Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

A Copper(I)-Catalyzed Three-Component Reaction of Triethoxysilanes, Sulfur Dioxide, and Alkyl Halides

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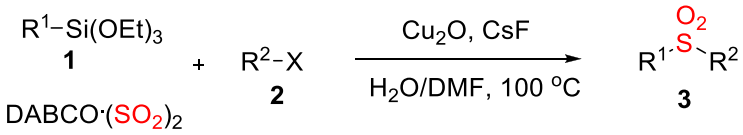
Supporting Information

General experimental methods:

Unless otherwise stated, all commercial reagents were used as received. All solvents were dried and distilled according to standard procedures. Flash column chromatography was performed using silica gel (60-Å pore size, 32–63μm, standard grade). Analytical thin–layer chromatography was performed using glass plates pre-coated with 0.25 mm 230–400 mesh silica gel impregnated with a fluorescent indicator (254 nm). Thin layer chromatography plates were visualized by exposure to ultraviolet light. Organic solutions were concentrated on rotary evaporators at ~20 Torr at 25–35°C. Nuclear magnetic resonance (NMR) spectra are recorded in parts per million from internal tetramethylsilane on the δ scale. ^{1}H and ^{13}C NMR spectra were recorded in $CDCl_3$ on a Bruker DRX-400 spectrometer operating at 400 MHz and 100 MHz, respectively. All chemical shift values are quoted in ppm and coupling constants quoted in Hz. High resolution mass spectrometry (HRMS) spectra were obtained on a micrOTOF II Instrument.

*General experimental procedure for the aminosulfonylation reaction of sulfonylation reaction of triethoxysilanes **1** with DABCO•$(SO_2)_2$ and alkyl halides **2***



Triethoxysilanes **1** (0.3 mmol) and alkyl halides **2** (0.6 mmol) were added to a solution of Cu_2O (0.03 mmol), CsF (0.6 mmol) and DABCO•$(SO_2)_2$ (0.3 mmol) in H_2O/DMF (0.1 mL/2.0 mL). The mixture was stirred at 100 °C for 10-15 hours. After completion of reaction as indicated by TLC, the mixture was extracted with ethyl acetate. The combined organic solution was dried over Na_2SO_4 and the solvent was evaporated under reduced pressure. The residue was purified directly by flash column chromatograph (EtOAc/*n*-hexane, 1:6) to give the desired product **3**.

1. Computational Details and References

The B3LYP density functional theory calculations were performed with the Gaussian09 package using 6-31+G(d,p) basis set for C, H, O, N, F, S, Br.[1, 2] B3LYP calculations utilize Becke's three parameter hybrid

exchange functional together with the correlation functional of Lee, Yang and Parr. For Cu and Cs, we used the Lanl2DZ pseudo potential with the associated double-z basis set.[3] The NBO program in Gaussian 09, Version 5.9, was used to obtain more information about some special bonds.[4] The geometry optimizations were performed without symmetry constraints, and the nature of the extrema was checked by analytical frequency calculations. The intrinsic reaction coordinate (IRC)[5] pathways have been traced to verify two desired minima connected by the transition states.

Solvent effects including contributions of non electrostatic terms have been considered at the same DFT level using N,N-dimethyl amide as solvent. Single point energies were calculated at B3LYP/6-311+G(d,p) (LANL2DZ for Cu and Cs) on the structures obtained in the gas-phase using a simple self-consistent reaction field (SCRF) method [6-8] based on the polarizable continuum model (PCM) [9-11] with UFF cavities.[12]

Table S1. Coordinate data sets and absolute energies for DFT optimized complexes at B3LYP/6-311+G(d,p) (LANL2DZ for Cu and Cs) level.

L-CuBr -3016.1839121 a.u.

O	0.028989	-0.117905	0.276230
N	-0.034853	2.147885	0.027638
C	1.397409	2.318375	0.267105
C	-0.820061	3.347652	-0.242609
C	-0.601158	0.935589	0.051426
Cu	-0.623448	-1.944742	0.313015
Br	-1.443691	-4.040622	0.338916
H	1.554231	2.960994	1.139985
H	1.845280	1.342023	0.446205
H	1.866828	2.783909	-0.606035
H	-0.757033	4.040622	0.603359
H	-0.445078	3.851606	-1.139985
H	-1.866828	3.080087	-0.400713
H	-1.681021	0.931180	-0.144095

CsF -119.7702549 a.u.

Cs	1.333335	0.000000	0.000000
F	-1.333335	0.000000	0.000000

PhSi(OEt)3 -984.6794033 a.u.

Si	0.574298	1.181584	0.220067
C	1.216258	-0.557508	0.034727
C	2.588306	-0.826077	0.202959
C	0.366667	-1.632966	-0.283335
C	3.094928	-2.119306	0.058233
C	0.868979	-2.929266	-0.429342
C	2.233903	-3.174425	-0.258782
O	1.034329	1.798957	1.678763
O	1.205408	2.238174	-0.899914
O	-1.071143	1.060474	0.061176
C	1.099944	2.092297	-2.320061

C	1.381785	3.148749	2.008052
C	-2.011855	2.110004	0.305008
C	1.894855	3.198281	-2.996478
C	2.270820	3.149700	3.242076
C	-3.421768	1.577895	0.100295
H	3.269436	-0.017406	0.456521
H	-0.696139	-1.450619	-0.411006
H	4.156671	-2.304833	0.195776
H	0.195347	-3.746513	-0.672476
H	2.625169	-4.182077	-0.369745
H	1.483765	1.107758	-2.620516
H	0.043737	2.142736	-2.618437
H	1.890702	3.617675	1.158181
H	0.461331	3.715936	2.204613
H	-1.890611	2.478906	1.332555
H	-1.817609	2.948688	-0.378321
H	2.951013	3.141618	-2.714724
H	1.820944	3.106685	-4.085959
H	1.513553	4.182077	-2.704614
H	3.199801	2.603686	3.049758
H	2.524620	4.178108	3.523767
H	1.761859	2.673551	4.085959
H	-3.623462	0.750357	0.787502
H	-4.156671	2.369687	0.284238
H	-3.552697	1.214792	-0.924058

DMF **-248.5333895** **a.u.**

O	2.073545	-0.095191	0.000036
N	-0.228602	-0.017793	0.000012
C	-0.304405	1.435380	-0.000023
C	-1.476450	-0.760190	-0.000005
C	0.980790	-0.647768	0.000023
H	-0.836135	1.792429	0.890658
H	0.710681	1.832986	-0.000097
H	-0.836248	1.792372	-0.890658
H	-2.073545	-0.522842	0.889660
H	-2.073469	-0.522940	-0.889746
H	-1.267160	-1.832986	0.000066
H	0.879476	-1.749152	0.000051

DABCO-SO2 **-893.9744057** **a.u.**

S	2.411164	0.000628	-0.479077
O	2.632826	1.258233	0.272119
O	2.632052	-1.257170	0.272048
N	-2.475522	0.000402	0.106852
C	-2.085484	1.197664	-0.654438
C	-0.536871	1.210713	-0.898575
N	0.046462	0.000944	-0.282994
C	-0.217088	0.004206	1.172715
C	-1.767181	0.003751	1.398699
C	-0.535498	-1.212357	-0.892933
C	-2.084118	-1.199880	-0.648983
H	-2.400804	2.082021	-0.091566
H	-2.632826	1.197292	-1.602688
H	-0.051877	2.081640	-0.448334
H	-0.290728	1.201472	-1.965711
H	0.267618	-0.878442	1.600212
H	0.266570	0.889439	1.596015
H	-2.081017	-0.878469	1.965711
H	-2.082144	0.888066	1.961812
H	-0.049460	-2.080543	-0.438563
H	-0.289282	-1.207854	-1.960085
H	-2.631385	-1.204332	-1.597260
H	-2.398559	-2.082021	-0.082163

DABSO **-1442.5898321** **a.u.**

S	-3.679906	-0.169094	0.356548
O	-3.925810	0.652792	-0.848095
O	-3.785475	-1.633902	0.186629
S	3.679914	-0.169094	-0.356537

O	3.925810	0.652797	0.848104
O	3.785494	-1.633900	-0.186614
N	-1.250215	-0.085606	0.193730
C	-0.770795	1.309079	0.138020
C	0.770810	1.309076	-0.137919
N	1.250210	-0.085612	-0.193714
C	0.958529	-0.767406	1.083554
C	-0.590477	-0.804496	1.301695
C	0.590462	-0.804423	-1.301725
C	-0.958544	-0.767327	-1.083581
H	-1.006413	1.789686	1.092410
H	-1.326576	1.827668	-0.647950
H	1.326599	1.827608	0.648083
H	1.006434	1.789739	-1.092282
H	1.389654	-1.771197	1.036792
H	1.469290	-0.220133	1.880622
H	-0.975448	-1.827668	1.316022
H	-0.873240	-0.323403	2.243022
H	0.975418	-1.827599	-1.316116
H	0.873231	-0.323274	-2.243022
H	-1.469301	-0.220001	-1.880616
H	-1.389679	-1.771116	-1.036876

BnBr -2842.7080401 a.u.

C	2.030101	0.878262	-0.000204
C	2.254106	-0.502869	-0.000201
C	1.164947	-1.374883	-0.000144
C	-0.142498	-0.877178	-0.000032
C	-0.372875	0.500064	-0.000064
C	0.726801	1.373621	-0.000179
C	-1.742036	1.139043	-0.000037
Br	-3.268031	-0.096801	-0.000188
H	2.868867	1.568364	-0.000259
H	3.268031	-0.891766	-0.000260
H	1.326890	-2.448934	-0.000138
H	-0.982602	-1.562300	0.000033
H	0.561499	2.448934	-0.000214
H	-1.887584	1.759291	-0.885724
H	-1.887615	1.759176	0.885724

T-CuBr -3264.7308748 a.u.

O	2.773562	-0.173744	0.613907
N	2.614497	2.085853	0.364027
C	4.036062	2.318066	0.601036
C	1.770975	3.247011	0.094691
C	2.088239	0.856581	0.387863
Cu	2.024991	-1.955134	0.647116
Br	0.935763	-3.943460	0.639338
H	4.168219	2.969521	1.472059
H	4.525427	1.361944	0.782210
H	4.486404	2.801793	-0.272810
H	1.805784	3.943460	0.939960
H	2.120429	3.767750	-0.803932
H	0.739713	2.923750	-0.058767
H	1.007414	0.802970	0.196098
O	-1.027920	0.463758	-0.125424
C	-1.424288	-0.708809	-0.070056
N	-2.704706	-1.109122	-0.239736
C	-3.764441	-0.149825	-0.513278
C	-3.066501	-2.518952	-0.149857
H	-0.739692	-1.548354	0.128729
H	-3.329280	0.848967	-0.552674
H	-4.246163	-0.377287	-1.472059
H	-4.525427	-0.186572	0.275840
H	-3.794915	-2.676856	0.654831
H	-3.509564	-2.861567	-1.092875
H	-2.175466	-3.115911	0.058908

L-CuPh -676.357153 a.u.

O	0.501916	1.505480	0.855599

N	0.349250	3.756077	1.205903
C	1.786840	3.930794	1.400248
C	-0.492950	4.942585	1.303173
C	-0.172885	2.548107	0.947934
Cu	-0.154500	-0.321550	0.496992
C	-0.840469	-2.069271	0.164808
C	-1.048100	-3.000304	1.207065
C	-1.184987	-2.506462	-1.133750
C	-1.555794	-4.284898	0.973101
C	-1.693550	-3.788142	-1.381664
C	-1.882423	-4.685320	-0.326093
H	1.981567	4.338046	2.398391
H	2.276831	2.963386	1.298143
H	2.183091	4.624585	0.650805
H	-0.397811	5.396470	2.295845
H	-0.198688	5.681273	0.549352
H	-1.538089	4.671283	1.139871
H	-1.263435	2.541911	0.821107
H	-0.805674	-2.726892	2.232581
H	-1.051590	-1.838072	-1.982687
H	-1.697167	-4.972472	1.804890
H	-1.943109	-4.085863	-2.398391
H	-2.276831	-5.681273	-0.513112

CsBr -2591.3729478 a.u.

Cs	1.678159	0.000000	0.000000
Br	-1.678160	0.000000	0.000000

FSi(OEt)3 -852.9212164 a.u.

Si	1.069330	-0.852384	0.141233
O	1.518321	-0.341130	1.626102
O	1.552682	0.272350	-0.953647
O	-0.532586	-1.176281	0.137169
C	1.522604	0.121538	-2.382418
C	2.803264	0.186917	1.995740
C	-1.559901	-0.324111	0.668502
C	2.116748	1.364604	-3.022971
C	2.720931	0.742845	3.407160
C	-2.896310	-1.038174	0.557848
F	1.774674	-2.255066	-0.248251
H	2.094216	-0.771133	-2.665313
H	0.485114	-0.022723	-2.711027
H	3.547709	-0.617697	1.942057
H	3.092013	0.969217	1.283796
H	-1.328794	-0.090299	1.714576
H	-1.578013	0.618439	0.105230
H	3.154464	1.504902	-2.704785
H	2.098354	1.271301	-4.114451
H	1.546164	2.255066	-2.741158
H	2.428854	-0.039458	4.114451
H	3.695577	1.140161	3.711603
H	1.984973	1.551114	3.462360
H	-2.879545	-1.975133	1.122814
H	-3.695577	-0.404317	0.957808
H	-3.126622	-1.270321	-0.486575

T-CuPh -924.9021831 a.u.

O	2.815975	1.461927	0.900668
N	2.466860	3.690275	1.244667
C	3.886670	4.005869	1.358965
C	1.512200	4.786106	1.380309
C	2.039226	2.439730	1.023214
Cu	2.171607	-0.359696	0.555497
C	1.373364	-2.065275	0.220045
C	1.031667	-2.956760	1.263571
C	1.044513	-2.495280	-1.086719
C	0.413986	-4.192064	1.025350
C	0.427171	-3.727762	-1.340245
C	0.105663	-4.583461	-0.281629
H	4.096332	4.441885	2.342288

H	4.462732	3.089425	1.235843
H	4.174066	4.727241	0.585654
H	1.615675	5.259409	2.363460
H	1.690406	5.542524	0.607334
H	0.495769	4.401827	1.275262
H	0.947858	2.329364	0.956374
H	1.257038	-2.690803	2.295026
H	1.280980	-1.860057	-1.938862
H	0.175541	-4.849545	1.859311
H	0.199497	-4.020805	-2.363460
H	-0.369896	-5.542524	-0.472500
O	-1.140425	1.949488	0.841560
C	-1.390774	0.755650	0.629049
N	-2.629607	0.213993	0.574792
C	-3.816365	1.032077	0.774939
C	-2.818282	-1.209782	0.322599
H	-0.591048	0.015014	0.464308
H	-3.504510	2.062044	0.949645
H	-4.462732	0.990652	-0.110375
H	-4.387396	0.671360	1.639376
H	-3.345822	-1.680444	1.161028
H	-3.408288	-1.362478	-0.589273
H	-1.849287	-1.698433	0.200362

L-A **-2118.945858 a.u.**

O	-0.905441	0.458074	-3.099217
S	-0.967211	-0.876844	-2.433948
O	0.075403	-1.093774	-1.394516
S	1.078640	2.001213	1.865971
O	1.870426	2.227595	3.099217
O	0.864181	3.208368	1.017750
N	4.671160	-0.050456	-0.681313
C	3.877843	-1.092617	-0.009397
C	2.739264	-0.445797	0.851800
N	2.757866	1.018222	0.621901
C	4.038330	1.589969	1.090318
C	5.205917	0.870383	0.332743
C	2.573810	1.301721	-0.819089
C	3.796654	0.701464	-1.596345
H	4.547637	-1.692709	0.615088
H	3.454918	-1.750753	-0.774111
H	2.885182	-0.617144	1.922824
H	1.754028	-0.822731	0.565915
H	4.016285	2.664624	0.885946
H	4.091456	1.460852	2.175010
H	5.853834	1.600224	-0.163659
H	5.827525	0.294848	1.026333
H	2.491249	2.386088	-0.938416
H	1.634497	0.842891	-1.134397
H	3.453607	0.026222	-2.386097
H	4.391584	1.490895	-2.067363
O	-2.658488	1.671908	-0.454030
N	-1.830645	3.789930	-0.603447
C	-2.413186	4.223161	0.664845
C	-0.932769	4.726591	-1.274189
C	-1.971620	2.544444	-1.045329
Cu	-2.988638	-0.193798	-0.891716
C	-3.554591	-2.008613	-1.102804
C	-3.054912	-3.034142	-0.278558
C	-4.560723	-2.344167	-2.029133
C	-3.561571	-4.337695	-0.352571
C	-5.070521	-3.646263	-2.107911
C	-4.571531	-4.647094	-1.268604
H	-2.991144	5.139632	0.507973
H	-3.064751	3.437504	1.044511
H	-1.609987	4.417659	1.382585
H	-1.463877	5.659627	-1.488960
H	-0.070844	4.929810	-0.631500
H	-0.583997	4.293393	-2.213690
H	-1.445728	2.303021	-1.976261

H	-2.259721	-2.825421	0.434019
H	-4.964466	-1.588205	-2.699613
H	-3.164452	-5.110610	0.301395
H	-5.853834	-3.878266	-2.825864
H	-4.961404	-5.659627	-1.332491

L-TSAB -2118.9371281 a.u.

O	-1.194571	-0.049885	-2.891196
S	-0.960456	-1.472102	-2.448937
O	0.031843	-1.587333	-1.328854
S	0.894988	1.744524	1.870725
O	1.723355	1.931782	3.087597
O	0.691951	2.971835	1.047690
N	4.355138	-0.353559	-0.790259
C	3.596999	-1.381150	-0.057011
C	2.497341	-0.716619	0.839982
N	2.503644	0.742762	0.577274
C	3.803163	1.325363	0.972978
C	4.934341	0.591758	0.175041
C	2.250696	0.994181	-0.860173
C	3.434801	0.373841	-1.680011
H	4.297728	-1.964291	0.549610
H	3.136619	-2.055779	-0.784177
H	2.690420	-0.862580	1.907374
H	1.503283	-1.100347	0.598700
H	3.769034	2.395790	0.748415
H	3.907766	1.216691	2.056240
H	5.554573	1.312238	-0.368453
H	5.591347	0.034125	0.850561
H	2.165829	2.076030	-0.999149
H	1.299476	0.525783	-1.120988
H	3.051819	-0.322632	-2.431628
H	4.004347	1.150386	-2.201608
O	-2.879623	1.554996	-0.244223
N	-1.977880	3.626885	-0.556128
C	-2.550724	4.176036	0.670398
C	-1.034629	4.471715	-1.283678
C	-2.150969	2.352856	-0.894656
Cu	-2.935857	-0.317149	-0.747307
C	-2.891984	-2.178086	-1.406739
C	-2.603841	-3.159647	-0.431259
C	-3.971510	-2.421294	-2.290883
C	-3.390808	-4.306594	-0.305378
C	-4.759573	-3.568111	-2.170376
C	-4.469914	-4.509286	-1.174587
H	-3.068547	5.113662	0.444375
H	-3.254881	3.457702	1.087851
H	-1.748270	4.367890	1.390285
H	-1.522395	5.408954	-1.570815
H	-0.167806	4.682457	-0.649849
H	-0.700088	3.955871	-2.185786
H	-1.618167	2.017128	-1.791929
H	-1.736883	-3.026443	0.212502
H	-4.186525	-1.711294	-3.087597
H	-3.161222	-5.046880	0.456833
H	-5.591347	-3.734790	-2.850149
H	-5.073438	-5.408954	-1.088100

L-B -2118.9806862 a.u.

O	-1.569635	-1.912051	-3.154555
S	-0.935766	-3.054812	-2.254161
O	-0.055109	-2.452793	-1.163068
O	-2.511123	1.467568	-1.733977
N	-2.452538	3.261677	-0.333142
C	-3.531642	3.962473	-1.023450
C	-1.849729	3.918618	0.827318
C	-2.023853	2.063761	-0.737385
Cu	-2.023418	-0.262206	-2.388025
C	-2.422743	-3.603943	-1.325510
C	-2.338728	-3.820722	0.050858

C	-3.607221	-3.867864	-2.020995
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C	-4.723362	-4.338716	-1.324678
C	-4.649820	-4.552150	0.056857
H	-3.166760	4.921069	-1.408473
H	-3.885997	3.347527	-1.849455
H	-4.355003	4.153386	-0.326598
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H	-2.610376	4.086210	1.597888
H	-1.053833	3.292920	1.234898
H	-1.212599	1.637249	-0.137642
H	-1.407844	-3.601112	0.564605
H	-3.658021	-3.686726	-3.090828
H	-3.403512	-4.453817	1.816191
H	-5.649021	-4.537774	-1.858003
H	-5.518166	-4.921069	0.595826
S	0.846772	0.132396	1.976375
O	1.712692	0.385648	3.154555
O	0.355561	1.370970	1.291024
N	4.367589	-1.043008	-1.085662
C	3.817102	-2.255871	-0.458903
C	2.692160	-1.885482	0.566933
N	2.478971	-0.417234	0.507898
C	3.707787	0.295833	0.917516
C	4.871975	-0.150619	-0.032730
C	2.094502	-0.022196	-0.868092
C	3.293235	-0.356650	-1.821914
H	4.633992	-2.795265	0.031844
H	3.414805	-2.898889	-1.246863
H	2.971537	-2.139122	1.594419
H	1.746732	-2.371743	0.315212
H	3.507973	1.369258	0.847259
H	3.902102	0.062902	1.968099
H	5.340273	0.719636	-0.504348
H	5.649021	-0.682068	0.526286
H	1.857724	1.045833	-0.852800
H	1.199418	-0.588260	-1.135795
H	2.958091	-1.005962	-2.636064
H	3.710454	0.552423	-2.268091

T-A **-2367.4839456 a.u.**

O	-0.051484	0.772454	-3.523688
S	0.128903	-0.490169	-2.739022
O	1.231155	-0.418536	-1.727696
S	2.455734	2.462939	1.713631
O	3.334882	2.540728	2.906601
O	2.295526	3.737256	0.957113
N	5.704757	0.321492	-1.192147
C	4.871952	-0.702343	-0.539193
C	3.853260	-0.034315	0.446210
N	3.968800	1.436705	0.306429
C	5.316883	1.880766	0.718549
C	6.373224	1.123515	-0.156557
C	3.713154	1.828389	-1.098600
C	4.838424	1.202538	-1.992928
H	5.528584	-1.400783	-0.009714
H	4.341334	-1.261835	-1.314975
H	4.062839	-0.286388	1.490587
H	2.825247	-0.320725	0.211792
H	5.367005	2.964593	0.577021
H	5.428473	1.681598	1.788141
H	7.050846	1.831674	-0.644910
H	6.982663	0.452195	0.457402
H	3.699637	2.921419	-1.143571
H	2.727908	1.448557	-1.377248
H	4.397403	0.616452	-2.804710
H	5.465008	1.979994	-2.442709
O	-1.466316	1.749578	-0.638340
N	-0.644632	3.871009	-0.753595
C	-1.144936	4.253316	0.564088

C	0.180978	4.846352	-1.459211
C	-0.831200	2.643444	-1.243765
Cu	-1.856120	-0.146218	-1.076855
C	-2.159267	-2.008843	-1.530871
C	-1.524092	-3.045881	-0.821982
C	-3.129302	-2.375194	-2.483262
C	-1.856139	-4.390719	-1.037638
C	-3.465399	-3.717922	-2.706220
C	-2.830616	-4.731460	-1.981049
H	-1.777339	5.143557	0.473078
H	-1.728580	3.428656	0.971927
H	-0.300038	4.477382	1.222771
H	-0.382559	5.773724	-1.610326
H	1.081938	5.055732	-0.873955
H	0.469379	4.446594	-2.433704
H	-0.390886	2.451634	-2.229684
H	-0.750865	-2.814010	-0.091657
H	-3.635994	-1.611047	-3.070117
H	-1.348872	-5.170520	-0.473495
H	-4.218319	-3.970782	-3.449753
H	-3.083972	-5.773724	-2.157080
O	-3.522429	0.085321	0.476528
C	-4.224823	-0.878021	0.810617
N	-5.201900	-0.827221	1.741777
C	-5.505629	0.413123	2.444333
C	-5.987218	-2.005479	2.080048
H	-4.091089	-1.869237	0.354128
H	-4.835189	1.191309	2.080241
H	-6.545263	0.709113	2.260423
H	-5.363722	0.282461	3.523688
H	-5.871401	-2.254305	3.141790
H	-7.050846	-1.831507	1.877253
H	-5.651843	-2.856267	1.482800

T-TSAB **-2367.4763973 a.u.**

O	-0.143528	0.272798	-3.495067
S	0.237937	-1.026376	-2.848292
O	1.221512	-0.874474	-1.723098
S	2.567445	2.546866	1.527908
O	3.501810	2.617473	2.679087
O	2.526022	3.762533	0.666189
N	5.405696	-0.204408	-1.279856
C	4.524380	-1.064011	-0.470906
C	3.642383	-0.195489	0.488672
N	3.880509	1.233093	0.172558
C	5.287680	1.586934	0.454783
C	6.210674	0.634661	-0.379791
C	3.569841	1.489927	-1.252212
C	4.574499	0.666375	-2.128437
H	5.145888	-1.765719	0.095580
H	3.887036	-1.639550	-1.147249
H	3.898719	-0.348956	1.541718
H	2.580093	-0.405626	0.343826
H	5.425933	2.637551	0.181921
H	5.449642	1.500456	1.533124
H	6.921310	1.212997	-0.979668
H	6.789634	-0.023191	0.276773
H	3.647178	2.568159	-1.420942
H	2.541505	1.169791	-1.433782
H	4.028436	0.042771	-2.841582
H	5.239679	1.326564	-2.695263
O	-1.496660	1.777004	-0.623454
N	-0.479849	3.776696	-1.041250
C	-0.932822	4.393951	0.201582
C	0.405330	4.567020	-1.890641
C	-0.782837	2.510190	-1.346667
H	-1.518533	5.293145	-0.021911
H	-1.552240	3.680187	0.743802
H	-0.064242	4.672272	0.806771
H	-0.096703	5.491239	-2.199144

H	1.319211	4.813535	-1.340786
H	0.664918	3.993305	-2.782957
H	-0.363505	2.134478	-2.288107
Cu	-1.852009	-0.178295	-0.935448
C	-1.670709	-1.958134	-1.817311
C	-1.263648	-3.022736	-0.980191
C	-2.692926	-2.228813	-2.757737
C	-1.876451	-4.278601	-1.042486
C	-3.312030	-3.481697	-2.824687
C	-2.905120	-4.510231	-1.965141
H	-0.439289	-2.867934	-0.286380
H	-2.996723	-1.452585	-3.458068
H	-1.545366	-5.080261	-0.385927
H	-4.099127	-3.662708	-3.553273
H	-3.368769	-5.491239	-2.030588
O	-3.456195	-0.323937	0.573190
C	-4.121313	-1.360096	0.711421
N	-5.116832	-1.514051	1.609053
C	-5.488292	-0.429831	2.510870
C	-5.854461	-2.764958	1.716043
H	-3.936217	-2.249436	0.091457
H	-4.853670	0.430952	2.301535
H	-6.539152	-0.156488	2.360168
H	-5.351944	-0.740752	3.553273
H	-5.743994	-3.192787	2.719661
H	-6.921310	-2.600407	1.523337
H	-5.472969	-3.481994	0.985847

T-B -2367.5176135 a.u.

