Electronic Supporting Information for:

Role of Imine Isomerization in the Stereocontrol of the Staudinger Reaction between Ketenes and Imines

Fernando P. Cossío,*[a,b] Abel de Cózar,[a,b,c] Miguel A. Sierra,*[b,d] Luis Casarrubios,[b,d] Jaime G. Muntaner,[b,d] Bimal K. Banik,*[e,f] and Debasish Bandyopadhyay[f]

a: Kimika Fakultatea , Kimika Organikoa I Saila, Universidad del País Vasco - Euskal Herriko Unibertsitaea, P. K. 1071, 28080 San Sebastián-Donostia, Spain and Donostia International Physics Centre (DIPC) P.O. Box 1072, 20018 San Sebastián-Donostia, Spain. Email: fp.cossio@ehu.es

b: Centro de Innovación en Química Avanzada (ORFEO–CINQA).

c: IKERBASQUE, Basque foundation for Science, 48011 Bilbao.

d: Departamento de Química Orgánica, Facultad de Ciencias Químicas, Universidad Complutense, 28040 Madrid, Spain. Email: sierraor@quim.ucm.es

e: Department of Mathematics and Natural Sciences, College of Sciences and Human Studies, Deanship of Research, Prince Mohammad Bin Fahd University, Al Khobar, Kingdom of Saudi Arabia. Email: bimalbanik10@gmail.com; bbanik@pmu.edu.sa

f: Department of Chemistry, The University of Texas-Pan American, 1201 West University Drive, Edinburg, Texas 78541, USA

Table of Contents

Computational data:

Table S1. Total electronic energies (E, in a.u.),[a,b] zero point correction of the energy (ZPCE),[c,d,e] thermal corrections to Gibbs free energies (TCGFE, in a.u.),[c,d,e] and number of imaginary frequencies (NIMAG)[a,b,f] of all stationary points discussed in the main text.

Structure	E	ZPCE	T□□□□	NIMAG(ν)
1a	-267.103330[a]	0.059255[b]	0.041870[b]	0 [a]
(*E*)**-2a**	-710.357520[a]	0.225007[b]	0.200577[b]	0 [a]
TSia	-710.325126[a]	0.223434[b]	0.199103[b]	1 (-225.8514)v
(*Z*)**-2a**	-710.349818[a]	0.225218[b]	0.200773[b]	0 [a]
(*E*)**-TS1aa**	-977.458477[a]	0.286034[b]	0.256071[b]	1 (-178.1595) [a]
(*E*)**-INTaa**	-977.470185[a]	0.288463[b]	0.260263[b]	0 [a]
cis-**TS2aa**	-977.459726[a]	0.287172[b]	0.258830[b]	1 (-211.6957) [a]
cis-**3aa**	-977.533952[a]	0.290182[b]	0.261521[b]	0 [a]
(*Z*)**-TS1aa**	-977.457404[a]	0.285691[b]	0.255594[b]	1 (-128.8489) [a]
(*Z*)**-INTaa**	-977.470078[a]	0.288087[b]	0.259217[b]	0 [a]
trans-**TS2aa**	-977.465736[a]	0.287657[b]	0.259942[b]	1 (-103.2789) [a]
trans-**3aa**	-977.534606[a]	0.290166[b]	0.261681[b]	0 [a]
TSRaa	-977.432212[a]	0.286053[b]	0.258339[b]	1 (-304.7075) [a]
1b	-380.471913[a]	0.067668[b] (0.075788)[c]	0.047357 [b] (0.041829)[c]	0 [a]
(*E*)**-2b**	-674.651920[a]	0.256509 [b] (0.28729)[c]	0.230152 [b] (0.241771)[c]	0 [a]
TSib	-674.622365[a]	0.255021 [b] (0.285623)[c]	0.228925 [b] (0.240619)[c]	1 (-244.8487) [a]
(*Z*)**-2b**	-674.648294[a]	0.256899 [b] (0.287727)[c]	0.230902 [b] (0.242849)[c]	0 [a]
(*E*)**-TS1bb**	-1055.127054[a]	0.325903 [b] (0.365012)[c]	0.29308 [b] (0.30729)[c]	1 (-157.2223) [a]
(*E*)**-INTbb**	-1055.142849[a]	0.328674 [b] (0.368115)[c]	0.296651 [b] (0.311821)[c]	0 [a]
cis-**TS2bb**	-1055.122549[a]	0.328032 [b] (0.367395)[c]	0.297082 [b] (0.313003)[c]	1 (-290.7745) [a]
cis-**3bb**	-1055.196610[a]	0.331312 [b] (0.371069)[c]	0.307643 [b] (0.318382)[c]	0 [a]
(*Z*)**-TS1bb**	-1055.128185[a]	0.325785 [b] (0.364879)[c]	0.291819 [b] (0.305362)[c]	1 (-105.4477) [a]
(*Z*)**-INTbb**	-1055.144473[a]	0.328542 [b] (0.367967)[c]	0.296130 [b] (0.311000)[c]	0 [a]
trans-**TS2bb**	-1055.131497 [a]	0.32827 [b] (0.367662)[c]	0.297404 [b] (0.313426)[c]	1 (-186.0801) [a]
trans-**3bb**	-1055.199283[a]	0.331221 [b] (0.370967)[c]	0.307119 [b] (0.317436)[c]	0 [a]
TSRbb	-1055.084226[a]	0.326291 [b] (0.365446) [c]	0.295634 [b] (0.311610) [c]	1 (-42.5178)
1b	-380.471913[a] (-380.469658)[d]	0.075788 [c] (0.067819)[e]	0.041829 [c] (0.020875)[e]	0 [a,d]

