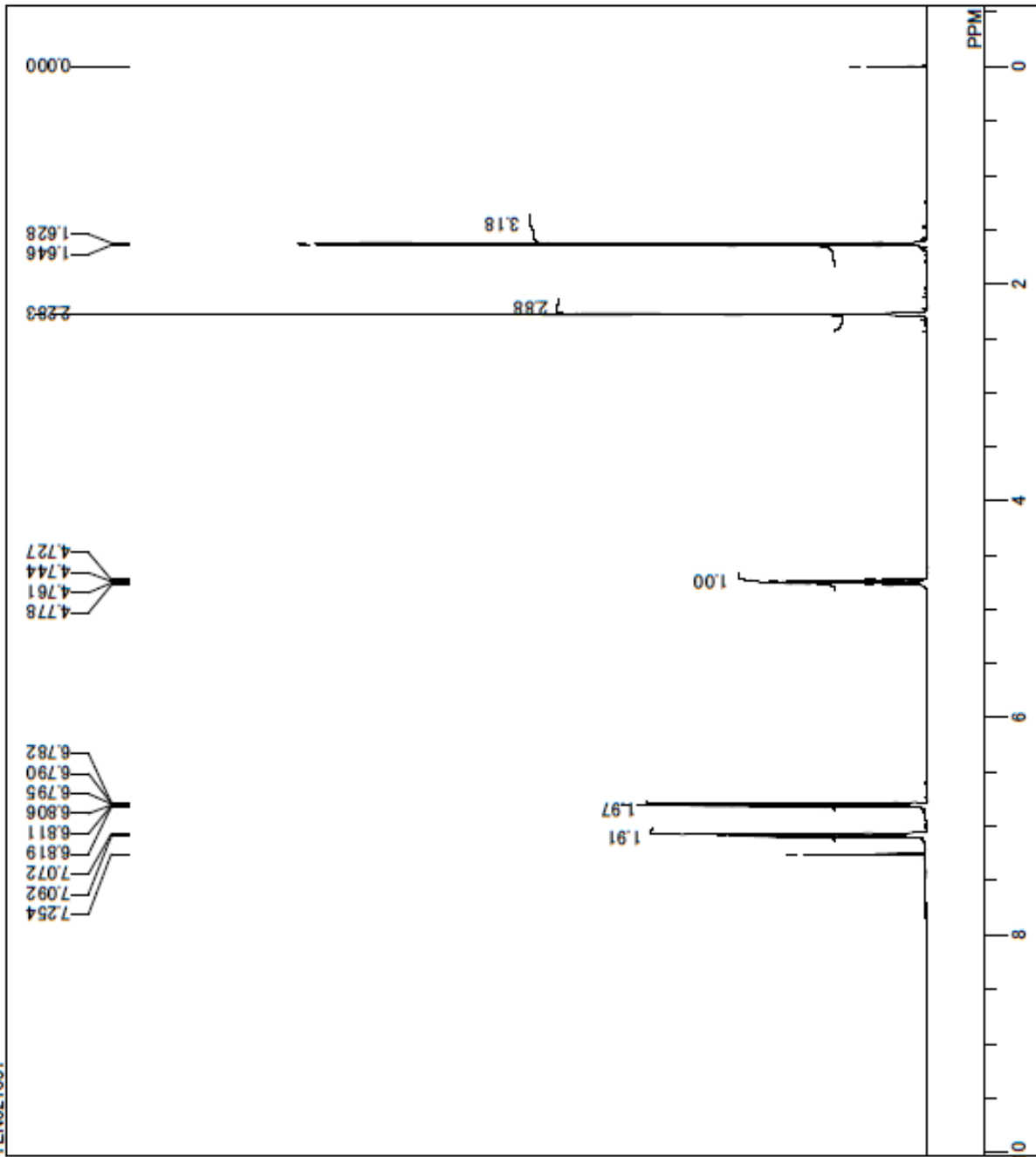


DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREOU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator\予
TEN050591C
2012/May/24 21:36:16
13C
ZGPG30
100.63 MHz
0.00 KHz
10060.25 Hz
32768
24038.46 Hz
512
0.0000 sec
0.0000 sec
7.10 usec
OFF
29.9 c
CDCL3
77.00 ppm
0.25 Hz
362



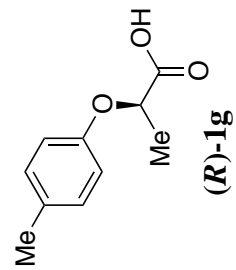
TEN021051



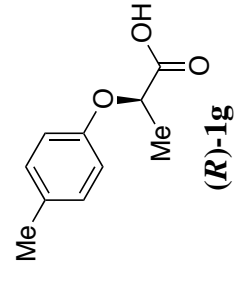
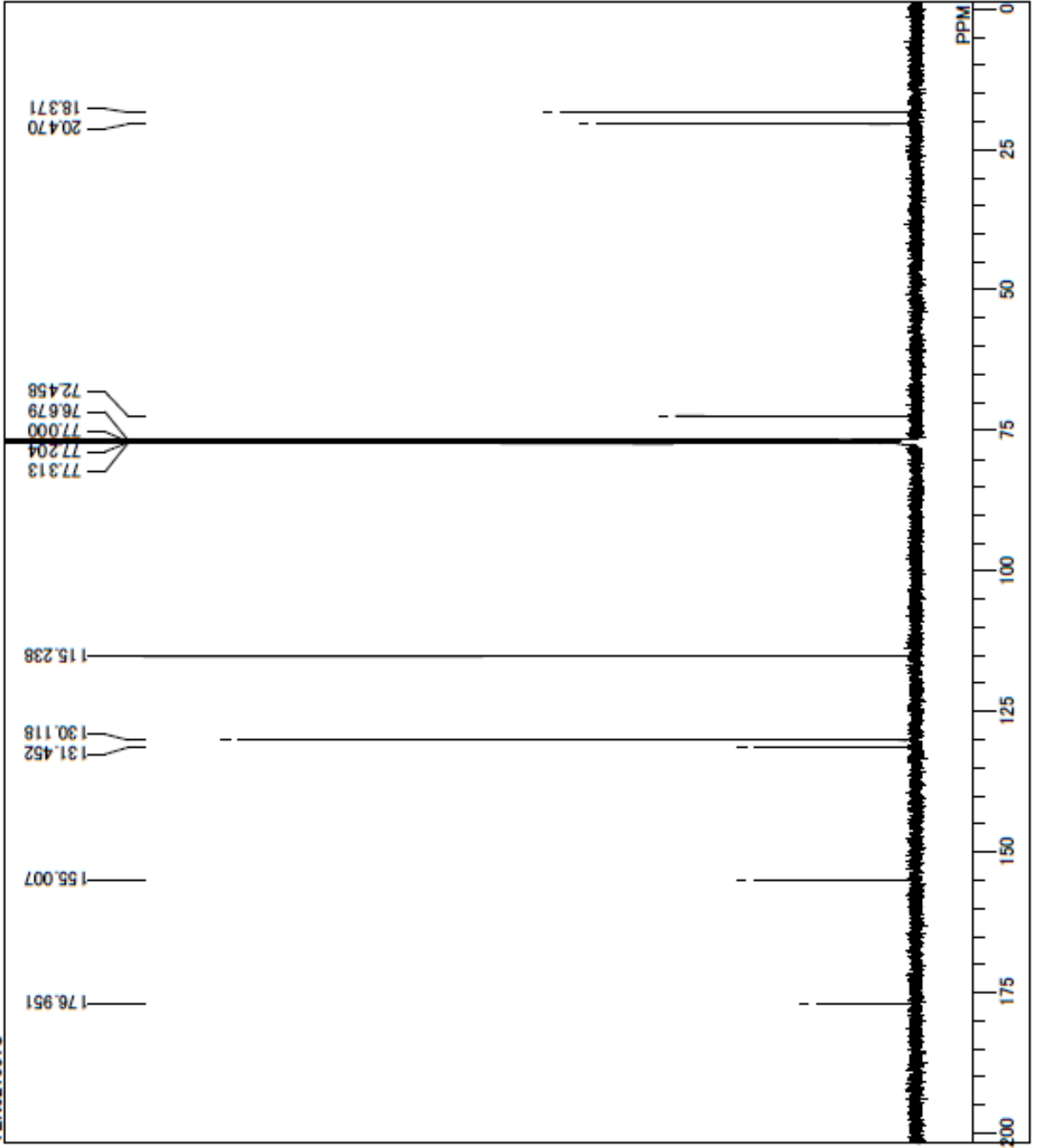
DFILE
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SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator\TEN021051
2012/Jun/20 21:50:08
1H
ZG30

400.18 MHz
0.00 KHz
2478.60 Hz
32768
8223.68 Hz
16
0.0000 sec
0.0000 sec
13.00 usec
OFF
29.9 c
CDCL3
0.00 ppm
0.25 Hz
406



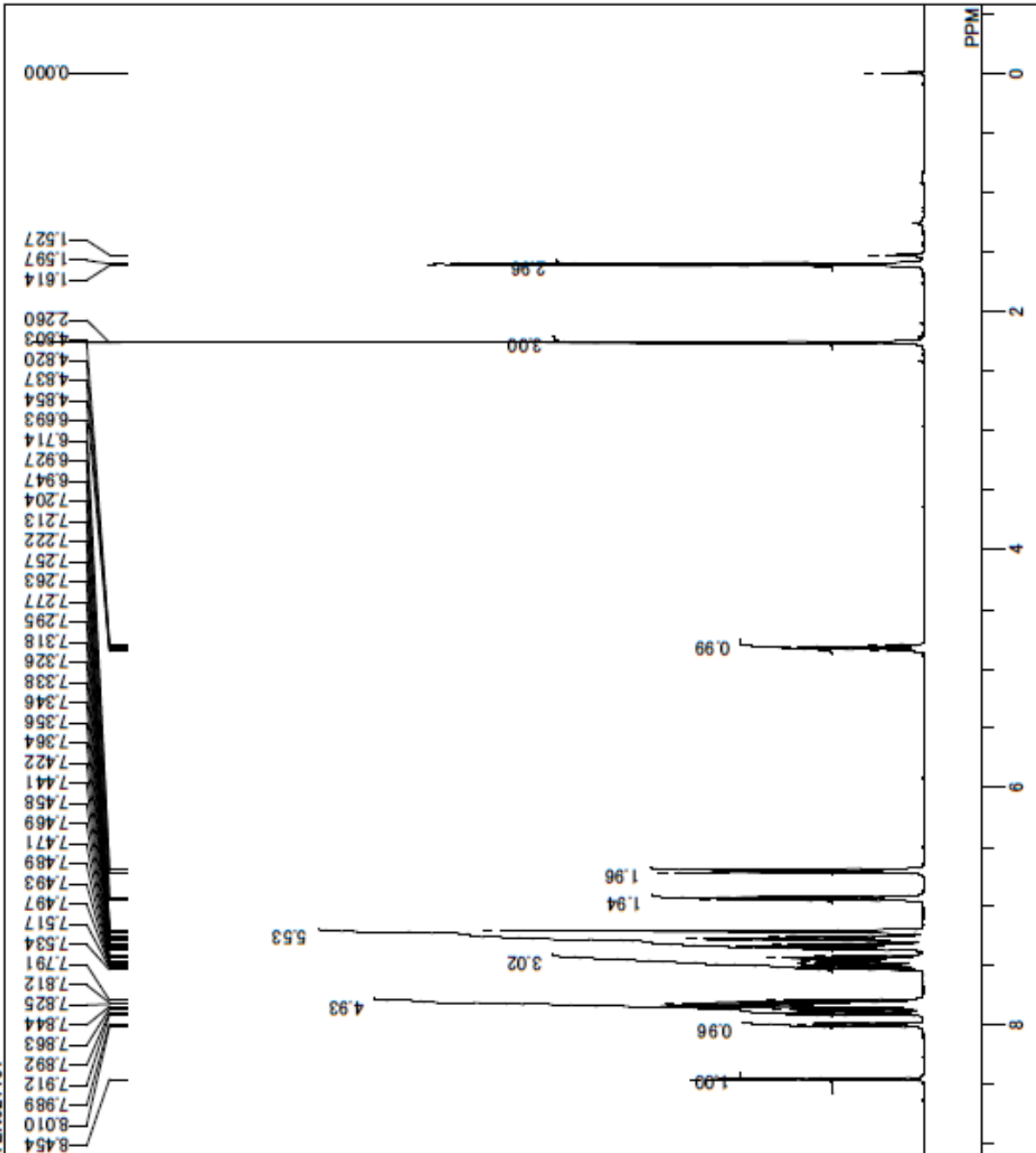
TEN021051C



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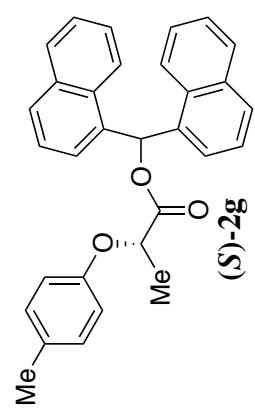
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TEN021051C
2012/Jun/20 22:50:21
13C
ZGPG30
100.63 MHz
0.00 KHz
10060.25 Hz
32768
24038.46 Hz
1024
0.0000 sec
0.0000 sec
7.10 usec
OFF
29.9 c
CDCL3
77.00 ppm
0.25 Hz
322

TEN021151

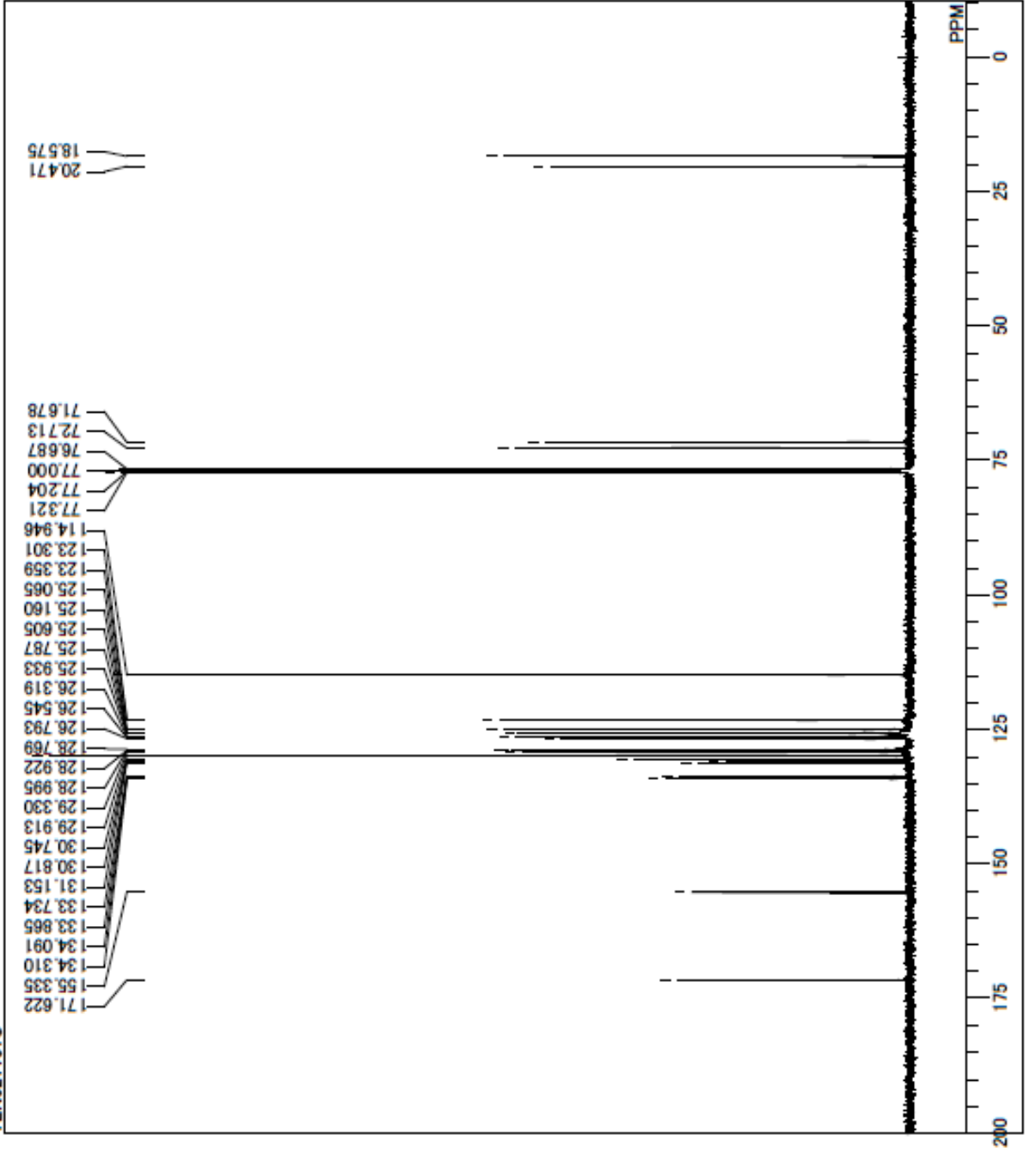


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TEN021151
2012/May/21 21:24:28
1H
ZG30
400.18 MHz
0.00 KHz
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32768
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0.0000 sec
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13.00 usec
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CDCL3
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0.25 Hz
101

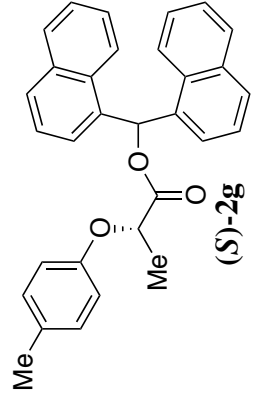


TEN021151C

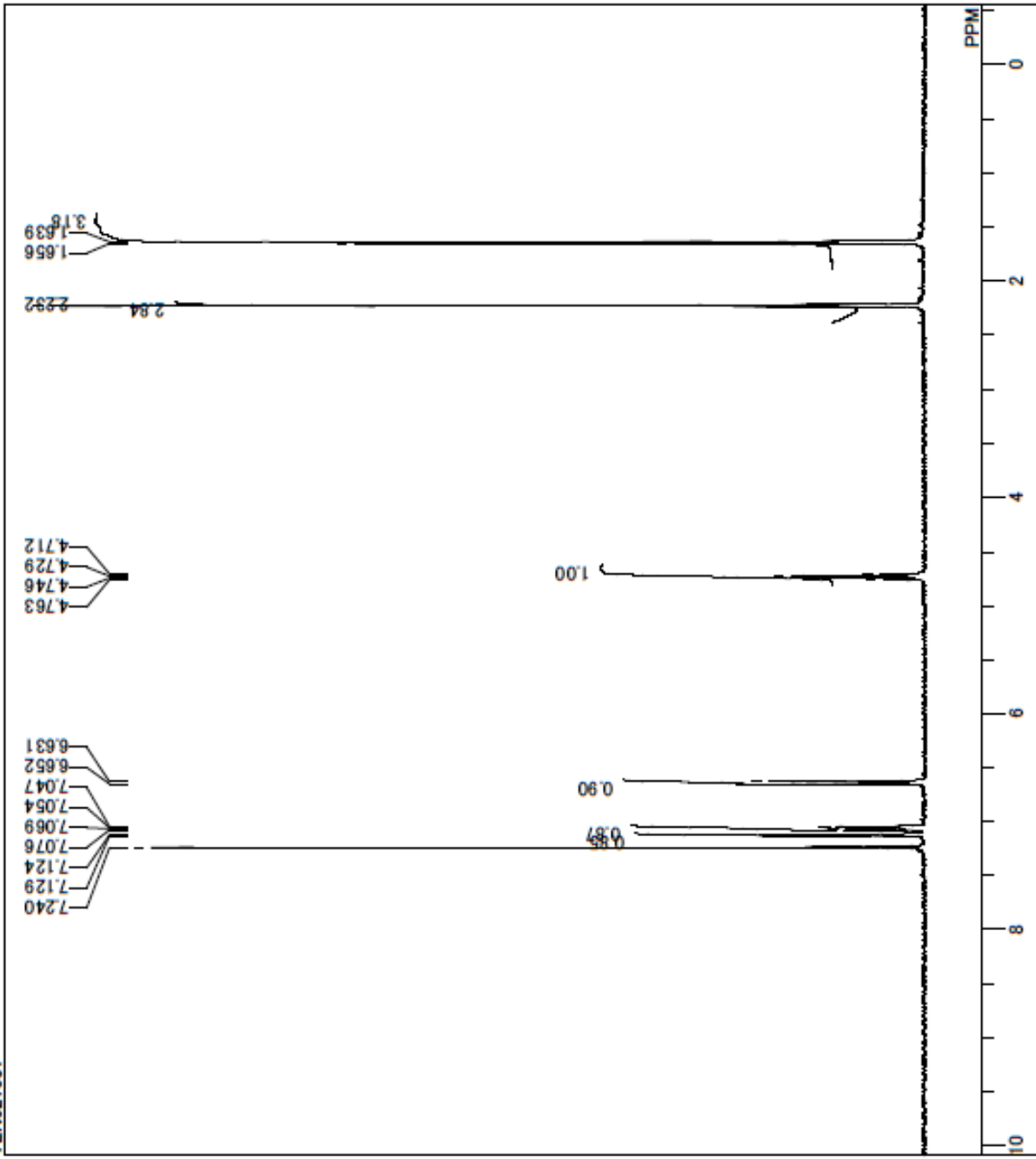


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2012/May/21 16:23:55
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0.0000 sec
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7.10 usec
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26.9 c
CDCL3
77.00 ppm
0.25 Hz
322

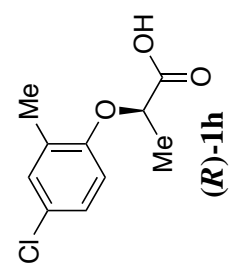


TEN021031

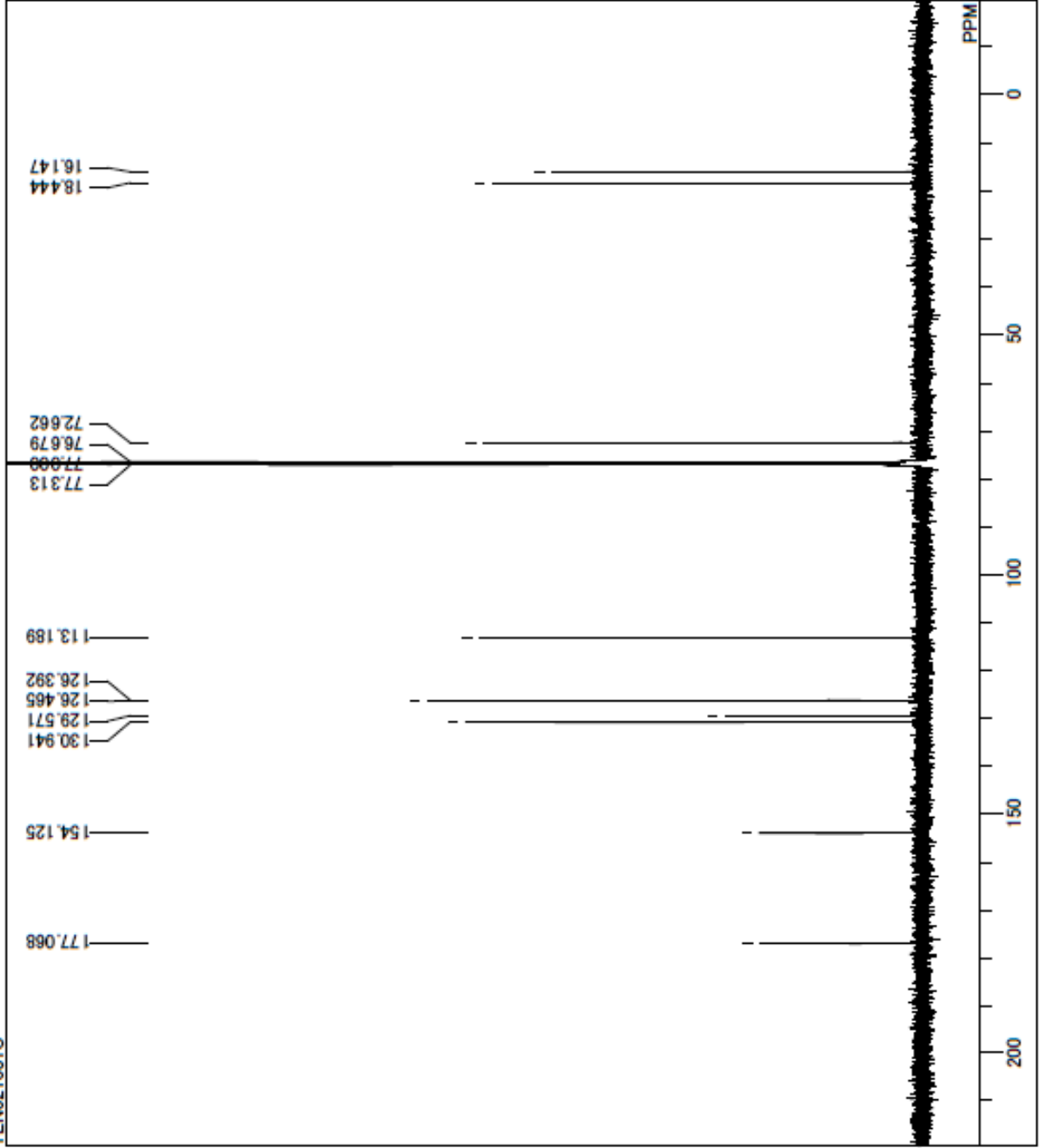


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TEN021031
2011/Sep/22 11:38:19
1H
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32768
8223.68 Hz
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0.0000 sec
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13.00 usec
OFF
30.9 c
CDCL3
7.24 ppm
0.25 Hz
724

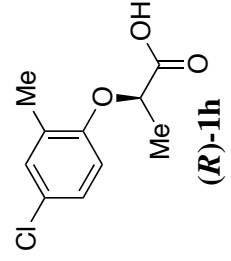


TEN021031C

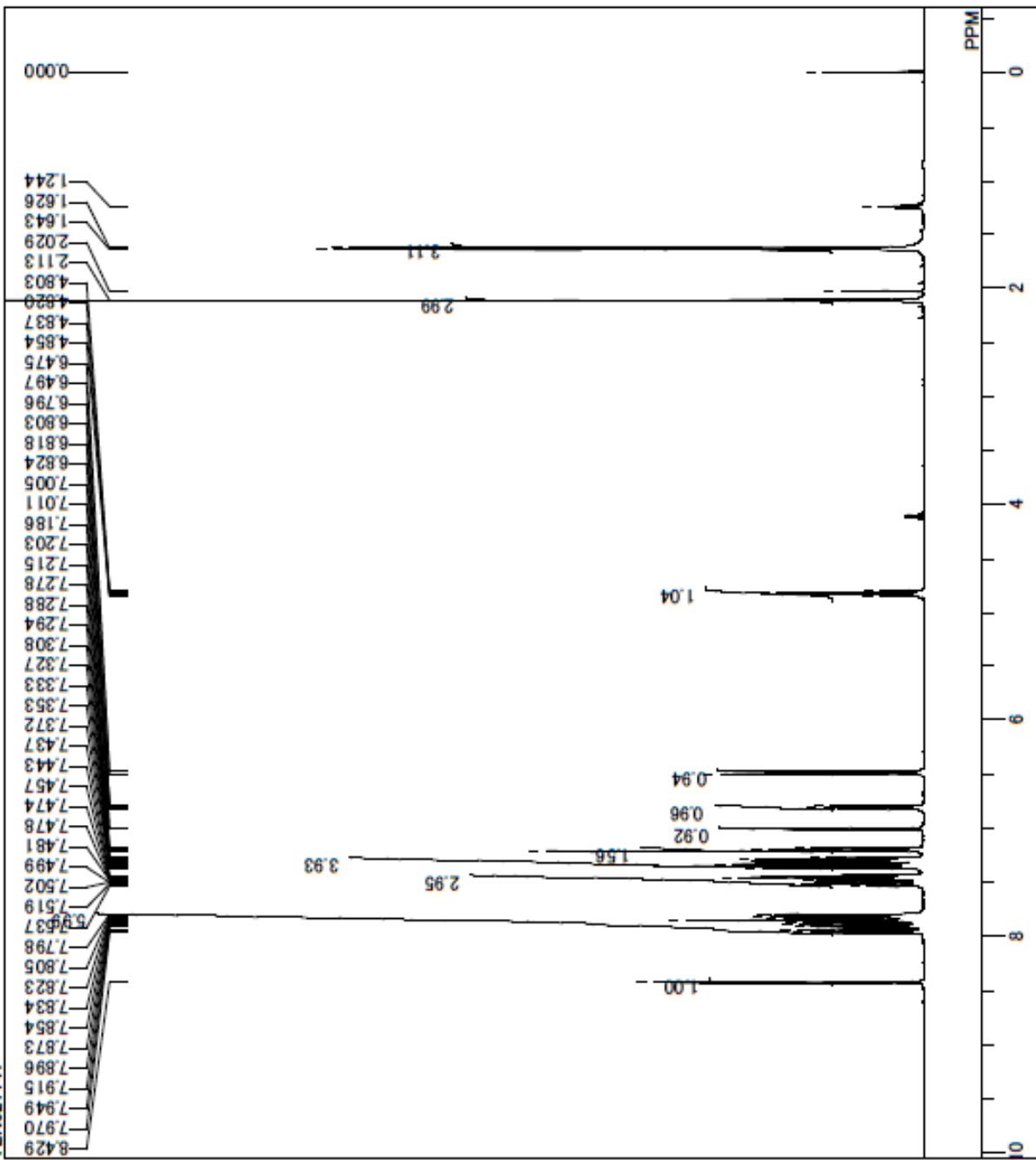


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10060.25 Hz
32768
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7.10 usec
OFF
29.9 c
CDCL3
77.00 ppm
0.25 Hz
57