O	-0.104725	-1.180601	-1.132769
S	-0.824854	-2.517596	-0.907354
O	-1.916576	-2.374698	0.214633
C	-1.883644	-2.656571	-2.405718
C	-3.131012	-3.281629	-2.328230
C	-1.390265	-2.205500	-3.633007
C	-3.896501	-3.441608	-3.487428
C	-2.158245	-2.369104	-4.789958
C	-3.410525	-2.988656	-4.718464
H	-3.501107	-3.614841	-1.363521
H	-0.422548	-1.714116	-3.670895
H	-4.872380	-3.916547	-3.429569
H	-1.781196	-2.012485	-5.744938
H	-4.006136	-3.116235	-5.618207
S	1.512825	2.481962	1.114173
O	2.239600	2.812867	2.365119
O	1.785286	3.385975	-0.038375
N	4.446066	-1.167708	-0.171697
C	3.409058	-1.666468	0.747316
C	2.456707	-0.502238	1.187715
N	2.863021	0.726933	0.466971
C	4.242192	1.105778	0.838718
C	5.193637	-0.089949	0.493705
C	2.773124	0.500116	-0.993534
C	3.796367	-0.624840	-1.376438
H	3.902341	-2.119981	1.613667
H	2.842960	-2.449715	0.234651
H	2.522822	-0.296882	2.260742
H	1.417775	-0.716650	0.924957
H	4.498819	2.011098	0.280106
H	4.247521	1.359506	1.902693
H	6.001671	0.235748	-0.169843
H	5.653771	-0.498799	1.399428
H	2.986620	1.450590	-1.492056
H	1.750639	0.190167	-1.221622
H	3.284247	-1.441695	-1.893673
H	4.577197	-0.241285	-2.041983
O	-2.480150	1.352071	-0.026154
N	-1.467995	2.883342	-1.385438
C	-2.105760	4.031530	-0.750207
C	-0.505581	3.155826	-2.448948

C	-1.685949	1.634986	-0.954225
H	-2.680987	4.597770	-1.491517
H	-2.771998	3.675842	0.035022
H	-1.341160	4.687071	-0.318933
H	-0.986523	3.731858	-3.247539
H	0.347117	3.712492	-2.047892
H	-0.145325	2.212105	-2.863529
H	-1.109605	0.847844	-1.458237
Cu	-2.595466	-0.531084	0.619352
O	-3.676488	-1.078981	2.403266
C	-3.546693	-2.254970	2.782163
N	-4.137247	-2.764095	3.882940
C	-4.992468	-1.939840	4.728484
C	-3.938770	-4.152882	4.272101
H	-2.923662	-2.963417	2.218494
H	-5.039186	-0.936945	4.304785
H	-6.001671	-2.365614	4.775614
H	-4.584719	-1.889142	5.744938
H	-3.481733	-4.212824	5.267138
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H	-3.280195	-4.646285	3.553914

P **-1051.2328583 a.u.**

S	-0.925881	-2.024797	0.220727
O	-1.826447	-2.994477	-0.433034
O	-0.388119	-2.281021	1.570352
C	-1.758121	-0.425981	0.249799
C	0.505490	-1.820281	-0.930033
C	-1.396151	0.514570	1.216986
C	-2.045334	1.751098	1.230047
C	-3.038803	2.032501	0.287377
C	-3.395319	1.077709	-0.670418
C	-2.754815	-0.163090	-0.693758
C	1.523699	-0.793941	-0.524519
C	2.440587	-1.060411	0.504593
C	3.388518	-0.104199	0.871588
C	3.436022	1.129009	0.213606
C	2.528948	1.401931	-0.813277
C	1.577646	0.446362	-1.177546
H	0.057963	-1.608274	-1.903828
H	0.913679	-2.836082	-0.948765
H	-0.634926	0.269932	1.949481
H	-1.778263	2.490666	1.978741
H	-3.542736	2.994477	0.304373
H	-4.178097	1.293527	-1.391293
H	-3.035405	-0.927342	-1.411055
H	2.399071	-2.012631	1.024341
H	4.092181	-0.323341	1.669315
H	4.178097	1.869871	0.496658
H	2.561971	2.355393	-1.332370
H	0.875635	0.662705	-1.978741

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J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J.Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, **2009**.

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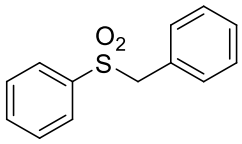
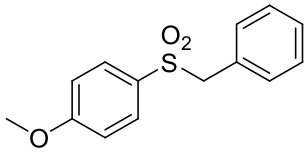
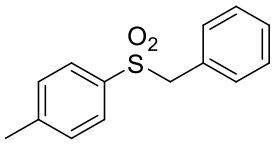


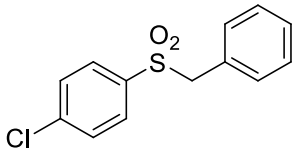
Benzylsulfonylbenzene (**3a**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59-7.65 (m, 3H), 7.45 (t, J = 8.0 Hz, 2H), 7.24-7.32 (m, 3H), 7.09 (d, J = 7.2 Hz, 2H), 4.32 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.8, 133.6, 130.7, 128.8, 128.7, 128.6, 128.5, 128.0, 62.8; HRMS (ESI) calcd for $C_{13}H_{12}O_2NaS^+$: 255.0450 ($M + Na^+$), found: 255.0464.



1-(Benzylsulfonyl)-4-methoxybenzene (**3b**)[1]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, J = 7.2Hz, 2H), 7.25-7.32 (m, 3H), 7.09 (d, J = 6.8Hz, 2H), 6.90 (d, J = 8.0Hz, 2H), 4.29 (s, 2H), 3.86 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.6, 130.7, 129.4, 128.9, 128.6, 128.4, 113.9, 63.0, 55.5; HRMS (ESI) calcd for $C_{14}H_{14}O_3NaS^+$: 285.0556 ($M + Na^+$), found: 285.0566.

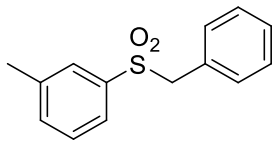


1-(Benzylsulfonyl)-4-methylbenzene (**3c**)[2]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, J = 8.0 Hz, 2H), 7.23-7.33 (m, 5H), 7.10 (d, J = 6.8 Hz, 2H), 4.30 (s, 2H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.6, 134.9, 134.1, 130.7, 129.4, 128.5, 128.4, 128.2, 62.8, 21.5; HRMS (ESI) calcd for $C_{14}H_{15}O_2S^+$: 247.0793 ($M + H^+$), found: 247.0803.

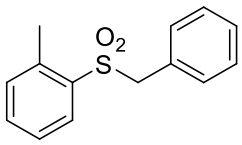


1-(Benzylsulfonyl)-4-chlorobenzene (**3d**)[1]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, J = 8.4 Hz, 2H), 7.42 (d, J = 8.4 Hz, 2H), 7.27-7.34 (m, 3H), 7.10 (d, J = 7.2 Hz, 2H), 4.32 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.4, 136.2, 130.7, 130.0, 129.1, 128.9,

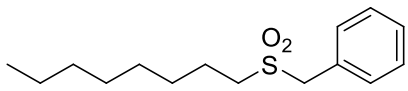
128.6, 116.6, 62.8; HRMS (ESI) calcd for $C_{13}H_{11}ClO_2NaS^+$: 289.0060 ($M + Na^+$), found: 289.0053.



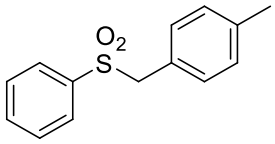
1-(Benzylsulfonyl)-3-methylbenzene (**3e**)[3]: ^1H NMR (400 MHz, $CDCl_3$) δ 7.39-7.45 (m, 3H), 7.25-7.35 (m, 4H), 7.10 (d, J = 7.2 Hz, 2H), 4.30 (s, 2H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.0, 134.8, 134.4, 131.1, 130.8, 128.9, 128.6, 128.4, 128.1, 125.6, 62.8, 21.0; HRMS (ESI) calcd for $C_{14}H_{18}NO_2S^+$: 264.1053 ($M + NH_4^+$), found: 264.1055.



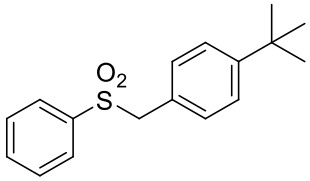
1-(Benzylsulfonyl)-2-methylbenzene (**3f**)[4]: ^1H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, J = 8.0 Hz, 1H), 7.47 (t, J = 8.0 Hz, 1H), 7.23-7.33 (m, 5H), 7.08 (d, J = 7.2 Hz, 2H), 4.34 (s, 2H), 2.53 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.6, 135.9, 133.6, 132.3, 130.8, 130.7, 128.6, 128.5, 127.9, 126.3, 62.2, 20.2; HRMS (ESI) calcd for $C_{14}H_{14}O_2NaS^+$: 269.0612 ($M + Na^+$), found: 269.0615.



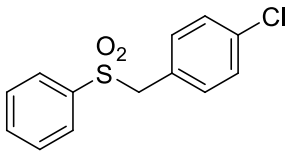
(Octylsulfonylmethyl)benzene (**3g**): ^1H NMR (400 MHz, $CDCl_3$) δ 7.41 (s, 5H), 4.22 (s, 2H), 2.81 (t, J = 8.0Hz, 2H), 1.76-1.84 (m, 2H), 1.26-1.37 (m, 10H), 0.88 (t, J = 7.2Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 130.4, 129.0, 128.9, 128.1, 59.3, 51.0, 31.6, 28.9, 28.9, 28.3, 22.5, 21.7, 13.9;



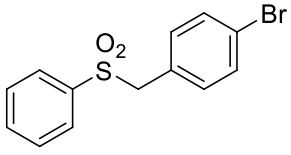
1-Methyl-4-(phenylsulfonylmethyl)benzene (**3h**)[5]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59-7.66 (m, 3H), 7.46 (t, J = 8.0 Hz, 2H), 7.07 (d, J = 8.0 Hz, 2H), 6.97 (d, J = 8.0 Hz, 2H), 4.28 (s, 2H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.6, 137.9, 133.5, 130.6, 129.2, 128.8, 128.5, 124.9, 62.5, 21.1; HRMS (ESI) calcd for $C_{14}H_{14}O_2NaS^+$: 269.0607 ($M + Na^+$), found: 269.0615.



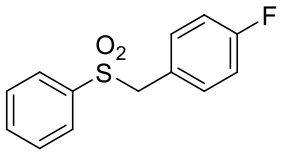
1-*tert*-Butyl-4-(phenylsulfonylmethyl)benzene (**3i**)[4]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, J = 8.0 Hz, 2H), 7.61 (t, J = 7.2 Hz, 1H), 7.46 (t, J = 8.0 Hz, 2H), 7.27-7.31 (m, 2H), 7.04 (d, J = 8.4 Hz, 2H), 4.29 (s, 2H), 1.30 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 133.5, 130.4, 128.7, 128.5, 125.4, 124.8, 62.4, 34.5, 31.1; HRMS (ESI) calcd for $C_{17}H_{20}O_2NaS^+$: 311.1082 ($M + Na^+$), found: 311.1089.



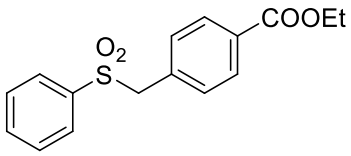
1-Chloro-4-(phenylsulfonylmethyl)benzene (**3j**)[4]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61-7.66 (m, 3H), 7.48 (t, J = 7.6 Hz, 2H), 7.26 (t, J = 8.0 Hz, 2H), 7.03 (d, J = 8.4 Hz, 2H), 4.28 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.0, 133.8, 132.0, 128.9, 128.7, 128.5, 126.5, 62.0; HRMS (ESI) calcd for $C_{13}H_{11}ClO_2NaS^+$: 289.0060 ($M + Na^+$), found: 289.0056.



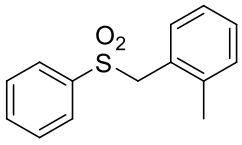
1-Bromo-4-(phenylsulfonylmethyl)benzene (**3k**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61-7.67 (m, 3H), 7.49 (t, J = 8.0 Hz, 2H), 7.40 (d, J = 8.4 Hz, 2H), 6.97 (d, J = 8.4 Hz, 2H), 4.26 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 133.8, 132.3, 131.7, 129.0, 128.5, 127.1, 123.2, 62.1; HRMS (ESI) calcd for $C_{13}H_{11}BrO_2NaS^+$: 332.9555 (M + Na^+), found: 332.9558.



1-Fluoro-4-(phenylsulfonylmethyl)benzene (**3l**)[4]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60-7.65 (m, 3H), 7.47 (t, J = 8.0 Hz, 2H), 7.05-7.09 (m, 2H), 6.96 (t, J = 8.4 Hz, 2H), 4.28 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.9 (d, J_F = 247.0 Hz), 137.6, 133.7, 132.5 (d, J_F = 8.3 Hz), 128.9, 128.5, 123.9, 115.6 (d, J_F = 21.7 Hz), 61.9; HRMS (ESI) calcd for $C_{13}H_{11}FO_2NaS^+$: 273.0356 (M + Na^+), found: 273.0352.

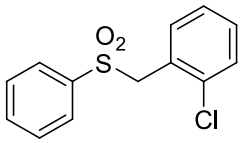


Ethyl 4-(phenylsulfonylmethyl)benzoate (**3m**)[6]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, J = 8.4 Hz, 2H), 7.60-7.64 (m, 3H), 7.46 (t, J = 8.0 Hz, 2H), 7.16 (d, J = 8.4 Hz, 2H), 4.34-4.40 (m, 4H), 1.39 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.9, 137.6, 133.8, 132.9, 130.7, 129.6, 128.9, 128.5, 126.3, 62.5, 61.1, 14.2; HRMS (ESI) calcd for $C_{16}H_{16}O_4NaS^+$: 327.0662 (M + Na^+), found: 327.0660.

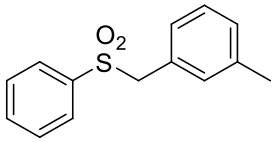


1-Methyl-2-(phenylsulfonylmethyl)benzene (**3n**)[7]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61-7.67 (m, 3H), 7.47 (t, J = 8.0 Hz, 2H), 7.23 (t, J = 7.6 Hz, 1H), 7.09-7.14 (m, 2H), 7.03 (d, J = 7.6 Hz, 1H), 4.39 (s, 2H), 2.12 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.2, 133.6, 131.8, 130.6, 128.9, 128.8, 128.6, 126.5, 126.0, 60.0, 19.2; HRMS (ESI)

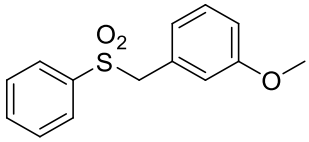
calcd for $C_{14}H_{14}O_2NaS^+$: 269.0607 ($M + Na^+$), found: 269.0605.



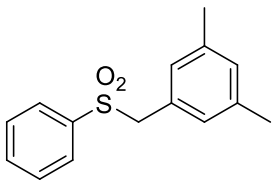
1-Chloro-2-(phenylsulfonylmethyl)benzene (**3o**): ^1H NMR (400 MHz, $CDCl_3$) δ 7.60-7.66 (m, 3H), 7.43-7.47 (m, 3H), 7.26-7.29 (m, 3H), 4.57 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 133.8, 132.8, 130.4, 130.2, 129.9, 129.5, 128.8, 128.6, 127.3, 127.0, 59.2; HRMS (ESI) calcd for $C_{13}H_{11}ClO_2NaS^+$: 289.0060 ($M + Na^+$), found: 289.0063.



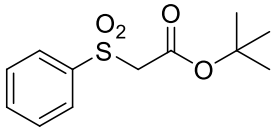
1-Methyl-3-(phenylsulfonylmethyl)benzene (**3p**)[4]: ^1H NMR (400 MHz, $CDCl_3$) δ 7.59-7.66 (m, 3H), 7.46 (t, J = 7.6 Hz, 2H), 7.13-7.14 (m, 2H), 6.91 (s, 1H), 6.86 (t, J = 6.0 Hz, 1H), 4.27 (s, 2H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.2, 137.9, 133.6, 131.5, 129.4, 128.7, 128.6, 128.3, 127.8, 62.8, 21.1; HRMS (ESI) calcd for $C_{14}H_{14}O_2NaS^+$: 269.0607 ($M + Na^+$), found: 269.0606.



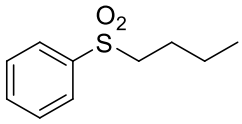
1-Methoxy-3-(phenylsulfonylmethyl)benzene (**3q**): ^1H NMR (400 MHz, $CDCl_3$) δ 7.59-7.67 (m, 3H), 7.46 (t, J = 8.0 Hz, 2H), 7.16 (t, J = 8.0 Hz, 1H), 6.86 (d, J = 8.0 Hz, 1H), 6.62-6.66 (m, 2H), 4.29 (s, 2H), 3.71 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.5, 137.8, 133.6, 129.4, 129.3, 128.8, 128.6, 123.1, 115.8, 114.7, 62.8, 55.1; HRMS (ESI) calcd for $C_{14}H_{14}O_3NaS^+$: 285.0556 ($M + Na^+$), found: 285.0555.



1,3-Dimethyl-5-(phenylsulfonylmethyl)benzene (**3r**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, J = 8.0 Hz, 2H), 7.61 (t, J = 8.0 Hz, 1H), 7.47 (t, J = 8.0 Hz, 2H), 6.95 (s, 1H), 6.68 (s, 2H), 4.23 (s, 2H), 2.22 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.0, 133.5, 130.3, 128.7, 128.6, 128.5, 127.6, 62.8, 21.0; HRMS (ESI) calcd for $C_{15}H_{16}O_2NaS^+$: 283.0763 ($M + Na^+$), found: 283.0768.



Tert-butyl 2-(phenylsulfonyl)acetate (**3s**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94-7.96 (m, 2H), 7.67 (t, J = 7.2Hz, 1H), 7.58 (t, J = 7.2 Hz, 2H), 4.04 (s, 2H), 1.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.1, 138.8, 134.0, 129.1, 128.4, 83.5, 62.0, 27.6; HRMS (ESI) calcd for $C_{12}H_{16}O_4NaS^+$: 279.0662 ($M + Na^+$), found: 279.0669.



Butylsulfonylbenzene (**3t**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, J = 8.0 Hz, 2H), 7.66 (t, J = 7.6Hz, 1H), 7.57 (t, J = 7.6 Hz, 2H), 3.07-3.11 (m, 2H), 1.65-1.73 (m, 2H), 1.34-1.44 (m, 2H), 0.89 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.1, 133.5, 129.2, 127.9, 56.0, 24.5, 21.4, 13.4; HRMS (ESI) calcd for $C_{10}H_{14}O_2NaS^+$: 221.0607 ($M + Na^+$), found: 221.0612.

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[2] J. L. Treece, J. R. Goodell, D. V. Velde, J. A. PorcoJr., J. Aubé, *J. Org. Chem*. **2010**, *75*, 2028.