(*E*)-**2c**	-878.064930[a] (-878.058848)[d]	0.271365[c] (0.242354)[e]	0.225487[c] (0.174179)[e]	0 [a,d]
TSic	-878.035307[a] (-878.030289)[d]	0.269716[c] (0.240859)[e]	0.224412[c] (0.173493)[e]	1 (-232.8344) [a] [-226.7432][d]
(*Z*)-**2c**	-878.063451[a] (-878.058442)[d]	0.271073[c] (0.242188)[e]	0.225498[c] (0.174477)[e]	0 [a,d]
(*E*)-**TS1bc**	-1258.538534[a] (-1258.528945)[d]	0.348954[c] (0.312013)[e]	0.290078[c] (0.223688)[e]	1 (-126.9503) [a] [-137.5918][d]
(*E*)-**INTbc**	-1258.547330[a] (-1258.535082)[d]	0.350752[c] (0.313293)[e]	0.293774[c] (0.226831)[e]	0 [a,d]
cis-**TS2bc**	-1258.549177 [a] (-1258.537735)[d]	0.350471[c] (0.313106)[e]	0.295229[c] (0.229263)[e]	1 (-23.7532)[a] [-20.3631][d]
cis-**3bc**	-1258.618993[a] (-1258.611394)[d]	0.353526[c] (0.315894)[e]	0.298734[c] (0.232925)[e]	0[a,d]
(*Z*)-**TS1bc**	-1258.537572[a] (-1258.530072)[d]	0.348516[c] (0.311617)[e]	0.289129 [c] (0.222784)[e]	1 (-136.1195) [a] [-122.2316][d]
(*Z*)-**INTbc**	-1258.549099[a] (-1258.537919)[d]	0.351108[c] (0.313424)[e]	0.295866[c] (0.227959)[e]	0[a,d]
trans-**TS2bc**	-1258.541983[a] (-1258.532623)[d]	0.350156[c] (0.312865)[e]	0.294627[c] (0.228413)[e]	1 (-121.6154)[a] [-94.9696][d]
trans-**3bc**	-1258.620975[a] (-1258.613522)[d]	0.353616[c] (0.315853)[e]	0.298555 [c] (0.231923)[e]	0[a,d]
TSRbc	-1258.530751[a] (-1258.523270)[e]	0.348907[c] (0.311835)[e]	0.293033 [c] (0.227181) [e]	1 (-42.1715) [a] [-38.7404][d]

[a] Computed at M06-2X(PCM, solvent=CH_2Cl_2)/def-TZVPP level. [b]Computed at 195.15 K at M06-2X(PCM, solvent=CH_2Cl_2)/def-TZVPP level. [c] Computed at 298.15 K at M06-2X(PCM, solvent=CH_2Cl_2)/def-TZVPP level. [d] Computed at M06-2X(PCM, solvent=toluene)/def-TZVPP level. [e] Computed at 384.15 K at M06-2X(PCM, solvent=toluene)/def-TZVPP level. [f]If NIMAG=1, the corresponding imaginary frequency ν (in parentheses) is given in cm^{-1}.