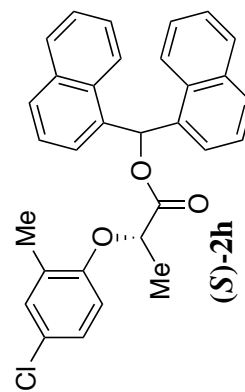


TEN021141

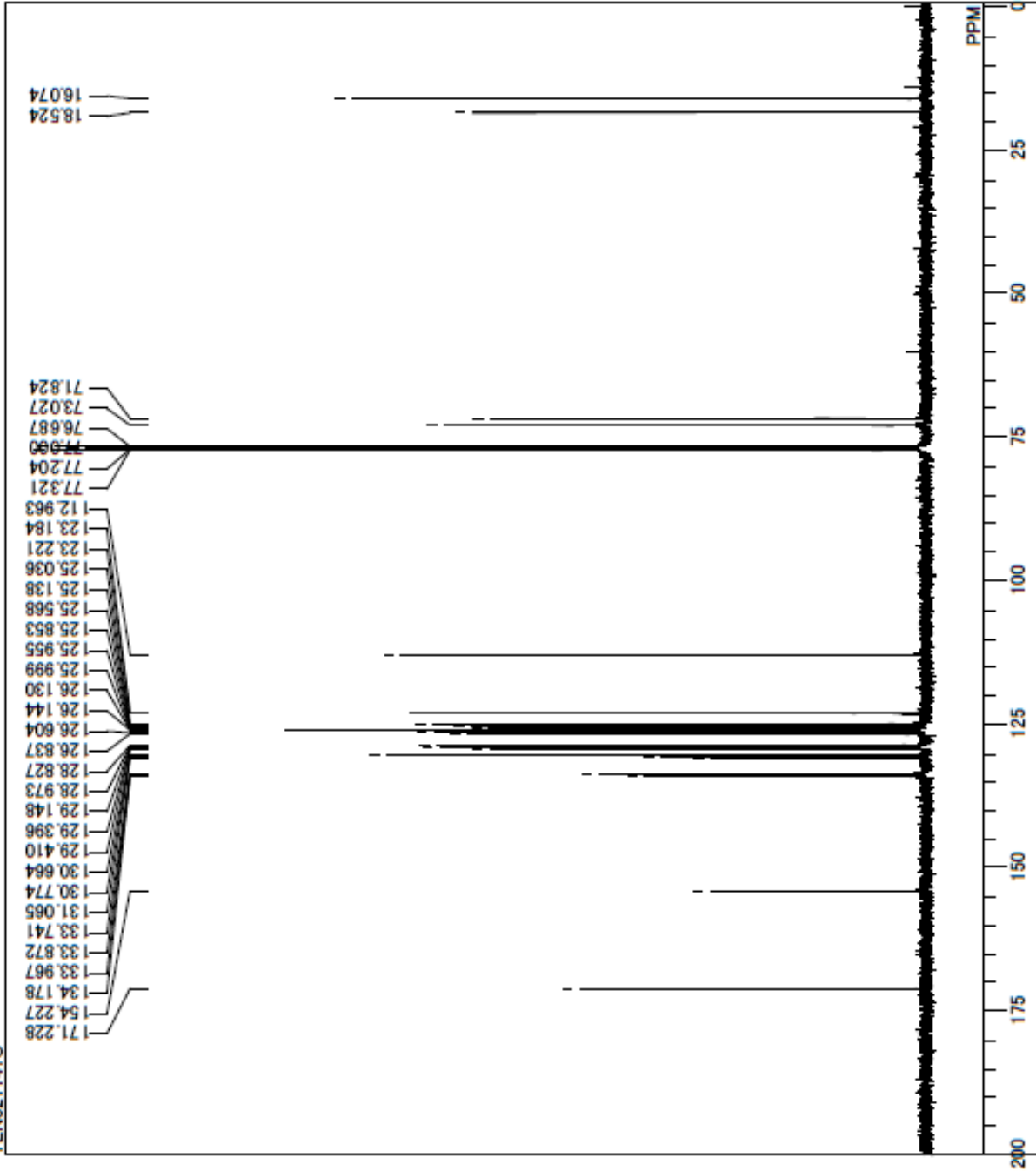


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2012/May/15 07:39:12
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8223.68 Hz
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13.00 usec
OFF
26.9 c
CDCL3
0.00 ppm
0.25 Hz
90

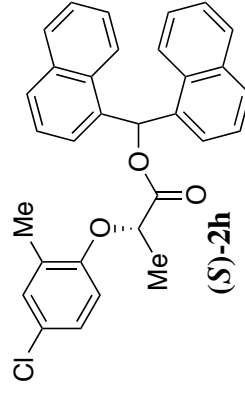


TEN021141C

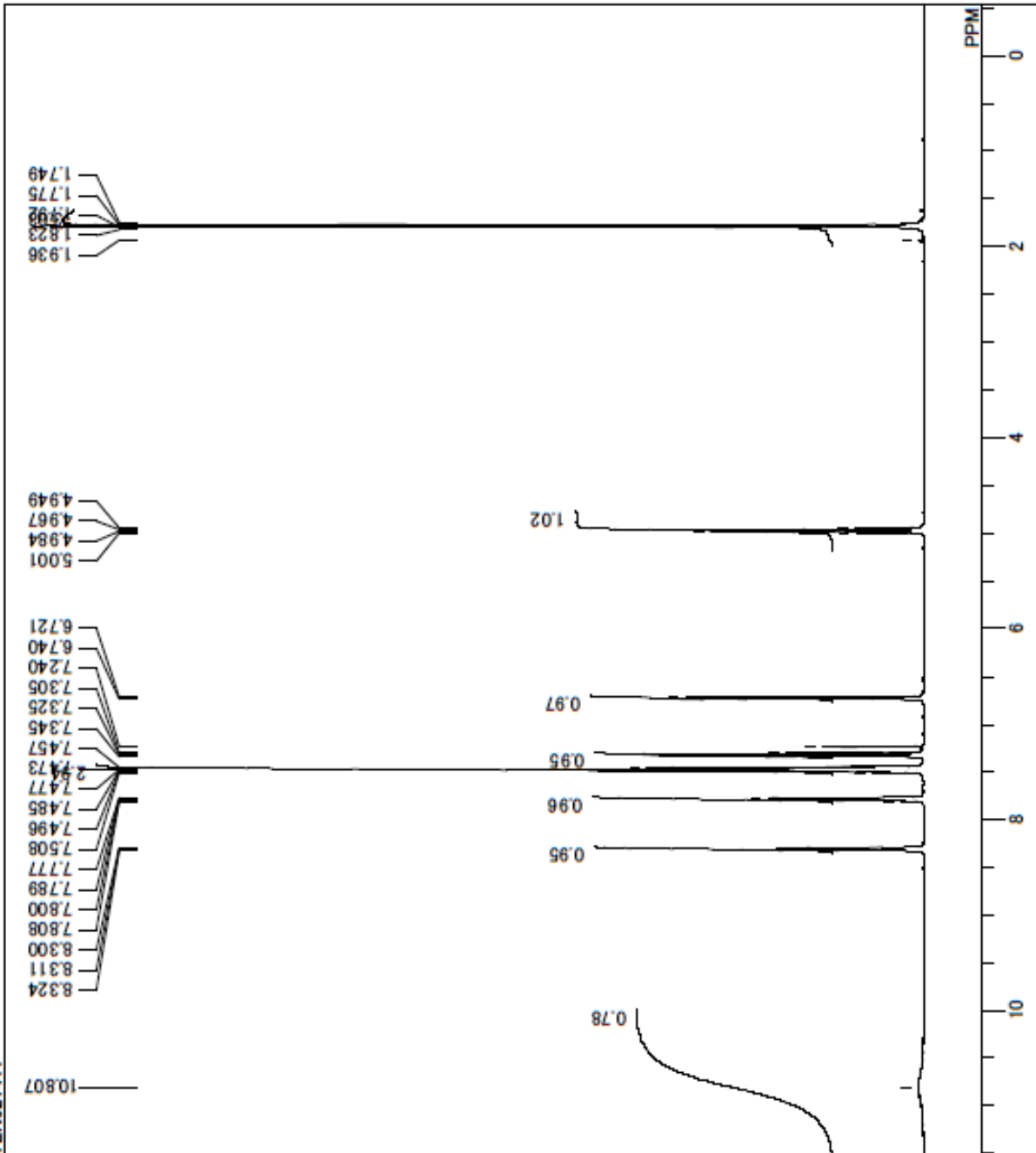


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TEN021141C
2012/May/15 23:42:46
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7.10 usec
OFF
26.9 c
CDCL3
77.00 ppm
0.25 Hz
57

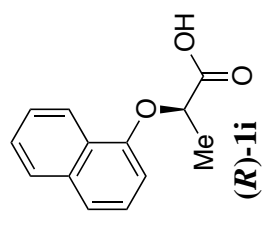


TEN021411

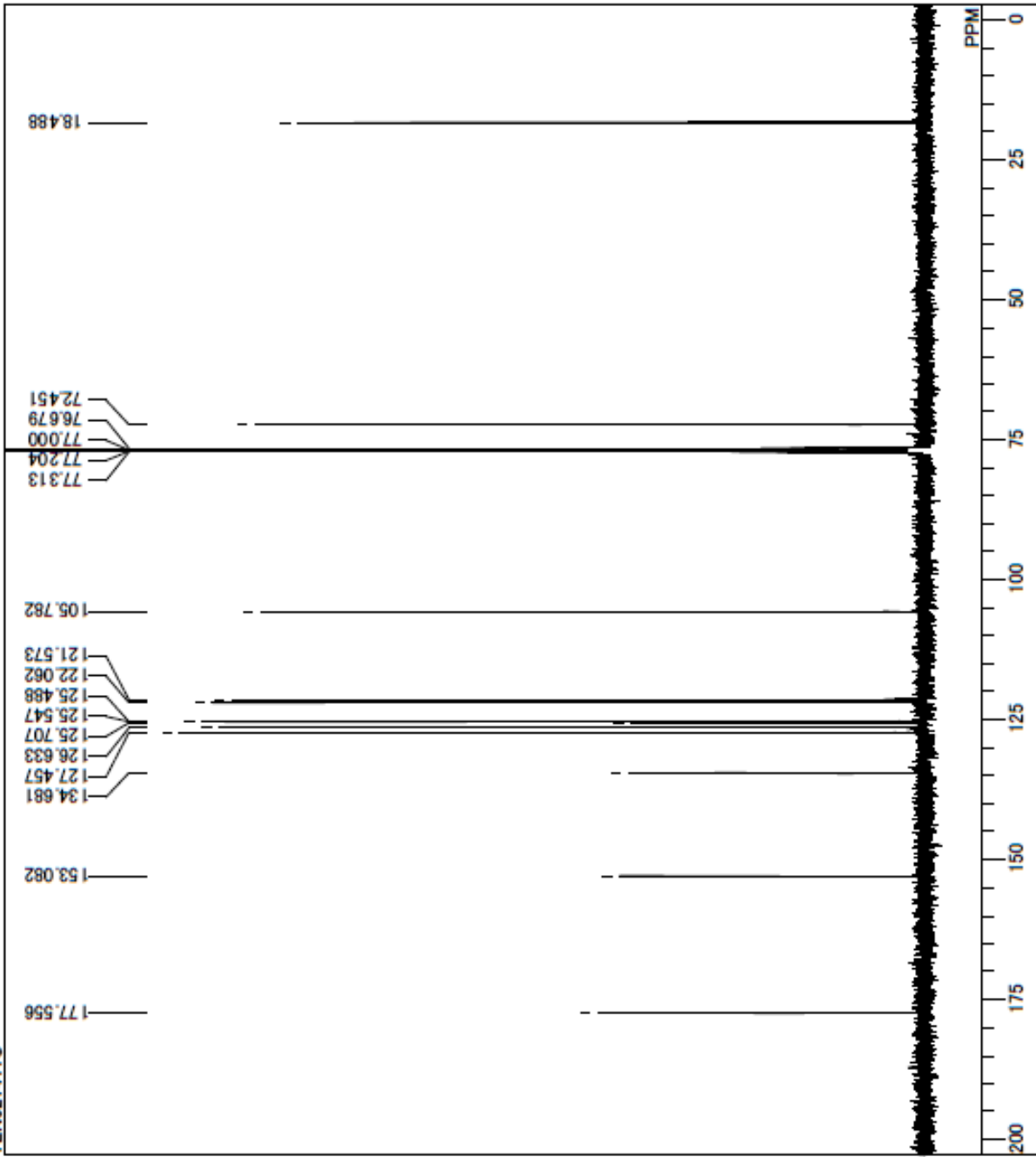


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TEN021411
2011/Oct/03 06:51:05
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13.00 usec
OFF
30.9 c
CDCL3
7.24 ppm
0.25 Hz
322

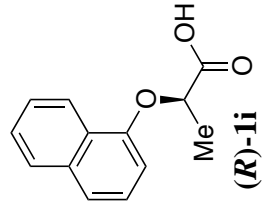


TEN021411C

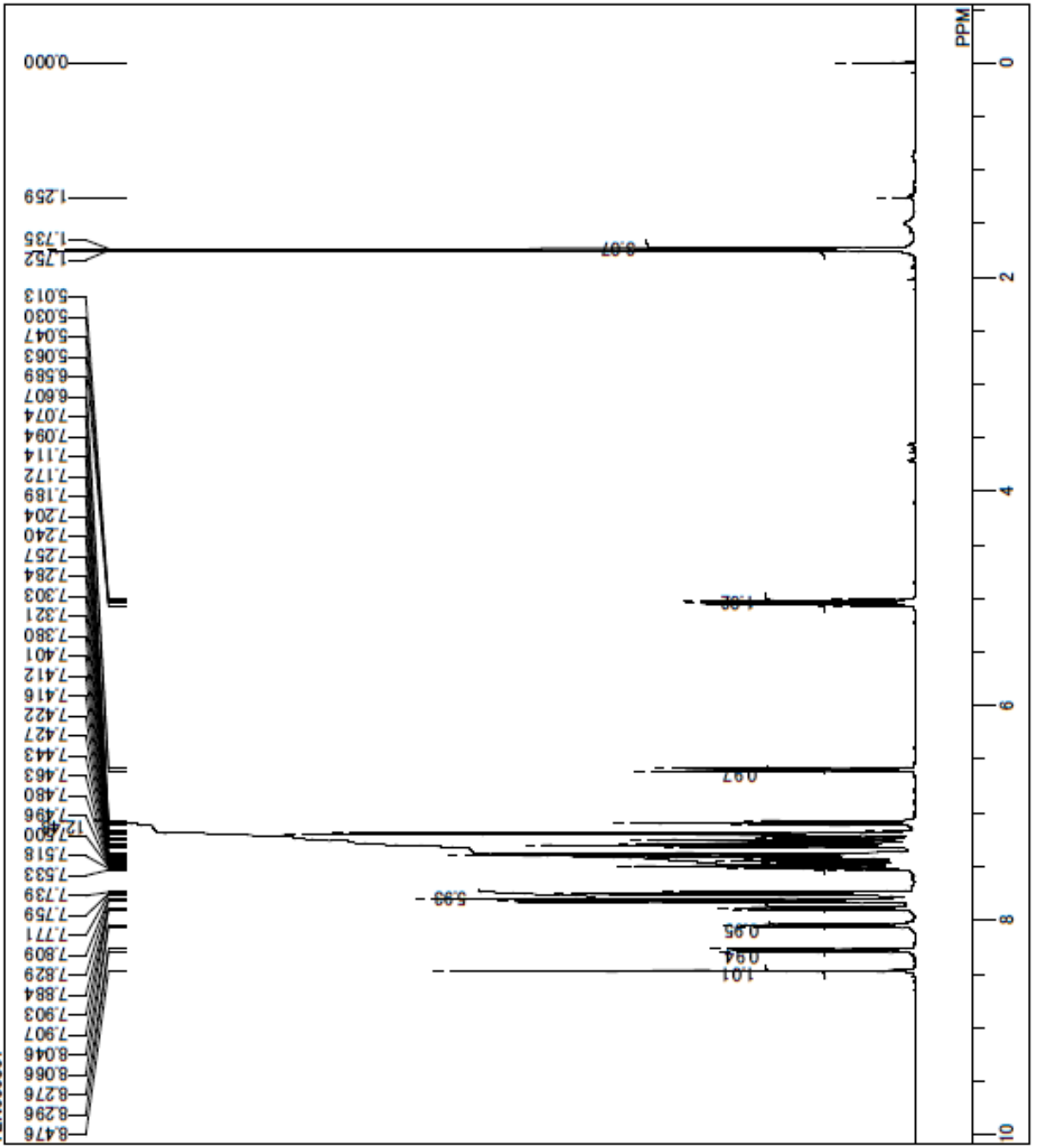


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10060.25 Hz
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7.10 usec
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29.9 c
CDCL3
77.00 ppm
0.25 Hz
64

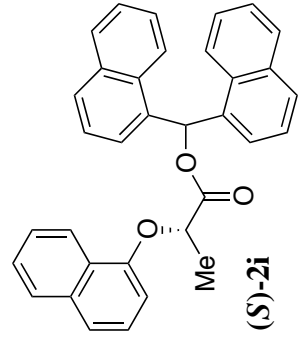


TEN050801

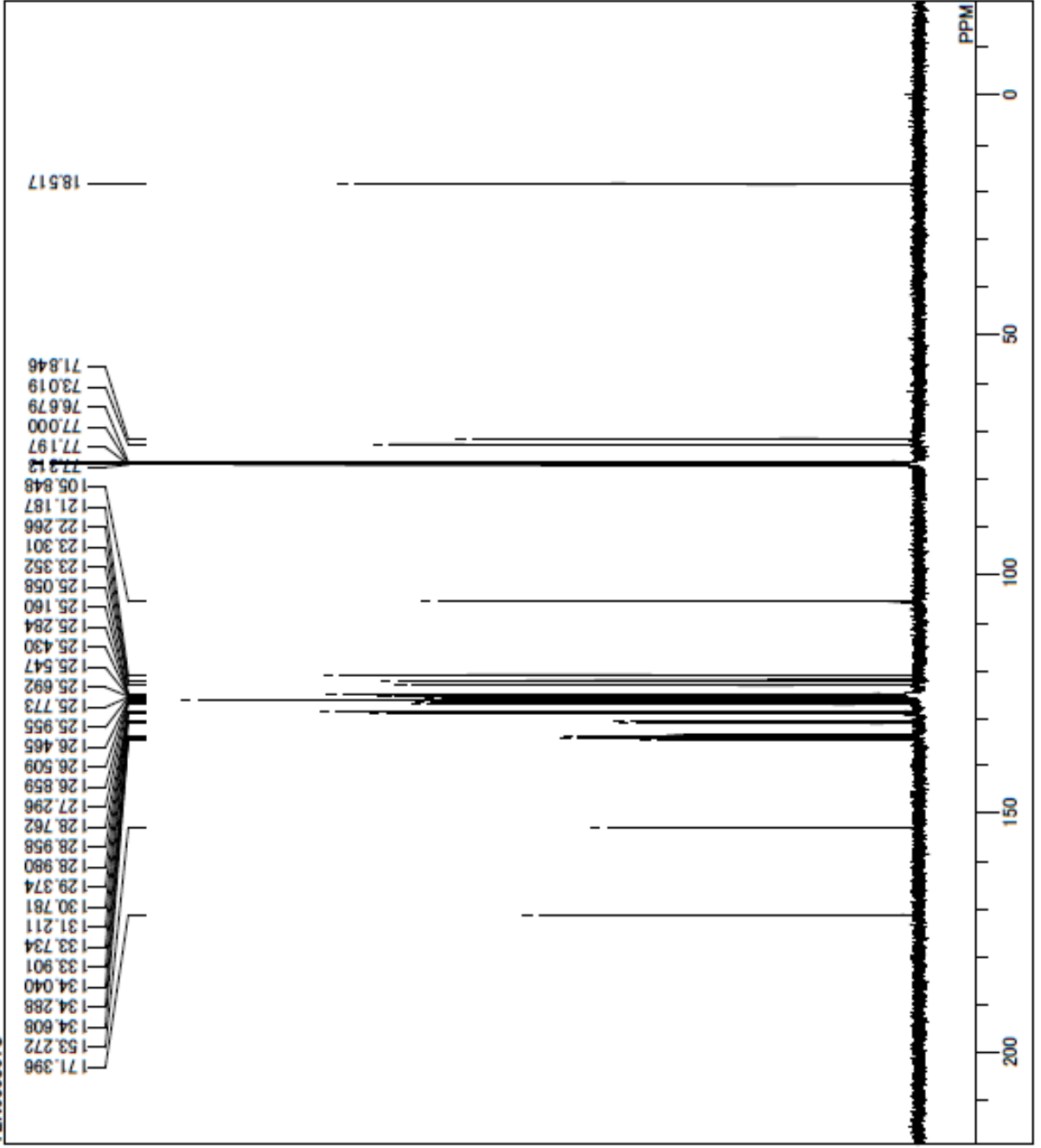


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13.00 usec
OFF
29.9 c
CDCL3
0.00 ppm
0.25 Hz
81

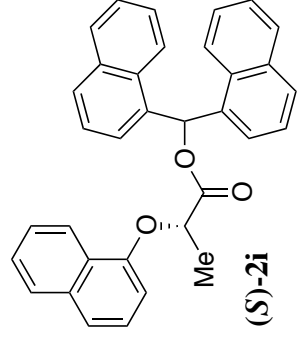


TEN050801C

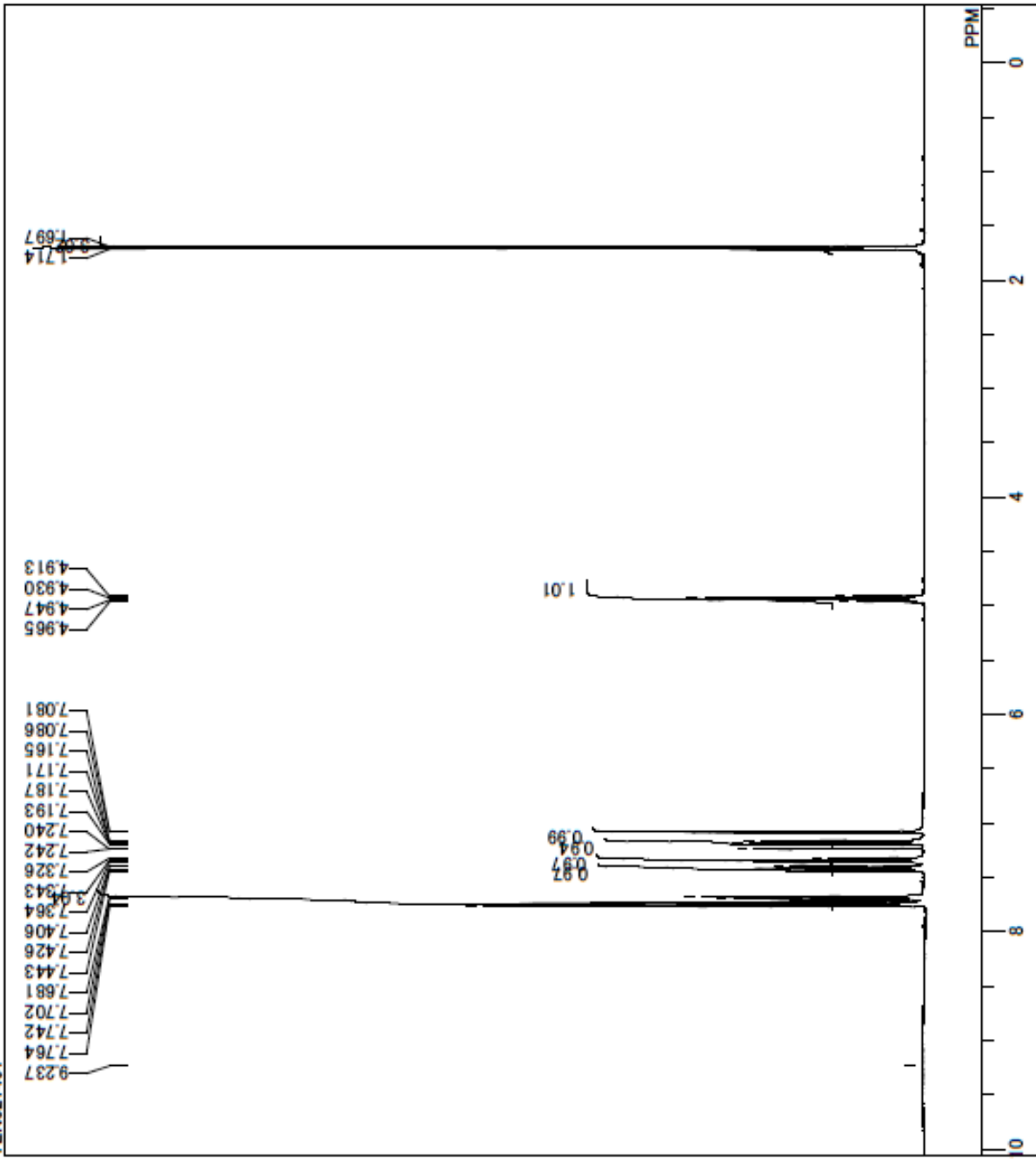


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TEN050801C
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7.10 usec
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29.9 c
CDCL3
77.00 ppm
0.25 Hz
362