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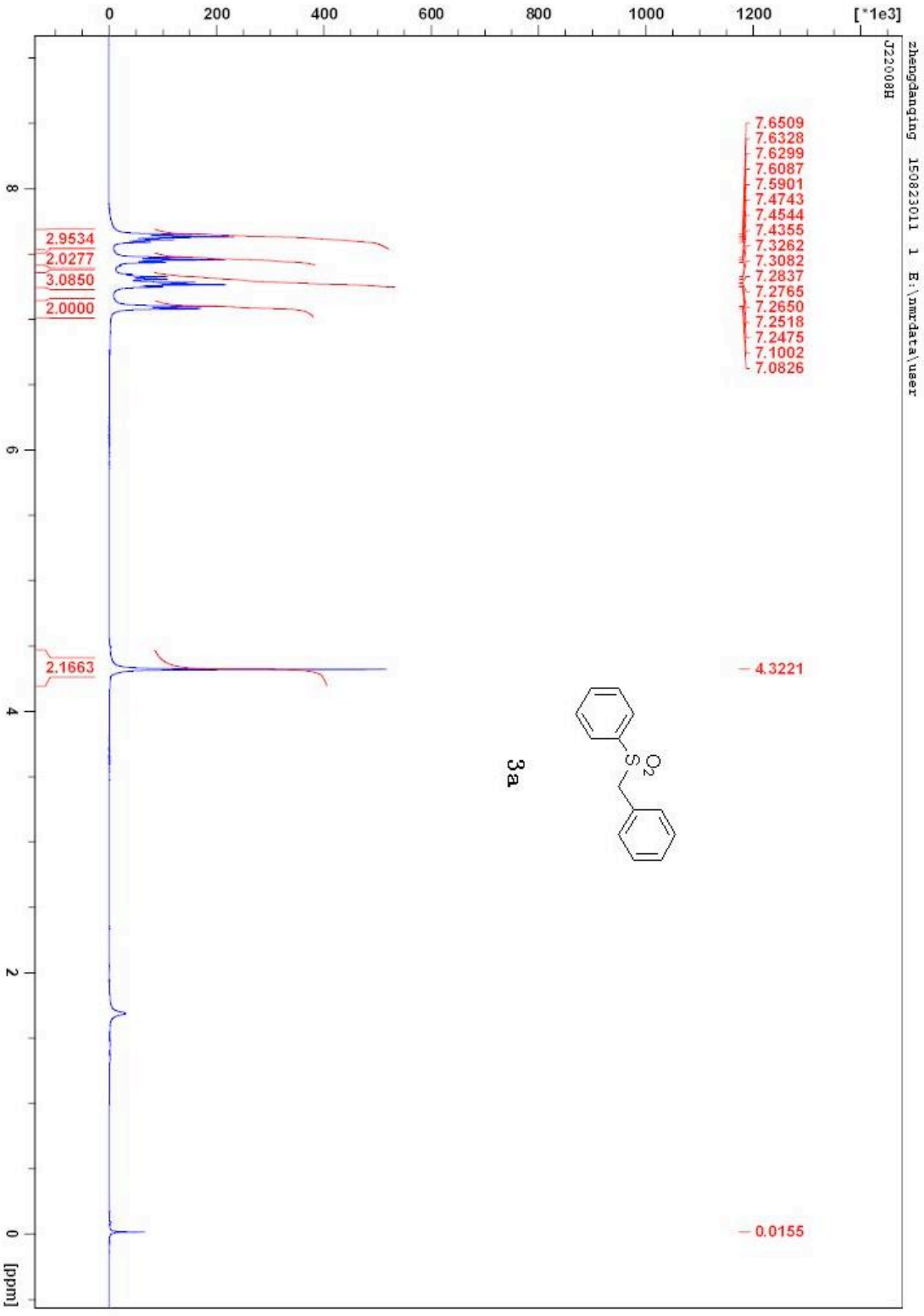
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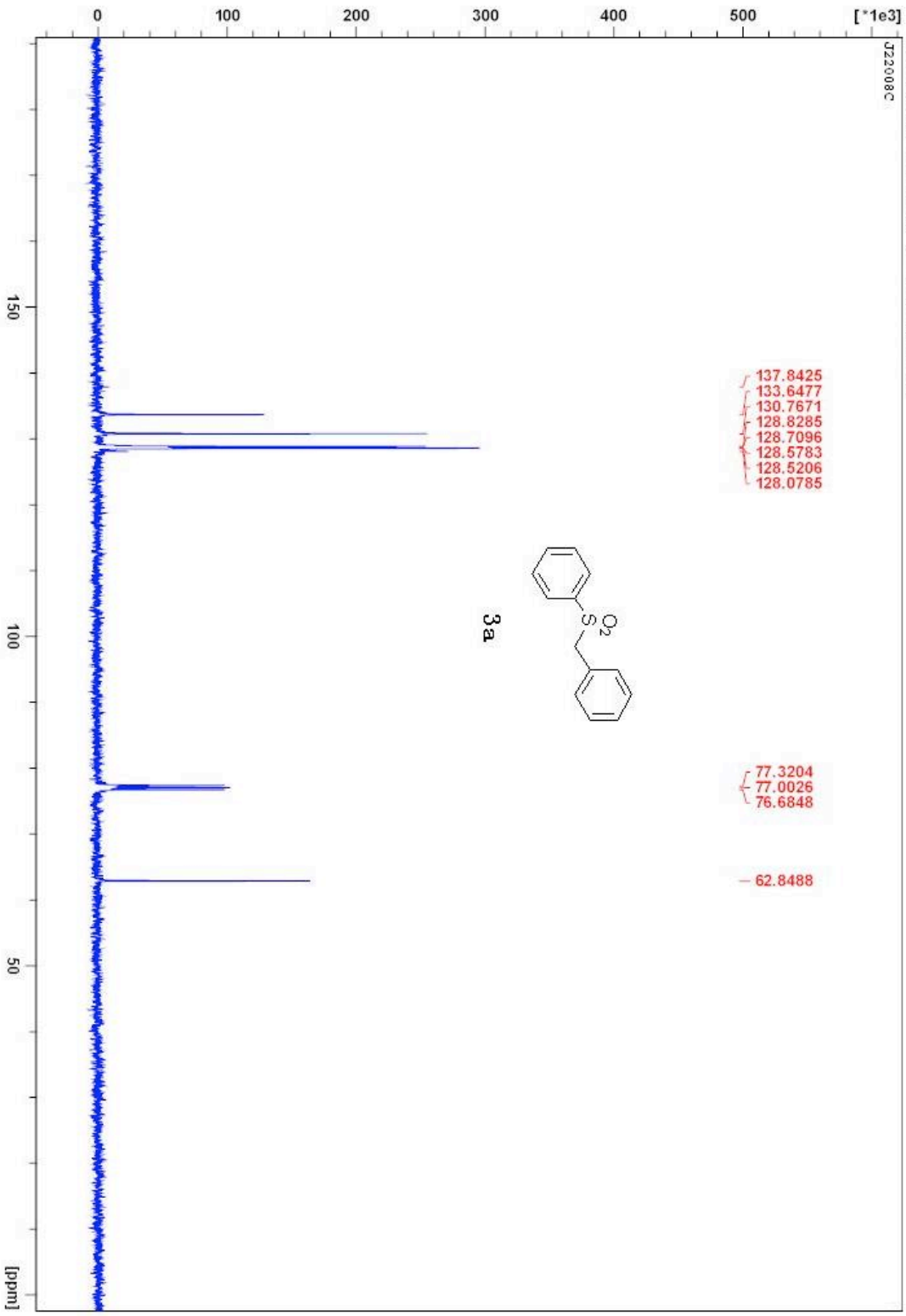
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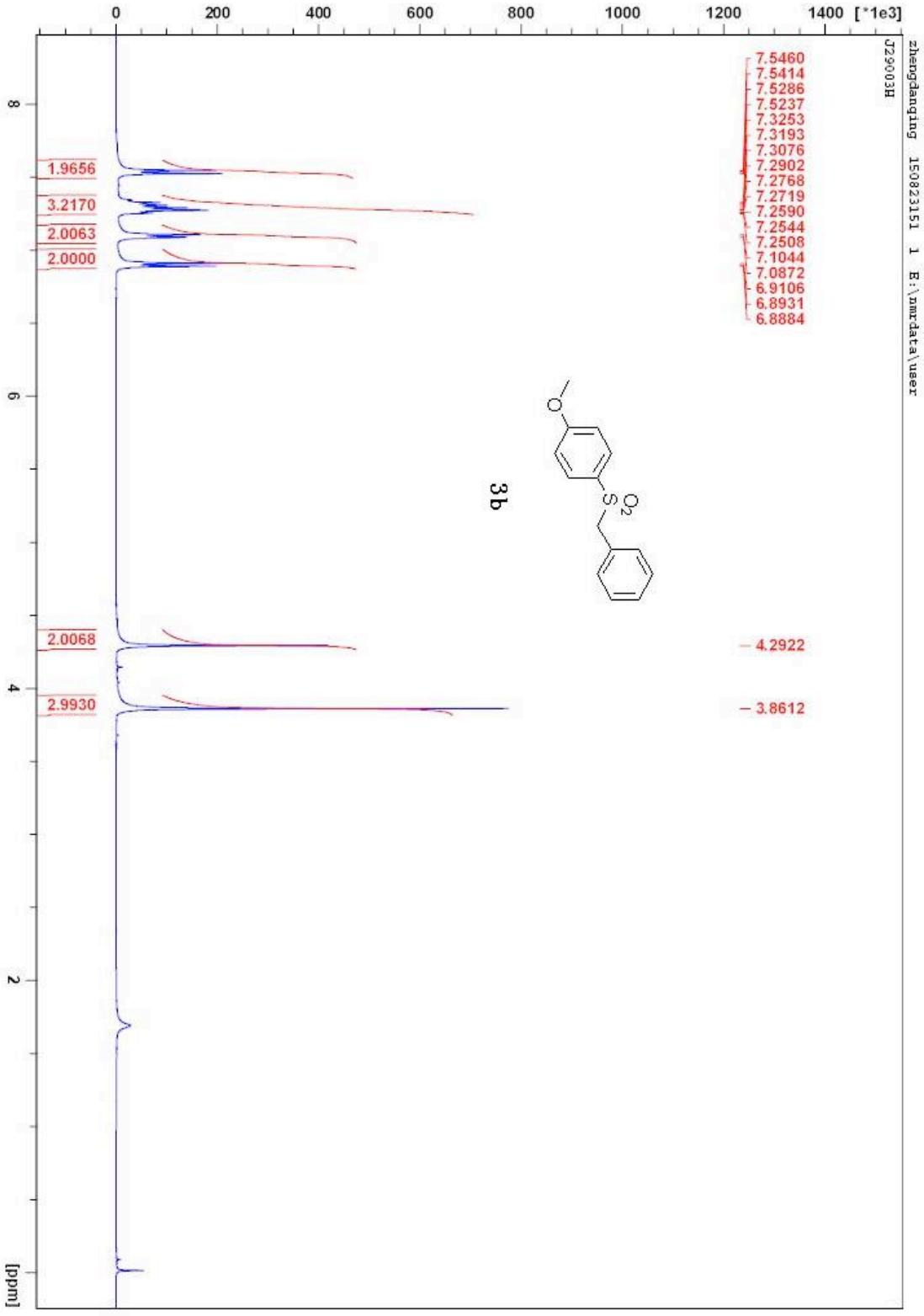
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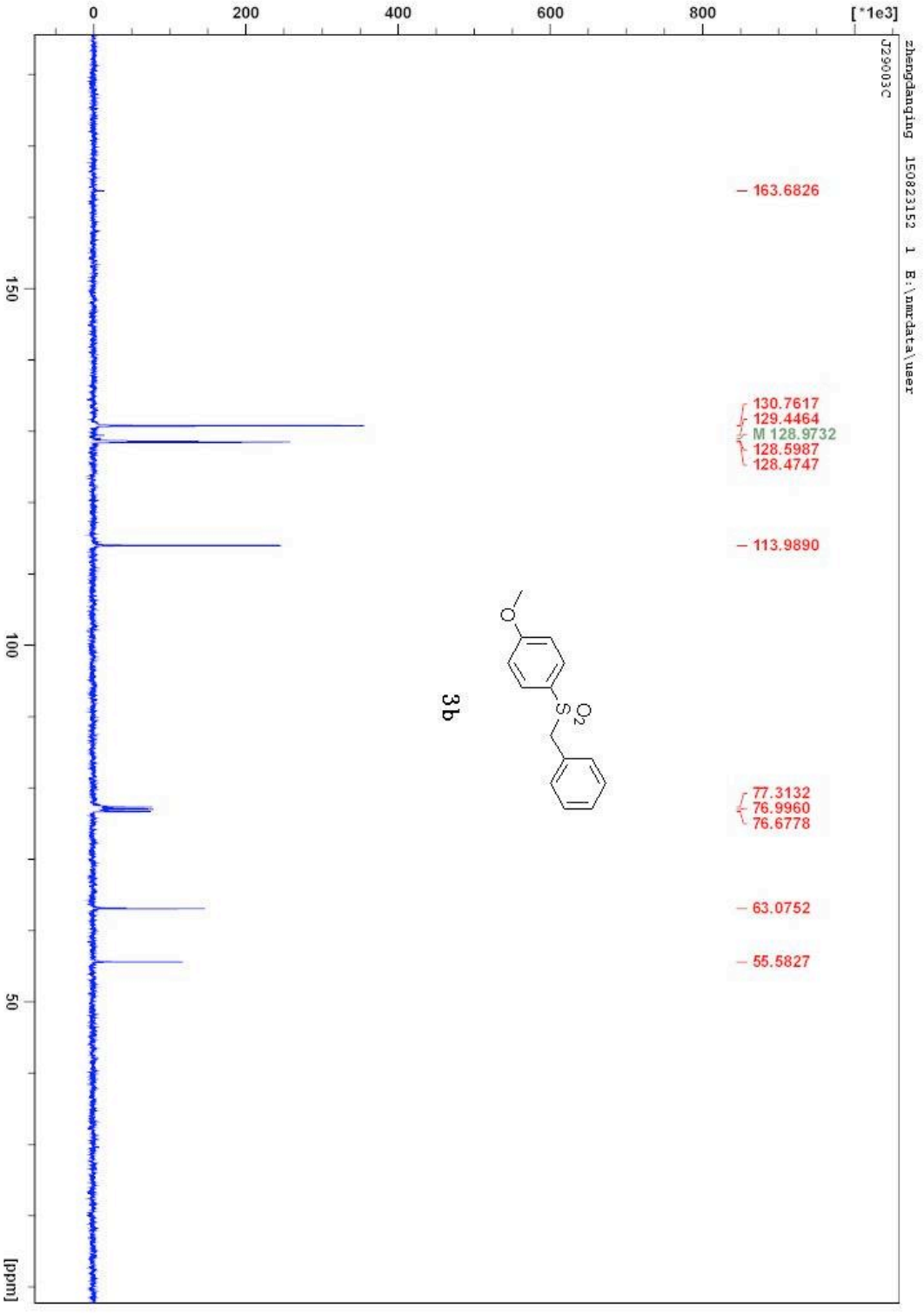
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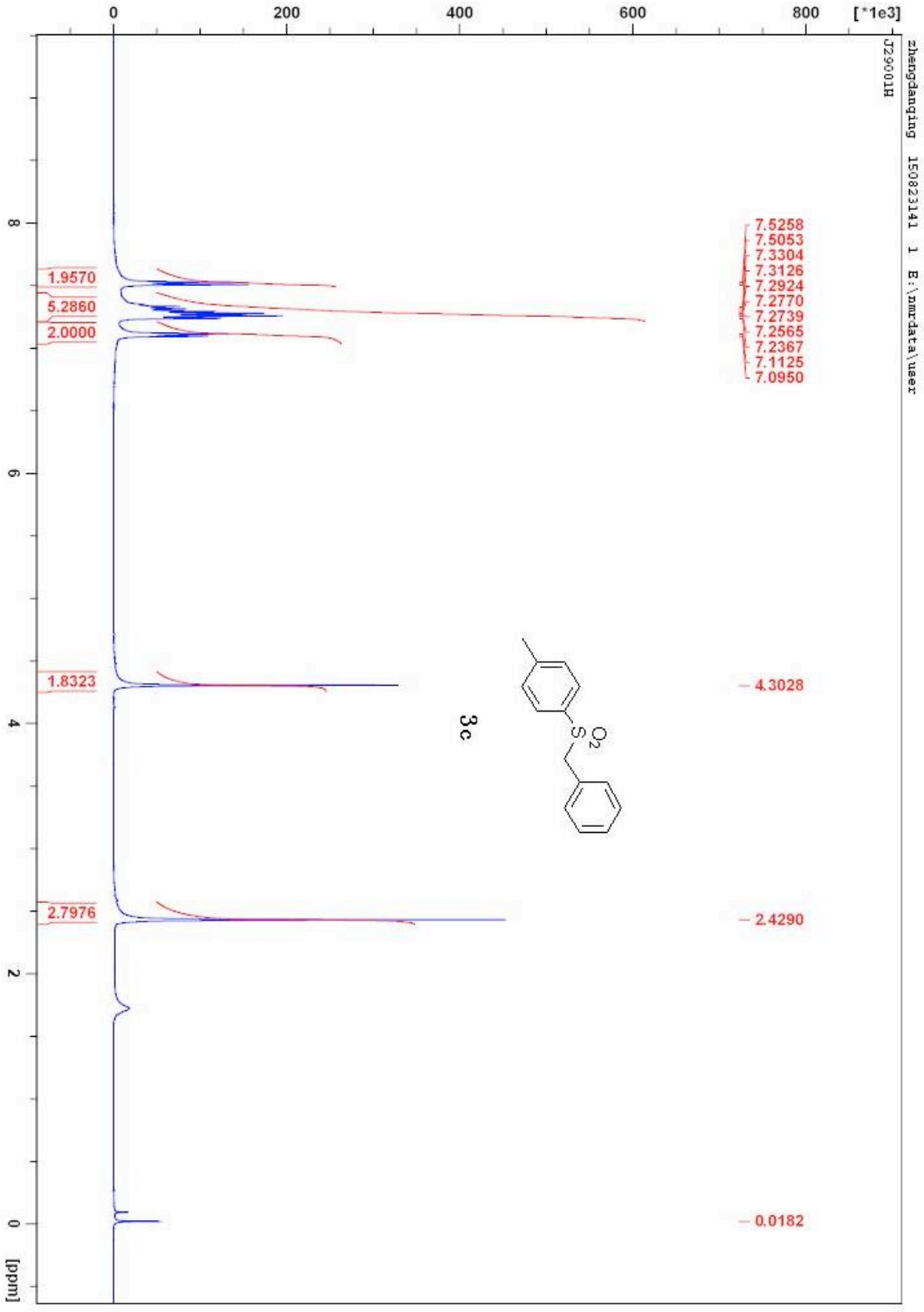
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7.5053
7.3304
7.3126
7.2924
7.2770
7.2739
7.2565
7.2367
7.1125
7.0950
1.9570
5.2860
2.0000
1.8323
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2.4290
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3c
O2
S
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6
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2
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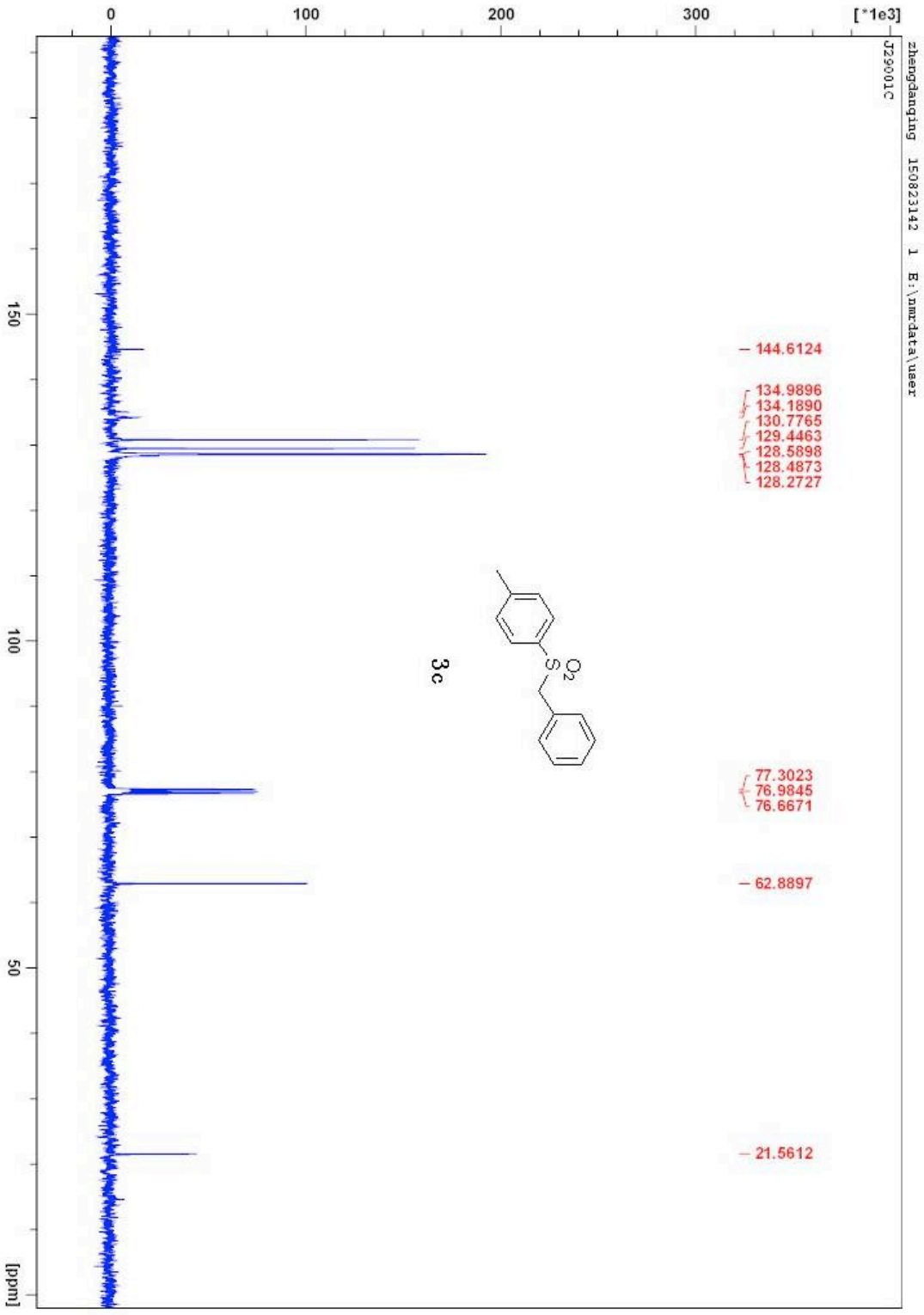
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128.4873
128.2727
77.3023
76.9845
76.6671
62.8897
21.5612
3c
O2
S
J29001C
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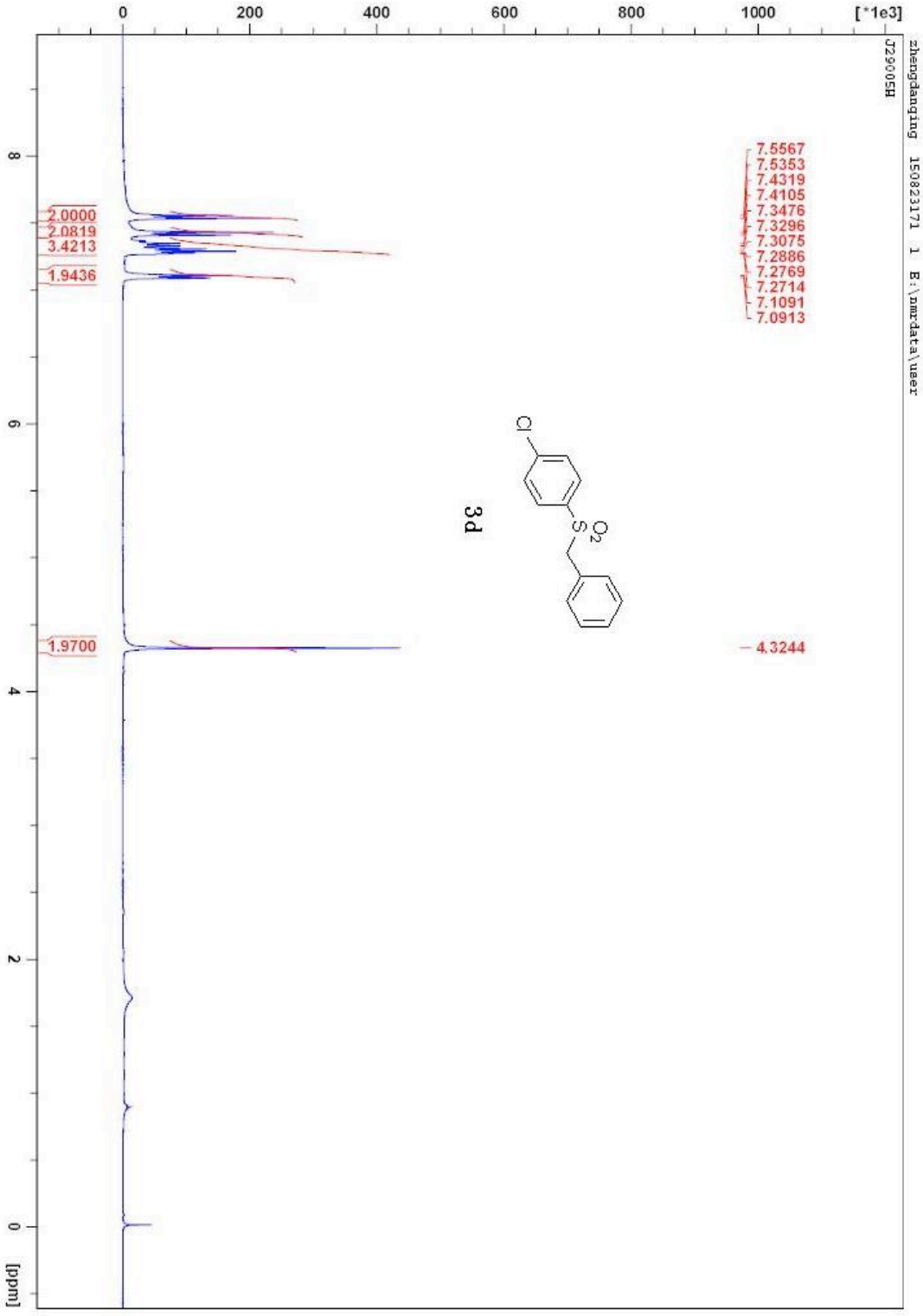
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7.3075
7.2886
7.2769
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7.1091
7.0913
2.0000
2.0819
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Cl
O2
S
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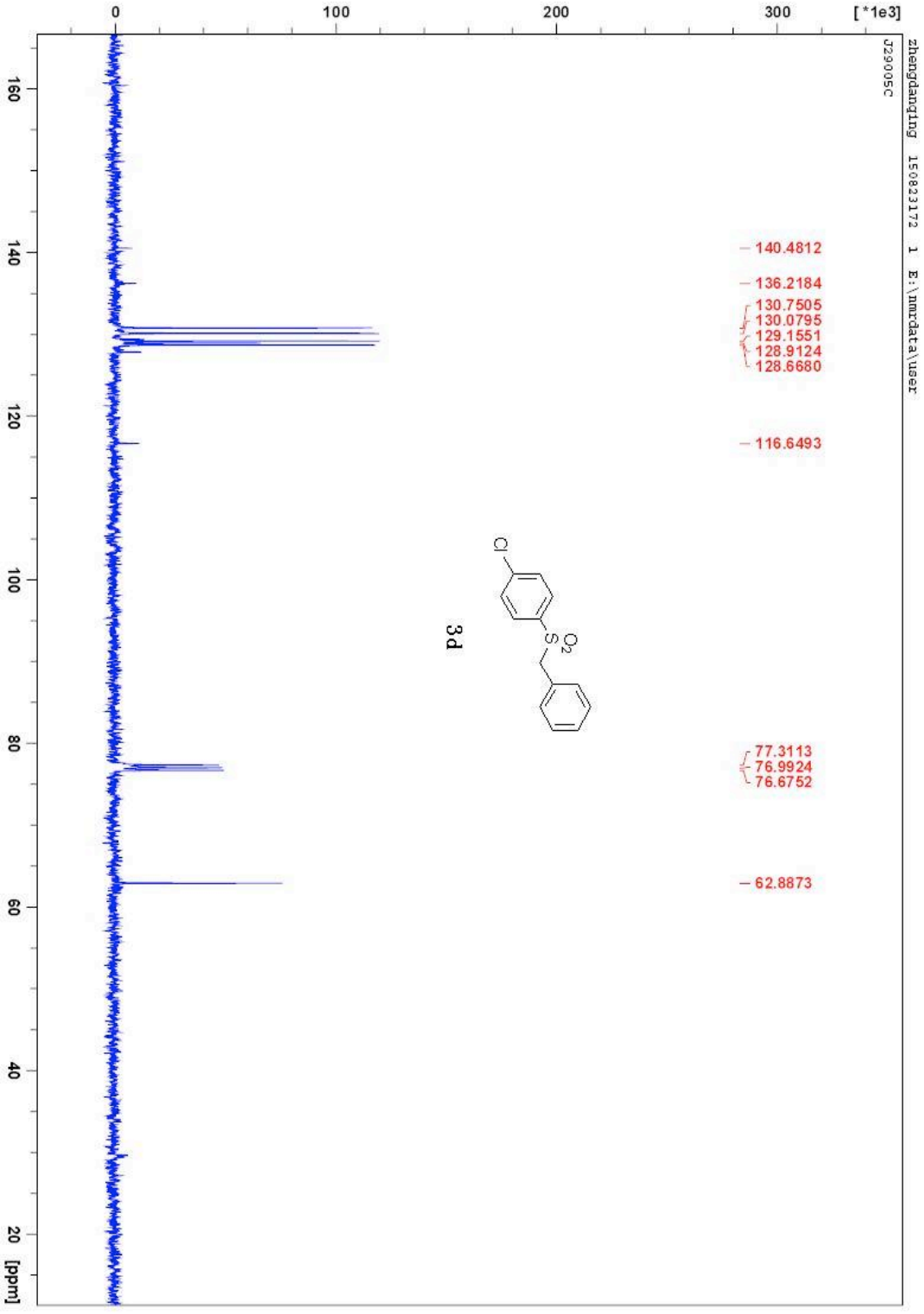
6
4
2
0
[ppm]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130.0795
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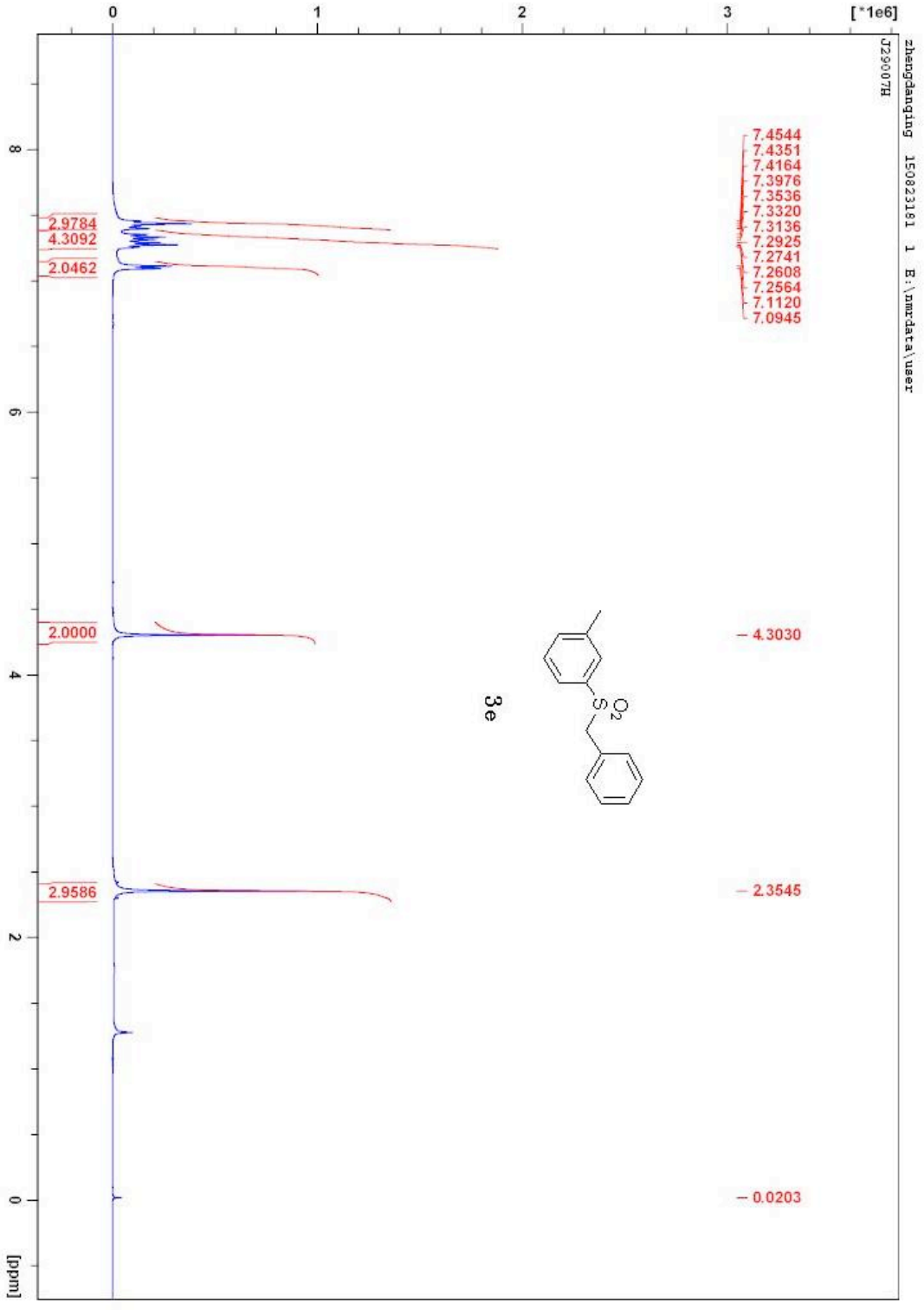
76.9924
76.6752
62.8873
Cl
S
O2
3d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7.3536
7.3320