Cartesian coordinates of all stationary points discussed in the main text

Cartesian coordinates (optimized at the M06-2X(PCM, solvent=CH_2Cl_2)/def-TZVPP level) of all the stationary points collected in the main text associated with the reaction of **1a** and **2a**.

1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.790554	-0.717870	0.422377
2	6	0	1.985804	-0.403781	-0.237165
3	1	0	1.591145	-1.264896	-0.779079
4	8	0	0.979108	0.171476	0.588143
5	6	0	-0.082507	0.663136	-0.135598
6	6	0	-1.259161	0.075299	-0.071550
7	8	0	-2.308914	-0.408847	0.003127
8	1	0	0.029767	1.542319	-0.756107
9	1	0	2.362157	0.331492	-0.951474

(*E*)-2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.724166	0.643127	0.293702
2	6	0	-3.314417	0.679134	0.173555
3	6	0	-2.621834	-0.501738	-0.198585
4	6	0	-3.366133	-1.682684	-0.443993
5	6	0	-4.727572	-1.688192	-0.318139
6	6	0	-5.416081	-0.512213	0.055466
7	6	0	-2.568229	1.864336	0.399598
8	6	0	-1.212162	1.874539	0.264551
9	6	0	-0.512370	0.687298	-0.076371
10	6	0	-1.211245	-0.470206	-0.314393
11	7	0	0.884684	0.777229	-0.210480
12	6	0	1.609892	-0.148781	0.264827
13	6	0	3.071693	-0.168835	0.123120
14	6	0	3.789940	-1.213849	0.699943
15	6	0	5.172485	-1.263012	0.585443
16	6	0	5.843007	-0.264778	-0.107037
17	6	0	5.130383	0.782519	-0.686031
18	6	0	3.752376	0.831737	-0.573482
19	1	0	1.172142	-0.983478	0.823081
20	1	0	3.260505	-1.989514	1.239723
21	1	0	5.723912	-2.077112	1.035478
22	1	0	6.920322	-0.299697	-0.197894
23	1	0	5.655786	1.558882	-1.225553
24	1	0	3.186407	1.638683	-1.018389
25	1	0	-3.096592	2.768833	0.674075
26	1	0	-0.640494	2.779076	0.422598
27	1	0	-2.836360	-2.582509	-0.730977
28	1	0	-5.285239	-2.595940	-0.505696
29	1	0	-6.493327	-0.530712	0.150385
30	1	0	-5.245404	1.548930	0.577855
31	1	0	-0.687840	-1.366479	-0.624363

TSia

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.160109	0.168707	-0.416743
2	6	0	-2.025163	0.713787	-1.199823
3	7	0	-0.837625	0.663956	-0.850450
4	6	0	1.274365	-0.438367	-0.806755
5	6	0	-4.449609	0.285721	-0.925069

6	6	0	-5.528899	-0.216471	-0.210689
7	6	0	-5.317007	-0.836135	1.013106
8	6	0	-4.027122	-0.954911	1.524601
9	6	0	-2.951294	-0.454211	0.812556
10	6	0	0.438920	0.614156	-0.466952
11	6	0	0.959640	1.687656	0.327130
12	6	0	2.255210	1.673282	0.740334
13	6	0	3.130796	0.607913	0.407072
14	6	0	2.618711	-0.458162	-0.379199
15	6	0	3.494162	-1.525067	-0.713346
16	6	0	4.794529	-1.525789	-0.289259
17	6	0	5.299340	-0.462886	0.492907
18	6	0	4.478791	0.579366	0.830389
19	1	0	-2.312295	1.185160	-2.151638
20	1	0	-4.604369	0.770943	-1.881315
21	1	0	-6.530909	-0.124761	-0.606810
22	1	0	-6.156033	-1.228245	1.572003
23	1	0	-3.866850	-1.438584	2.478541
24	1	0	-1.942526	-0.538939	1.196837
25	1	0	0.299169	2.503320	0.586586
26	1	0	2.634601	2.492335	1.339407
27	1	0	3.112768	-2.342538	-1.312823
28	1	0	5.446200	-2.348206	-0.554174
29	1	0	6.329769	-0.477652	0.820600
30	1	0	4.851507	1.401785	1.429375
31	1	0	0.890778	-1.253845	-1.405010