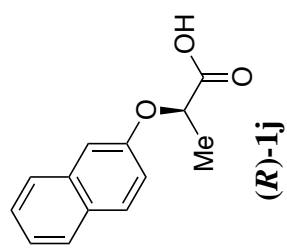


TEN021491

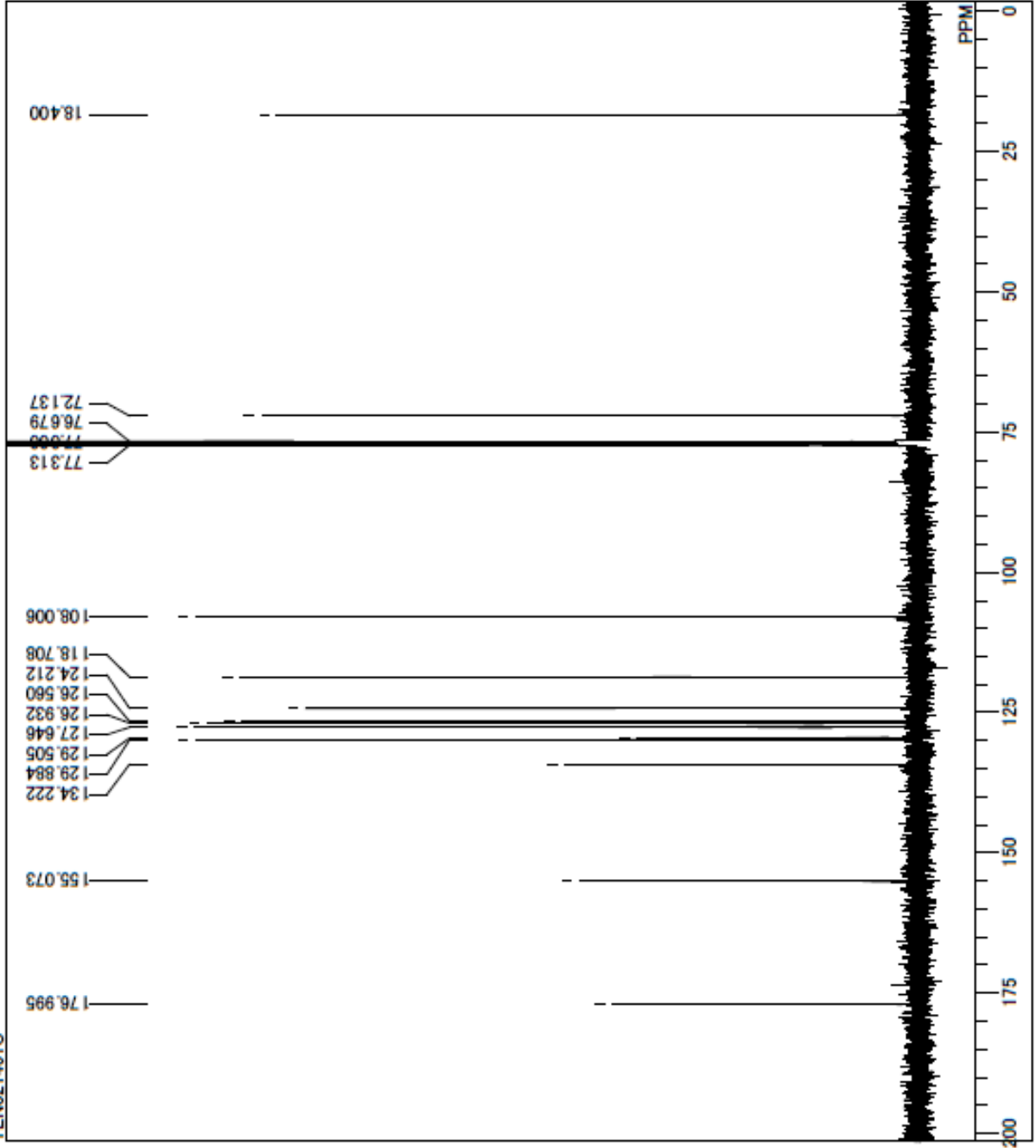


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2478.60 Hz
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13.00 usec
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29.9 c
CDCL3
7.24 ppm
0.25 Hz
406



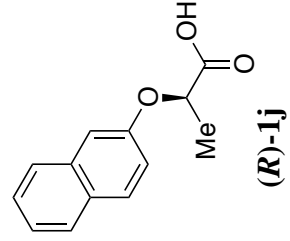
TEN021491C



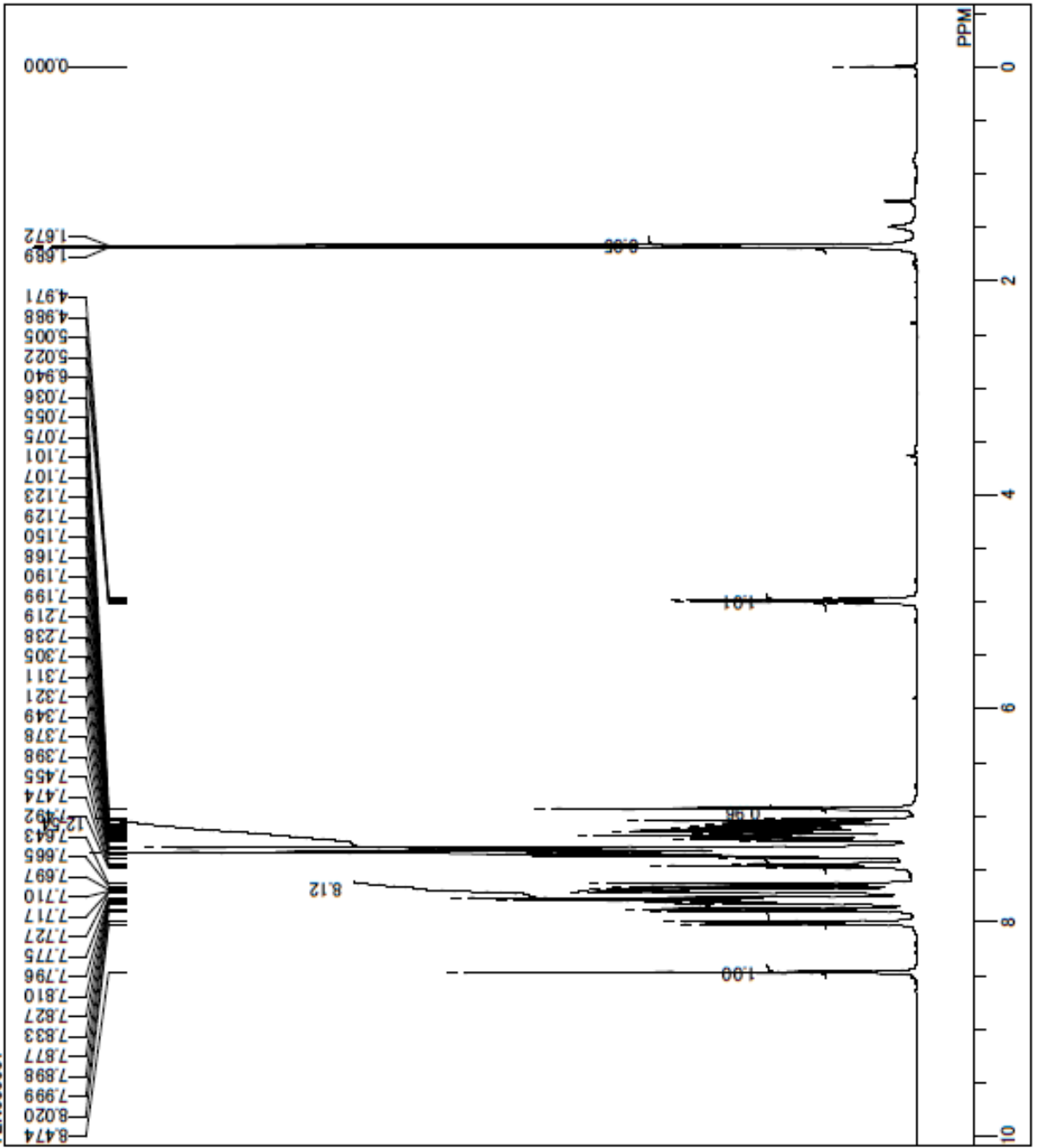
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24038.46 Hz
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0.0000 sec
7.10 usec
OFF
29.9 c
CDCL3
77.00 ppm
0.25 Hz
203

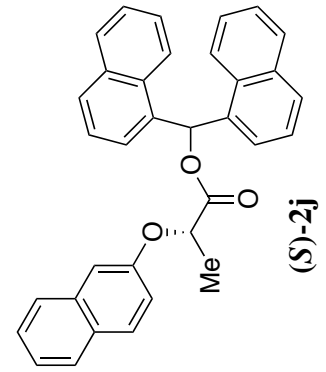


TEN050601

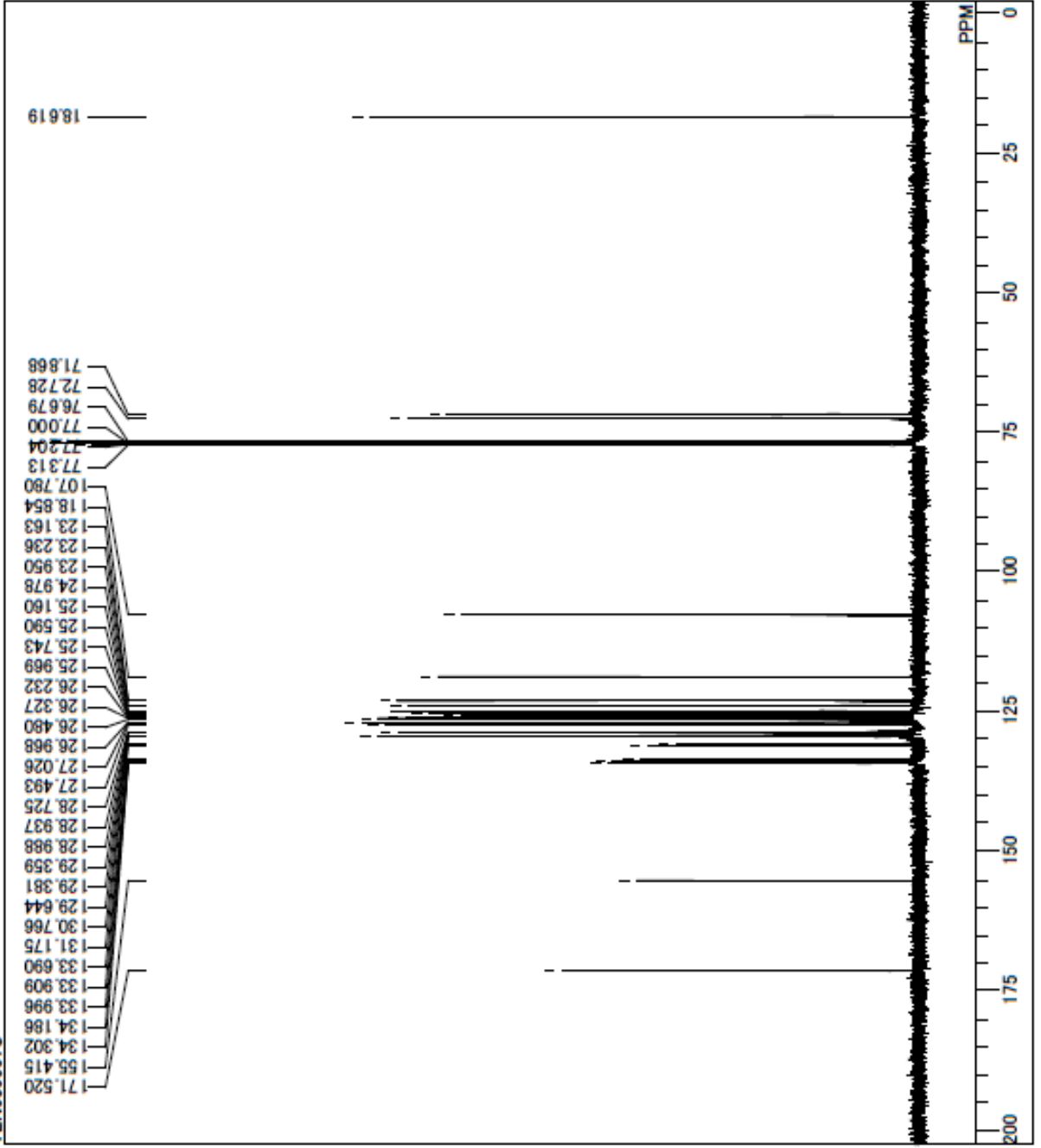


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TEN050601
2012/May/24 04:27:38
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8223.68 Hz
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0.0000 sec
13.00 usec
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CDCL3
0.00 ppm
0.25 Hz
128

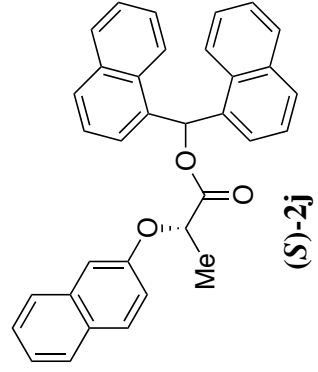


TEN050601C

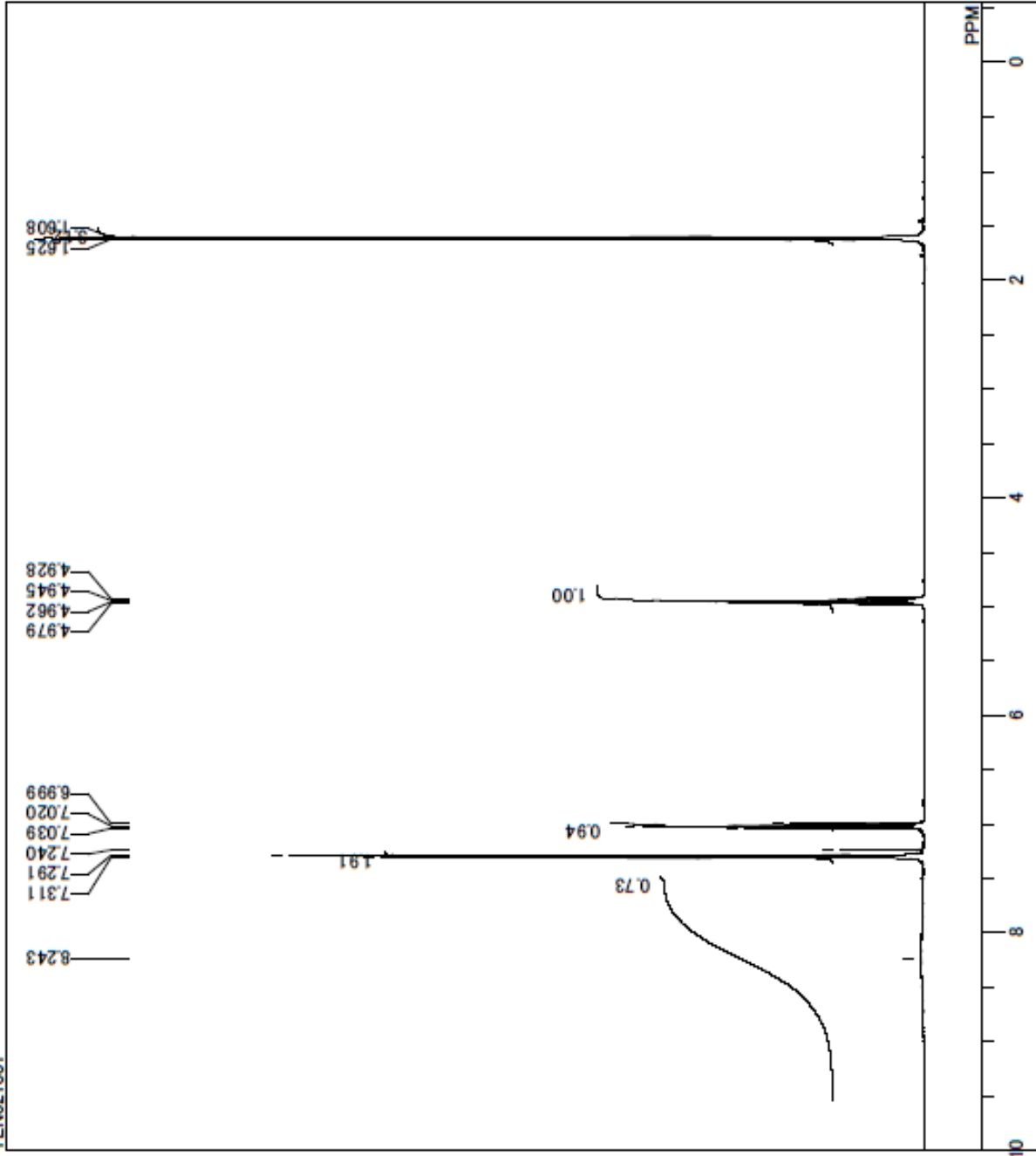


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0.0000 sec
7.10 usec
OFF
29.9 c
CDCL3
77.00 ppm
0.25 Hz
64

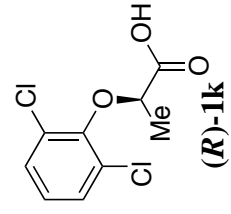


TEN021331

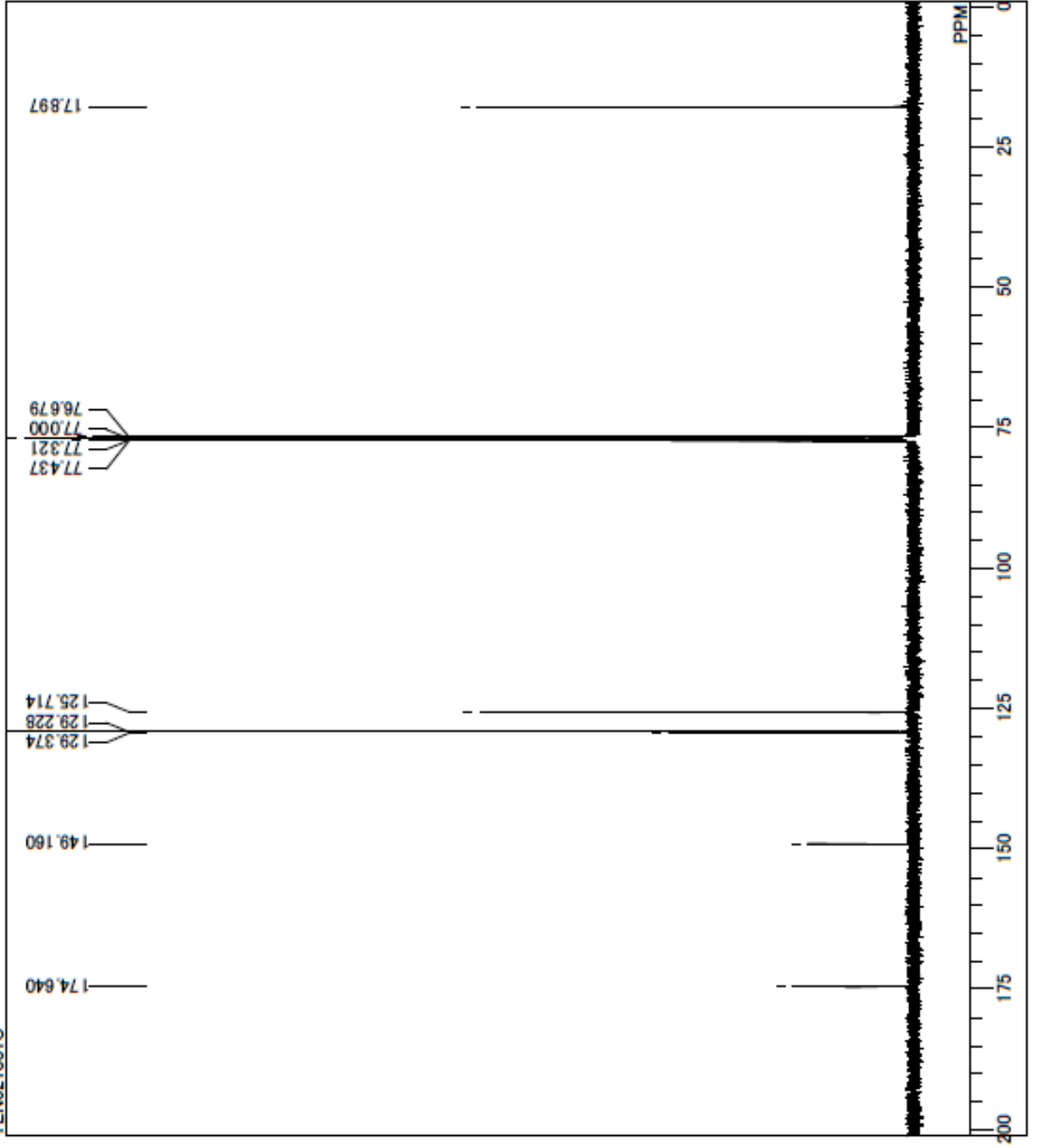


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2011/Sep/30 06:13:12
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13.00 usec
OFF
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CDCL3
7.24 ppm
0.25 Hz
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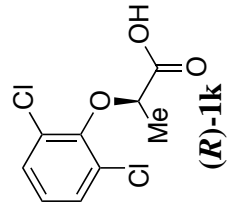


TEN021331C

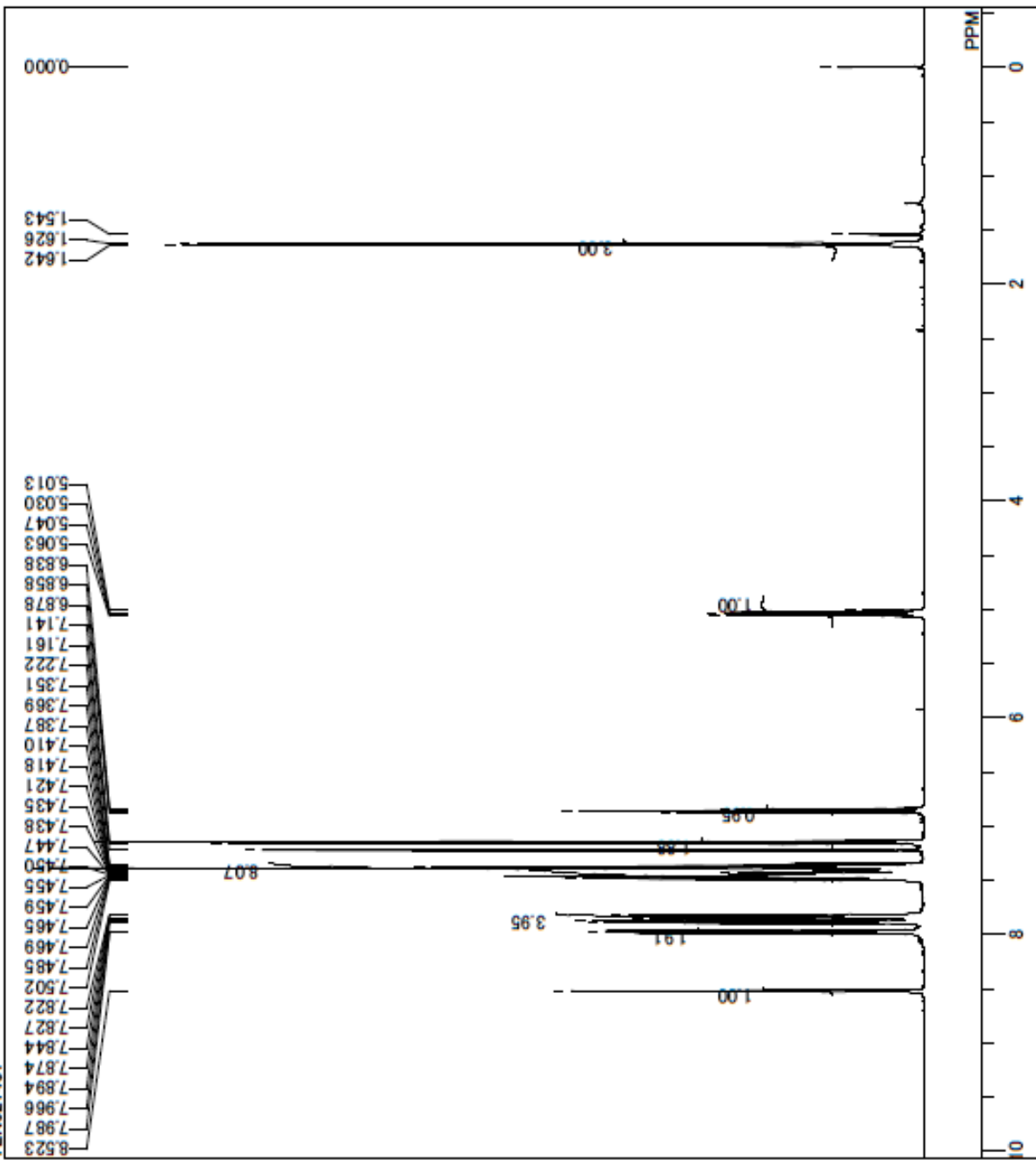


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TEN021331C
2011/Oct/01 00:35:27
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7.10 usec
OFF
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CDCL3
77.00 ppm
0.25 Hz
57

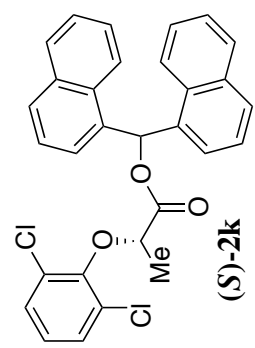


TEN021431

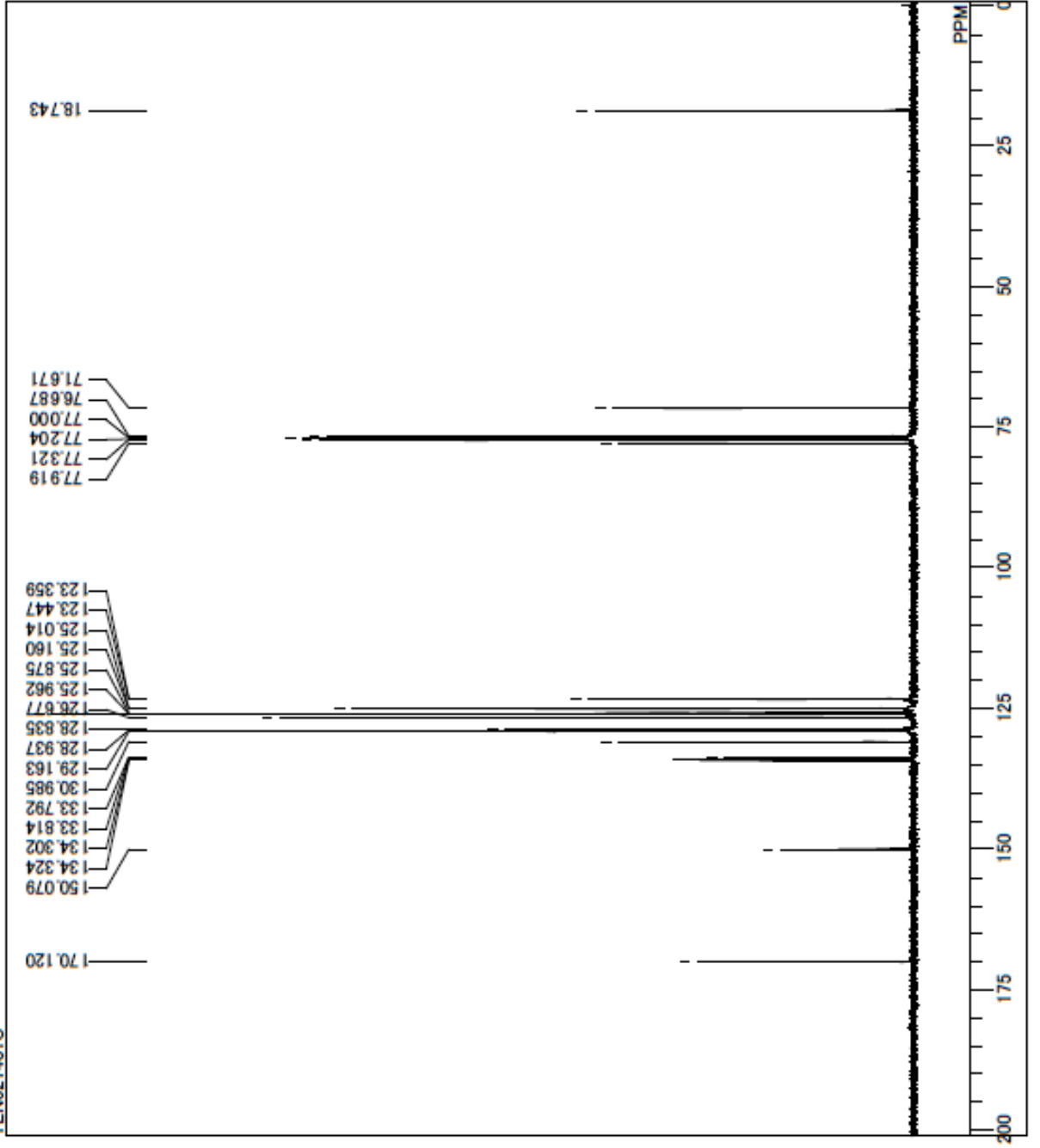


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TEN021431
2012/May/21 21:32:18
1H
ZG30
400.18 MHz
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2478.60 Hz
32768
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13.00 usec
OFF
26.9 c
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0.25 Hz
114