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7.2925
7.2741
7.2608
7.2564
7.1120
7.0945
2.9784
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2.0000
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4.3030
2.3545
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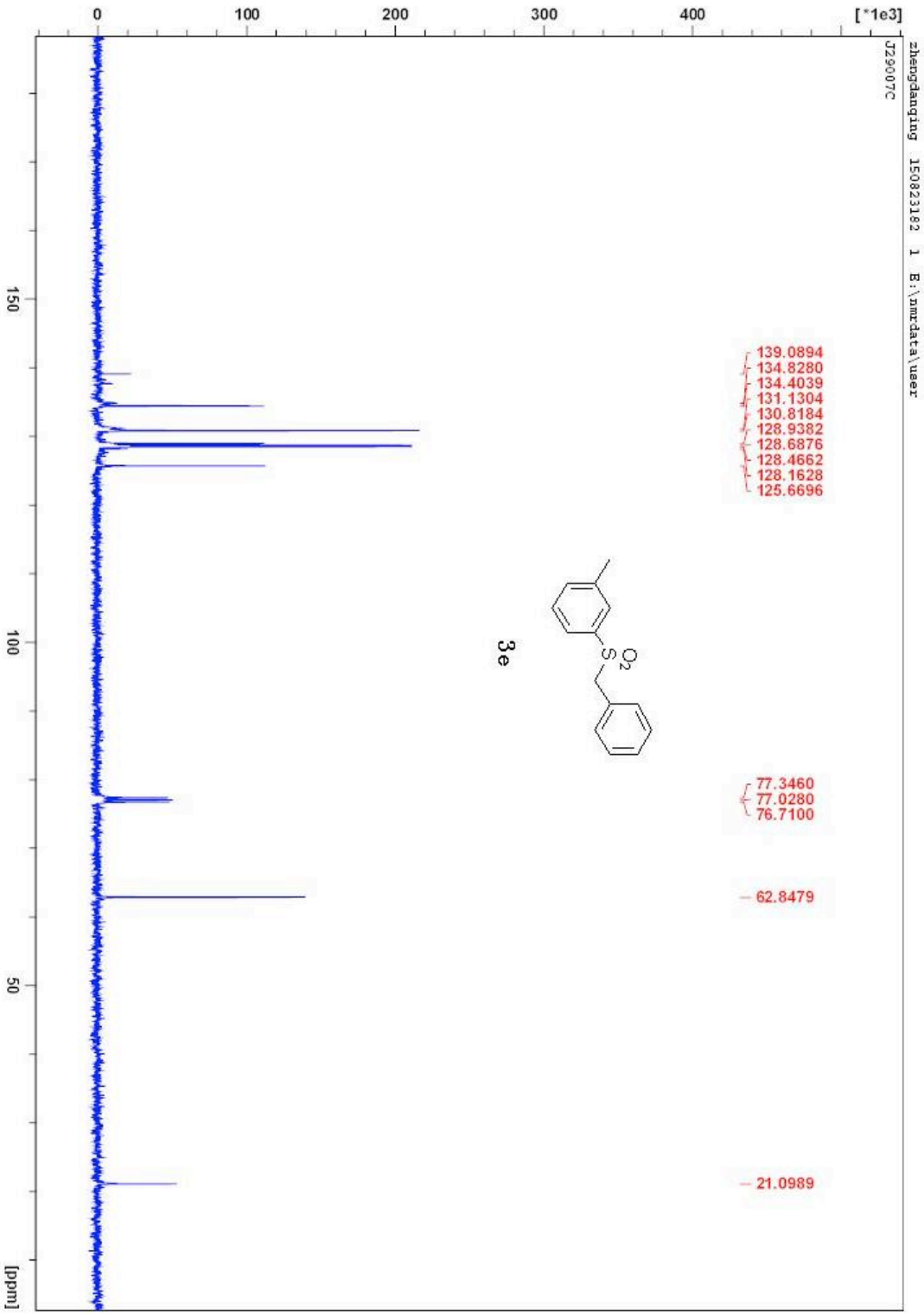
O2
S
[ppm]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134.8280
134.4039
131.1304
130.8184
128.9382
128.6876
128.4662
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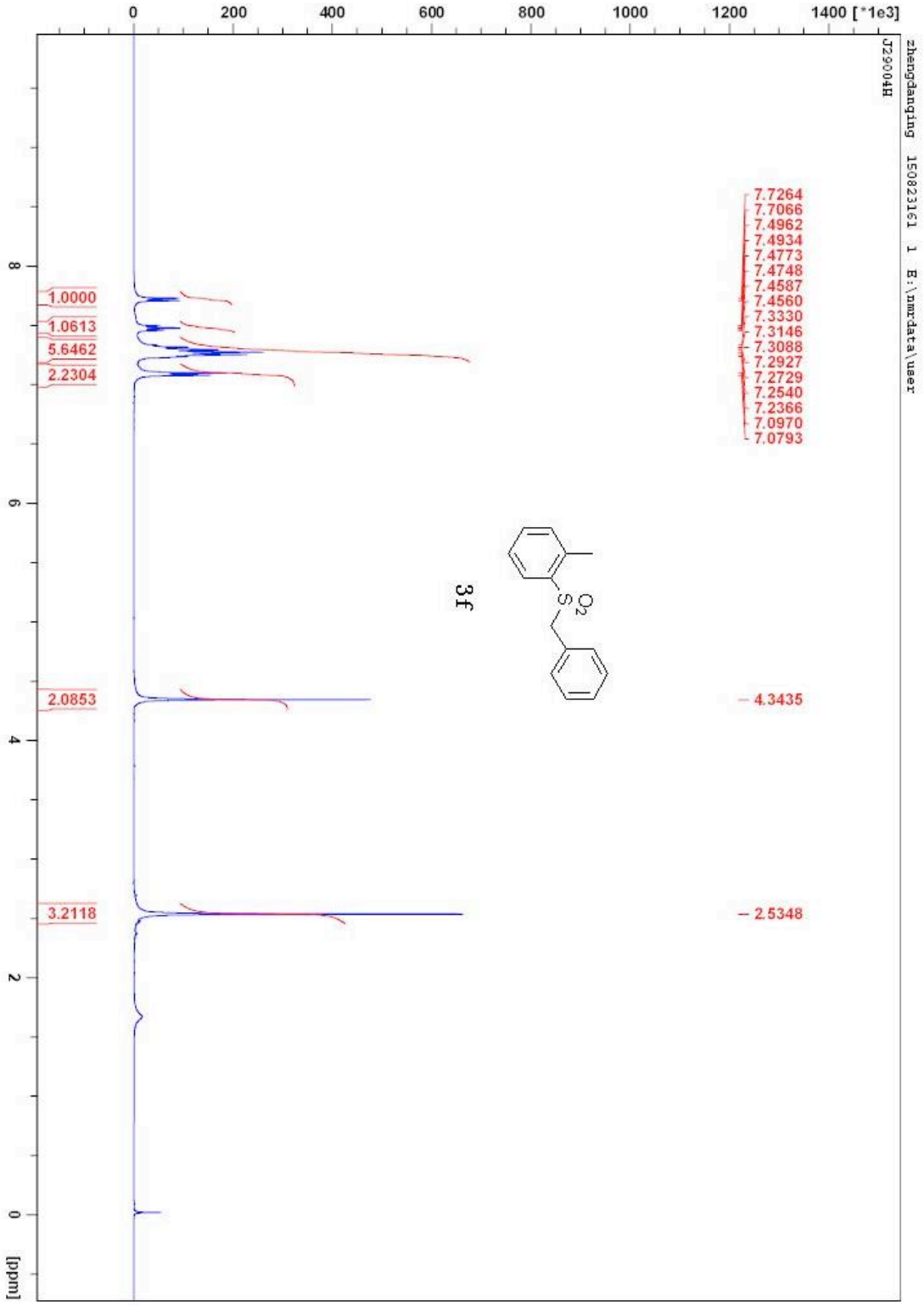
125.6696
77.3460
77.0280
76.7100
62.8479
21.0989
3e
O2
S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7.4773
7.4748
7.4587
7.4560
7.3330
7.3146
7.3088
7.2927
7.2729
7.2540
7.2366
7.0970
7.0793
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3.2118
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O2
S
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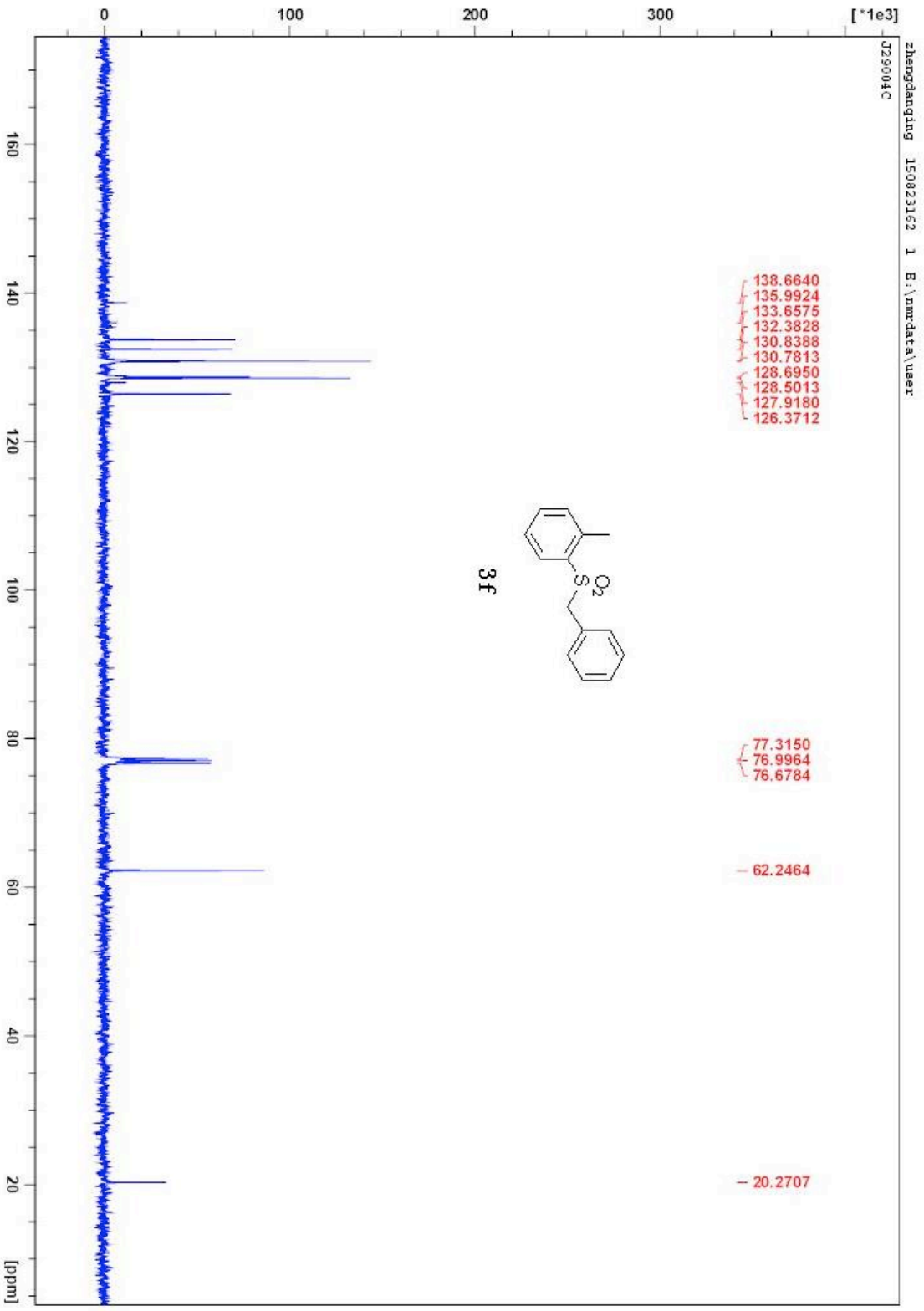
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80
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133.6575
132.3828
130.8388
130.7813
128.6950
128.5013
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126.3712
77.3150
76.9964
76.6784
62.2464
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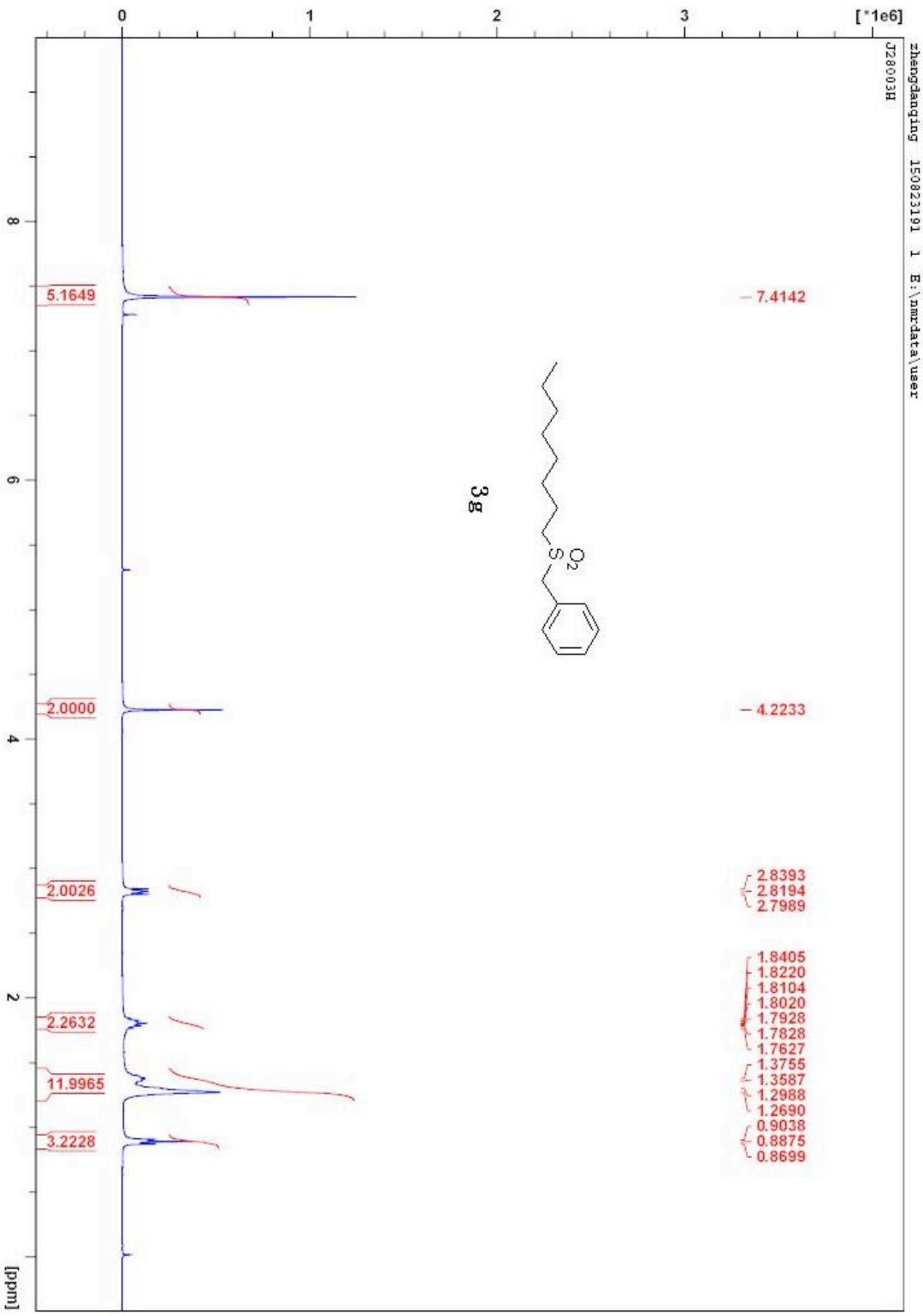
3f
O2
S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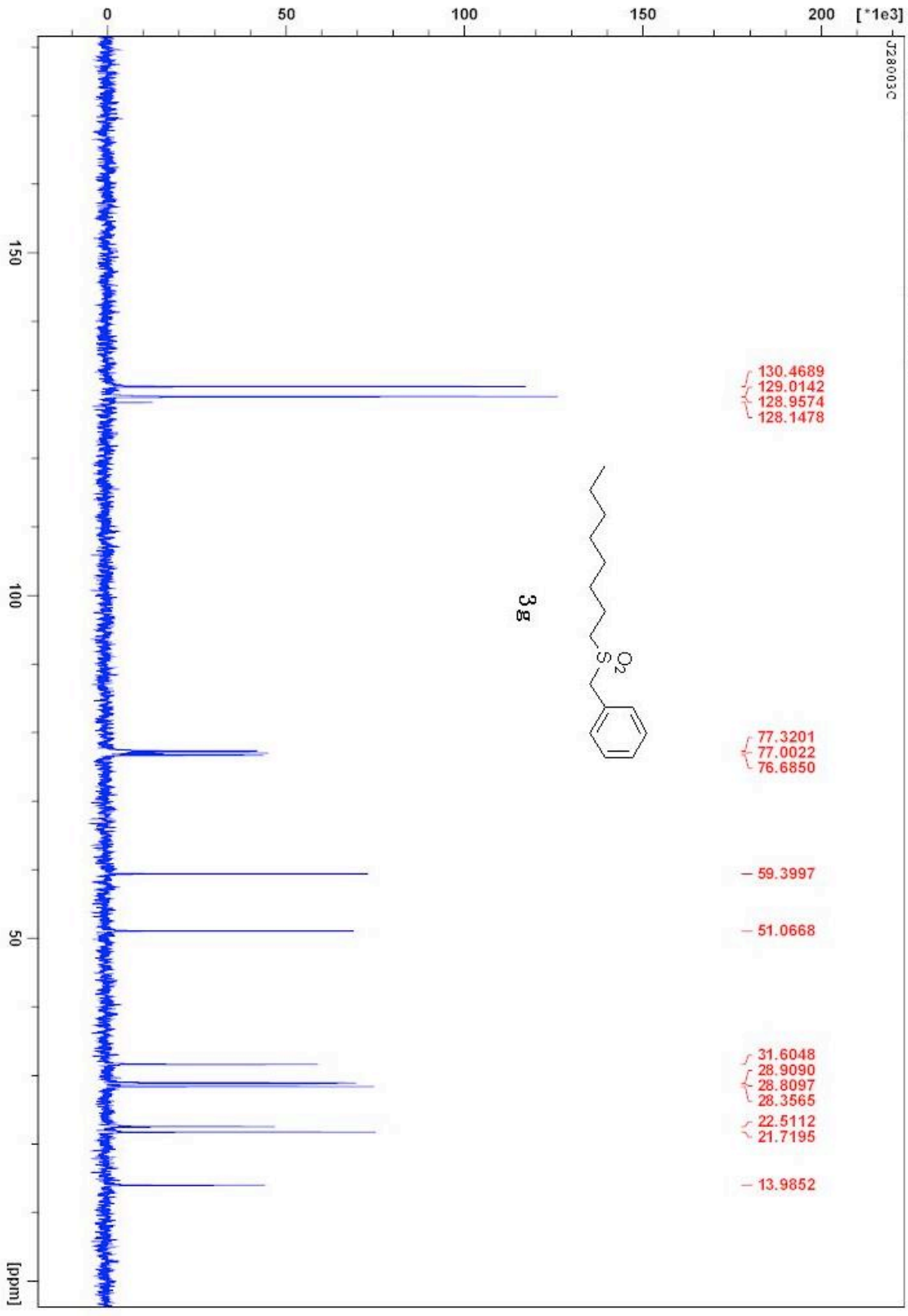
2.0026
2.2632
11.9965
3.2228
7.4142
4.2233
2.8393
2.8194
2.7989
1.8405
1.8220
1.8104
1.8020
1.7928
1.7828
1.7627
1.3755
1.3587
1.2988
1.2690
0.9038
0.8875
0.8699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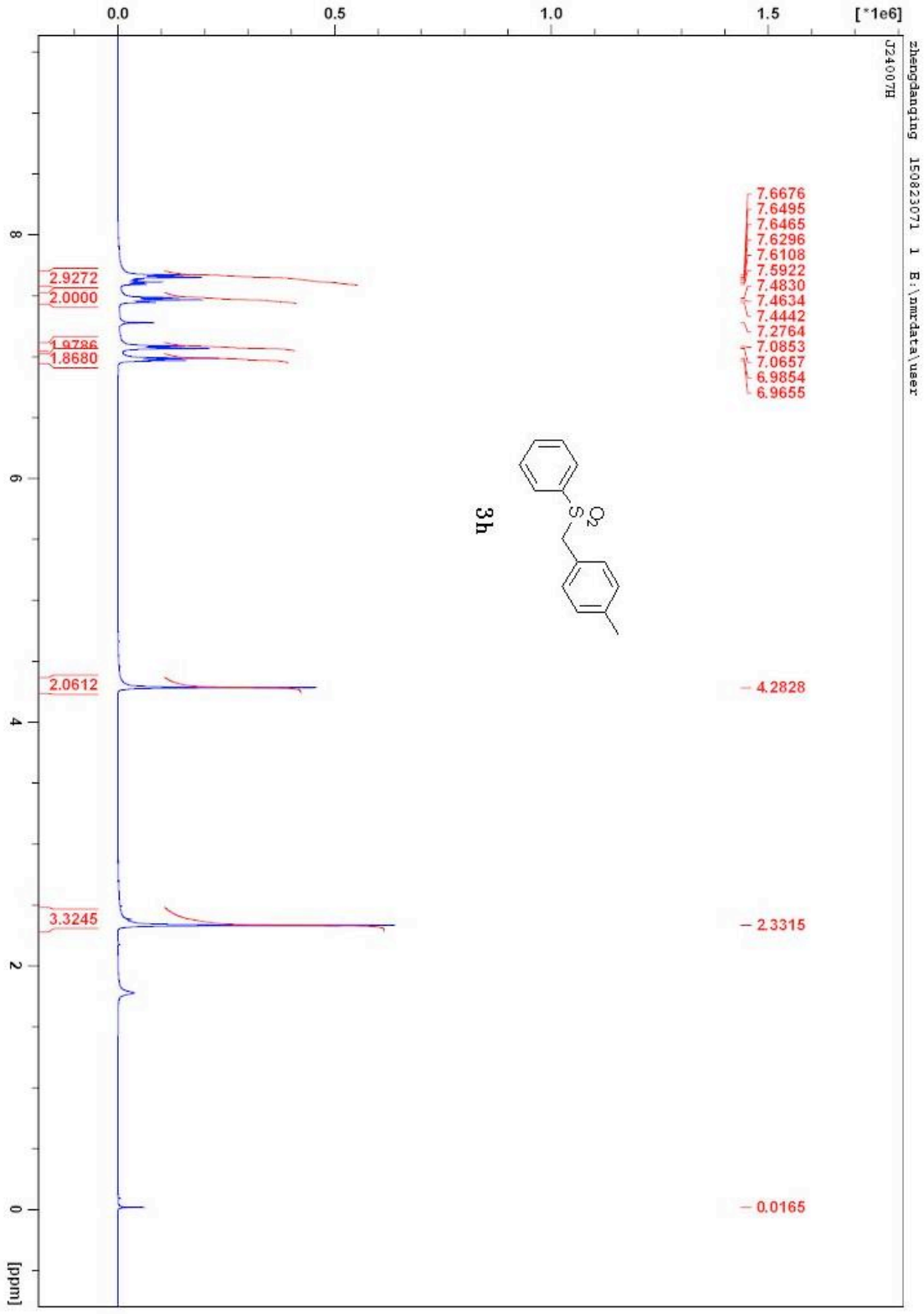
128.1478
77.3201
77.0022
76.6850
59.3997
51.0668
31.6048
28.9090
28.8097
28.3565