(*Z*)-2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.772067	-0.268911	0.855791
2	6	0	-2.567777	0.371481	0.476548
3	6	0	-1.831568	-0.134385	-0.626063
4	6	0	-2.327611	-1.270218	-1.314519
5	6	0	-3.492698	-1.869278	-0.923929
6	6	0	-4.225558	-1.363895	0.173860
7	6	0	-2.073440	1.512944	1.157016
8	6	0	-0.913445	2.115782	0.767515
9	6	0	-0.160278	1.588609	-0.312832
10	6	0	-0.622180	0.496398	-1.000581
11	7	0	1.005499	2.269526	-0.708751
12	6	0	2.157057	1.742120	-0.669264
13	6	0	2.590671	0.428138	-0.137674
14	6	0	3.725306	-0.147211	-0.708989
15	6	0	4.202124	-1.369976	-0.259592
16	6	0	3.564776	-2.014328	0.791424
17	6	0	2.453064	-1.431588	1.390211
18	6	0	1.962679	-0.221169	0.927506
19	1	0	2.967527	2.337784	-1.090408
20	1	0	4.232439	0.368128	-1.515540
21	1	0	5.074320	-1.812277	-0.721174
22	1	0	3.938288	-2.963144	1.152222
23	1	0	1.966941	-1.922930	2.221990
24	1	0	1.101677	0.223905	1.405359
25	1	0	-2.638577	1.908237	1.991968
26	1	0	-0.541930	2.994195	1.278103
27	1	0	-1.764925	-1.656246	-2.155331
28	1	0	-3.860398	-2.736253	-1.456363
29	1	0	-5.146254	-1.847545	0.470807
30	1	0	-4.327854	0.125527	1.697596
31	1	0	-0.054079	0.106855	-1.836540

(*E*)-TS1aa

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.792838	-1.682862	0.420276
2	6	0	-3.420606	-1.343604	0.329464

3	6	0	-3.039159	-0.205418	-0.426899
4	6	0	-4.044104	0.558171	-1.073186
5	6	0	-5.359653	0.205027	-0.969633
6	6	0	-5.739272	-0.928683	-0.214320
7	6	0	-1.671832	0.142098	-0.515448
8	6	0	-0.718607	-0.623582	0.102114
9	6	0	-1.098509	-1.751770	0.871963
10	6	0	-2.414052	-2.098138	0.979365
11	7	0	0.651891	-0.257343	0.001415
12	6	0	1.508913	-1.173580	-0.225350
13	6	0	2.964802	-1.044401	-0.280790
14	6	0	3.683515	-2.226602	-0.477564
15	6	0	5.068105	-2.211571	-0.529365
16	6	0	5.747801	-1.009815	-0.387972
17	6	0	5.040242	0.172905	-0.196984
18	6	0	3.657390	0.161859	-0.143130
19	6	0	0.911890	1.534130	0.876221
20	8	0	0.999364	1.319961	2.035309
21	6	0	0.891045	2.346182	-0.184724
22	8	0	0.974999	3.706694	0.044617
23	6	0	-0.281931	4.357518	-0.059647
24	1	0	-0.714495	4.204817	-1.052017
25	1	0	-0.111298	5.419705	0.102132
26	1	0	-0.975522	3.976276	0.693508
27	1	0	0.815147	1.980857	-1.195655
28	1	0	1.143154	-2.187594	-0.400112
29	1	0	3.148995	-3.162017	-0.586691
30	1	0	5.613568	-3.132737	-0.679735
31	1	0	6.828541	-0.991722	-0.428358
32	1	0	5.571507	1.108752	-0.091281
33	1	0	3.115257	1.085669	-0.009407
34	1	0	-1.379605	1.013580	-1.085112
35	1	0	-6.119595	0.793523	-1.465667
36	1	0	-3.749380	1.426518	-1.648919
37	1	0	-6.784971	-1.195075	-0.141398
38	1	0	-5.077357	-2.551136	1.001323
39	1	0	-0.337161	-2.315683	1.394287
40	1	0	-2.703777	-2.952749	1.577437