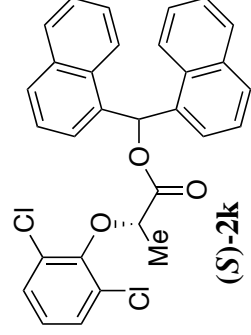


TEN021431C

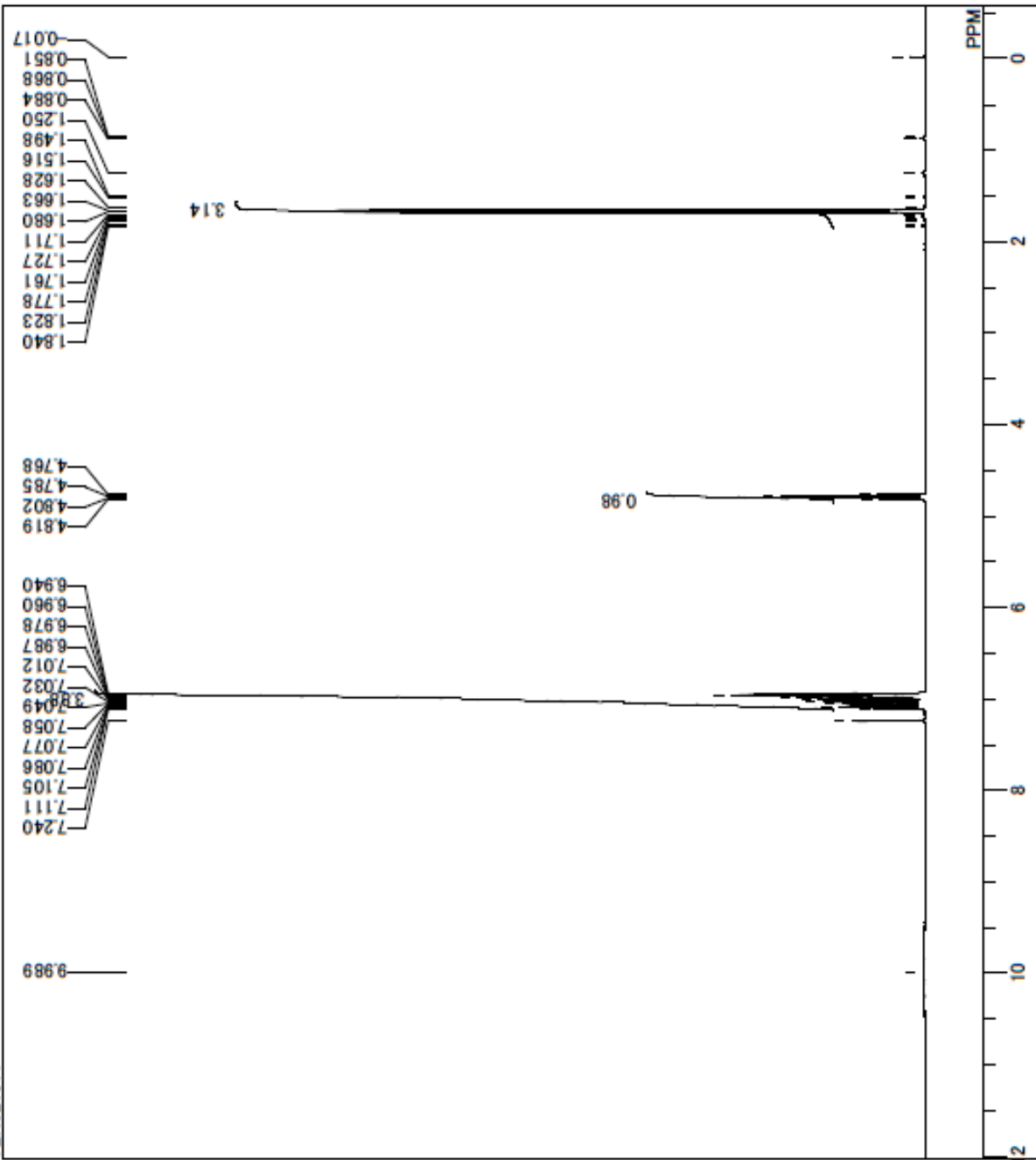


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TEN021431C
2012/May/21 17:28:57
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7.10 usec
OFF
26.9 c
CDCL3
77.00 ppm
0.25 Hz
406



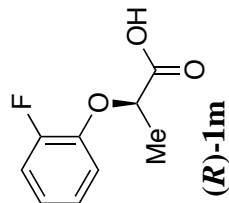
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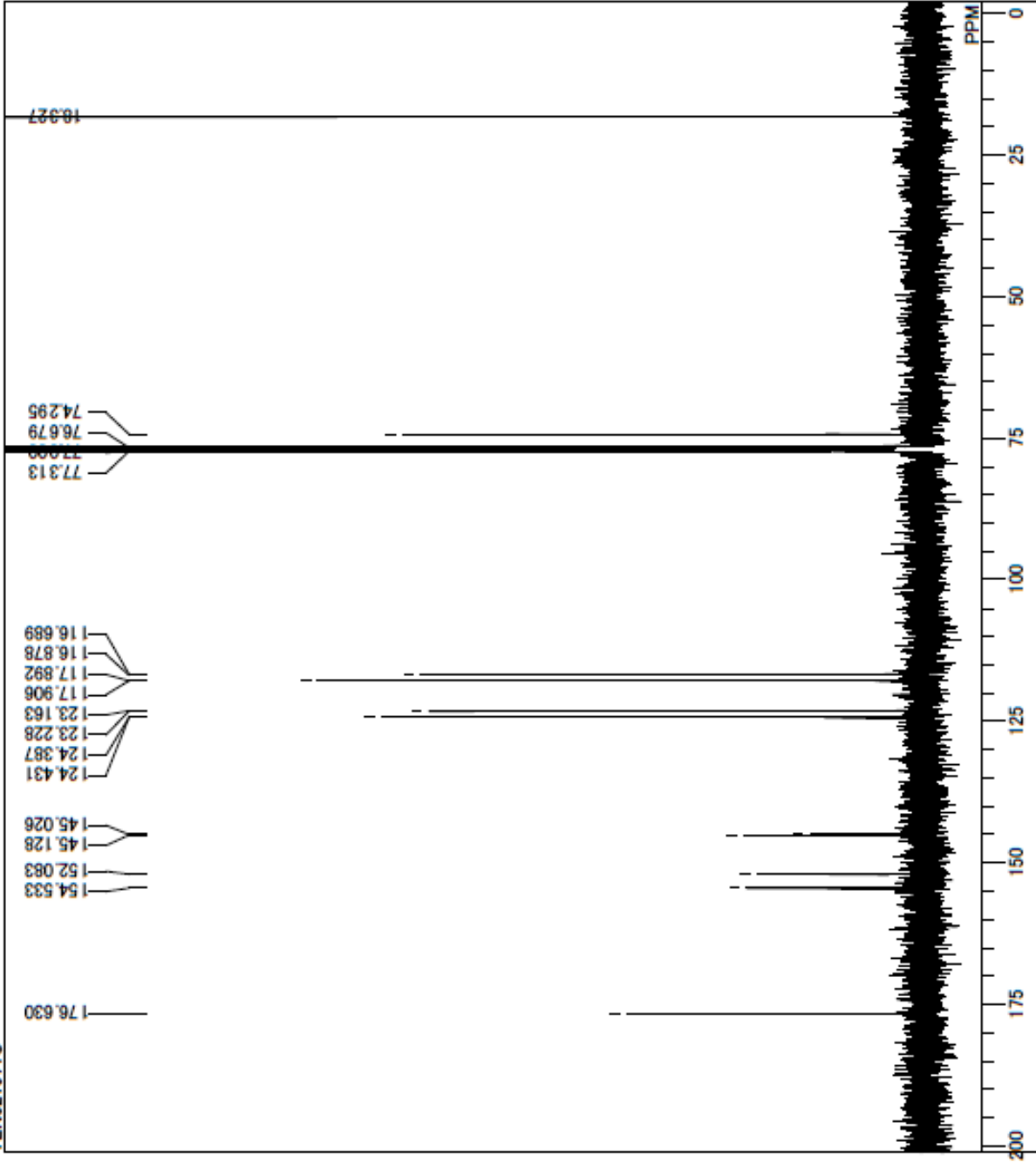
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TEN021971
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8223.68 Hz
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13.00 usec
OFF
30.9 c
CDCL3
7.24 ppm
0.25 Hz
322

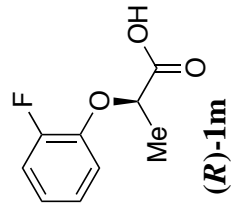


TEN021971C

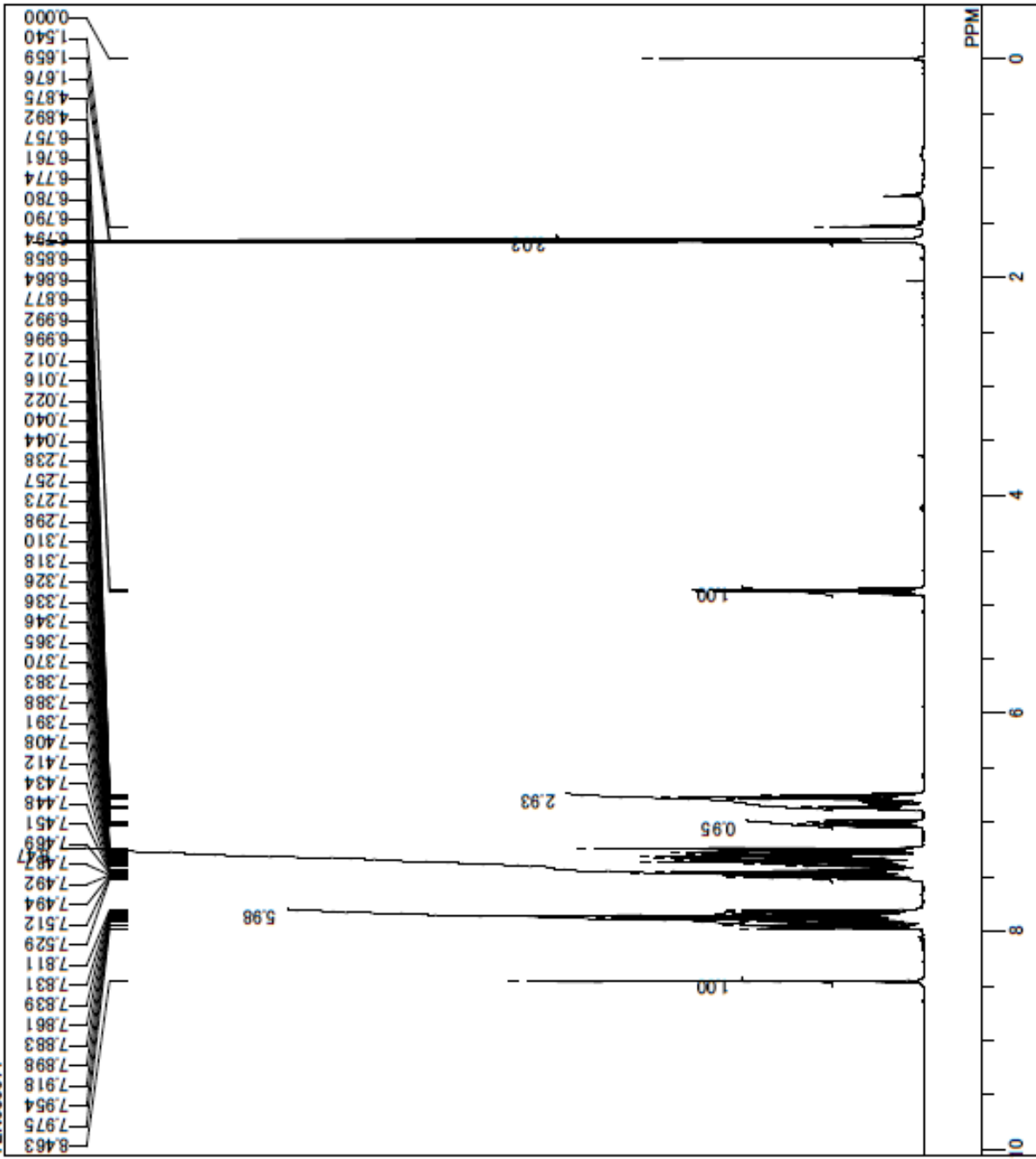


DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREOU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator\...
TEN021971C
2011/Oct/21 00:07:05
13C
ZGPG30
100.63 MHz
0.00 KHz
10060.25 Hz
32768
24038.46 Hz
512
0.0000 sec
0.0000 sec
7.10 usec
OFF
29.9 c
CDCL3
77.00 ppm
0.25 Hz
57

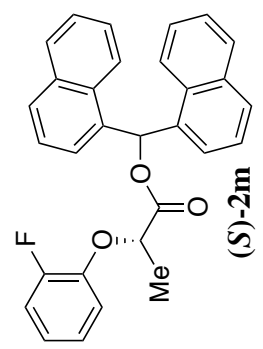


TEN030071

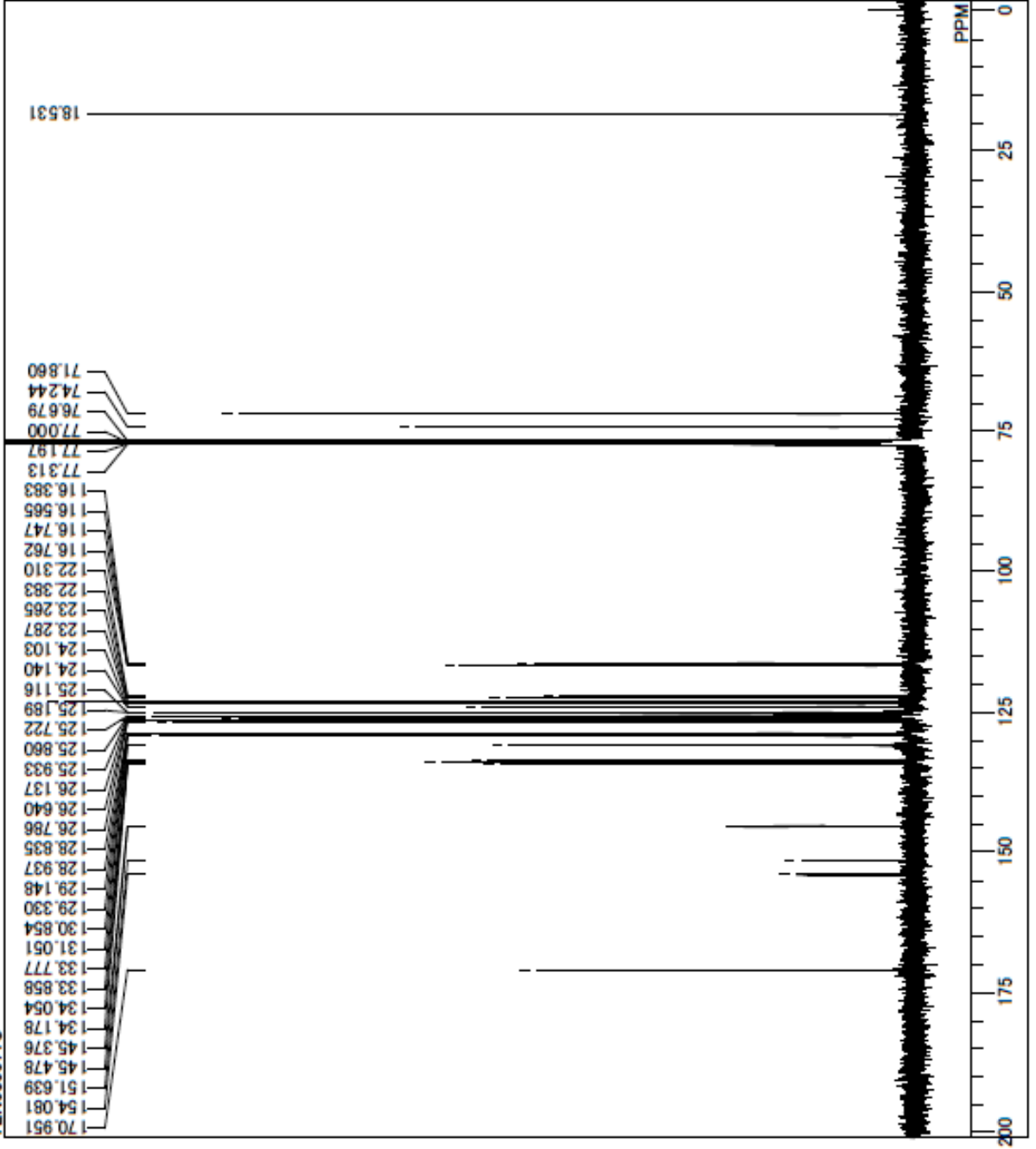


DFILE
COMNT
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PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator*子*
TEN030071
2012/May/07 09:57:10
1H
ZG30
400.18 MHz
0.00 KHz
2478.60 Hz
32768
8223.68 Hz
16
0.0000 sec
0.0000 sec
13.00 usec
OFF
26.9 c
CDCL3
0.00 ppm
0.25 Hz
203

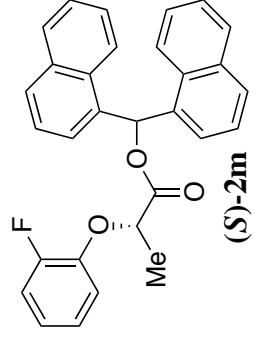


TEN030071C

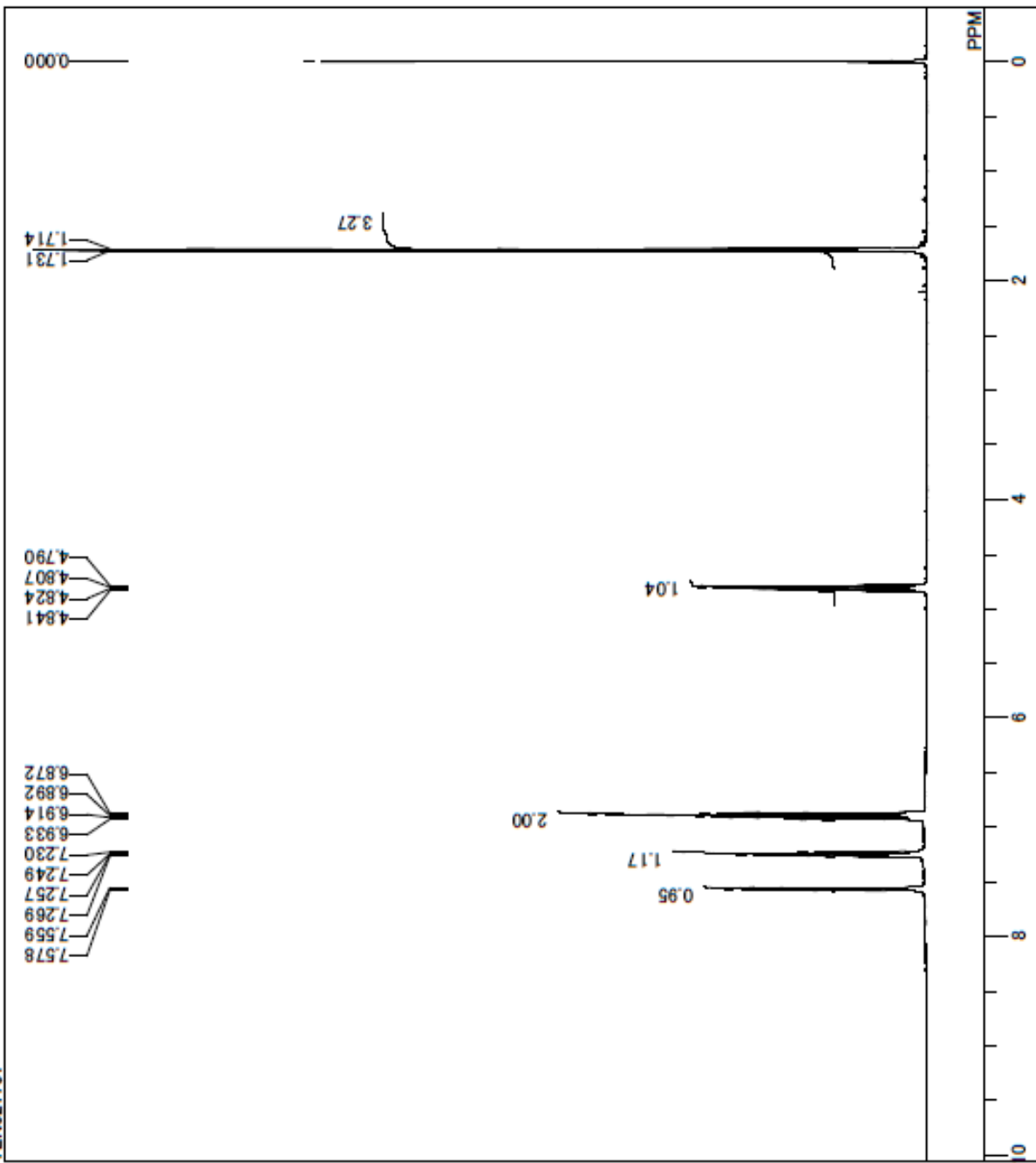


DFILE
COMNT
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EXMOD
OBFRQ
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OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
GTEMP
SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator\...
TEN030071C
2012/May/08 22:18:49
13C
ZGPG30
100.63 MHz
0.00 KHz
10060.25 Hz
32768
24038.46 Hz
1024
0.0000 sec
0.0000 sec
7.10 usec
OFF
26.9 c
CDCL3
77.00 ppm
0.25 Hz
362



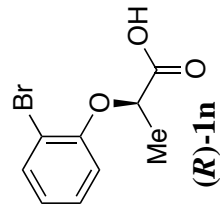
TEN021751



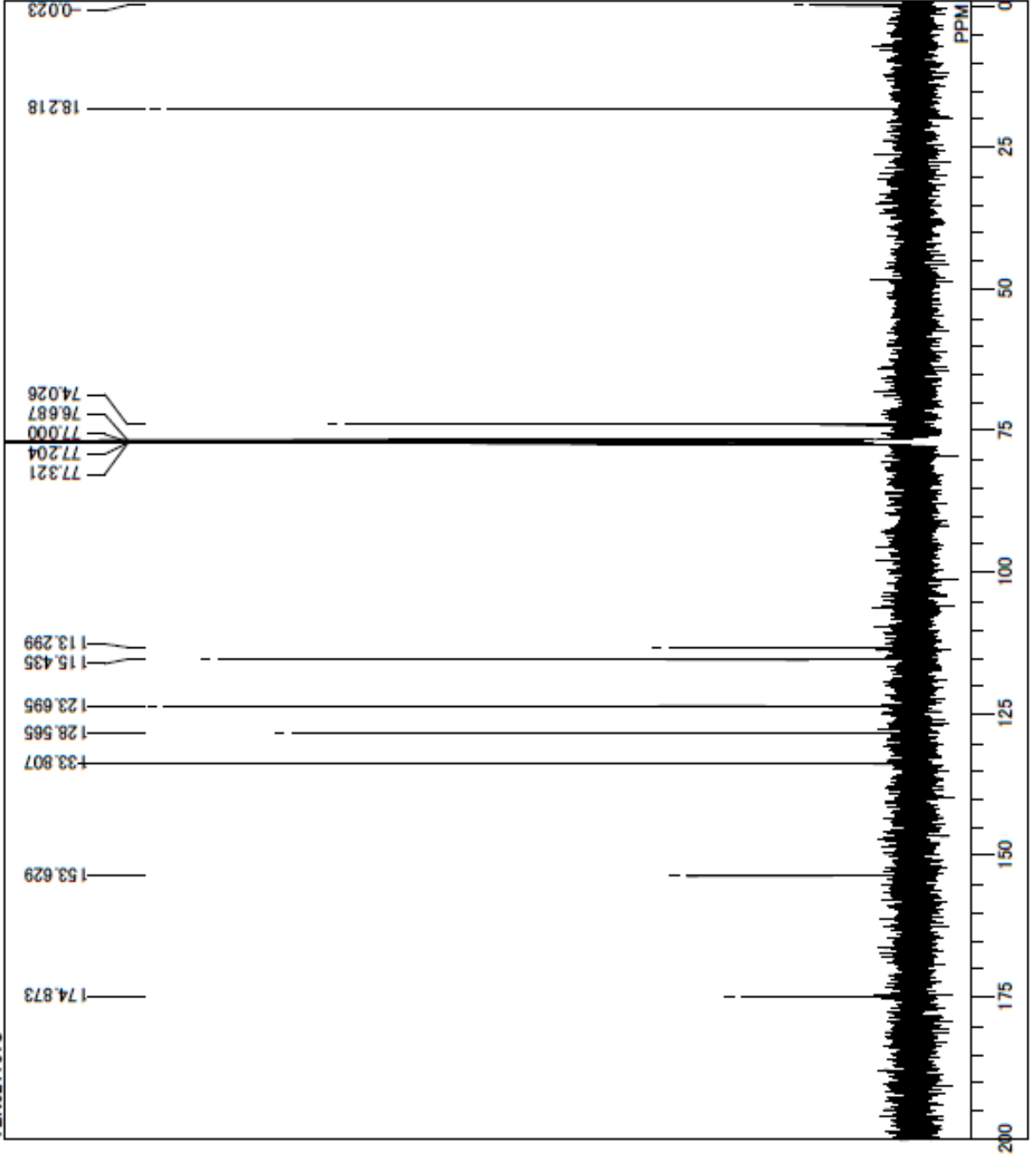
DFILE
COMNT
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SCANS
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PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator*子*
TEN021751
2011/Oct/14 04:01:50
1H
ZG30

400.18 MHz
0.00 KHz
2478.60 Hz
32768
8223.68 Hz
16
0.0000 sec
0.0000 sec
13.00 usec
OFF
30.9 c
CDCL3
0.00 ppm
0.25 Hz
456