22.5112
21.7195
13.9852
3g
O
O
S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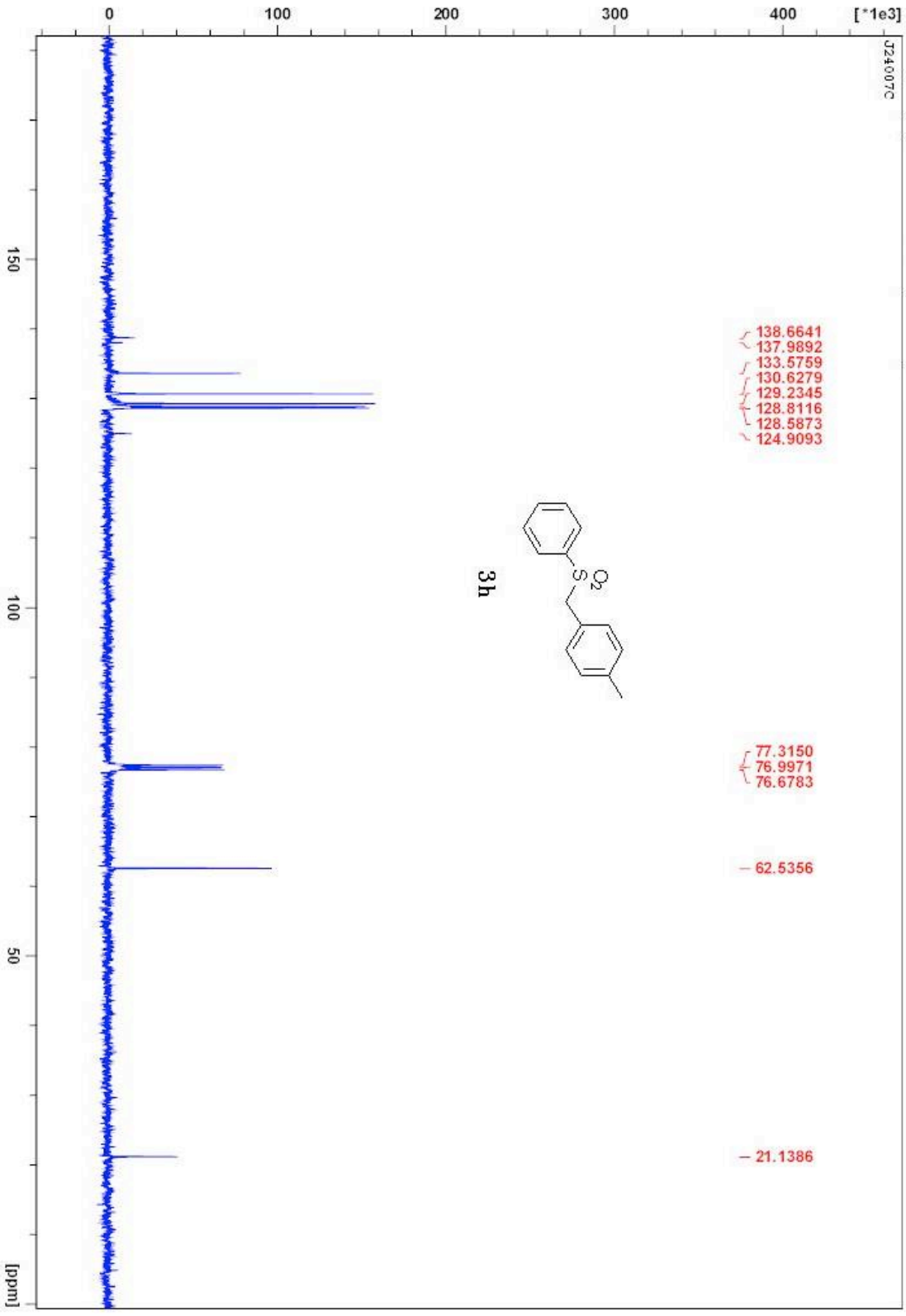
7.6465
7.6296
7.6108
7.5922
7.4830
7.4634
7.4442
7.2764
7.0853
7.0657
6.9854
6.9655
2.9272
2.0000
1.9786
1.8680
2.0612
3.3245
4.2828
2.3315
0.0165
3h
O2
S
8
6
4
2
0
[ppm]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129.2345
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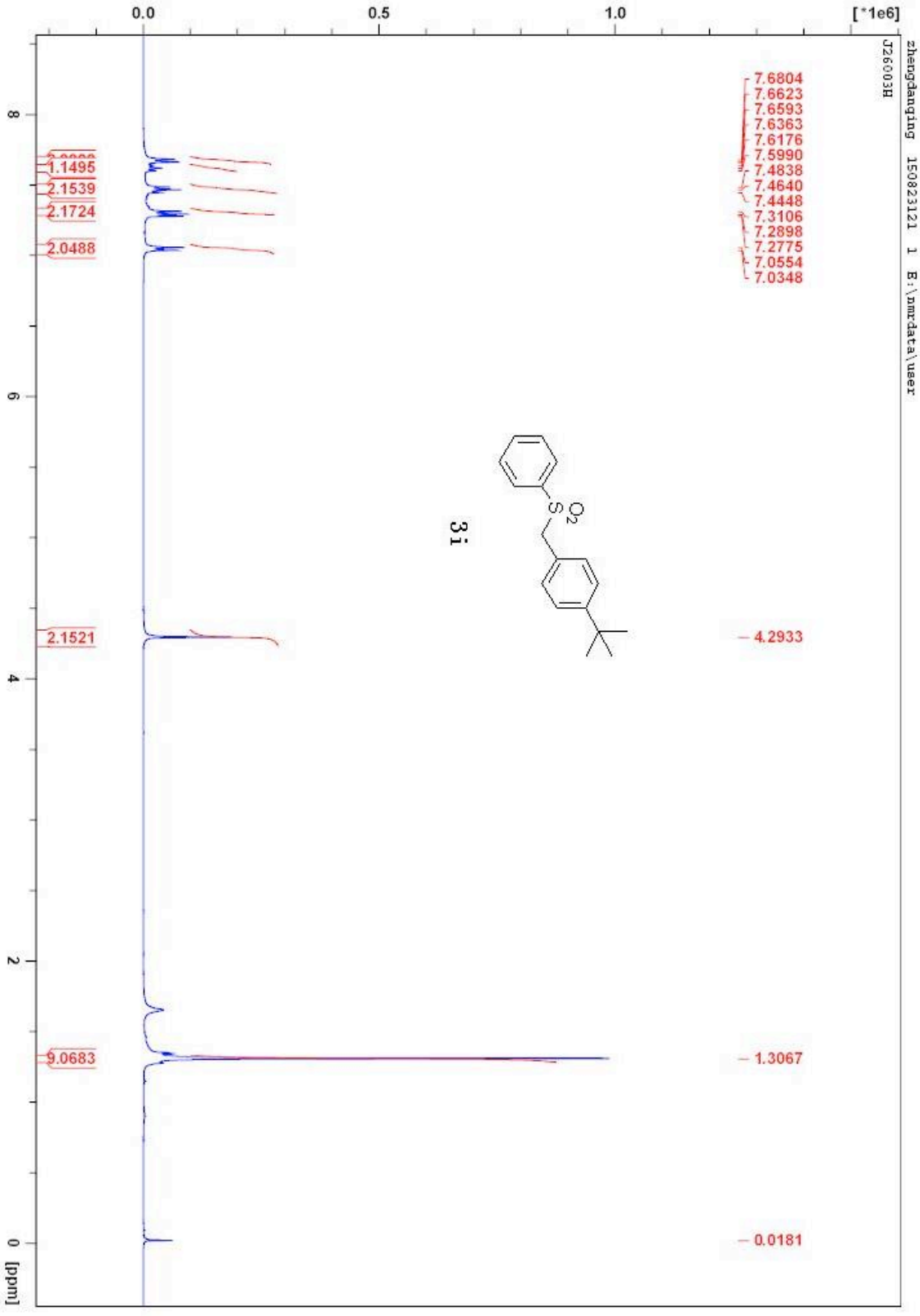
62.5356
21.1386
3h
O2
S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7.6176
7.5990
7.4838
7.4640
7.4448
7.3106
7.2898
7.2775
7.0554
7.0348
1.1495
2.1539
2.1724
2.0488
2.1521
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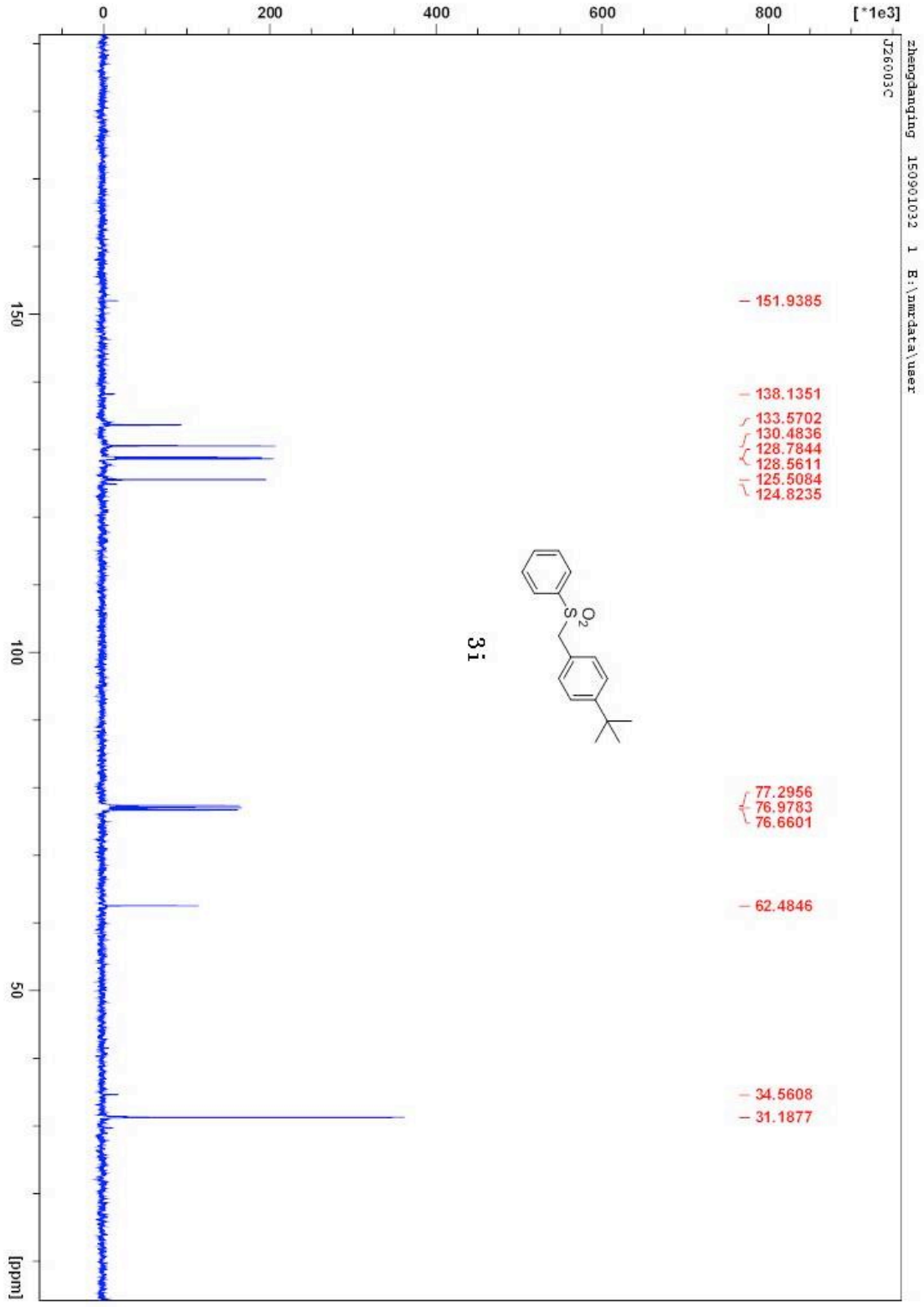
1.3067
0.0181
3i
O2
S
8
6
4
2
0
[ppm]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128.5611
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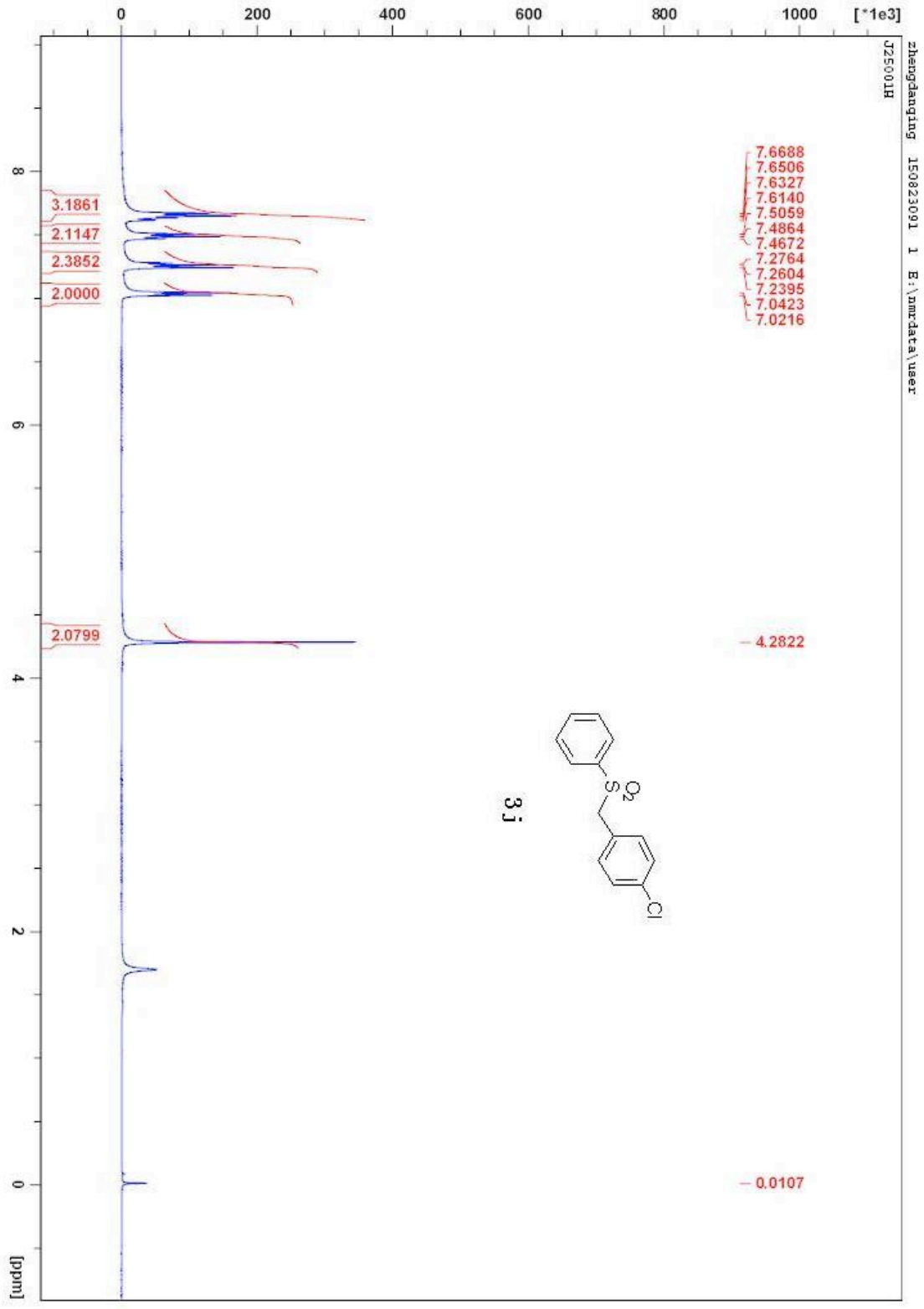
76.6601
62.4846
34.5608
31.1877
3i
O2
S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7.5059
7.4864
7.4672
7.2764
7.2604
7.2395
7.0423
7.0216
4.2822
0.0107
3.1861
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2.0799
8
6
4
2
0
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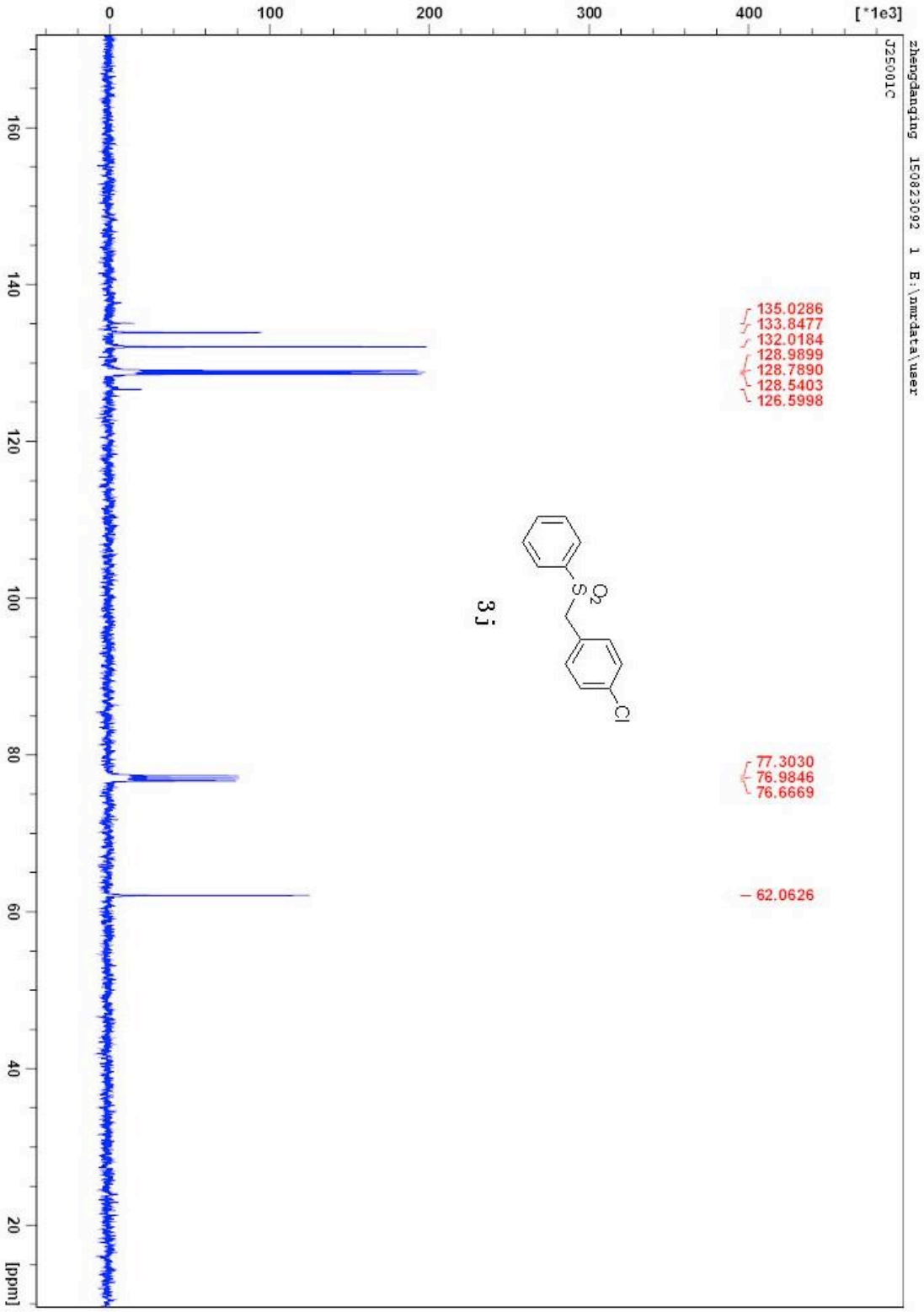
3j
O2
S
Cl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80
60
40
20
[ppm]
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132.0184
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128.7890
128.5403
126.5998
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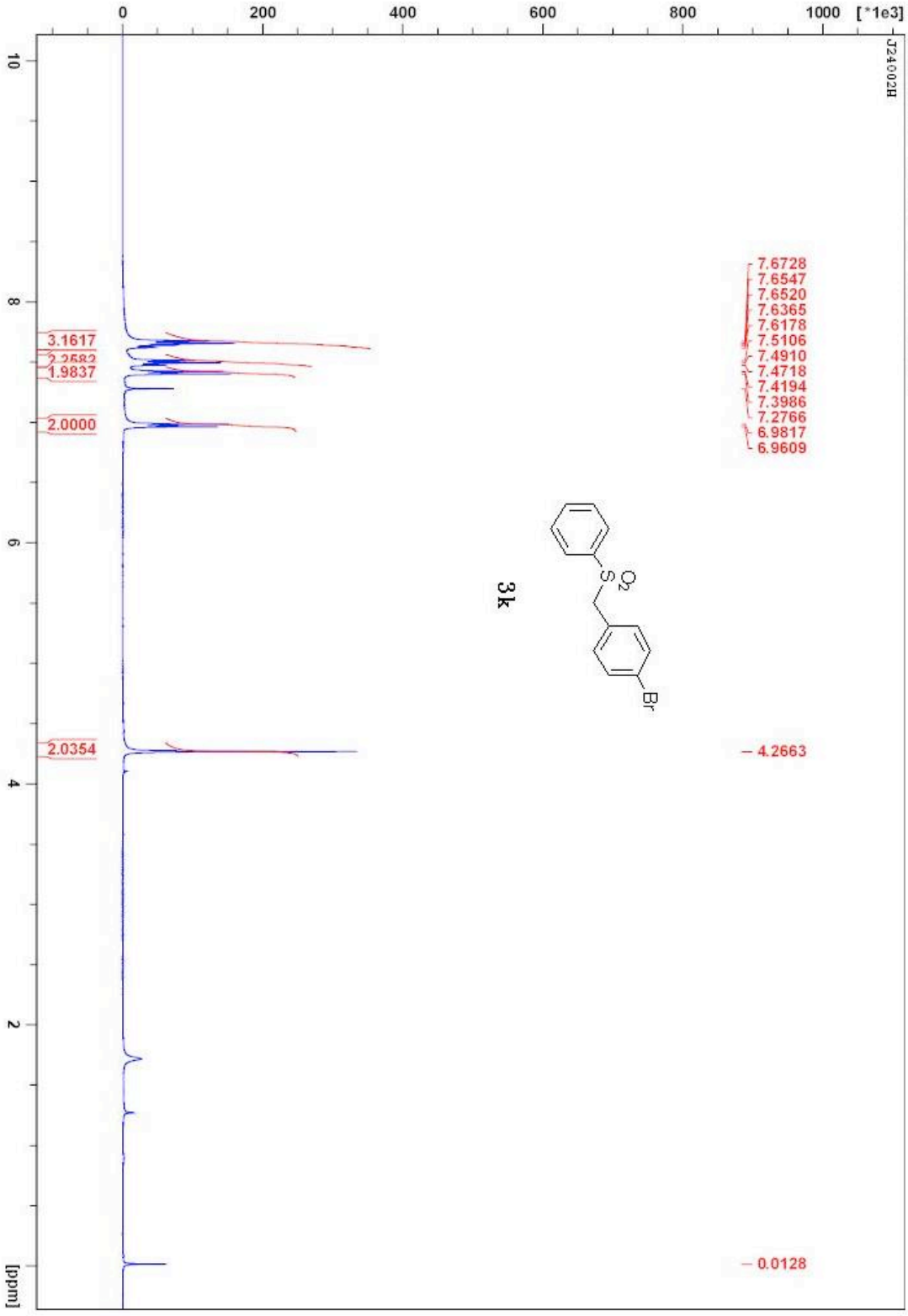
76.6669
62.0626
3j
O2
S
Cl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600
800
1000
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8
6
4
2
[ppm]