(*E*)-INTaa

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.009619	-1.228521	-0.684272
2	6	0	-3.625828	-0.971404	-0.525643
3	6	0	-3.209133	-0.012099	0.434215
4	6	0	-4.187728	0.657676	1.211330
5	6	0	-5.514584	0.385340	1.037613
6	6	0	-5.930275	-0.567834	0.078907
7	6	0	-2.645708	-1.635155	-1.302283
8	6	0	-1.317524	-1.371092	-1.130437
9	6	0	-0.914766	-0.422572	-0.163971
10	6	0	-1.831149	0.252684	0.593828
11	7	0	0.482284	-0.163581	0.026654
12	6	0	0.911567	1.275512	0.321625
13	6	0	0.507574	2.107390	-0.670512
14	8	0	0.802598	3.449861	-0.650438
15	6	0	2.192149	3.738766	-0.641327
16	6	0	1.304208	-1.159028	0.095373
17	6	0	2.749878	-1.139651	0.136977
18	6	0	3.363377	-2.361821	0.445547
19	6	0	4.741257	-2.472151	0.474721
20	6	0	5.523492	-1.366747	0.163658
21	6	0	4.925650	-0.157577	-0.175052
22	6	0	3.547943	-0.031418	-0.180533
23	8	0	1.581073	1.432875	1.358775
24	1	0	-5.323276	-1.958377	-1.419756
25	1	0	-3.863434	1.387552	1.941913
26	1	0	-6.256115	0.900057	1.633204
27	1	0	-6.985057	-0.771022	-0.046863
28	1	0	-2.964301	-2.348890	-2.050798
29	1	0	-0.572728	-1.856873	-1.746093
30	1	0	-0.132095	1.776842	-1.476153

31	1	0	2.673402	3.306069	0.237294
32	1	0	2.293151	4.821580	-0.619564
33	1	0	2.666777	3.347496	-1.545721
34	1	0	0.846162	-2.142605	0.099686
35	1	0	2.746923	-3.224073	0.665916
36	1	0	5.203848	-3.415508	0.728003
37	1	0	6.602010	-1.448366	0.177921
38	1	0	5.539708	0.695147	-0.429291
39	1	0	3.098200	0.911978	-0.445806
40	1	0	-1.503207	0.980380	1.324238

cis-TS2aa

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.362749	-1.684050	-0.369696
2	6	0	1.001765	-0.345966	-0.086651
3	6	0	1.959812	0.605182	0.146495
4	6	0	3.327034	0.259841	0.101130
5	6	0	3.699004	-1.075609	-0.207162
6	6	0	2.681105	-2.030881	-0.440025
7	6	0	5.073514	-1.413692	-0.260335
8	6	0	6.031666	-0.469463	-0.022127
9	6	0	5.661944	0.861643	0.282746
10	6	0	4.345099	1.217936	0.342890
11	7	0	-0.369215	-0.001707	-0.044809
12	6	0	-1.321377	-0.608977	-0.758953
13	6	0	-2.643430	-0.964567	-0.267285
14	6	0	-2.978120	-0.930810	1.095316
15	6	0	-4.232547	-1.338218	1.509218
16	6	0	-5.172860	-1.789763	0.586228
17	6	0	-4.842251	-1.842726	-0.761050
18	6	0	-3.585576	-1.440285	-1.184839
19	6	0	-0.871235	1.190431	0.586153
20	8	0	-0.705147	1.458121	1.779392
21	6	0	-1.598556	1.864271	-0.406788
22	8	0	-2.366284	2.900491	-0.066154
23	6	0	-2.661257	3.812064	-1.117336
24	1	0	-1.394914	1.699144	-1.456813
25	1	0	-1.007008	-1.067258	-1.694309
26	1	0	-2.251690	-0.590066	1.821240
27	1	0	-4.479190	-1.313018	2.562080
28	1	0	-6.150978	-2.108168	0.919658
29	1	0	-5.562388	-2.201693	-1.483791
30	1	0	-3.328416	-1.483272	-2.235829
31	1	0	0.588606	-2.427221	-0.505710
32	1	0	2.961978	-3.053486	-0.656789
33	1	0	5.349615	-2.434588	-0.492582
34	1	0	7.079132	-0.735275	-0.064896
35	1	0	6.431438	1.598307	0.469893
36	1	0	4.058051	2.234984	0.577687
37	1	0	1.671577	1.625690	0.363568
38	1	0	-1.748152	4.296646	-1.464622
39	1	0	-3.139503	3.290596	-1.947877
40	1	0	-3.341106	4.553559	-0.710721