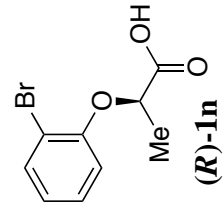


TEN021751C

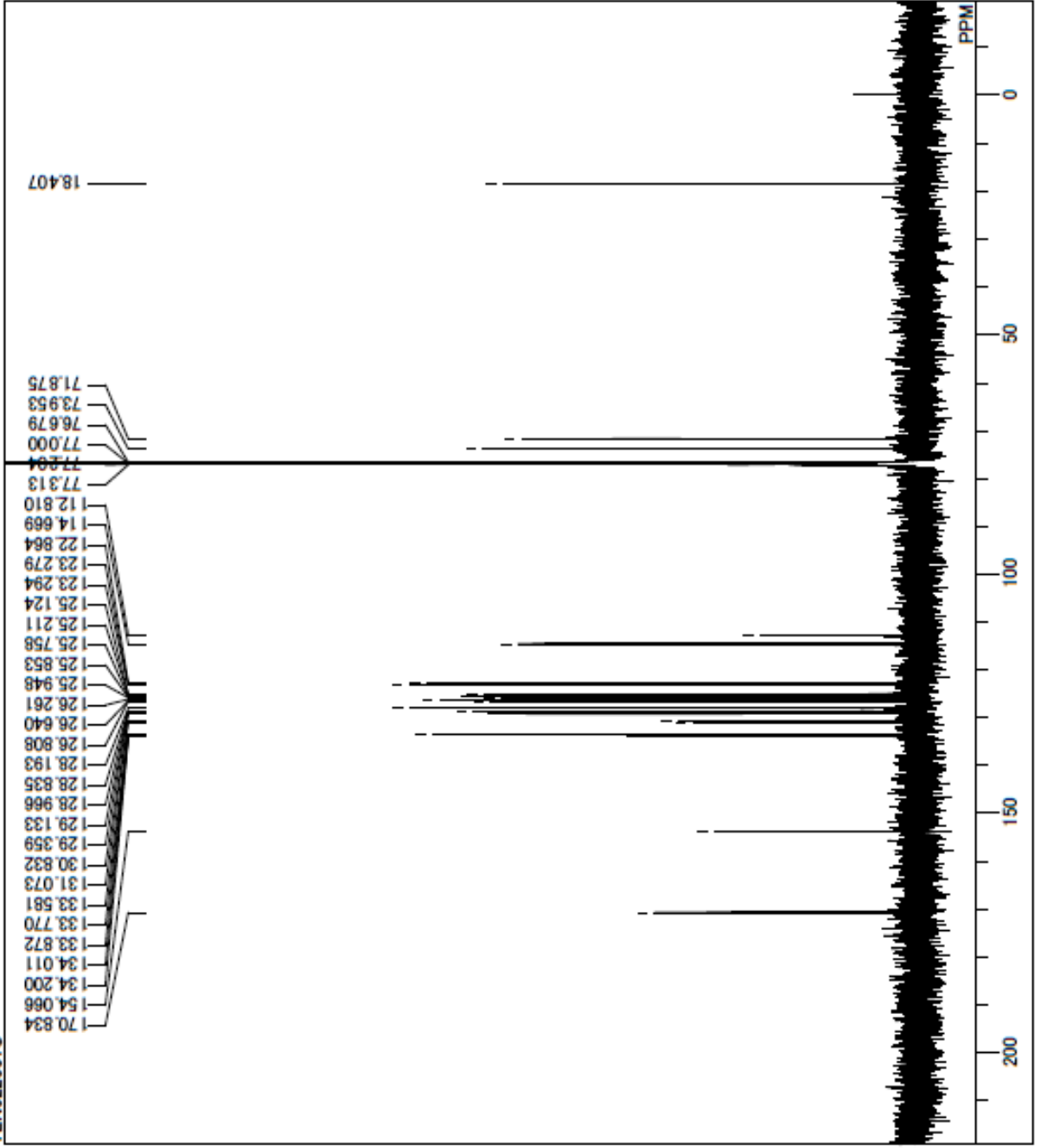


DFILE
COMINT
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SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator\...
TEN021751C
2012/Jun/19 23:41:33
13C
ZGPG30
100.63 MHz
0.00 KHz
10060.25 Hz
32768
24038.46 Hz
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0.0000 sec
0.0000 sec
7.10 usec
OFF
29.9 c
CDCL3
77.00 ppm
0.25 Hz
322

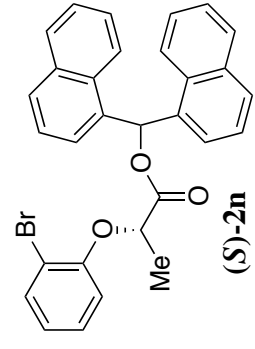


TEN022001C

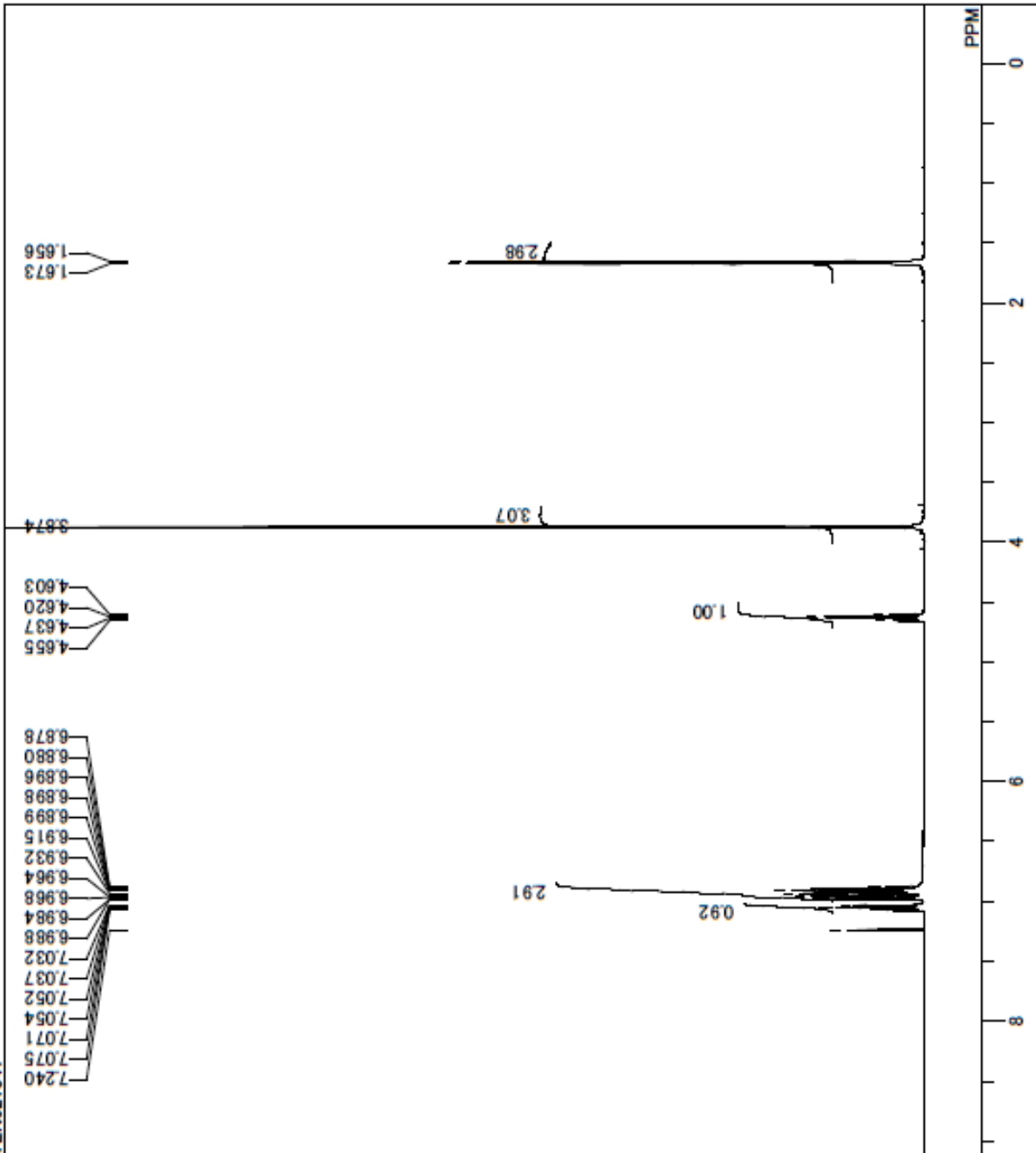


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PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

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TEN022001C
2012/May/16 00:20:01
13C
ZGPG30
100.63 MHz
0.00 KHz
10060.25 Hz
32768
24038.46 Hz
512
0.0000 sec
0.0000 sec
7.10 usec
OFF
26.9 c
CDCL3
77.00 ppm
0.25 Hz
57

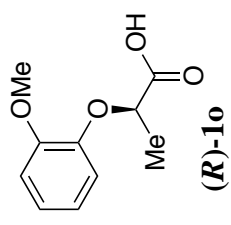


TEN021341

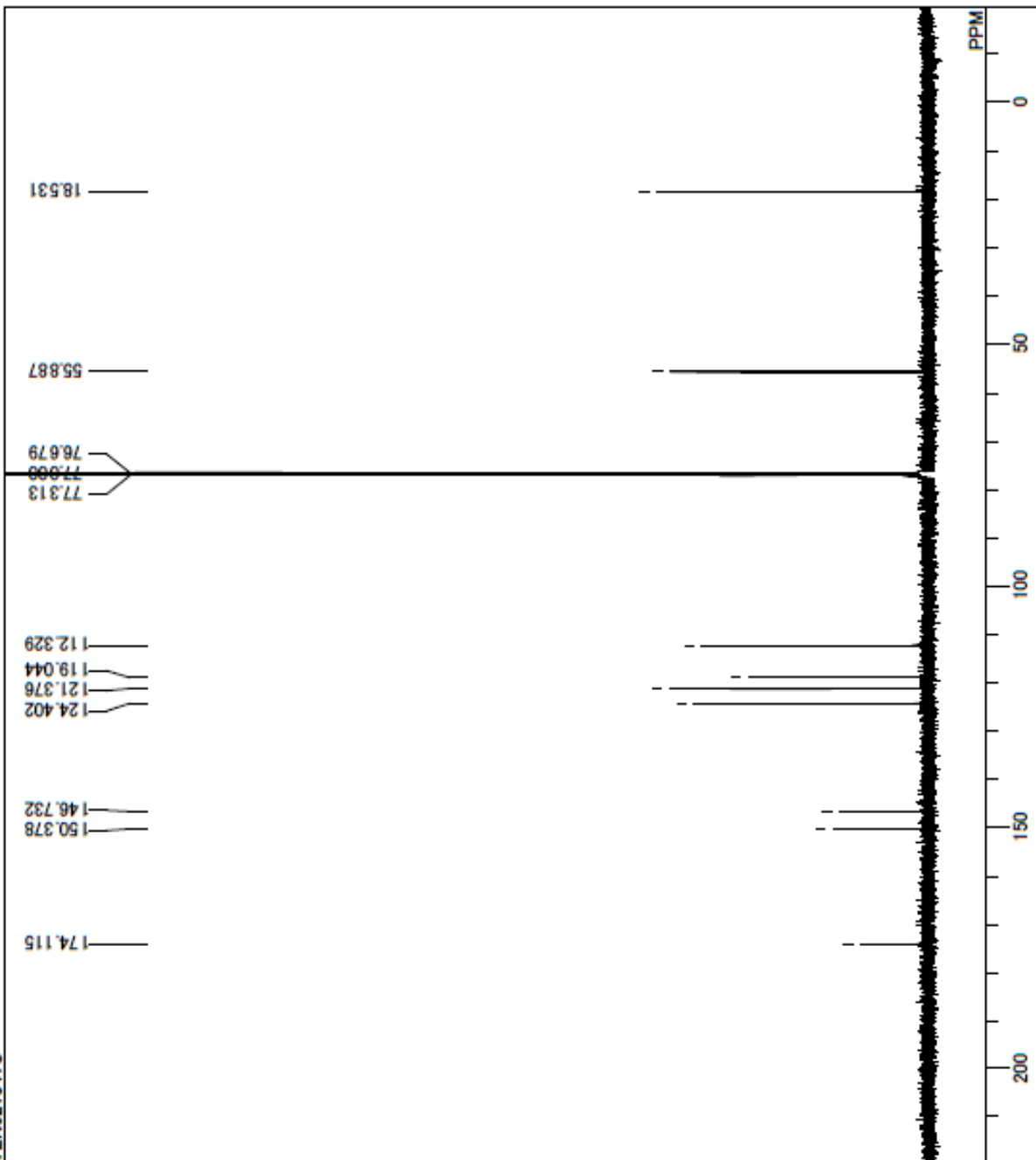


DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREOU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator*
TEN021341
2011/Sep/30 06:20:52
1H
ZG30
400.18 MHz
0.00 KHz
2478.60 Hz
32768
8223.68 Hz
16
0.0000 sec
0.0000 sec
13.00 usec
OFF
29.9 c
CDCL3
7.24 ppm
0.25 Hz
406

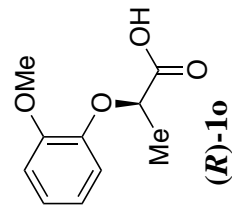


TEN021341C

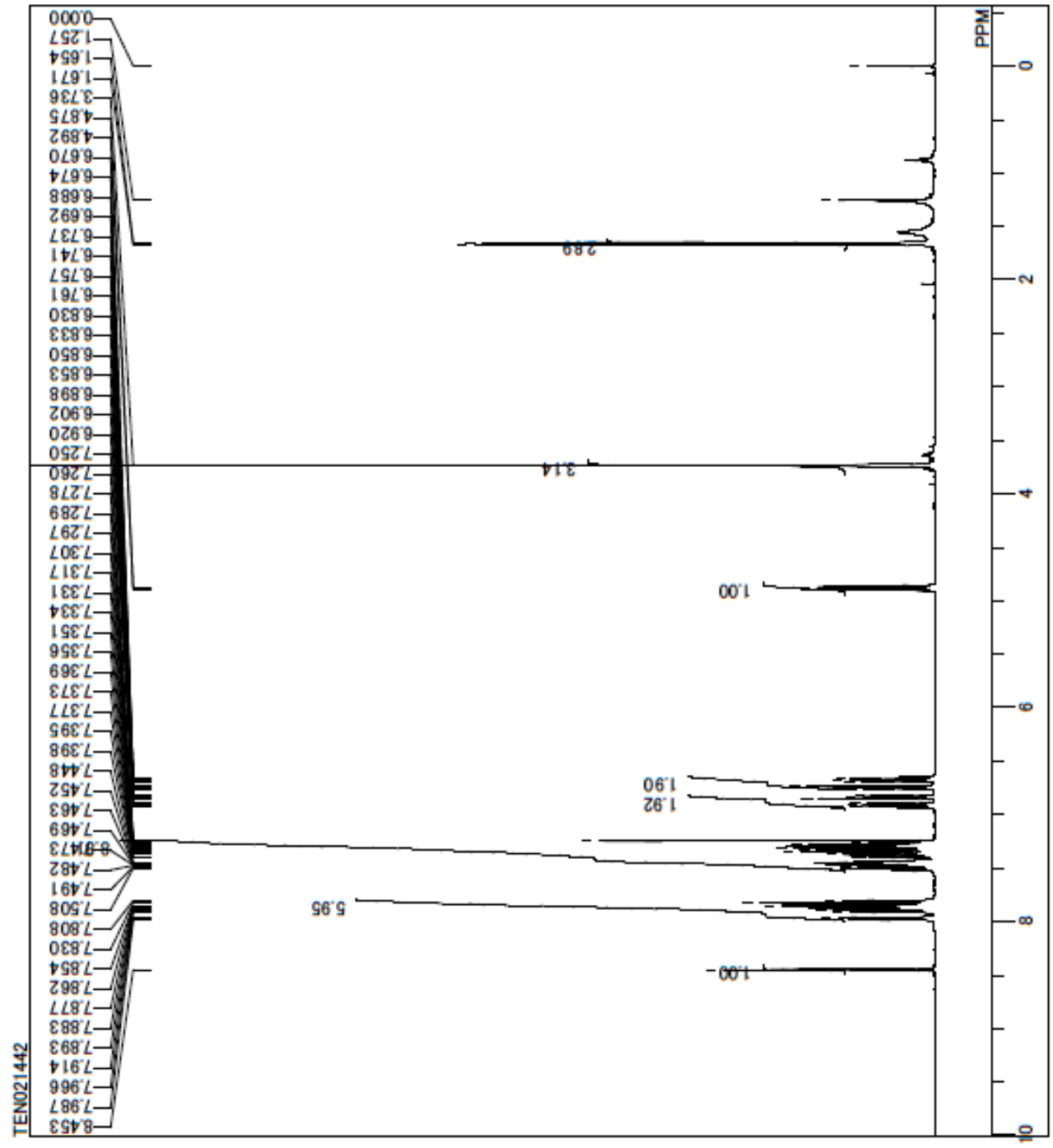
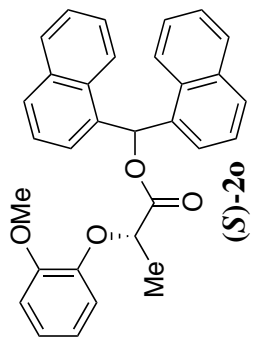


DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREOU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

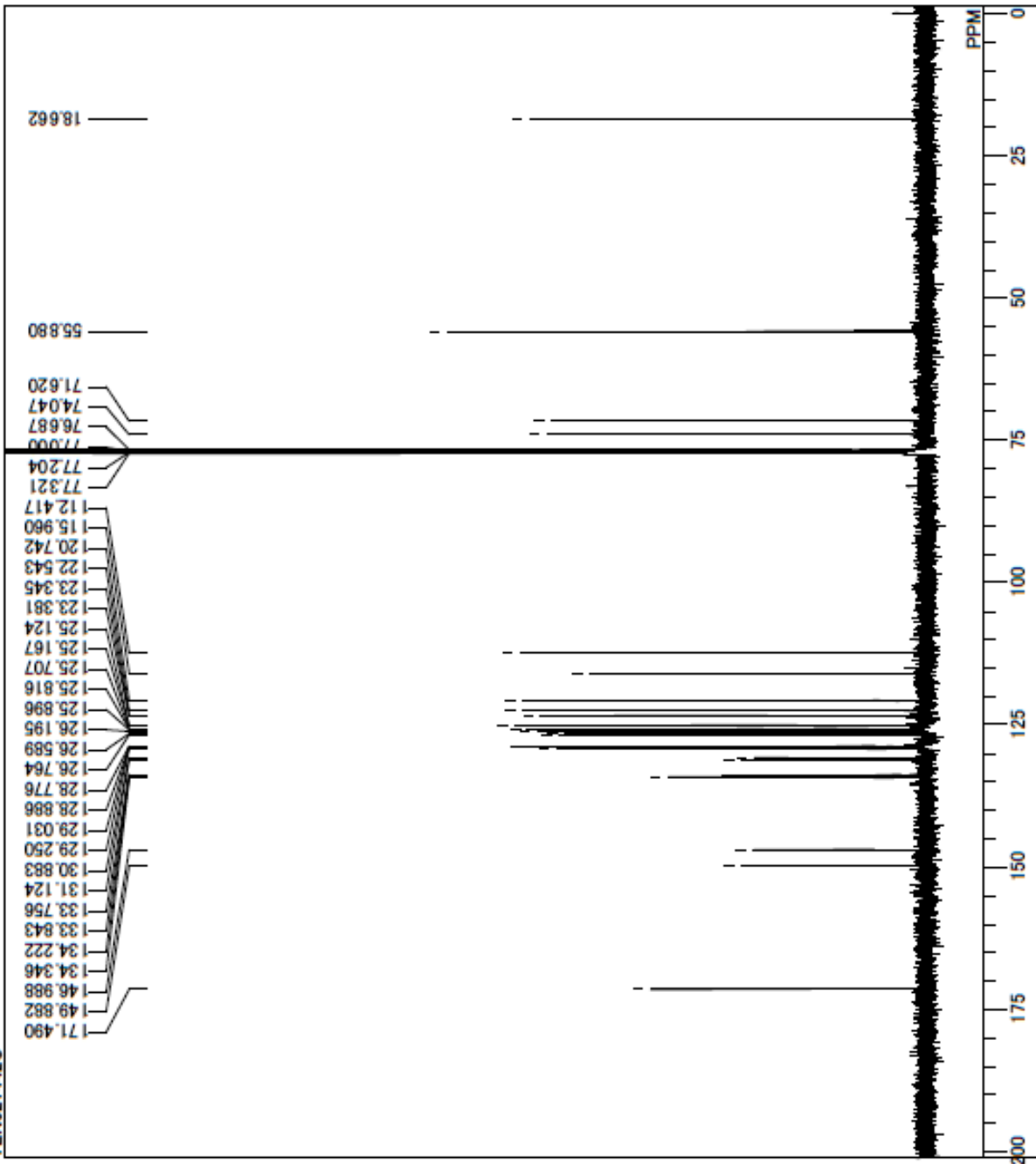
C:\Documents and Settings\Administrator*子*
TEN021341C
2011/Oct/01 01:12:02
13C
ZGPG30
100.63 MHz
0.00 KHz
10060.25 Hz
32768
24038.46 Hz
512
0.0000 sec
0.0000 sec
7.10 usec
OFF
29.9 c
CDCL3
77.00 ppm
0.25 Hz
57



F:\TEN021442.als
 TEN021442
 2012/Jun/21 08:24:16
 1H
 ZG30
 400.18 MHz
 0.00 KHz
 2478.60 Hz
 32768
 8223.68 Hz
 64
 0.0000 sec
 0.0000 sec
 13.00 usec
 PW1
 OFF
 IRNUC
 CTEMP 29.9 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.25 Hz
 RGAIN 362

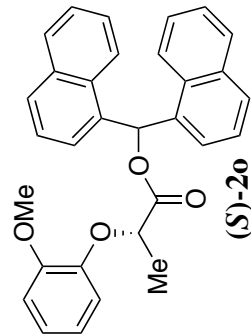


TEN021442C

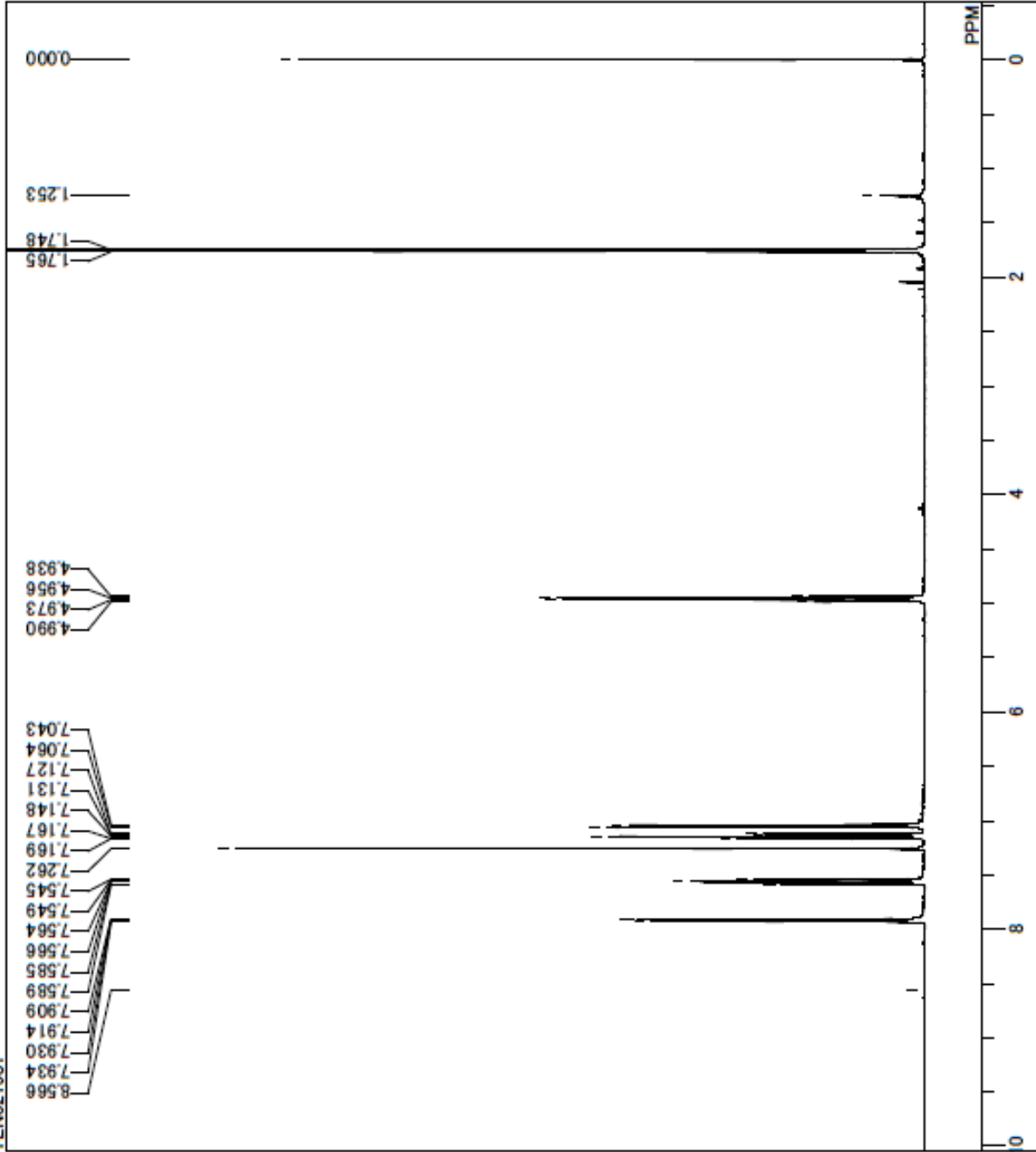


DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREOU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

TEN021442C
2012/May/15 23:05:44
13C
ZGPG30
100.63 MHz
0.00 KHz
10060.25 Hz
32768
24038.46 Hz
512
0.0000 sec
0.0000 sec
7.10 usec
OFF
26.9 c
CDCL3
77.00 ppm
0.25 Hz
406

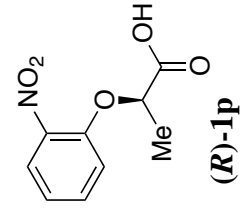


TEN021981

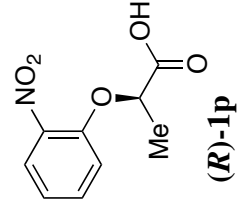
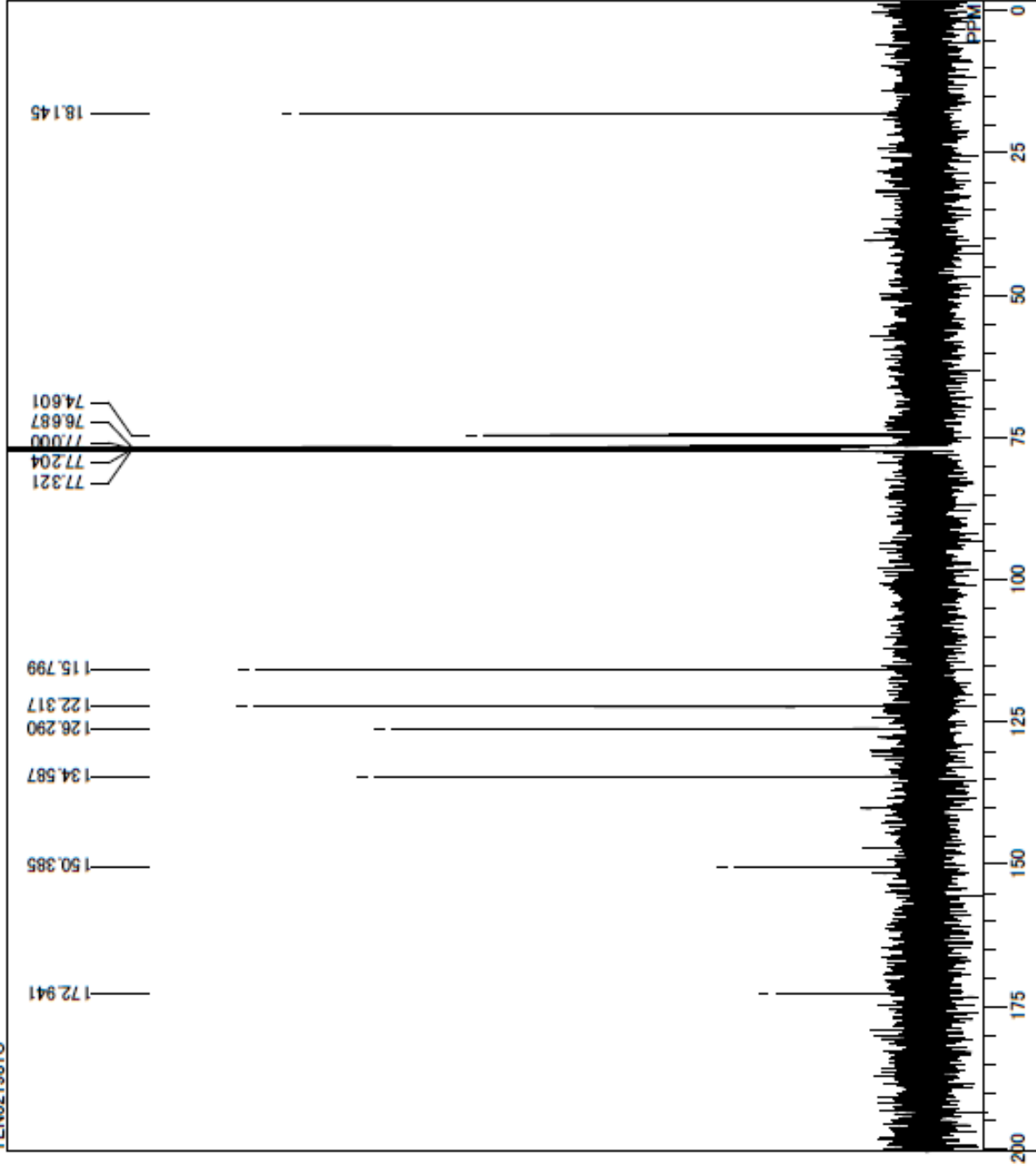