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7.6178
7.5106
7.4910
7.4718
7.4194
7.3986
7.2766
6.9817
6.9609
3.1617
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1.9837
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2.0354
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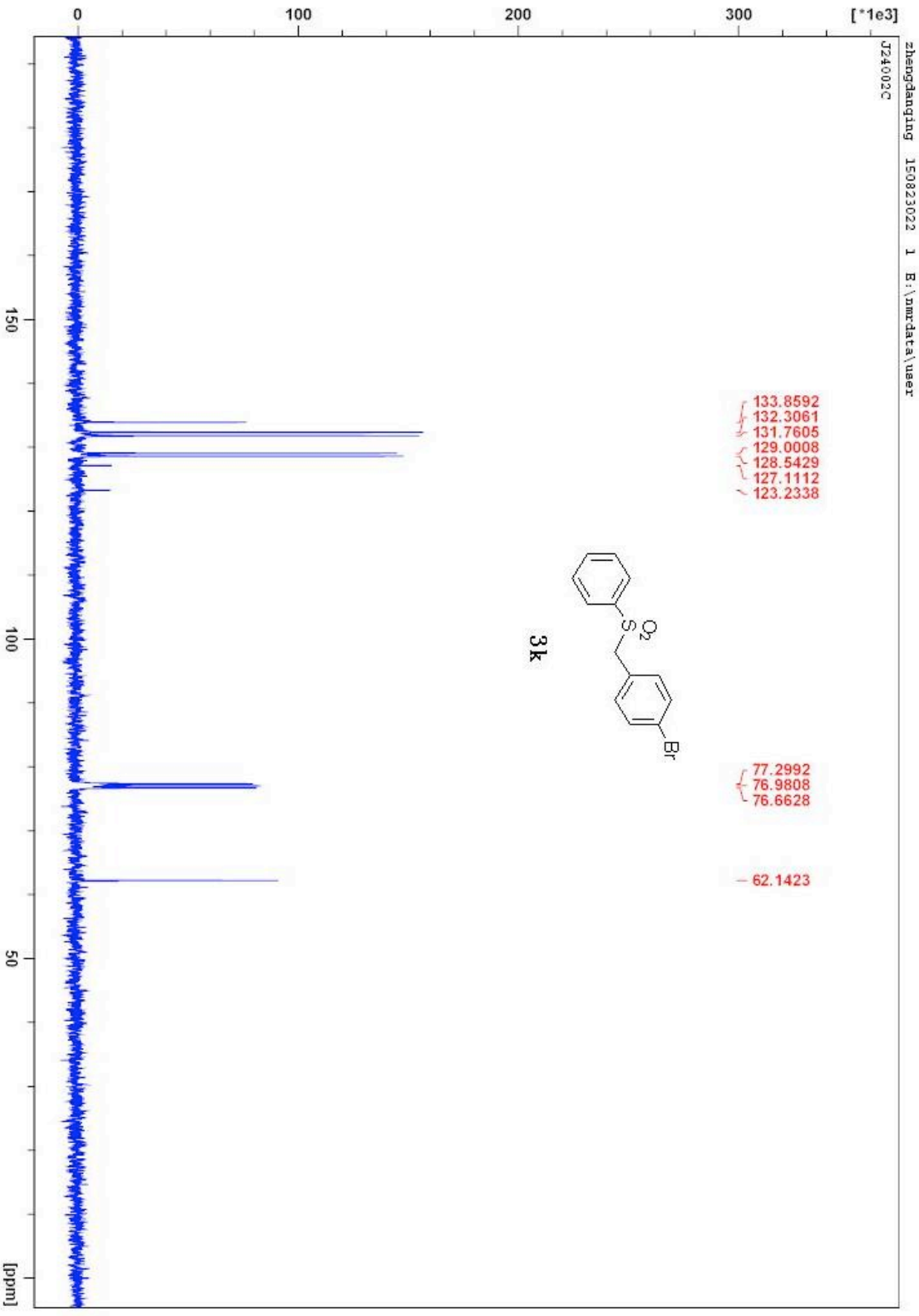
3k
O2
S
Br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131.7605
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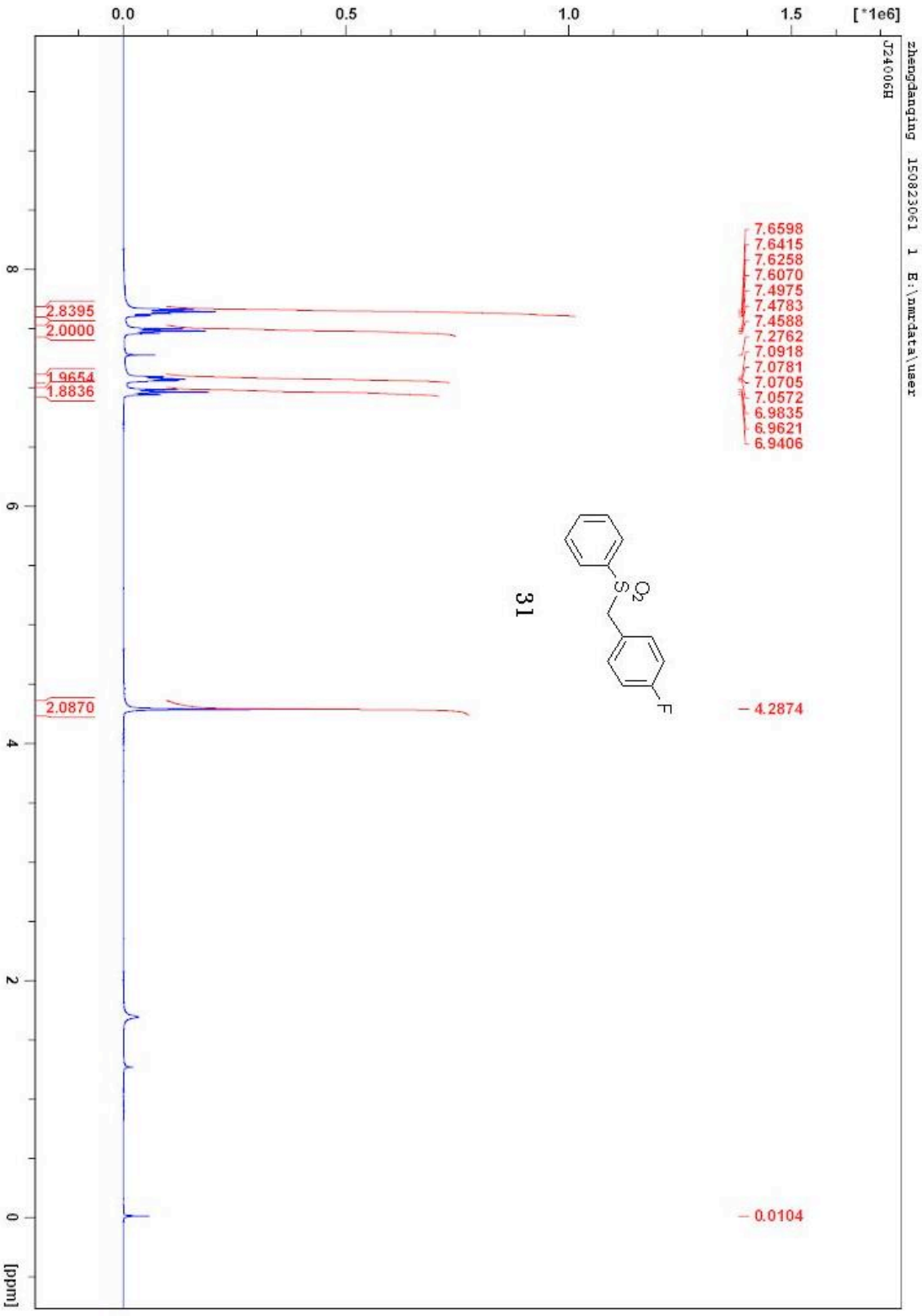
3k
O2
S
Br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1.5
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7.4975
7.4783
7.4588
7.2762
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7.0705
7.0572
6.9835
6.9621
6.9406
2.8395
2.0000
1.9654
1.8836
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4.2874
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31
O2
S
F
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6
4
2
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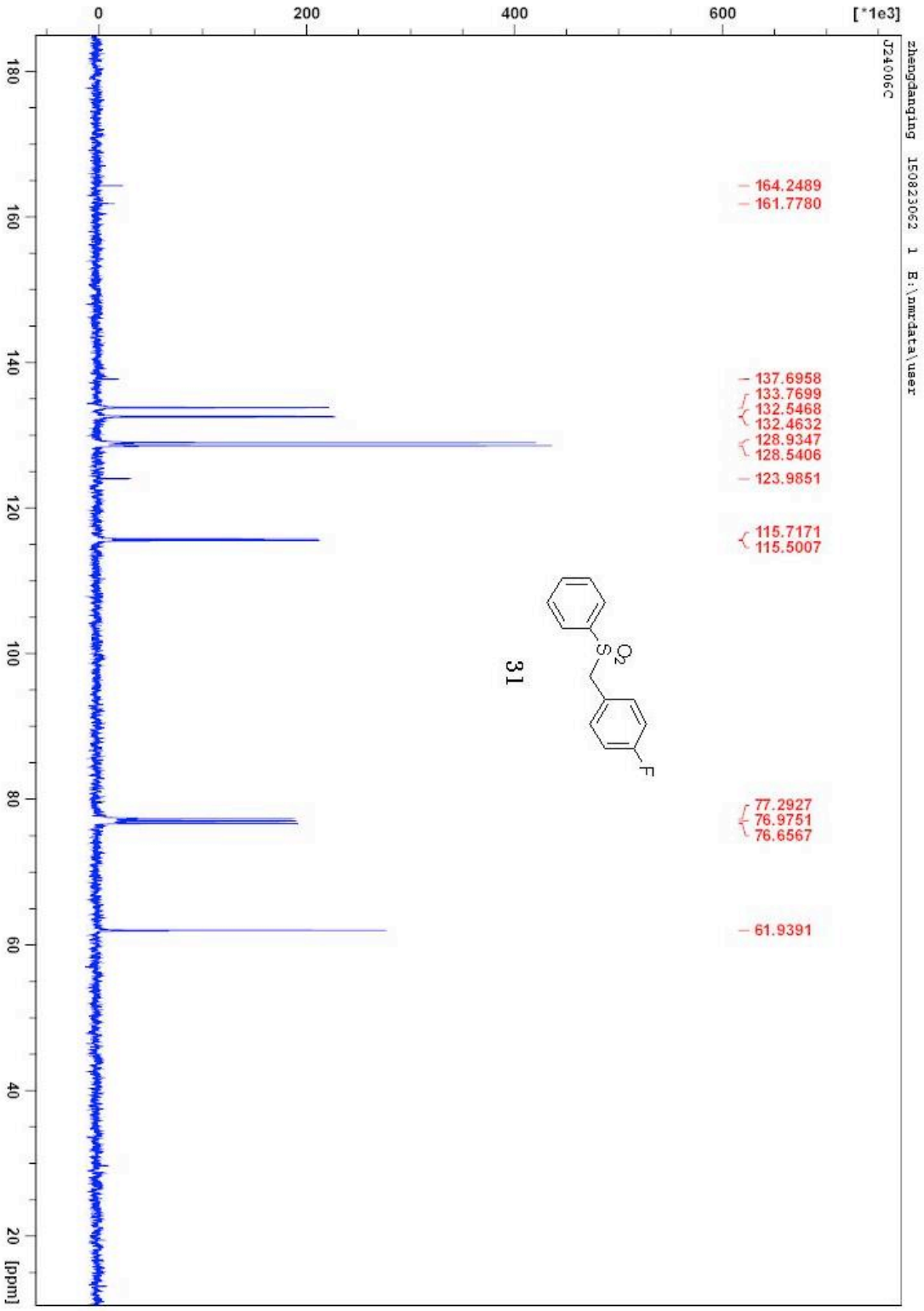
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20
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137.6958
133.7699
132.5468
132.4632
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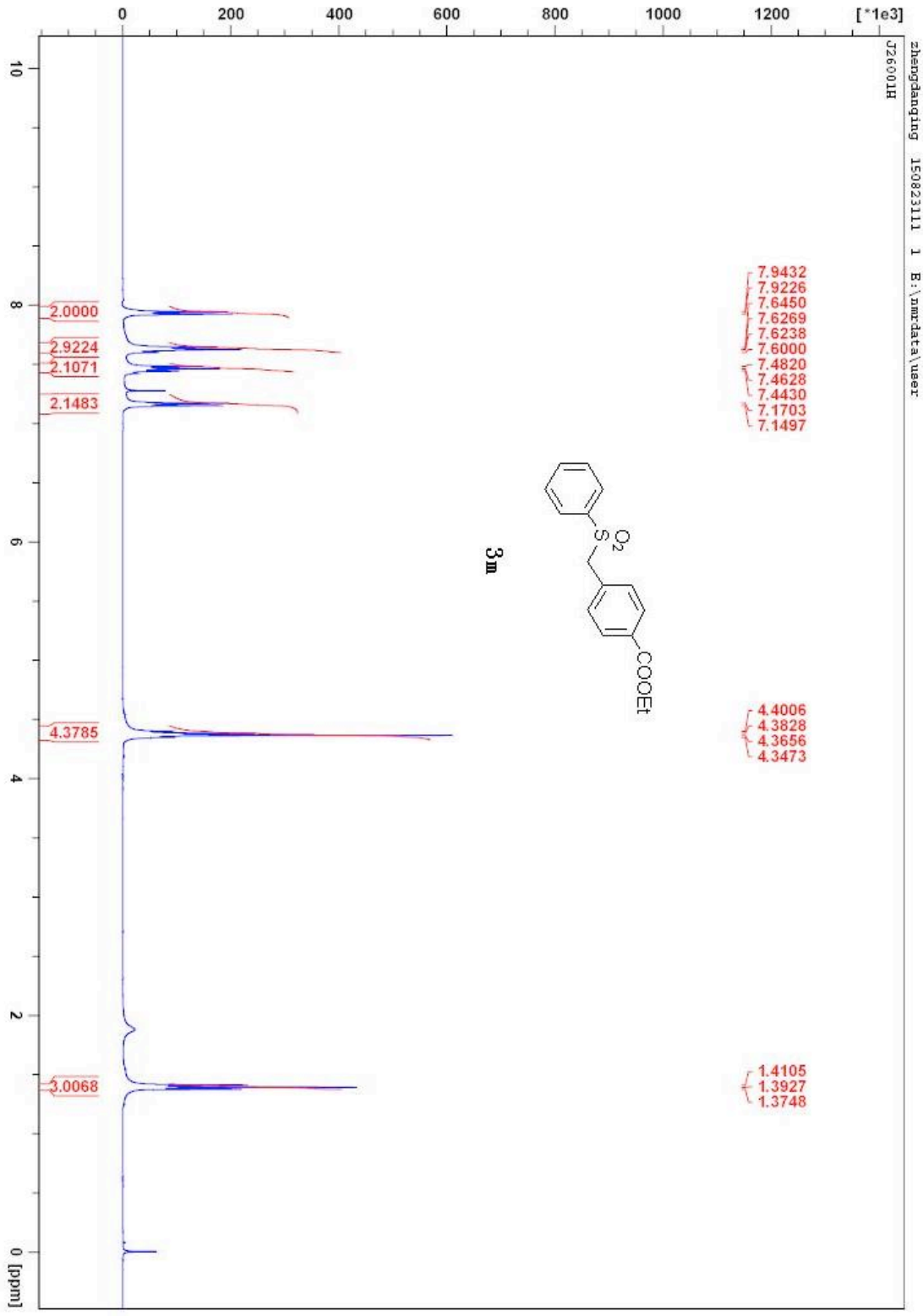
115.7171
115.5007
77.2927
76.9751
76.6567
61.9391
O2
S
F
31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800
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8
6
4
2
0 [ppm]
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2.1483
4.3785
3.0068
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7.4430
7.1703
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1.3748
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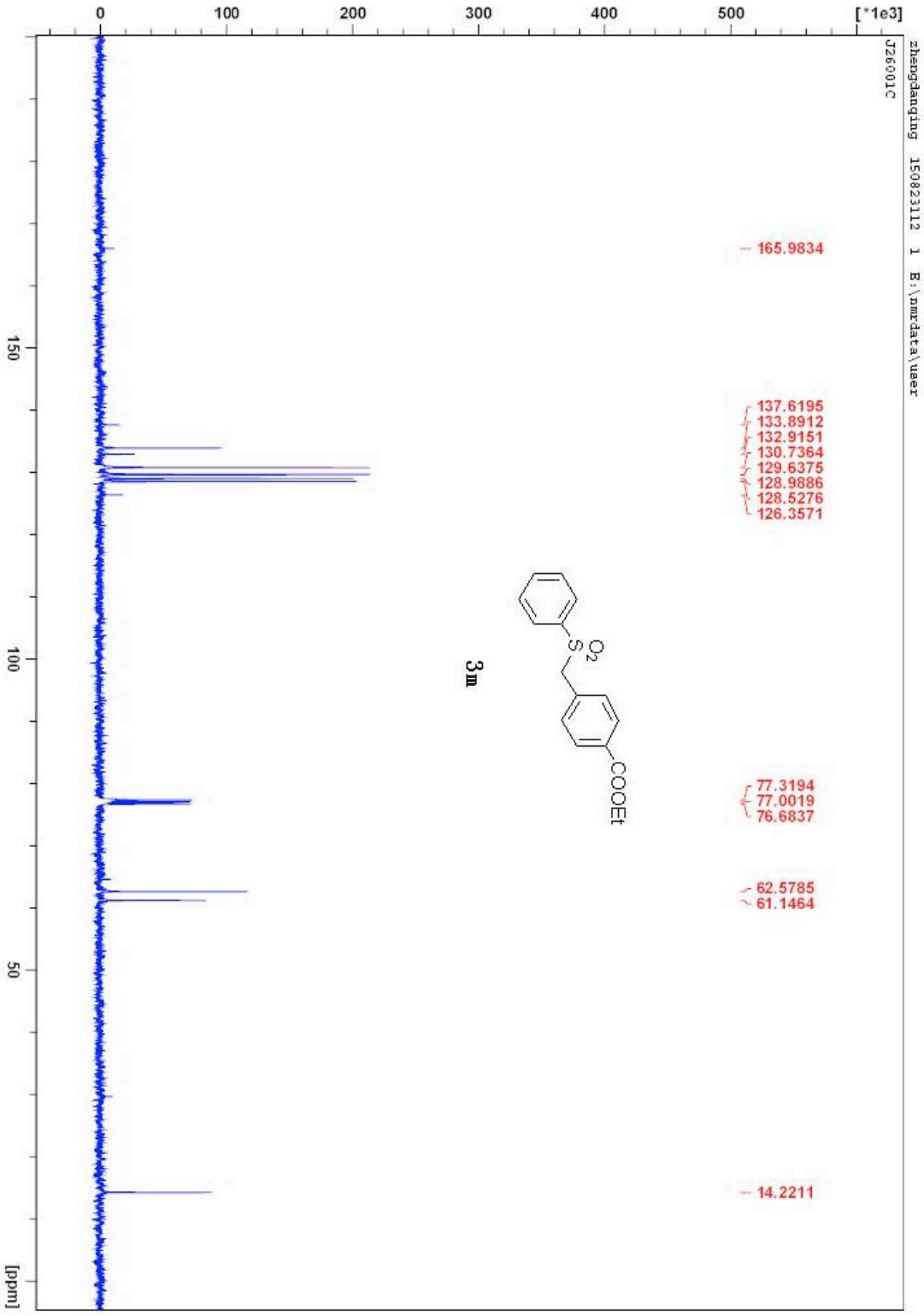
O2
S