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COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREOU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

TEN021981
2012/May/21 10:46:32
1H
ZG30
400.18 MHz
0.00 KHz
2478.60 Hz
32768
8223.68 Hz
64
0.0000 sec
0.0000 sec
13.00 usec
OFF
26.9 c
CDCL3
0.00 ppm
0.25 Hz
645



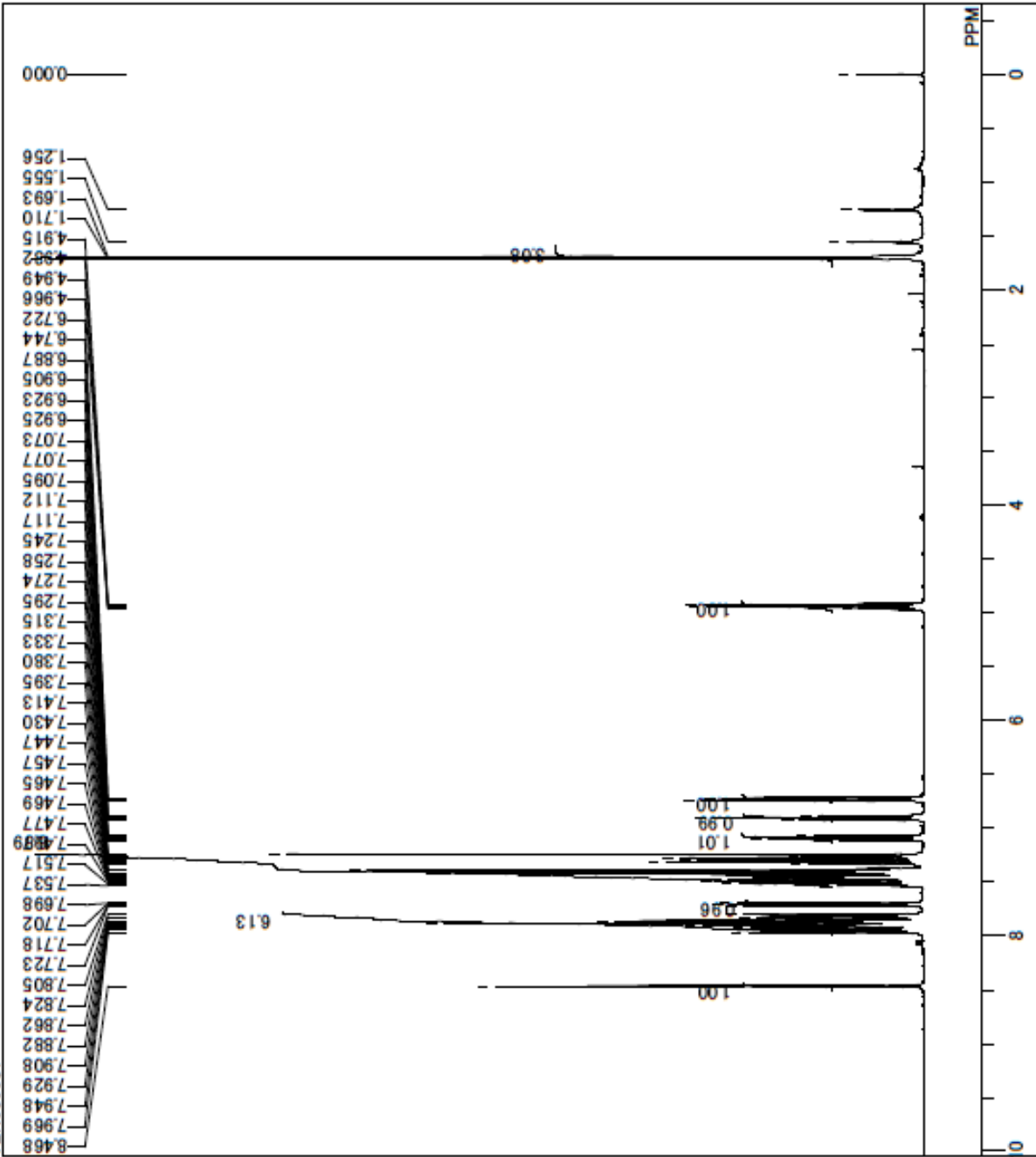
TEN021981C



DFILE
COMINT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

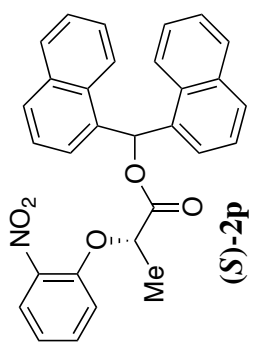
C:\Documents and Settings\Administrator\...
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2011/Oct/20 23:07:42
13C
ZGPG30
100.63 MHz
0.00 KHz
10060.25 Hz
32768
24038.46 Hz
1024
0.0000 sec
0.0000 sec
7.10 usec
OFF
29.9 c
CDCL3
77.00 ppm
0.25 Hz
114

TEN030081

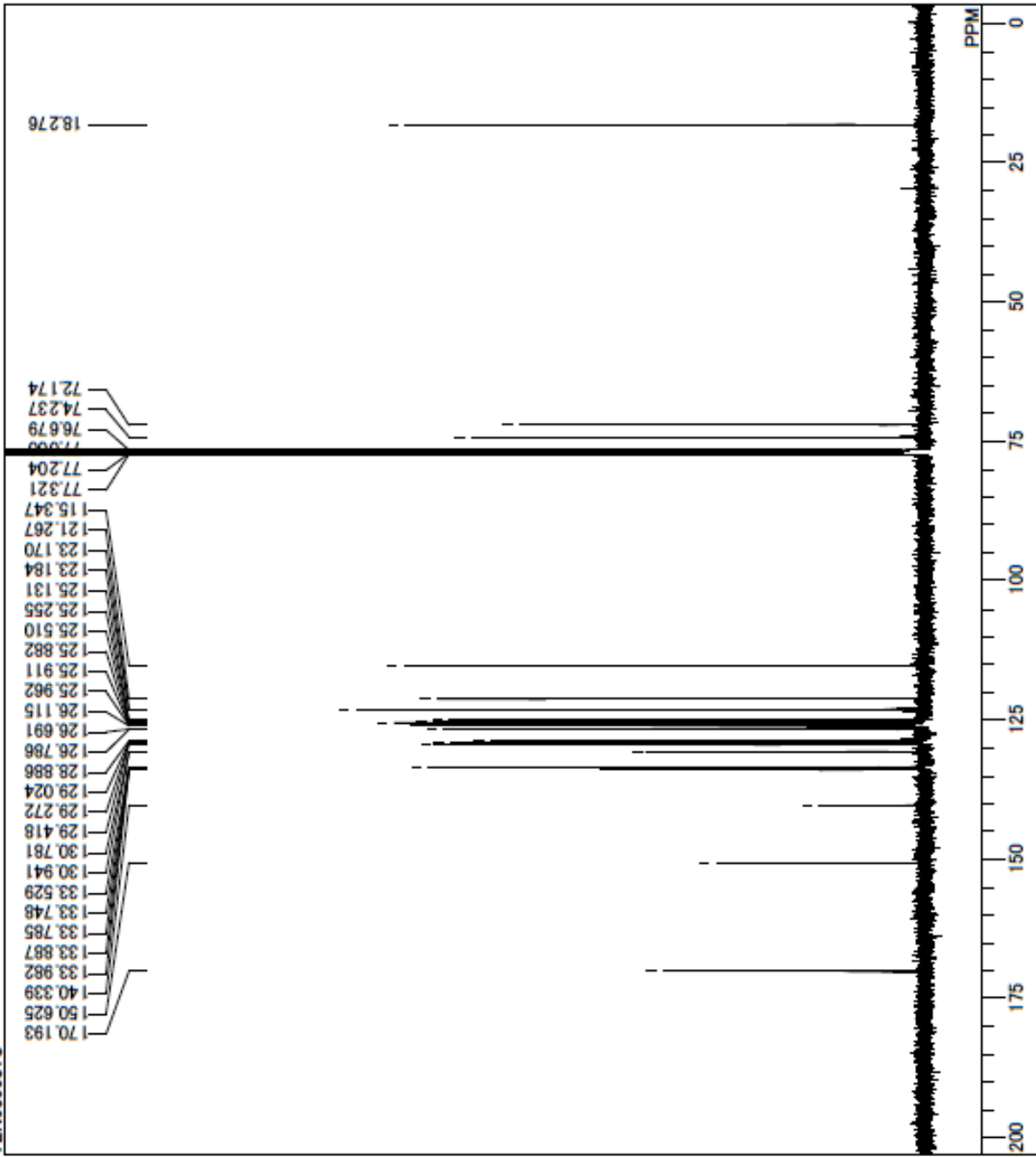


DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREOU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator\TEN030081
2012/May/07 10:05:08
1H
ZG30
400.18 MHz
0.00 KHz
2478.60 Hz
32768
8223.68 Hz
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0.0000 sec
13.00 usec
OFF
26.9 c
CDCL3
0.00 ppm
0.25 Hz
228

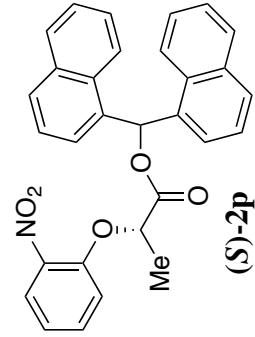


TEN030081C

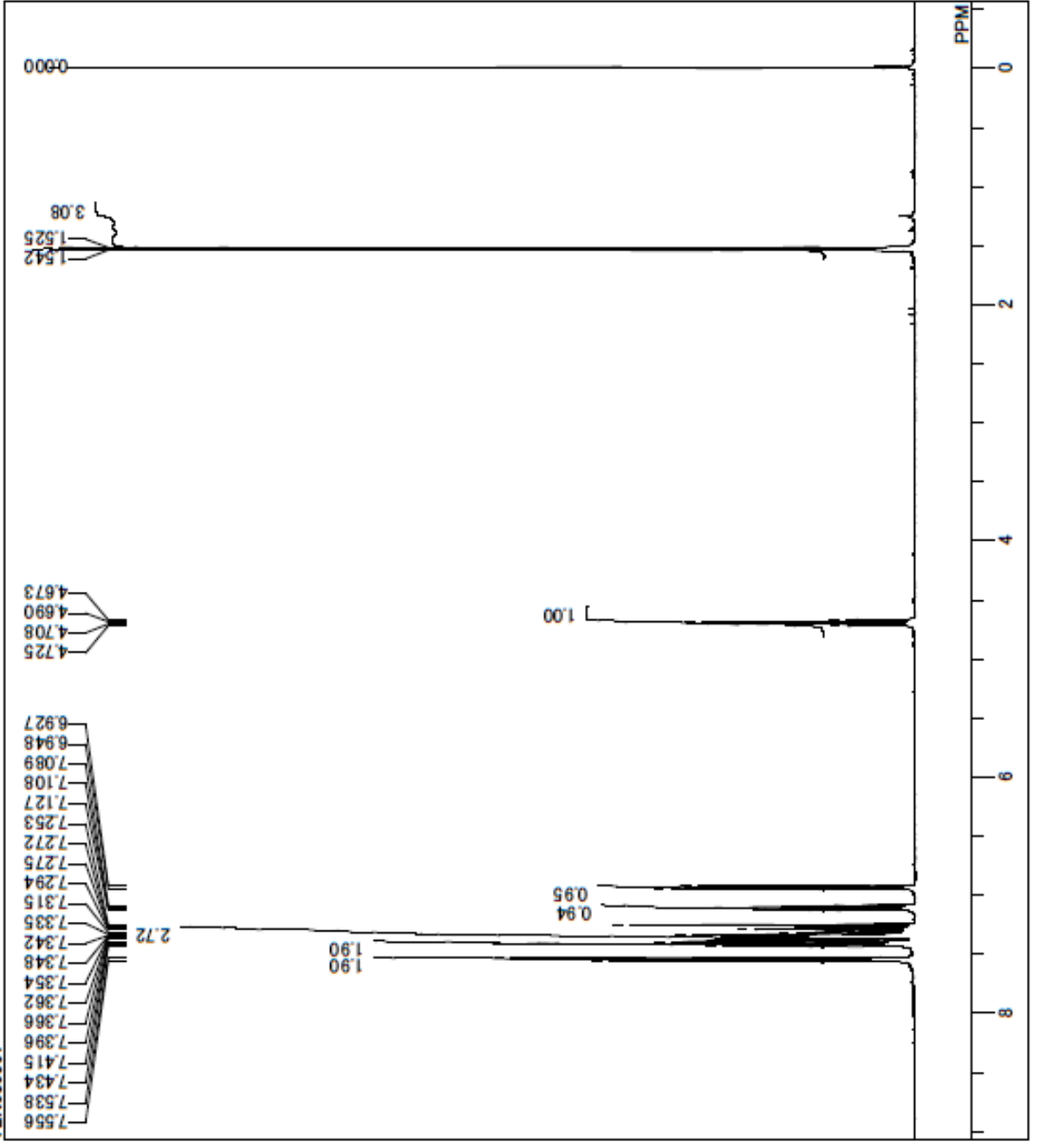


DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREOU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator*子*
TEN030081C
2012/May/08 23:24:17
13C
ZGPG30
100.63 MHz
0.00 KHz
10060.25 Hz
32768
24038.46 Hz
1024
0.0000 sec
0.0000 sec
7.10 usec
OFF
26.9 c
CDCL3
77.00 ppm
0.25 Hz
456

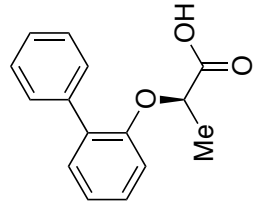


TEN030561



DFILE
COMNT
DATIM
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EXMOD
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OBSET
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FREQU
SCANS
ACQTM
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PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

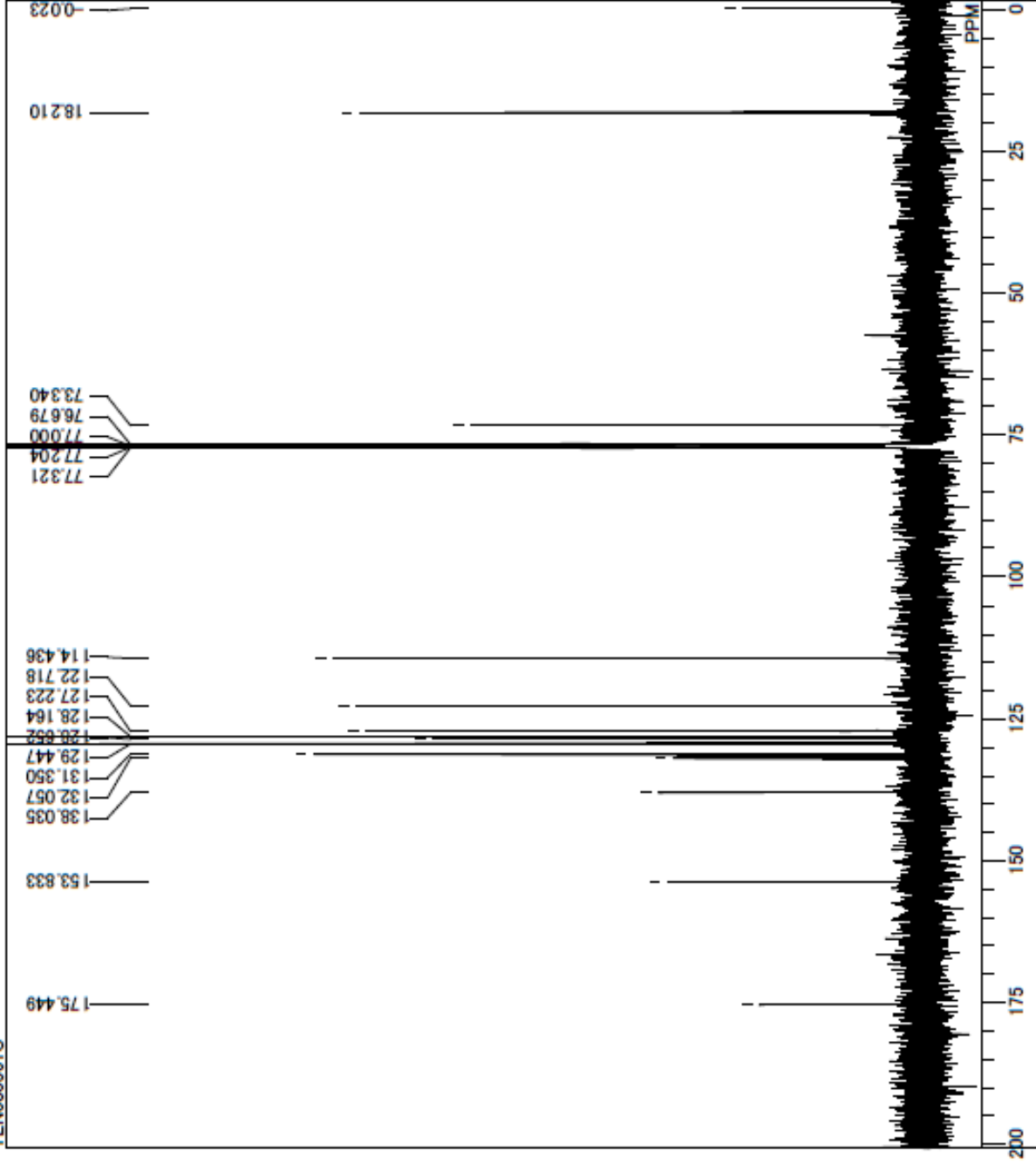
TEN030561
2011/Nov/12 02:19:54
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32768
8223.68 Hz
16
0.0000 sec
0.0000 sec
13.00 usec
OFF
30.9 c
CDCL3
0.00 ppm
0.25 Hz
456



(R)-1q

C:\Documents and Settings\Administrator\...

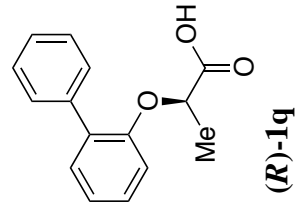
TEN030561C



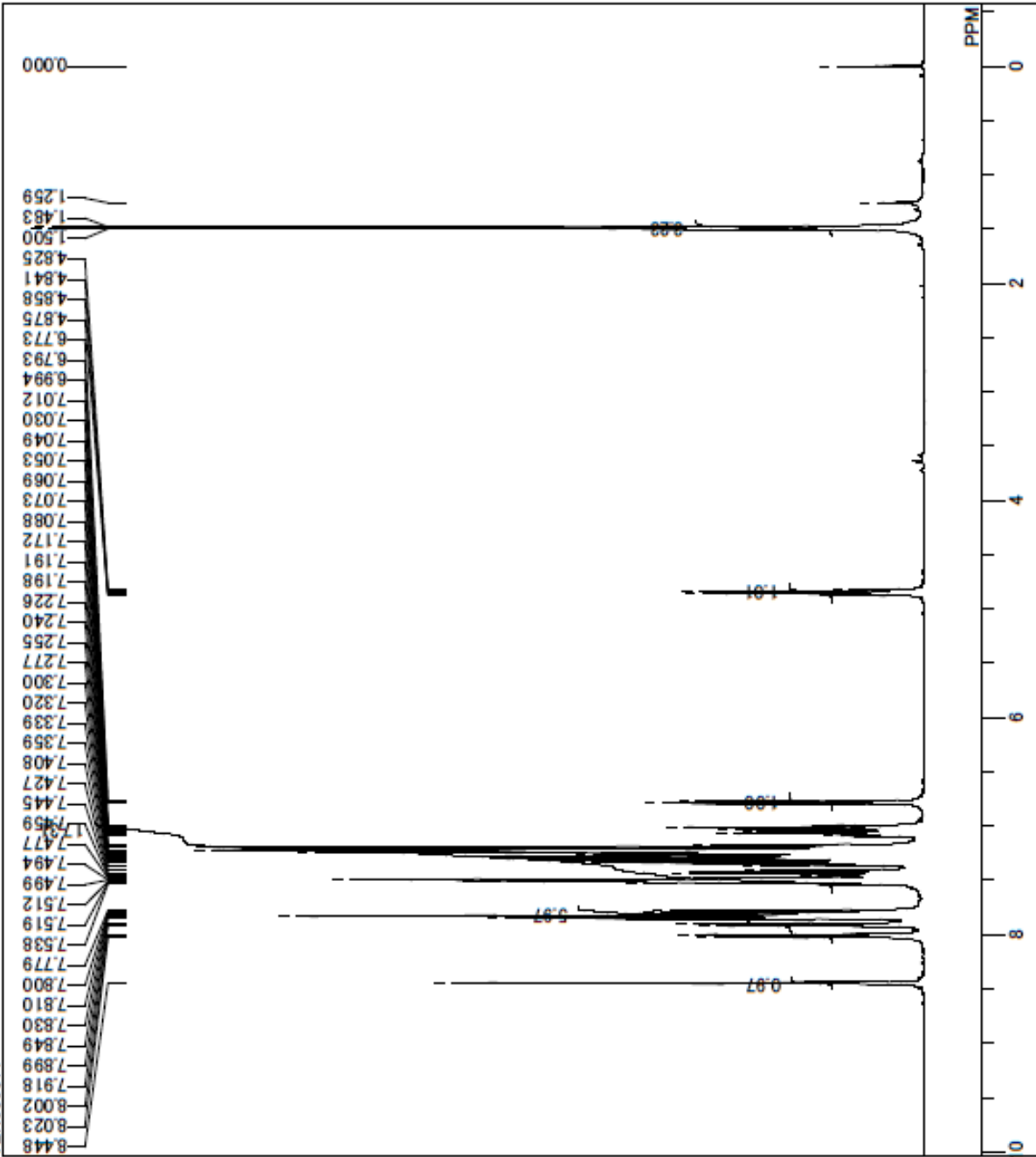
DFILE
COMINT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator\...
TEN030561C
2011/Nov/13 00:20:37
13C

ZGPG30
100.63 MHz
0.00 KHz
10060.25 Hz
32768
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0.0000 sec
0.0000 sec
7.10 usec
OFF
29.9 c
CDCL3
77.00 ppm
0.25 Hz
228

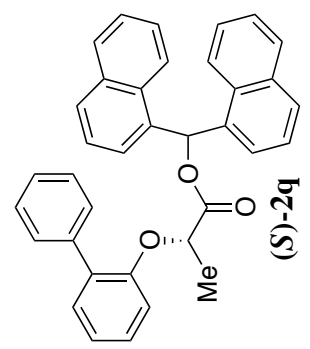


TEN050671

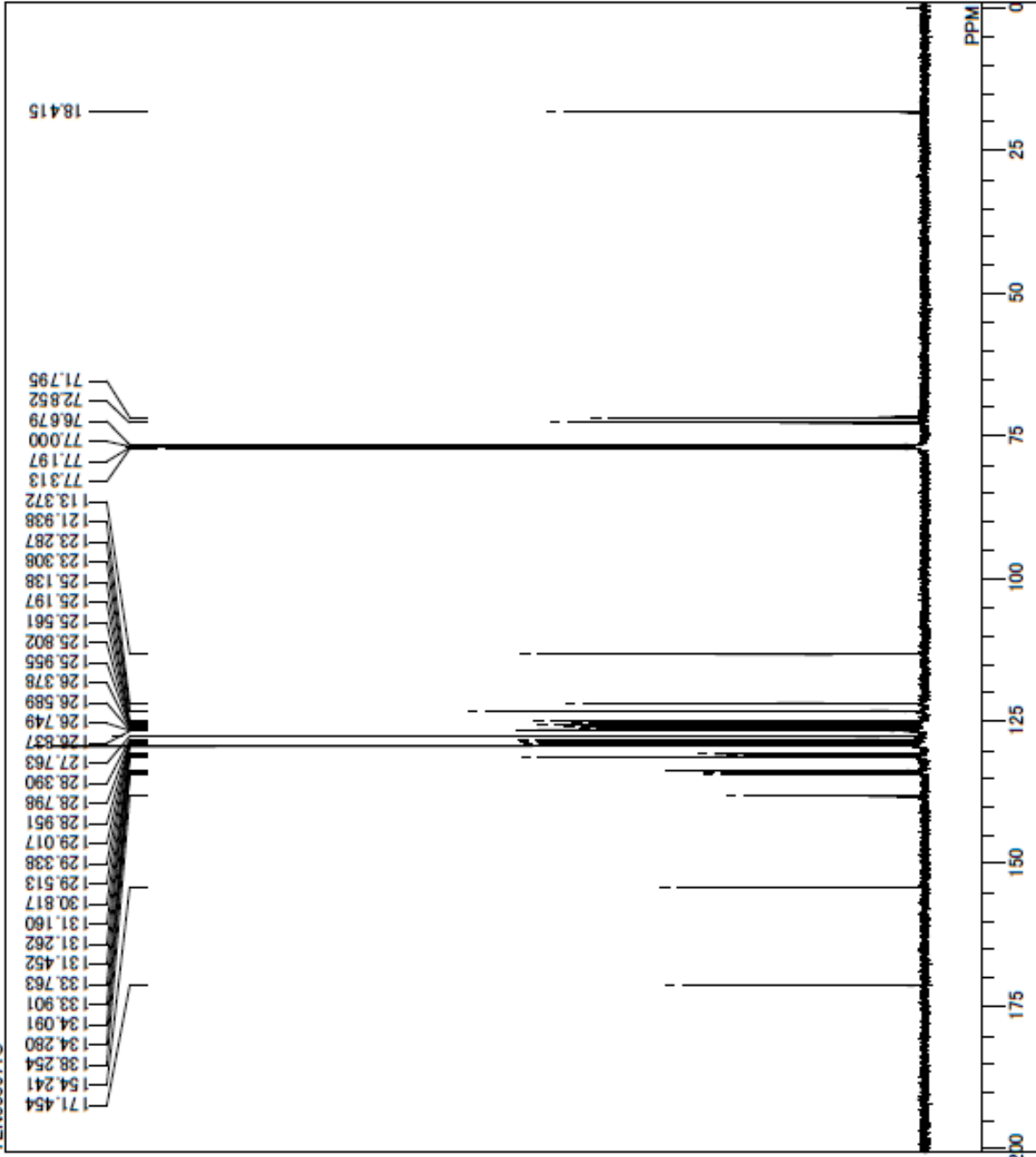


DFILE
COMNT
DATIM
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EXMOD
OBFRQ
OBSET
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POINT
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PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator\...
TEN050671
2012/Jun/03 23:24:05
1H
ZG30
400.18 MHz
0.00 KHz
2478.60 Hz
32768
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0.0000 sec
0.0000 sec
13.00 usec
OFF
29.9 c
CDCL3
0.00 ppm
0.25 Hz
90

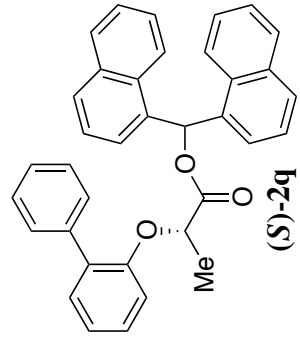


TEN050671C

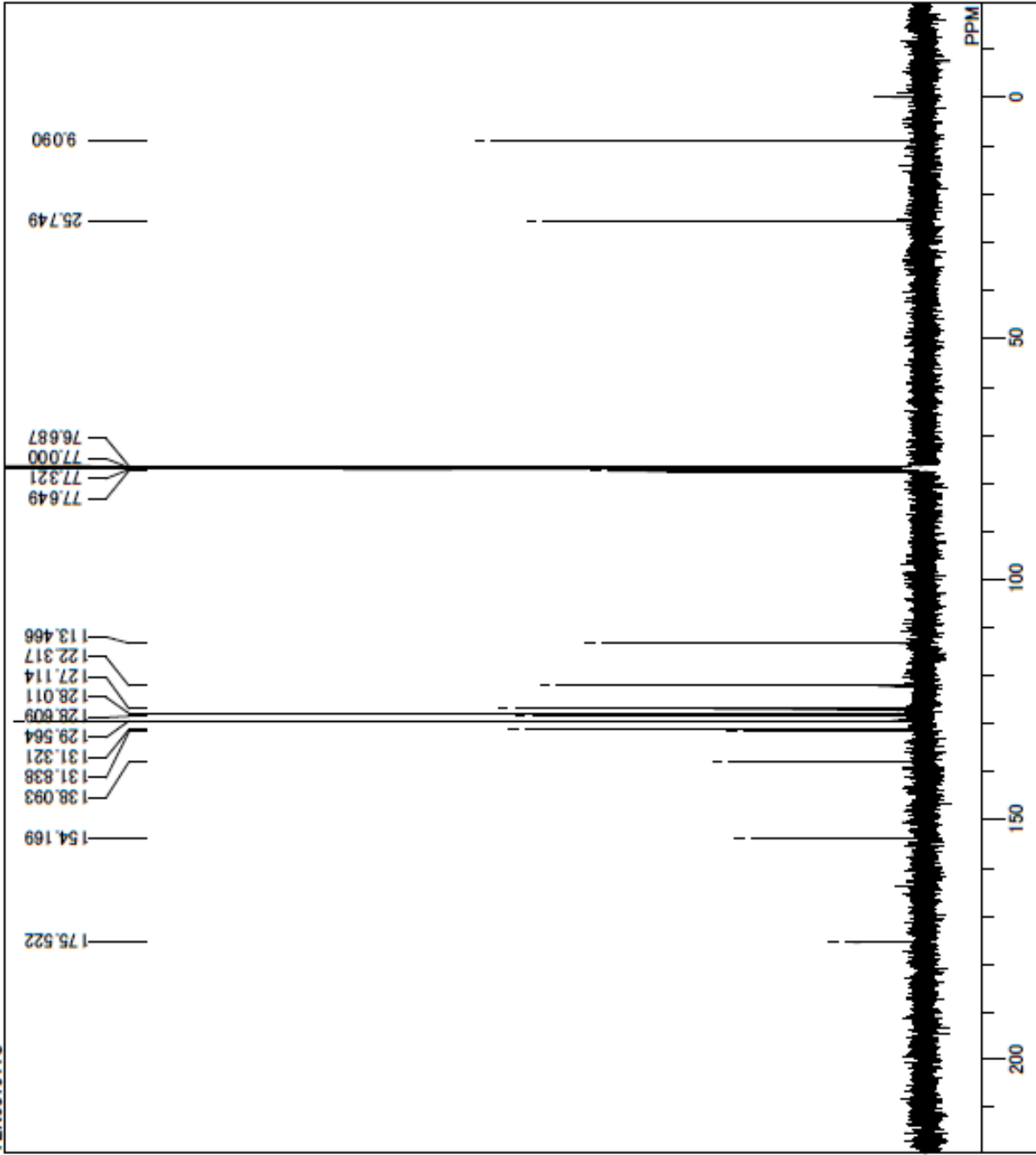


DFILE
COMNT
DATIM
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OBSET
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ACQTM
PD
PW1
IRNUC
GTEMP
SLVNT
EXREF
BF
RGAIN

TEN050671C
2012/Jun/04 00:24:46
13C
ZGPG30
100.63 MHz
0.00 KHz
10060.25 Hz
32768
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0.0000 sec
7.10 usec
OFF
29.9 c
CDCL3
77.00 ppm
0.25 Hz
57

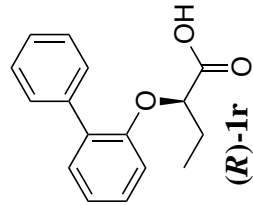


TEN031511C



DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
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FREOU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

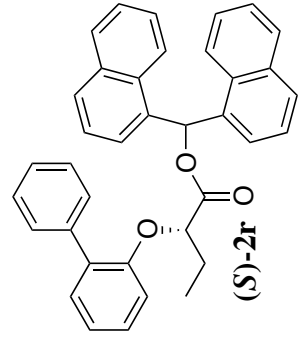
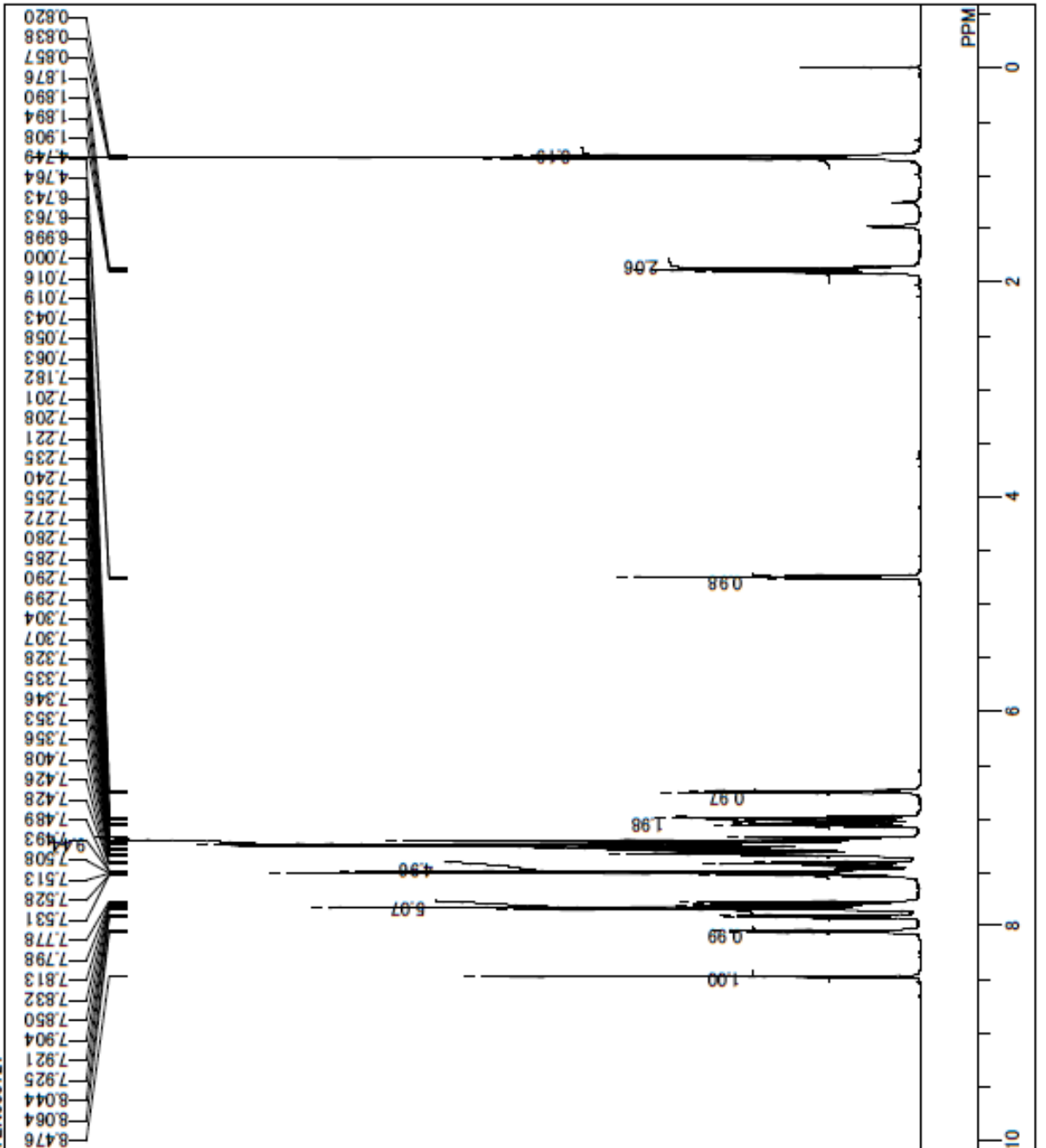
C:\Documents and Settings\Administrator*子*
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2011/Dec/22 01:18:41
13C
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100.63 MHz
0.00 KHz
10060.25 Hz
32768
24038.46 Hz
512
0.0000 sec
0.0000 sec
7.10 usec
OFF
29.9 c
CDCL3
77.00 ppm
0.25 Hz
64



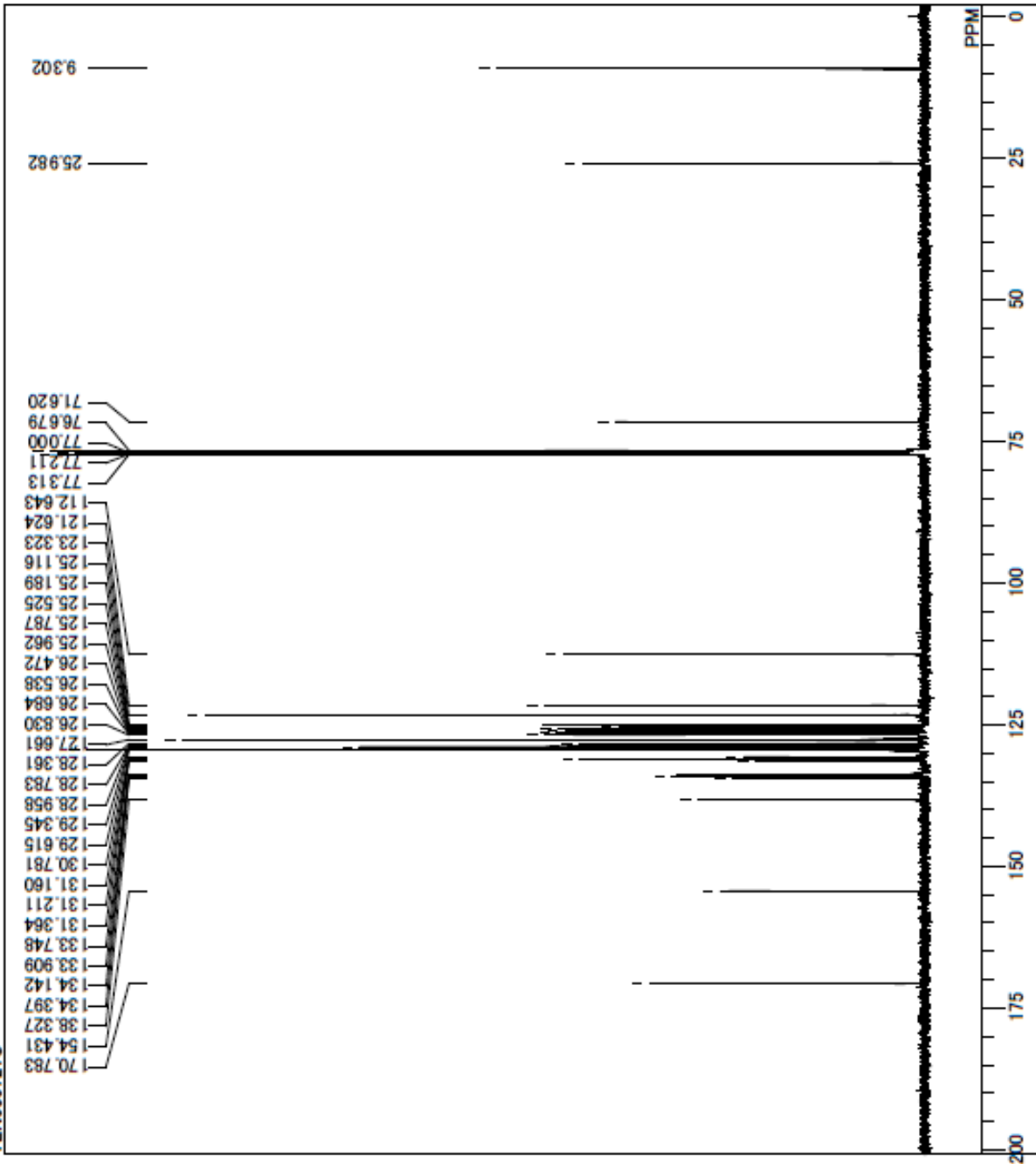
TEN050721

DFILE
 COMNT
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 EXMOD
 OBFRQ
 OBSET
 OBFIN
 POINT
 FREOU
 SCANS
 ACQTM
 PD
 PW1
 IRNUC
 CTEMP
 SLVNT
 EXREF
 BF
 RGAIN

C:\Documents and Settings\Administrator\...
 TEN050721
 2012/Jun/07 23:25:20
 1H
 ZG30
 400.18 MHz
 0.00 KHz
 2478.60 Hz
 32768
 8223.68 Hz
 16
 0.0000 sec
 0.0000 sec
 13.00 usec
 OFF
 29.9 c
 CDCL3
 0.00 ppm
 0.25 Hz
 101



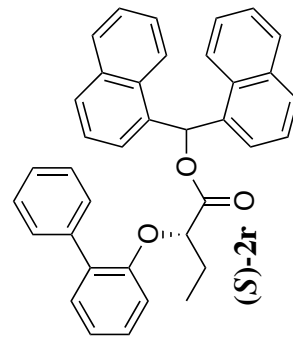
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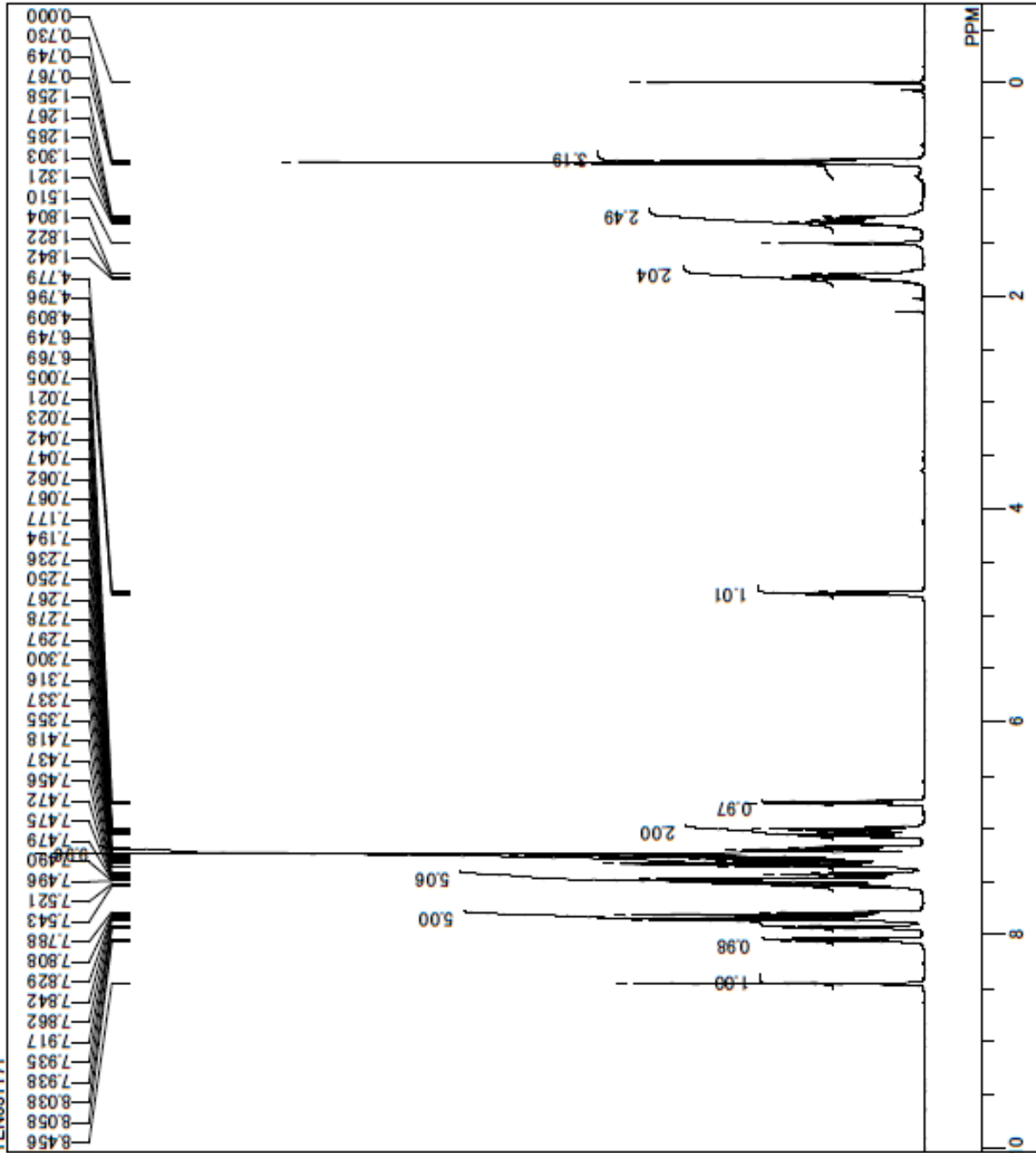
DFILE
COMINT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator\...
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2012/Jun/08 00:26:00
13C
ZGPG30

100.63 MHz
0.00 KHz
10060.25 Hz
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OFF
29.9 c
CDCL3
77.00 ppm
0.25 Hz
64



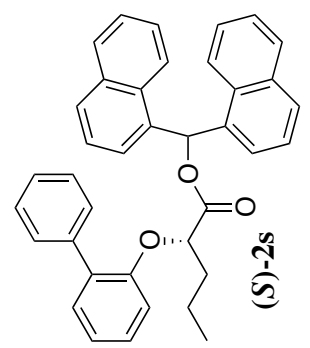
TEN031171



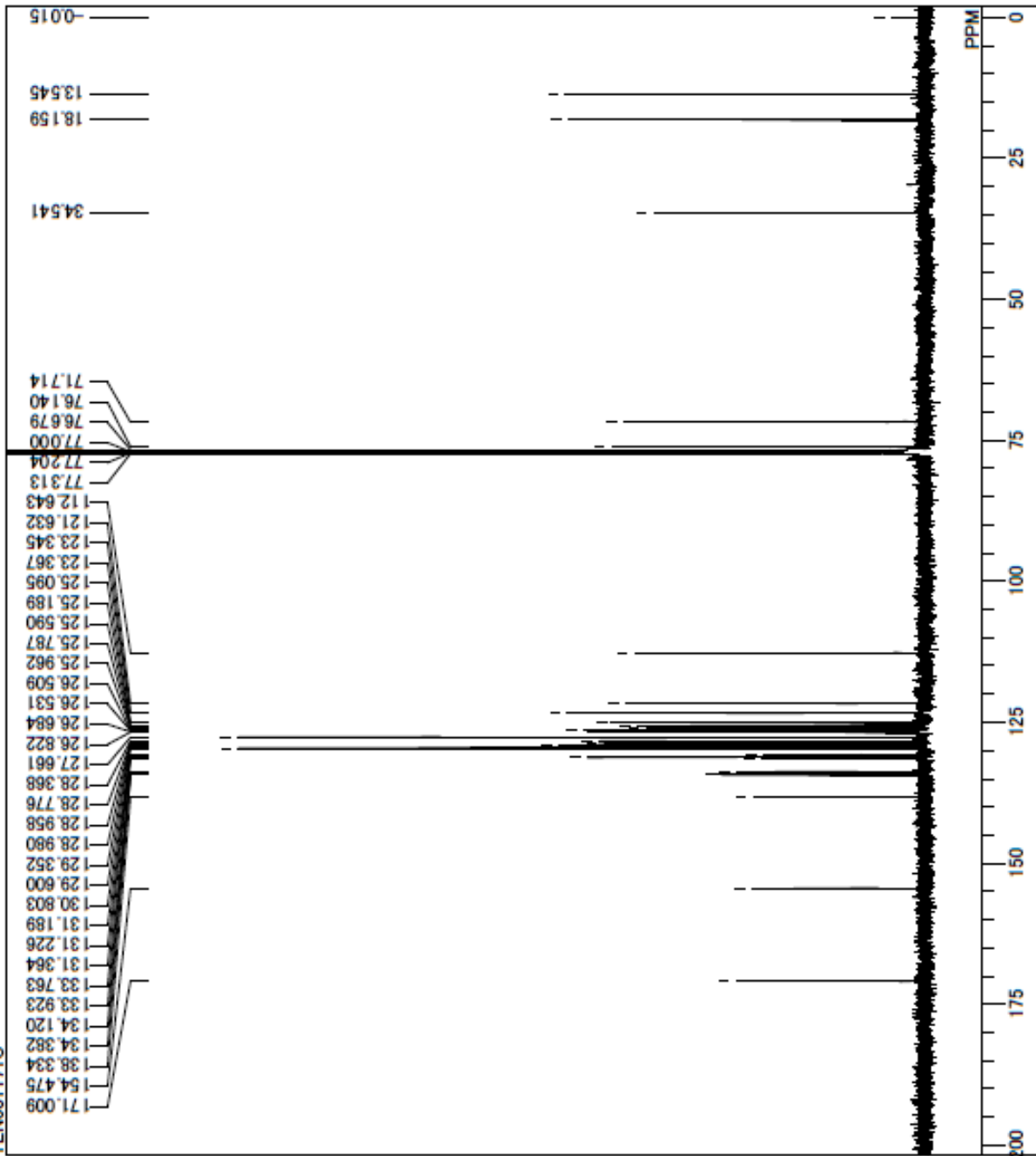
DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREOU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator\...
TEN031171
2012/Jun/01 07:41:25
1H
ZG30

400.18 MHz
0.00 KHz
2478.60 Hz
32768
8223.68 Hz
16
0.0000 sec
0.0000 sec
13.00 usec
OFF
29.9 c
CDCL3
0.00 ppm
0.25 Hz
181

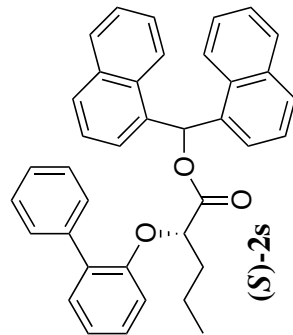


TEN031171C

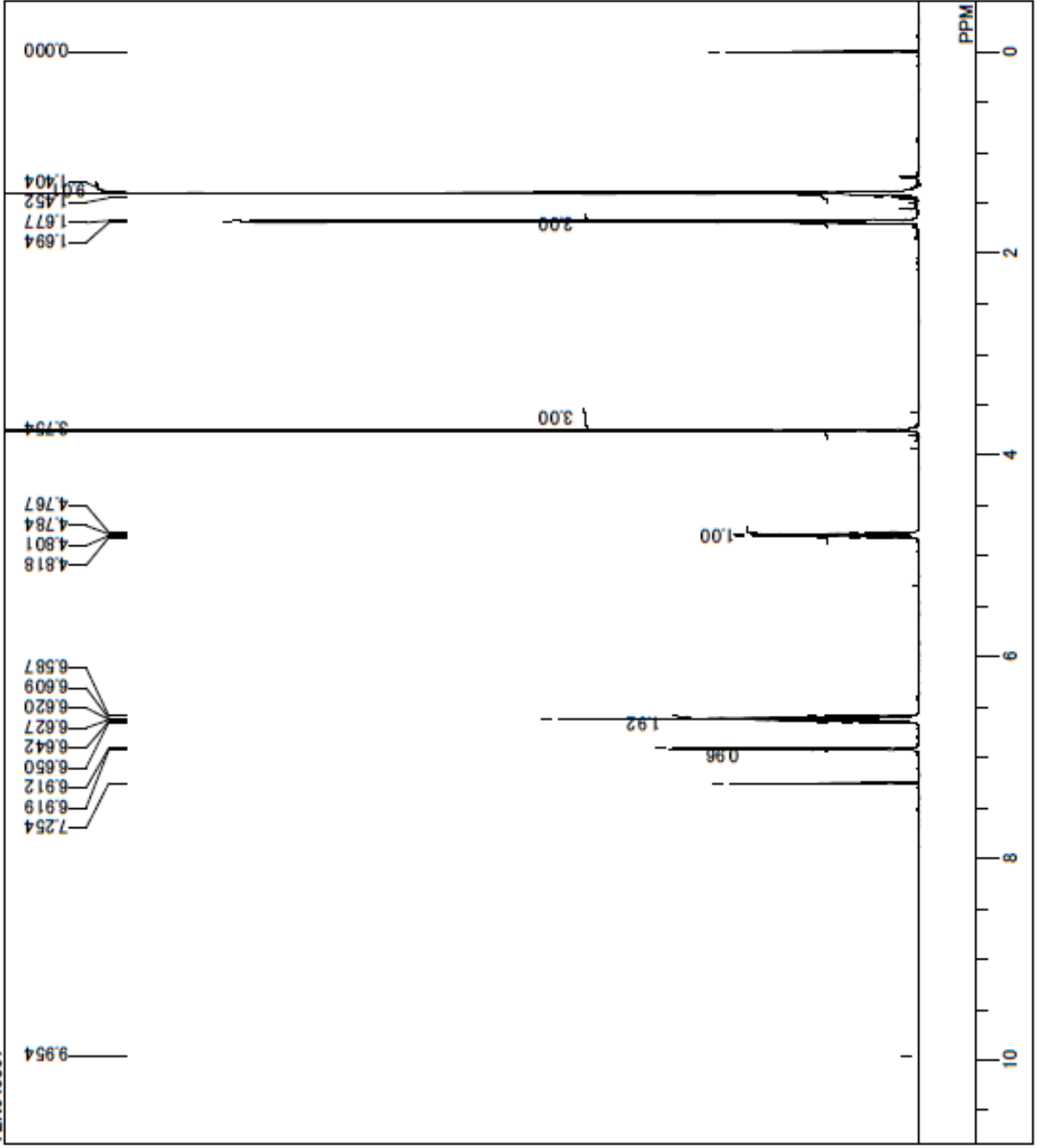


C:\Documents and Settings\Administrator\...