COOEt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133.8912
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130.7364
129.6375
128.9886
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77.0019
76.6837
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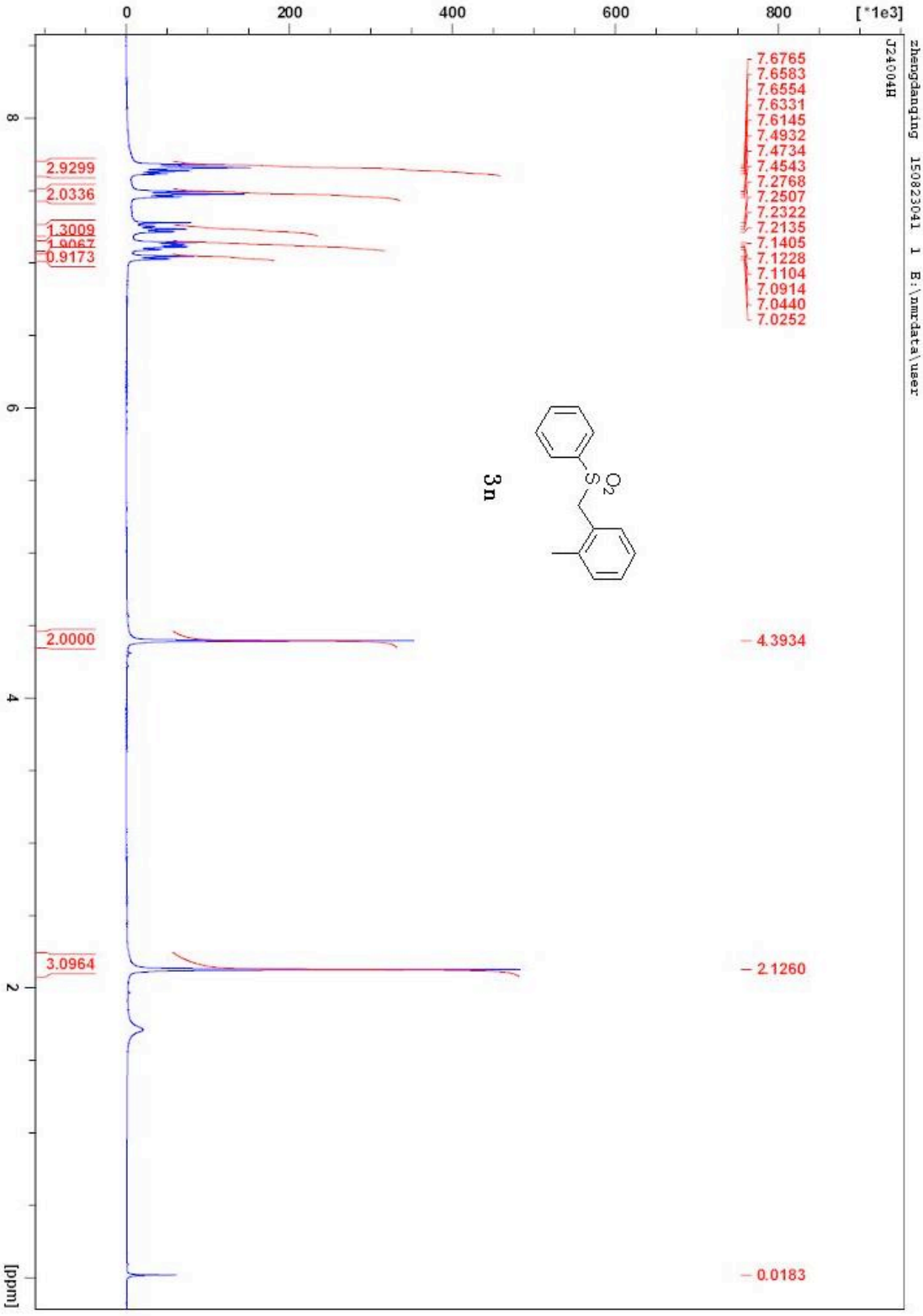
61.1464
14.2211
3m
O2
S
COOEt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800
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7.6554
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7.6145
7.4932
7.4734
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7.2507
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7.2135
7.1405
7.1228
7.1104
7.0914
7.0440
7.0252
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2.0336
1.3009
1.9067
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2.0000
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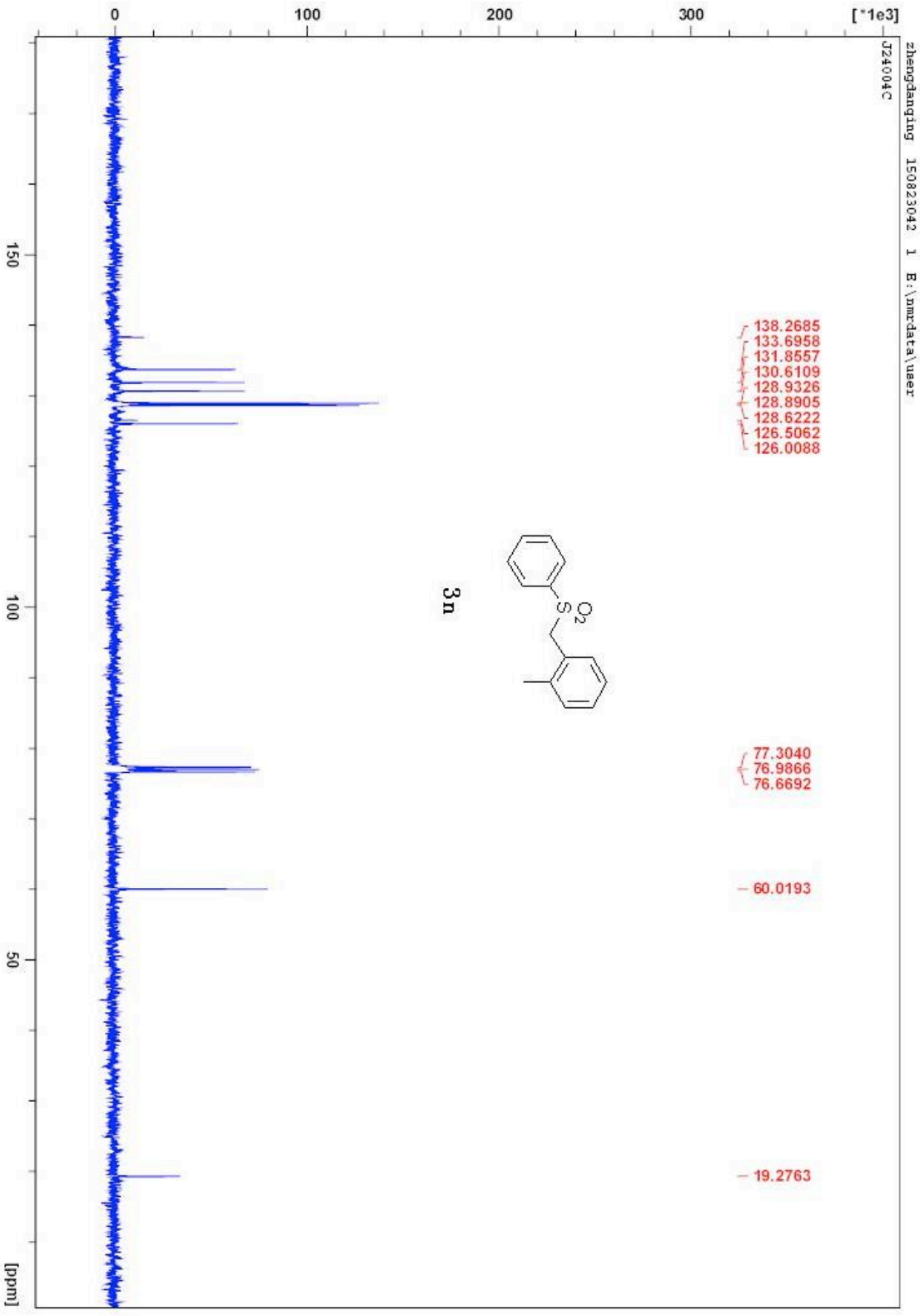
O2
S
8
6
4
2
[ppm]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100
50
[ppm]
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131.8557
130.6109
128.9326
128.8905
128.6222
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126.0088
77.3040
76.9866
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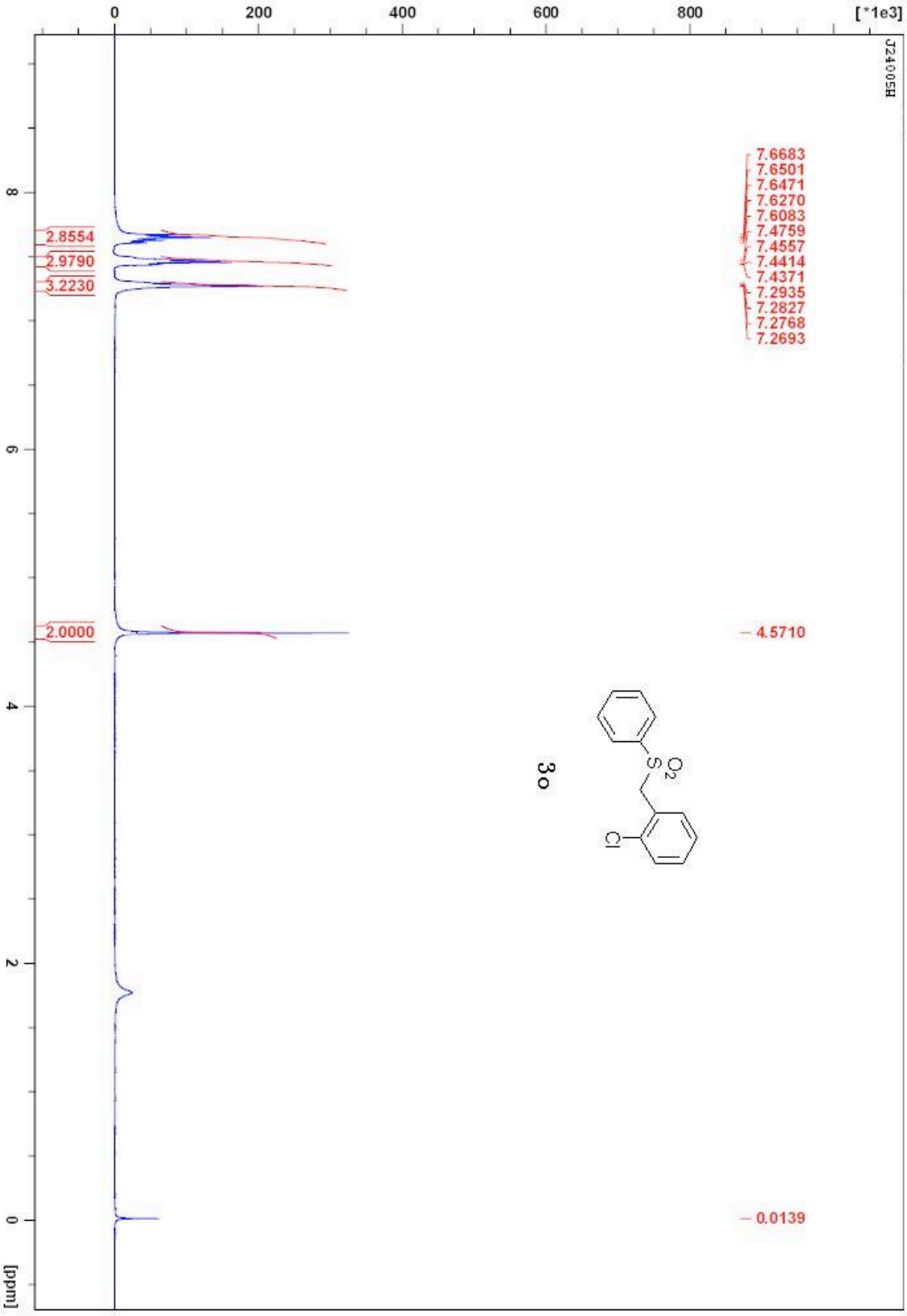
60.0193
19.2763
3n
O2
S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7.6083
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7.4557
7.4414
7.4371
7.2935
7.2827
7.2768
7.2693
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0.0139
2.8554
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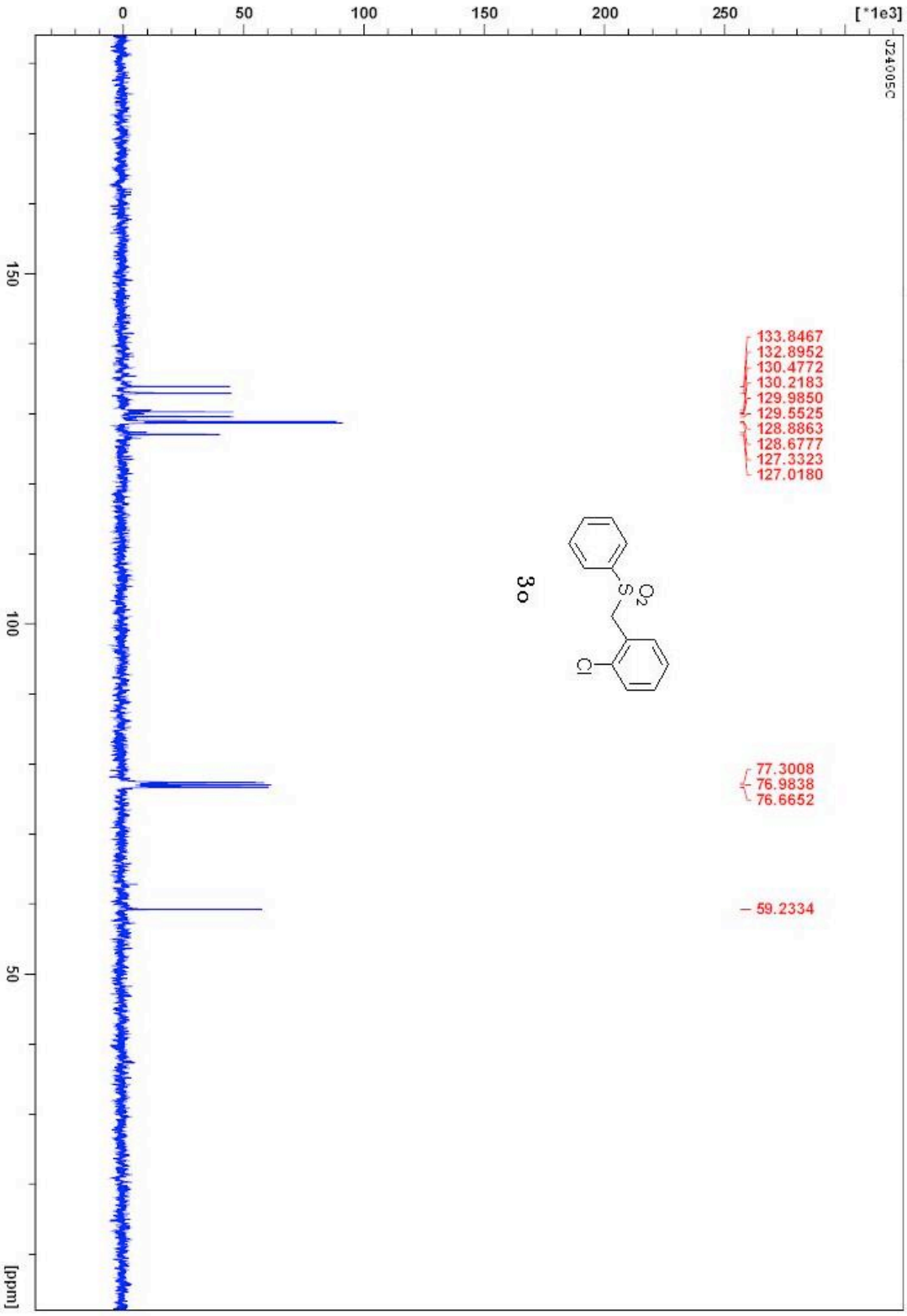
3.2230
2.0000
3o
O2
S
Cl
[*1e3]
[ppm]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200
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100
50
[ppm]
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130.2183
129.9850
129.5525
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127.3323
127.0180
77.3008
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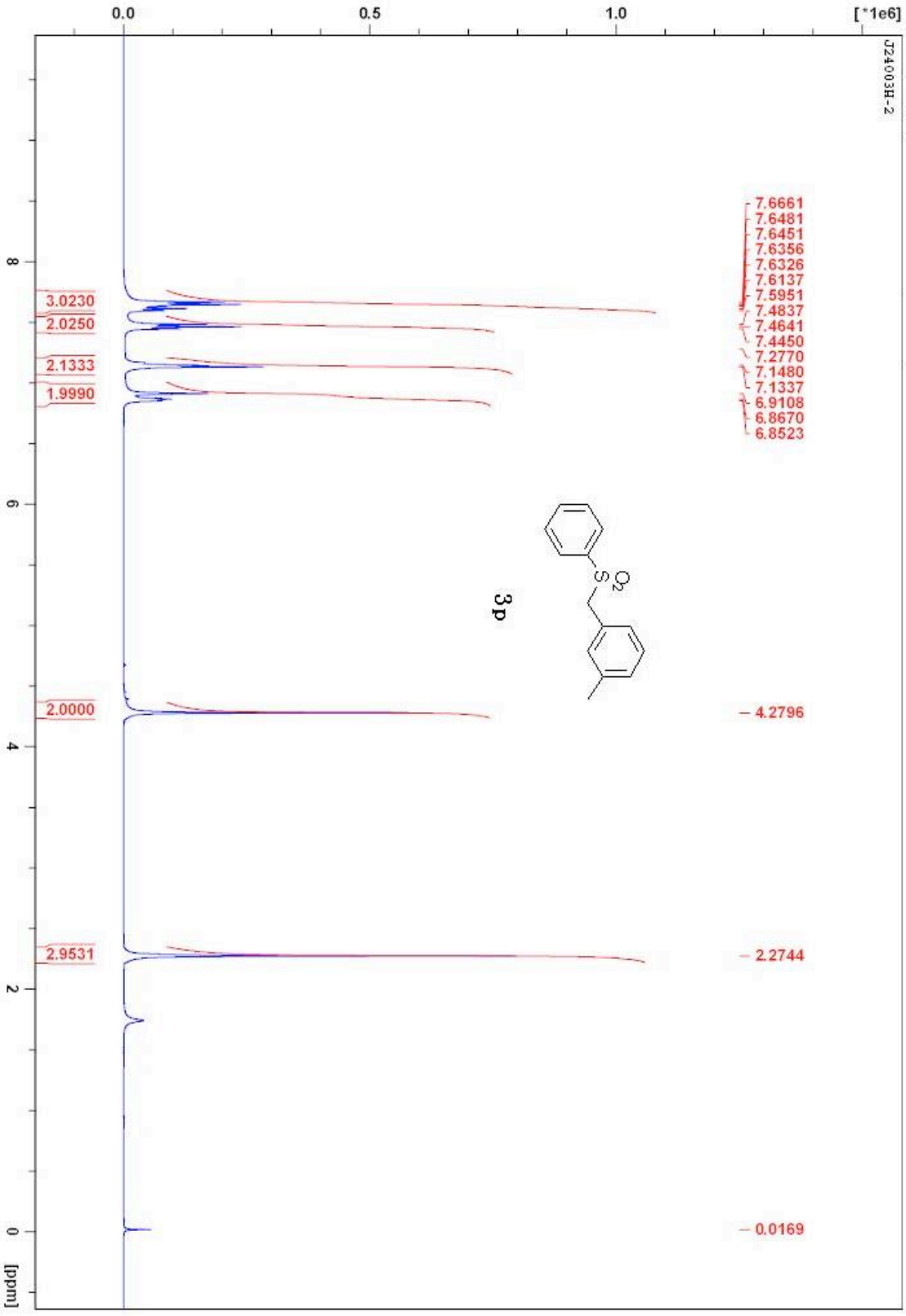
76.6652
59.2334
3o
O2
S
Cl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7.6137
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7.4837
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7.1337
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6.8523
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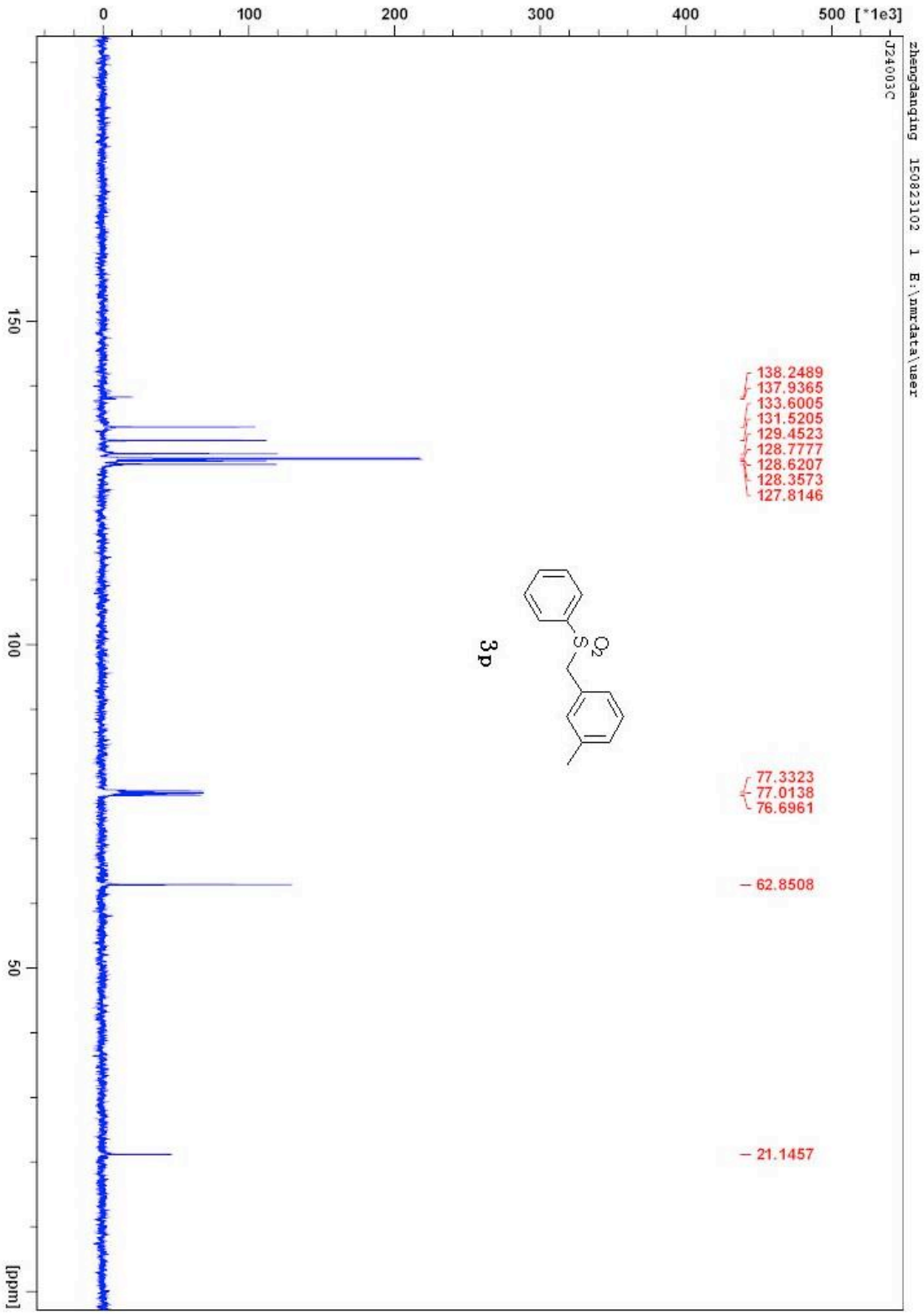
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O2
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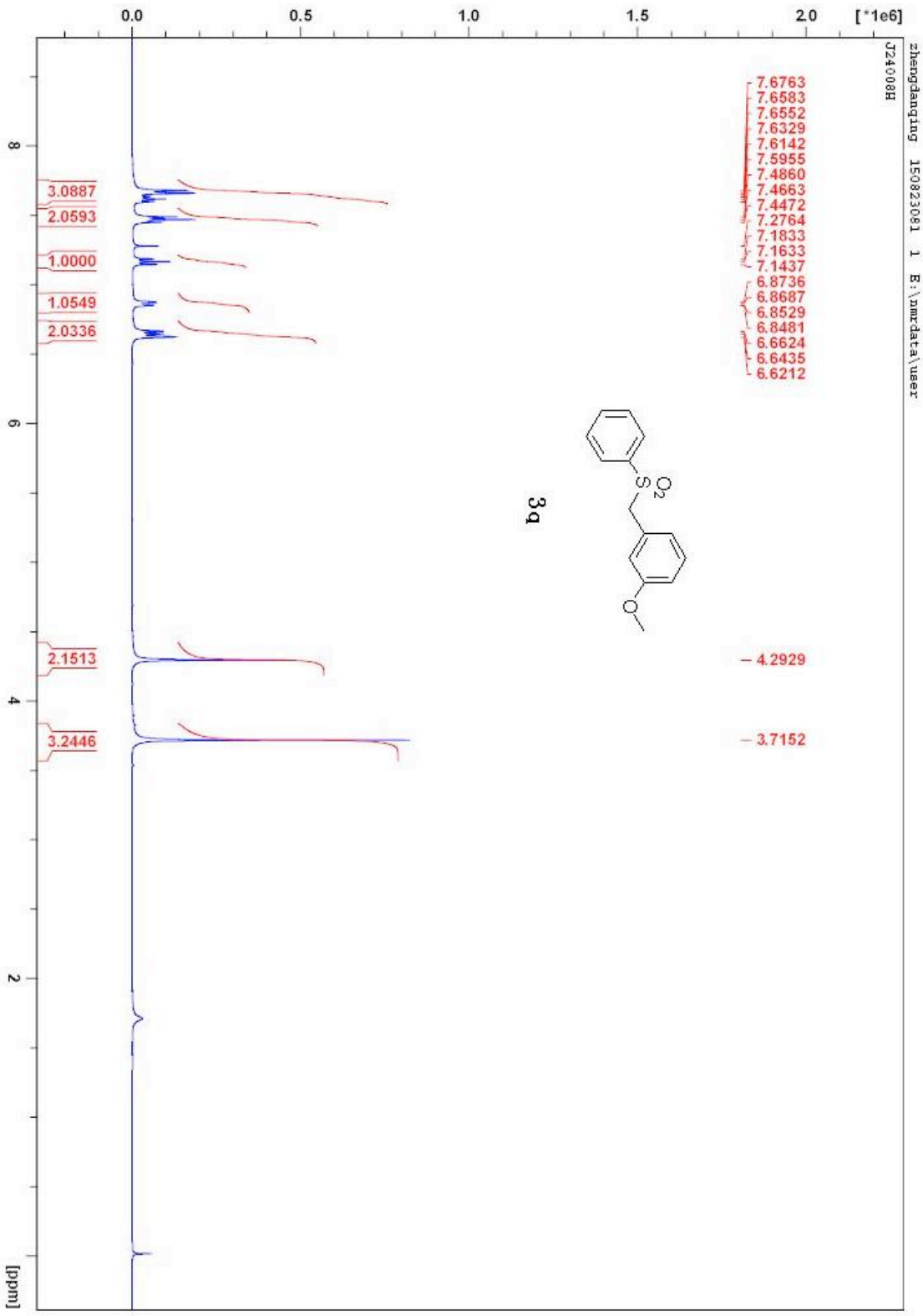
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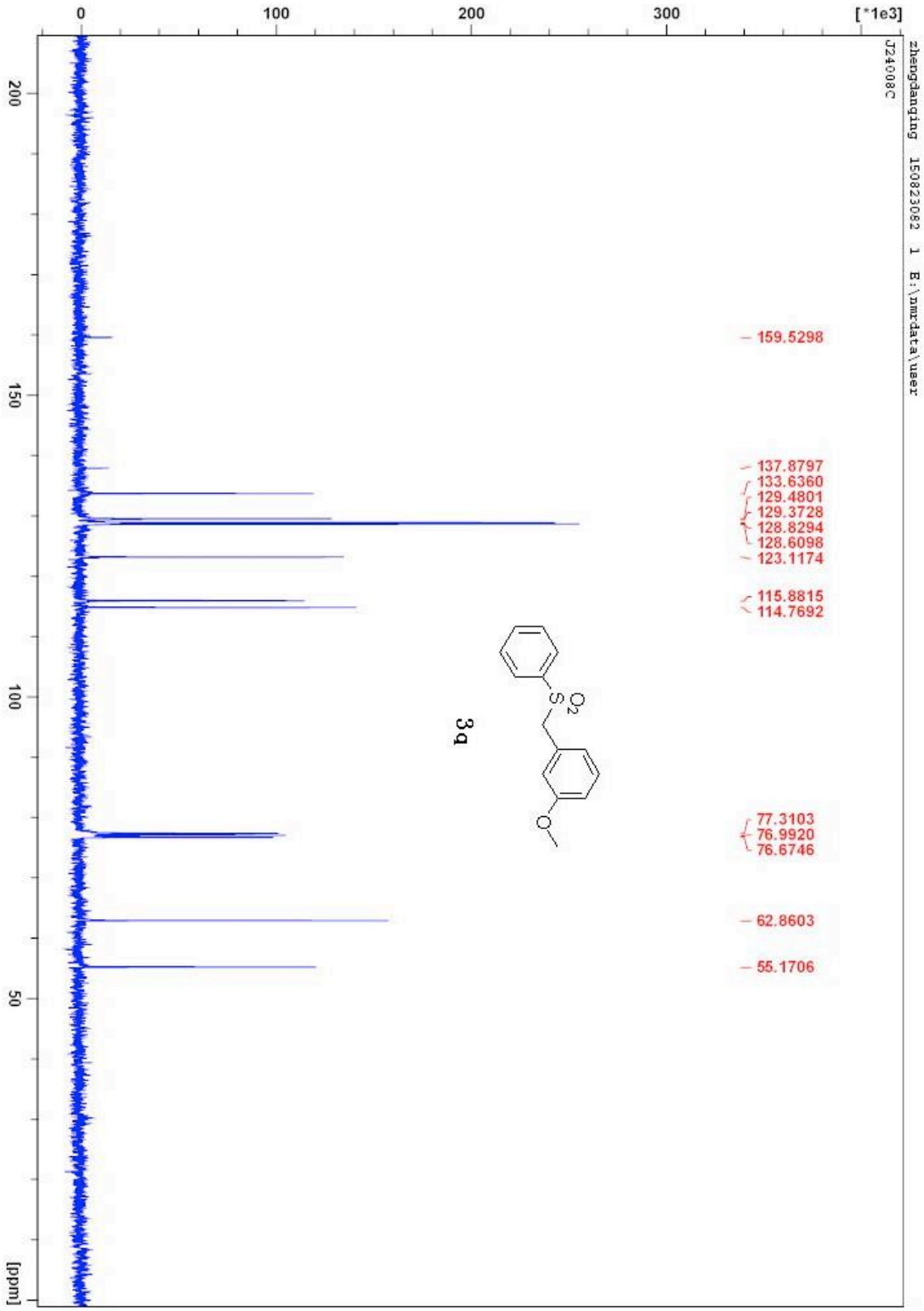
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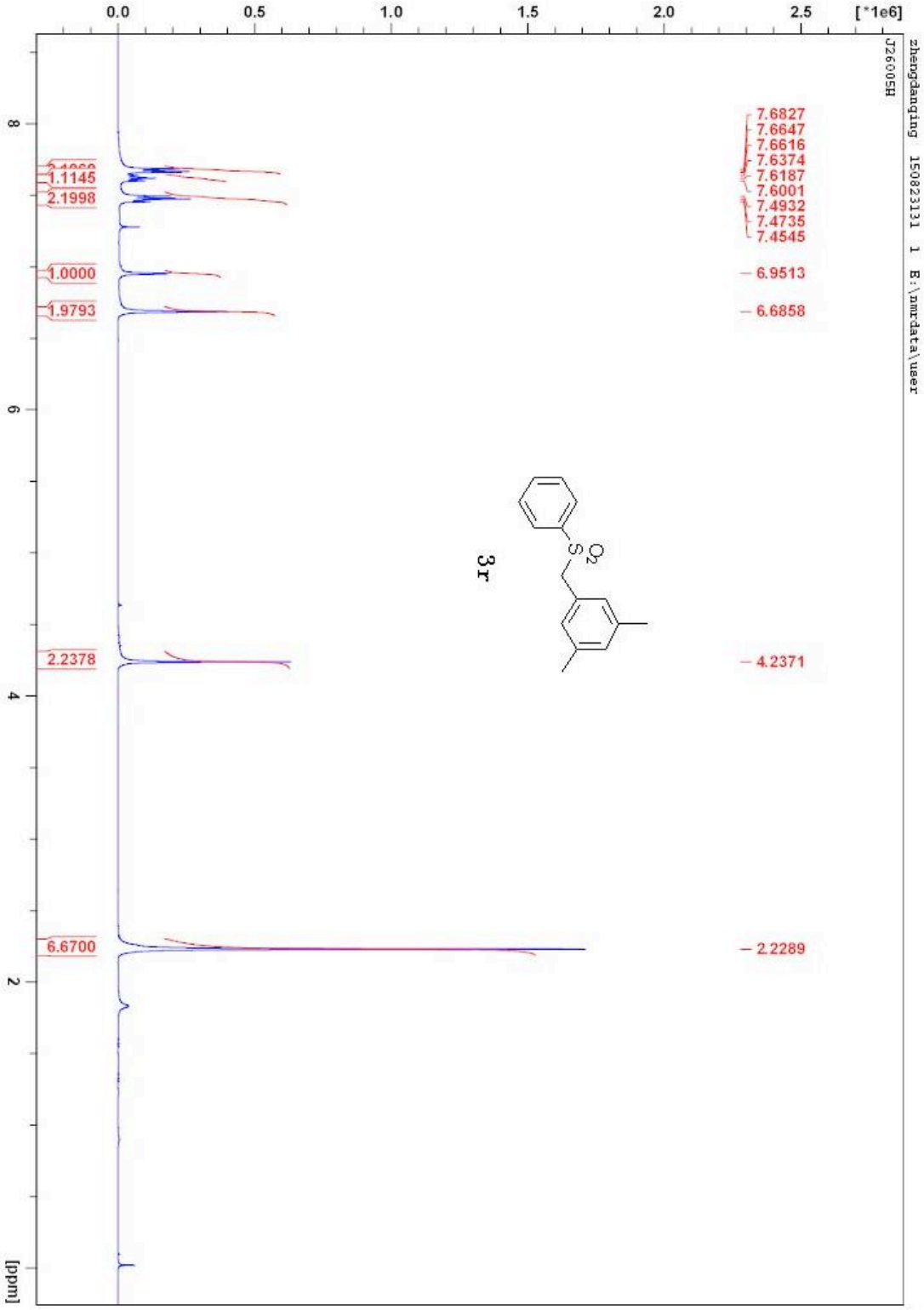
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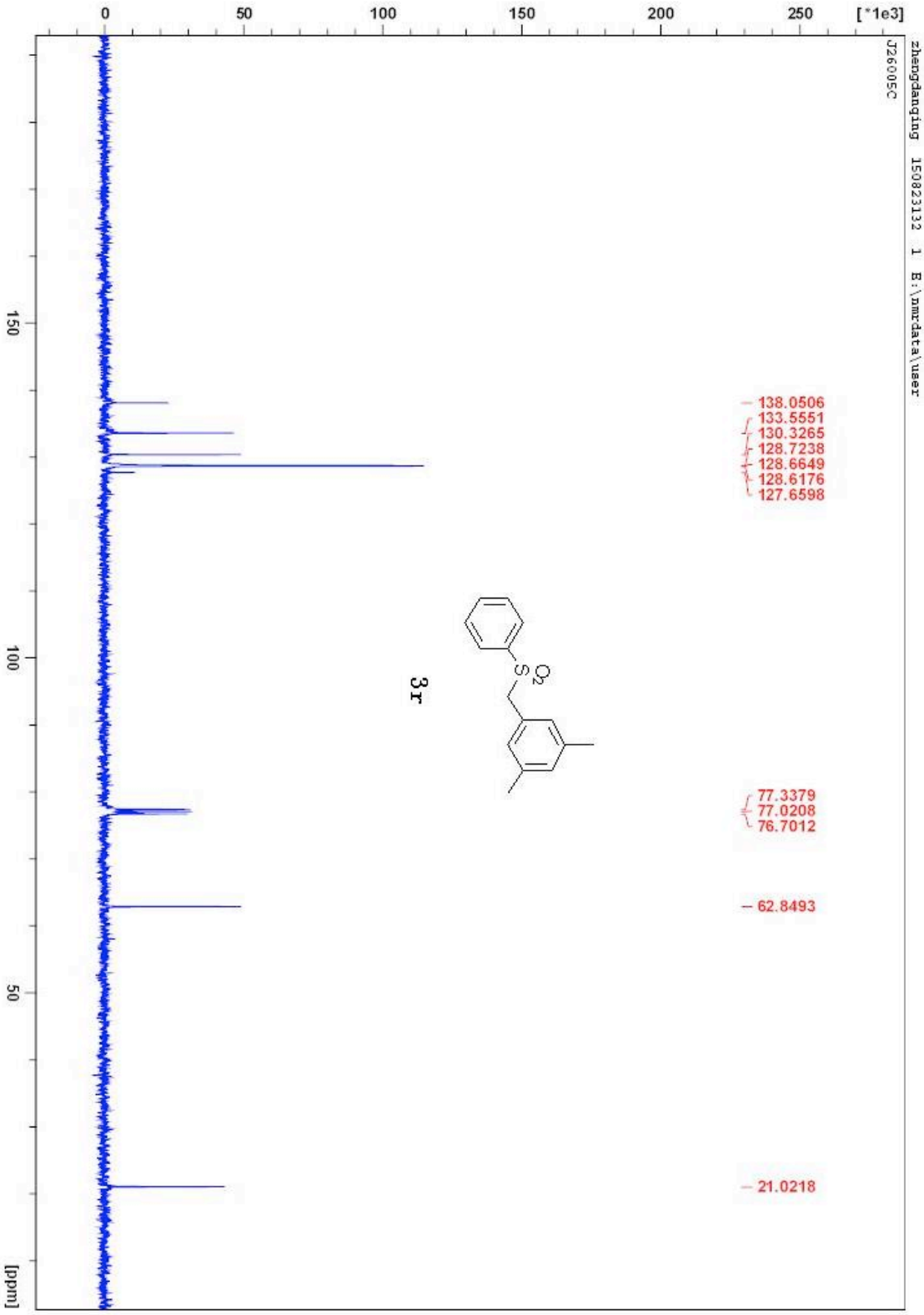
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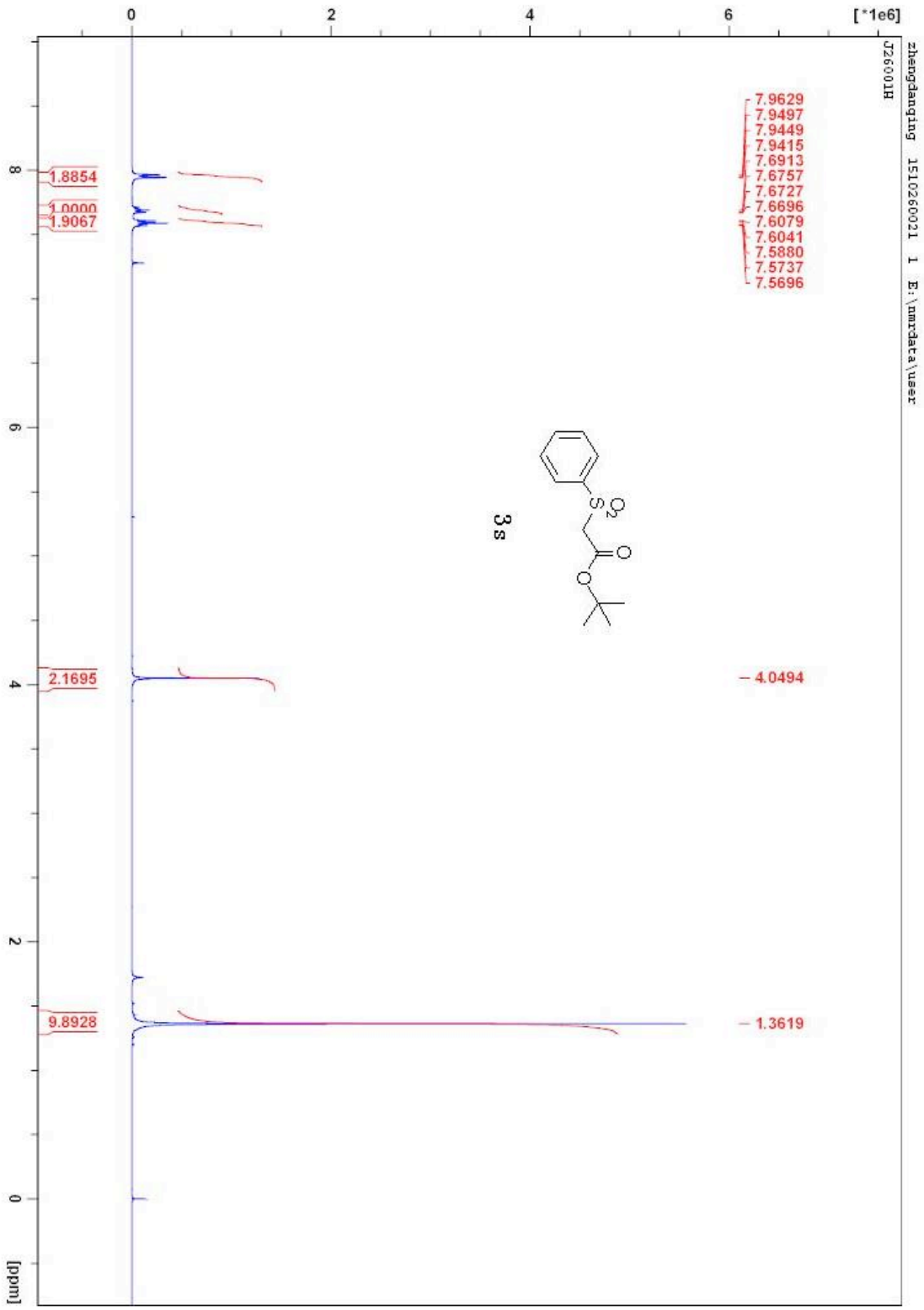
O2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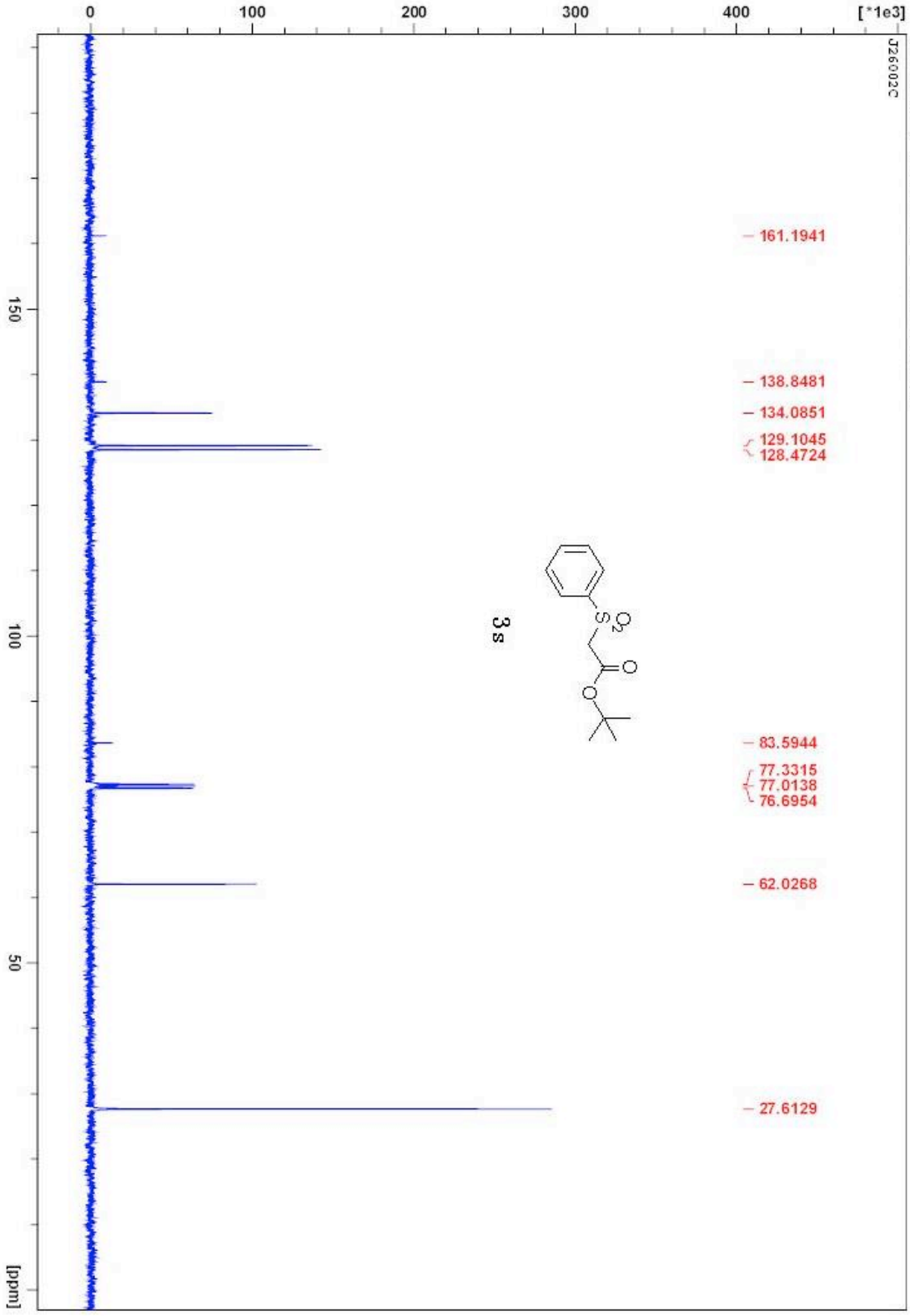
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O2
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O
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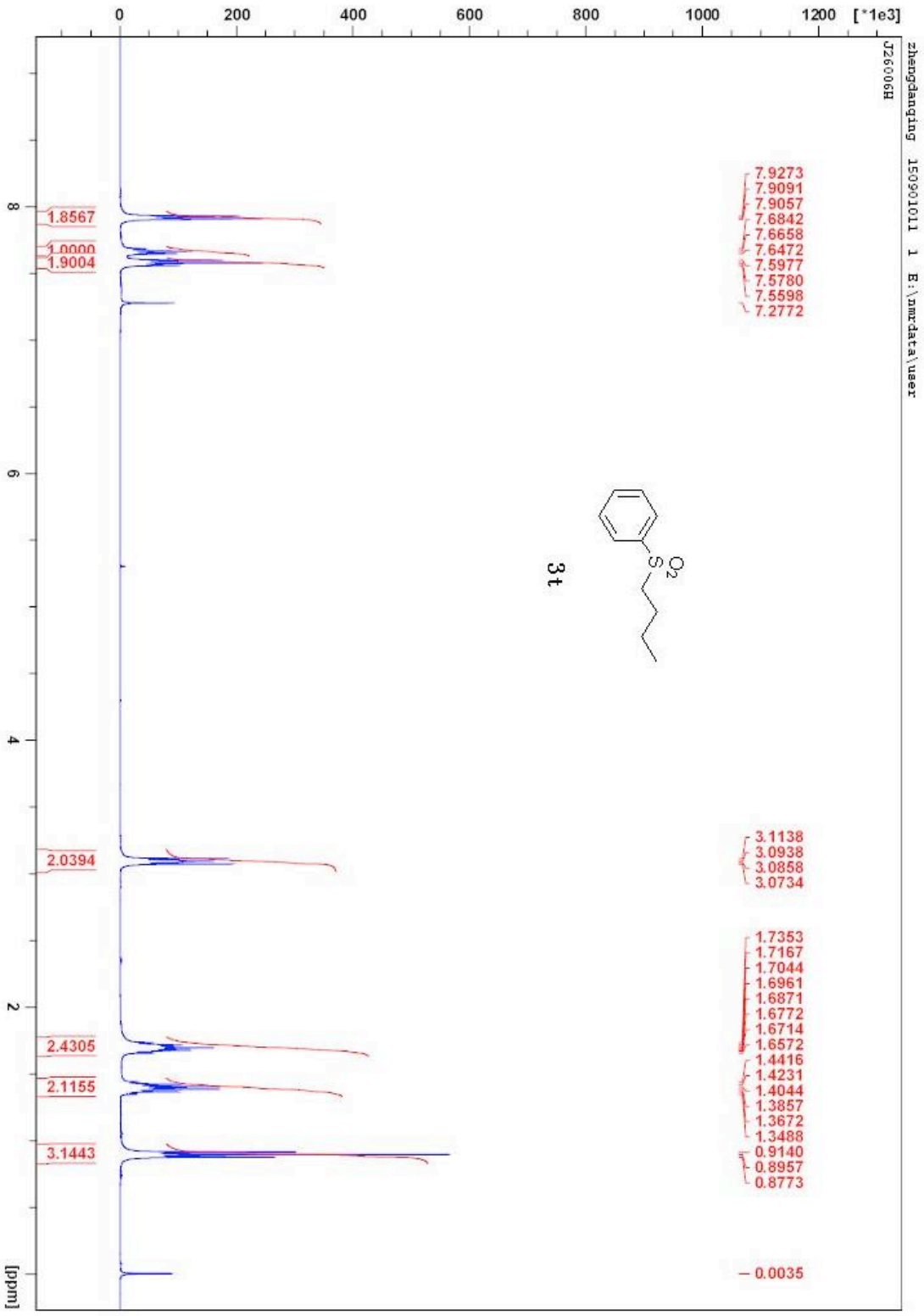
J26002C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1.7167
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O2
S
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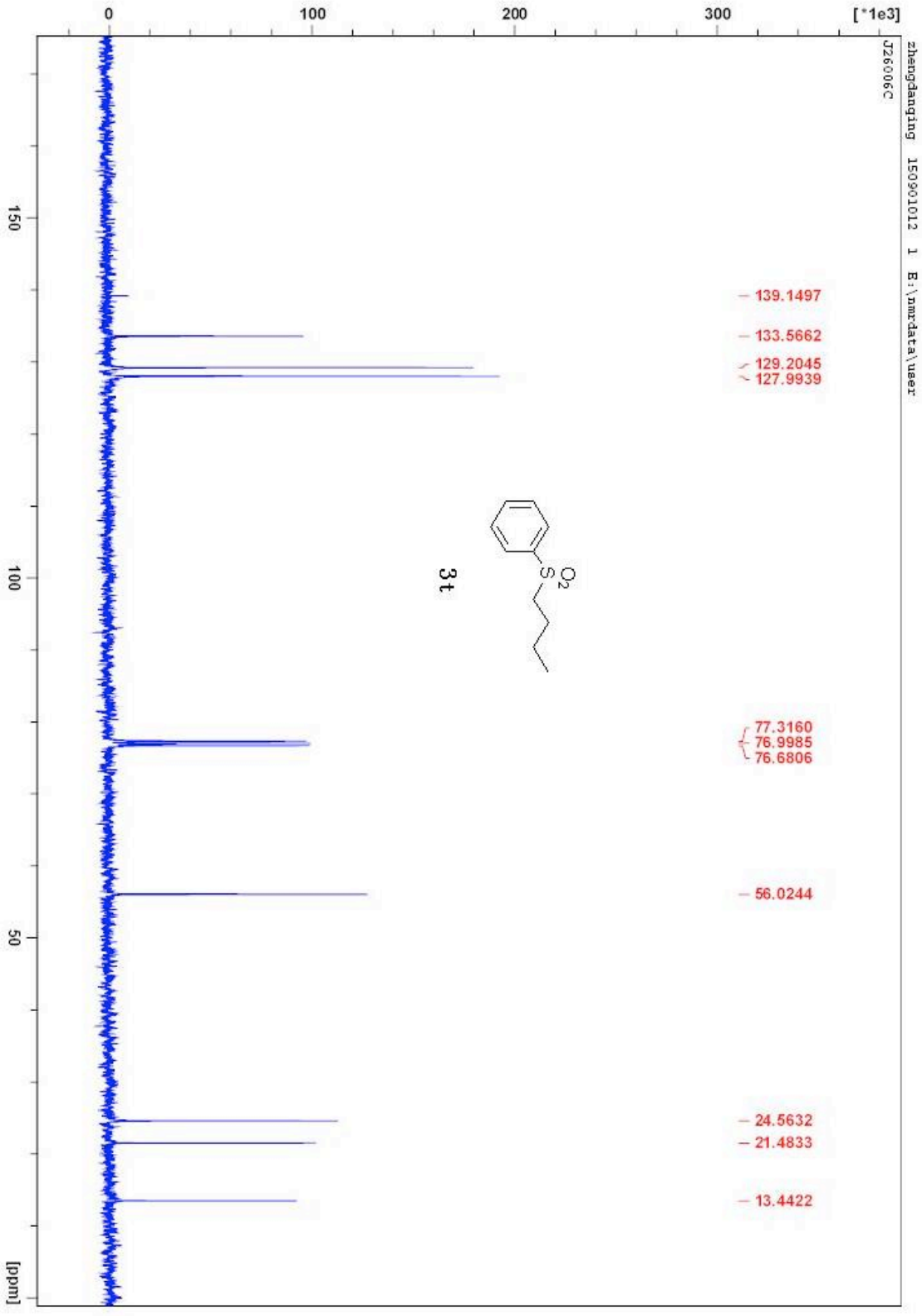
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O2
S