DFILE TEN031171C
COMNT 2012/Jun/01 22:57:23
DATIM 13C
OBNUC ZGPG30
EXMOD 100.63 MHz
OBFRQ 0.00 KHz
OBSET 10060.25 Hz
OBFIN 32768
POINT 24038.46 Hz
FREOU 1024
SCANS 0.0000 sec
ACQTM 0.0000 sec
PD 7.10 usec
PW1 OFF
IRNUC 29.9 c
CTEMP CDCL3
SLVNT 77.00 ppm
EXREF 0.25 Hz
BF 362
RGAIN

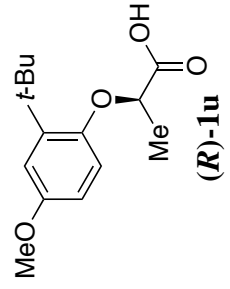


TEN040301

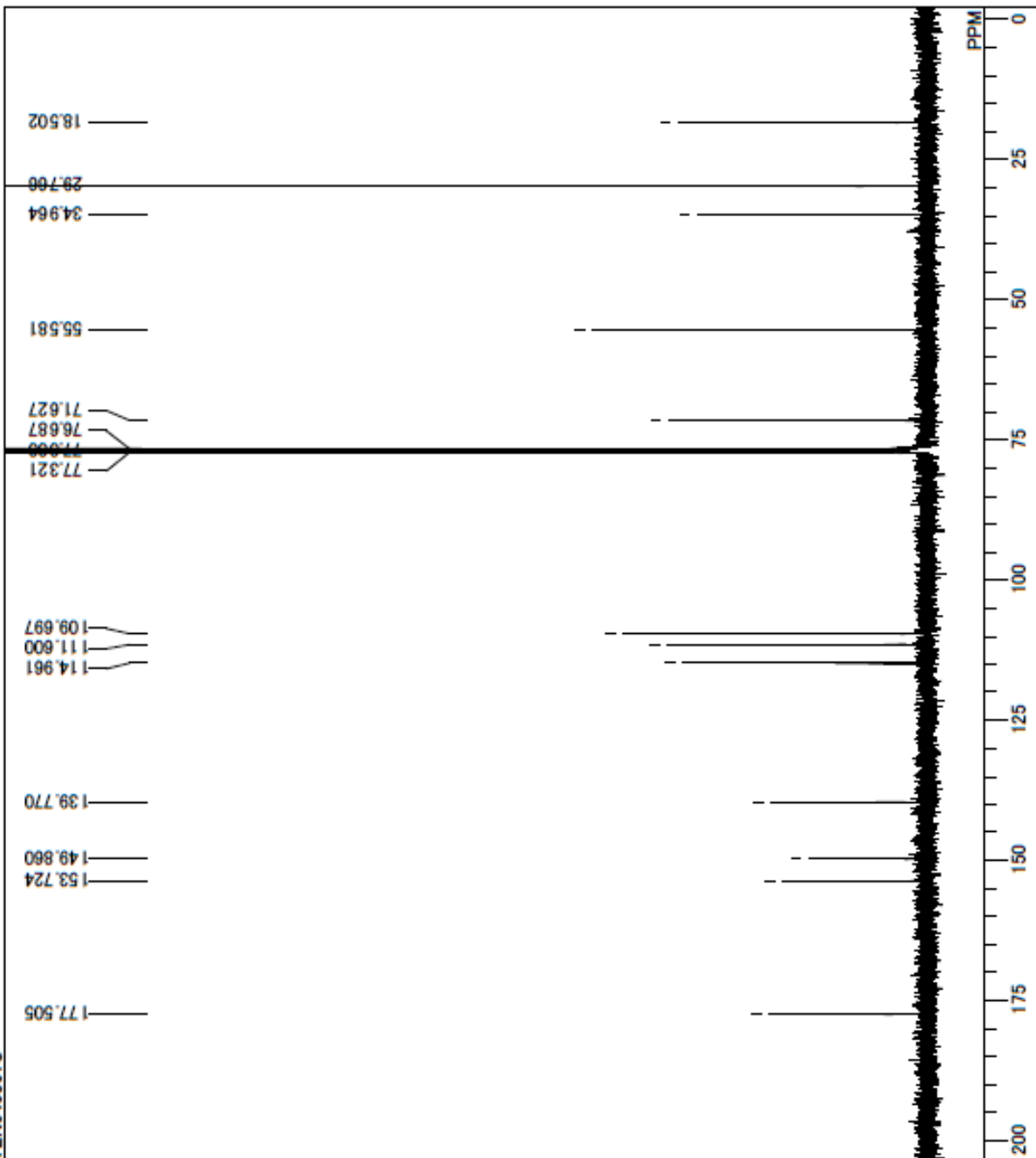


DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREOU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator*
TEN040301
2012/Jan/25 08:32:46
1H
ZG30
400.18 MHz
0.00 KHz
2478.60 Hz
32768
8223.68 Hz
16
0.0000 sec
0.0000 sec
13.00 usec
OFF
30.9 c
CDCL3
0.00 ppm
0.25 Hz
362

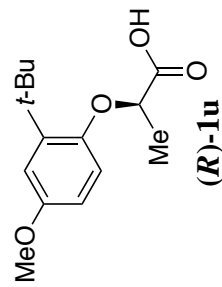


TEN040301C

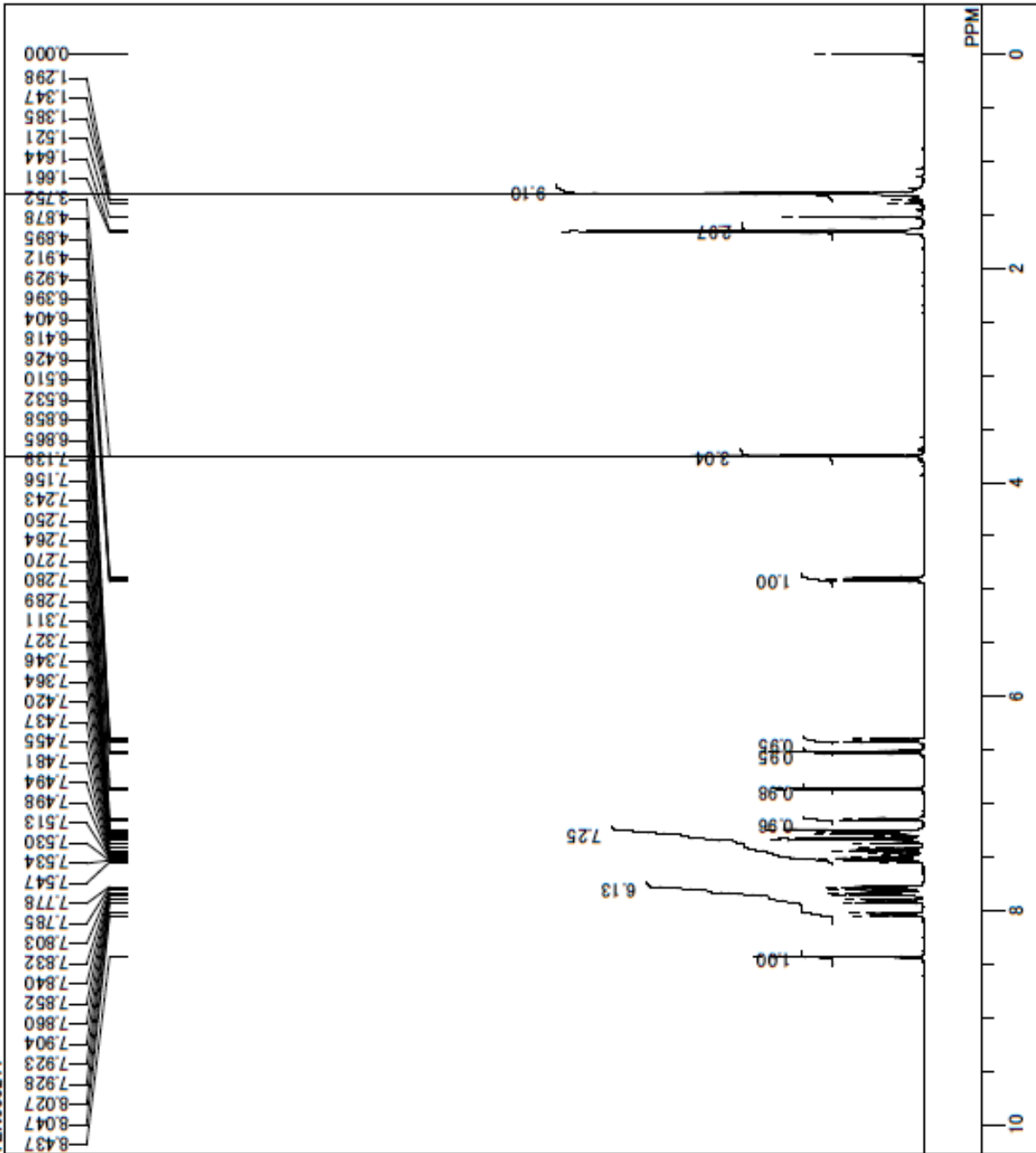


DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREOU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator*子*
TEN040301C
2012/Jan/26 00:24:58
13C
ZGPG30
100.63 MHz
0.00 KHz
10060.25 Hz
32768
24038.46 Hz
512
0.0000 sec
0.0000 sec
7.10 usec
OFF
29.9 c
CDCL3
77.00 ppm
0.25 Hz
64

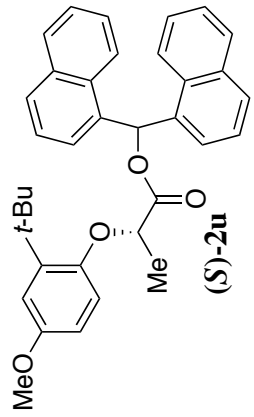


TEN050211

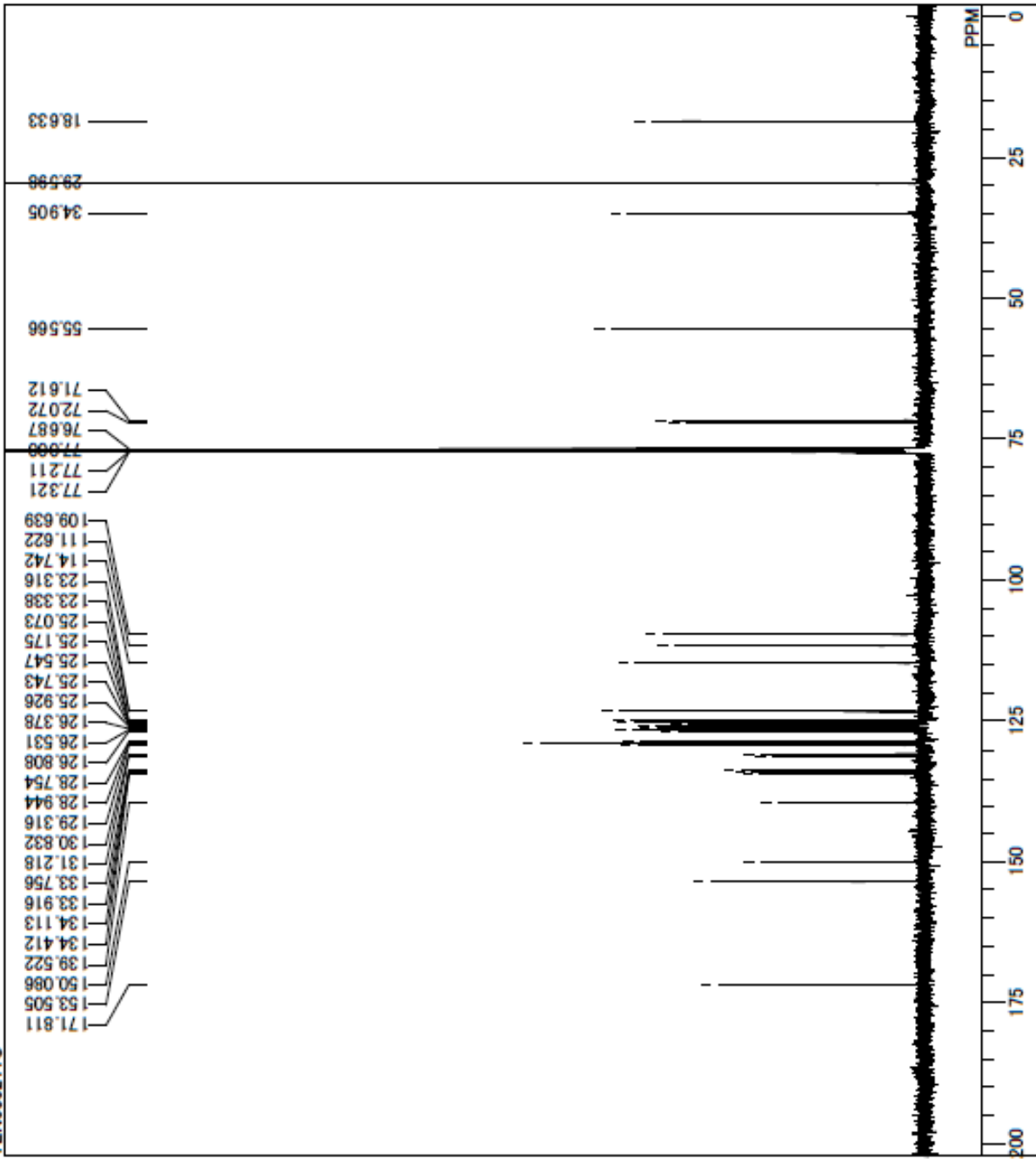


DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREOU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator*
TEN050211
2012/Jun/15 13:24:34
1H
ZG30
400.18 MHz
0.00 KHz
2478.60 Hz
32768
8223.68 Hz
16
0.0000 sec
0.0000 sec
13.00 usec
OFF
29.9 c
CDCL3
0.00 ppm
0.25 Hz
181

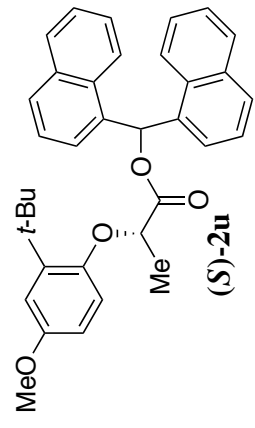


TEN050211C

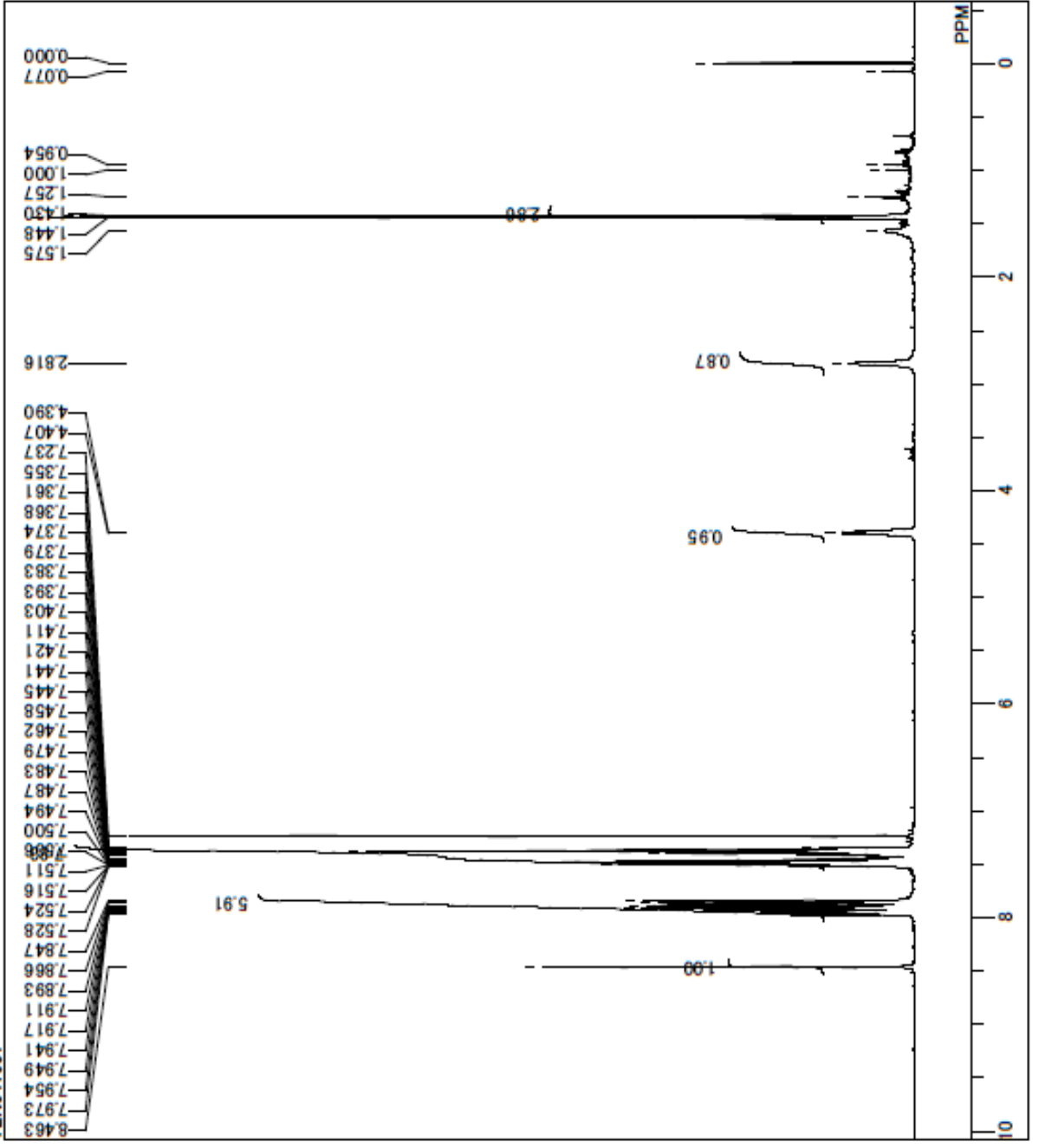


DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREOU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator*子*
TEN050211C
2012/Jun/15 14:24:26
13C
ZGPG30
100.63 MHz
0.00 KHz
10060.25 Hz
32768
24038.46 Hz
1024
0.0000 sec
0.0000 sec
7.10 usec
OFF
29.9 c
CDCL3
77.00 ppm
0.25 Hz
362

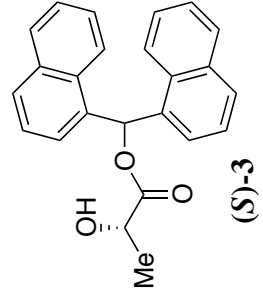


TEN041651

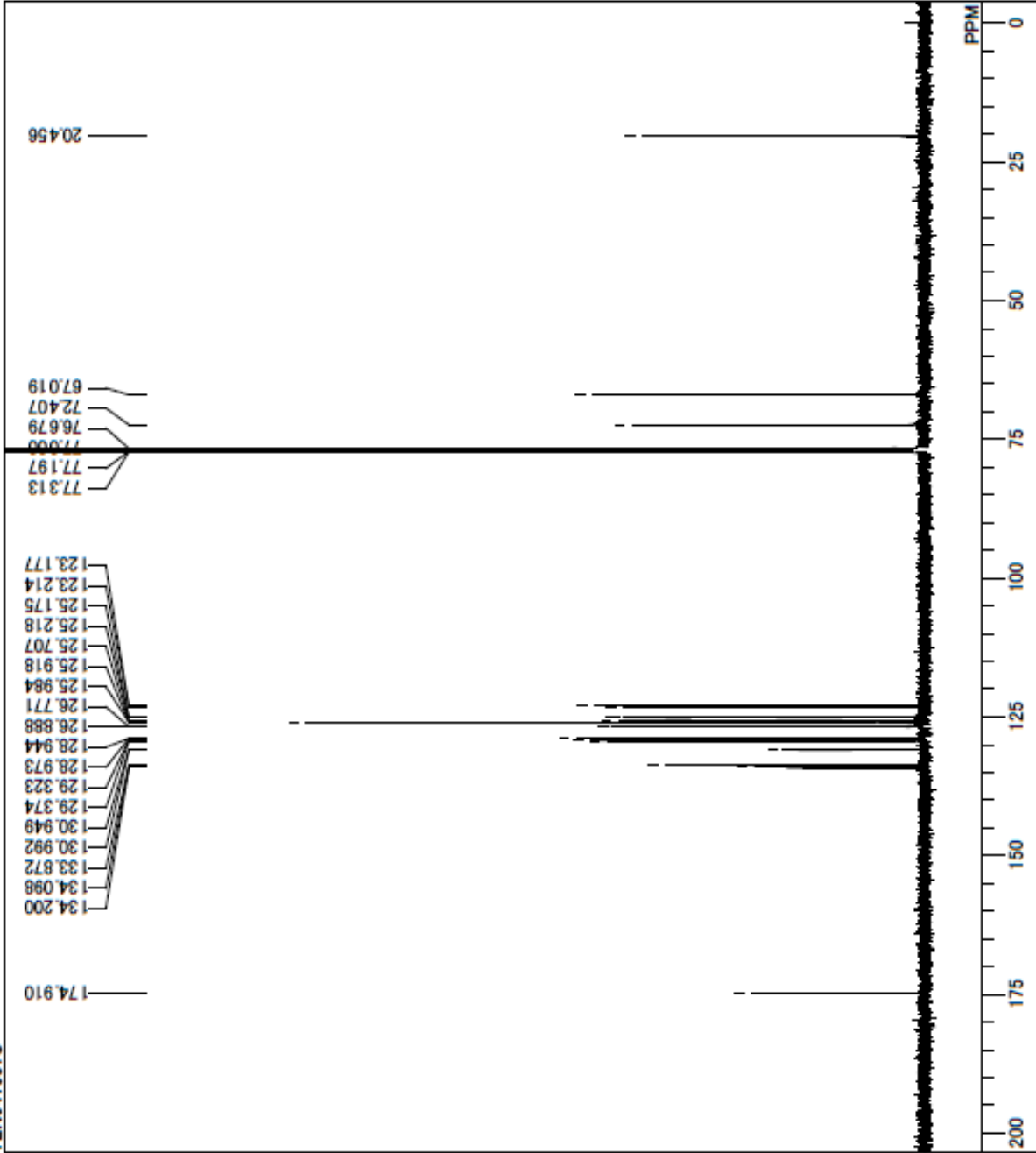


DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator\予,
TEN041651
2012/Jun/19 00:23:05
1H
ZG30
400.18 MHz
0.00 KHz
2478.60 Hz
32768
8223.68 Hz
16
0.0000 sec
0.0000 sec
13.00 usec
OFF
29.9 c
CDCL3
0.00 ppm
0.25 Hz
228

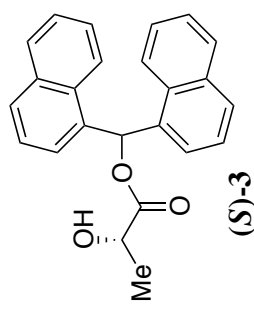


TEN041651C



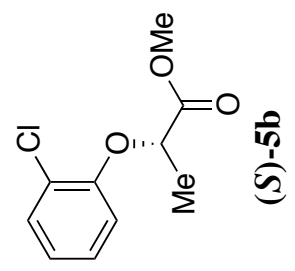
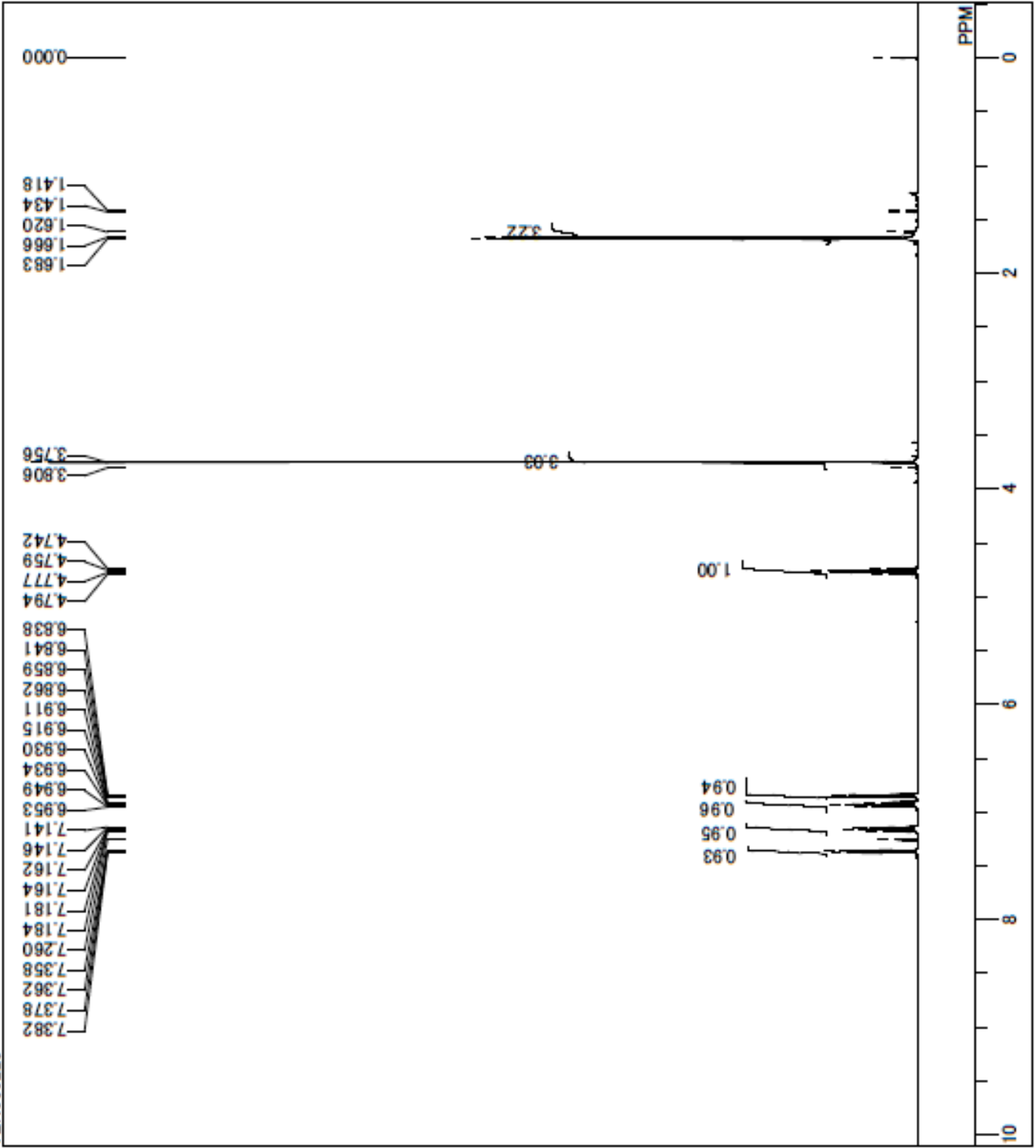
DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

C:\Documents and Settings\Administrator\予,
TEN041651C
2012/Jun/19 00:54:07
13C
ZGPG30
100.63 MHz
0.00 KHz
10060.25 Hz
32768
24038.46 Hz
512
0.0000 sec
0.0000 sec
7.10 usec
OFF
29.9 c
CDCL3
77.00 ppm
0.25 Hz
322



TEN060223

DFILE F:\TEN060223.als
COMNT TEN060223
DATIM 2012/Aug/13 05:05:46
OBNUC 1H
ZG30
EXMOD 400.18 MHz
OBFRQ 0.00 KHz
OBSET 2478.60 Hz
OBFIN 32768
POINT 8223.68 Hz
FREQU 16
SCANS 0.0000 sec
ACQTM 0.0000 sec
PD 13.00 usec
PW1
IRNUC OFF
CTEMP 29.9 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.25 Hz
RGAIN 203



TEN060223C

DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

F:\TEN060223C.als
TEN060223C
2012/Aug/13 05:22:35
13C
ZGPG30
100.63 MHz
0.00 KHz
10060.25 Hz
32768
24038.46 Hz
256
0.0000 sec
0.0000 sec
7.10 usec
OFF
29.9 c
CDCL3
77.00 ppm
0.25 Hz
64