cis-3aa

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.811811	0.322488	-0.467011
2	6	0	-1.030764	-0.972092	-1.002427
3	6	0	-2.275709	-1.526801	-0.954184
4	6	0	-3.364535	-0.831365	-0.373688
5	6	0	-3.137650	0.462864	0.161968
6	6	0	-1.842163	1.025995	0.106214
7	6	0	-4.226041	1.161034	0.744597
8	6	0	-5.470533	0.598569	0.789935
9	6	0	-5.694986	-0.691166	0.255680

10	6	0	-4.665106	-1.387788	-0.311938
11	1	0	-4.051981	2.148448	1.153257
12	1	0	-6.293161	1.140447	1.236962
13	1	0	-6.685761	-1.122647	0.298795
14	1	0	-4.827876	-2.376208	-0.723451
15	1	0	-2.444047	-2.515276	-1.362380
16	1	0	-0.204657	-1.513848	-1.443134
17	1	0	-1.665116	2.010649	0.514853
18	7	0	0.474457	0.861914	-0.540464
19	6	0	1.010306	2.071778	-0.197503
20	8	0	0.536214	3.046332	0.331417
21	6	0	2.389391	1.664576	-0.746097
22	8	0	3.433760	1.613923	0.165332
23	6	0	3.968814	2.897934	0.444307
24	1	0	4.778290	2.756450	1.154717
25	1	0	4.360030	3.356373	-0.468179
26	1	0	3.210515	3.551713	0.878398
27	1	0	2.662175	2.216566	-1.650974
28	6	0	1.726175	0.283543	-1.047420
29	6	0	2.254892	-0.898017	-0.284758
30	6	0	1.935336	-1.100079	1.054174
31	6	0	2.458477	-2.185830	1.741443
32	6	0	3.308755	-3.076583	1.097890
33	6	0	3.630119	-2.879453	-0.238259
34	6	0	3.100494	-1.796389	-0.926672
35	1	0	1.679881	0.062033	-2.114229
36	1	0	3.343779	-1.648092	-1.971831
37	1	0	4.287549	-3.571547	-0.746960
38	1	0	3.714726	-3.923226	1.634774
39	1	0	2.201423	-2.337368	2.781121
40	1	0	1.272482	-0.409211	1.560026

(*Z*)-TS1aa

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.124510	-2.610048	0.262970
2	6	0	2.023221	-1.854506	-0.140981
3	6	0	0.965462	-2.484921	-0.801066
4	6	0	1.006714	-3.850717	-1.026670
5	6	0	2.092046	-4.601979	-0.588698
6	6	0	3.152721	-3.980595	0.056117
7	6	0	2.078850	-0.401604	0.106981
8	7	0	1.139063	0.440455	0.239089
9	6	0	-0.228768	0.113437	0.330828
10	6	0	-0.681977	-0.784390	1.331451
11	6	0	-2.012877	-1.049866	1.457397
12	6	0	-2.963609	-0.440724	0.599057
13	6	0	-2.509098	0.475770	-0.384126
14	6	0	-1.124810	0.751118	-0.483554
15	6	0	-3.458024	1.097427	-1.233253
16	6	0	-4.790441	0.817602	-1.110521
17	6	0	-5.242530	-0.095991	-0.131768
18	6	0	-4.349580	-0.708365	0.703241
19	6	0	1.420197	2.563384	0.773181
20	6	0	2.431386	2.799037	-0.058889
21	8	0	3.034488	4.042669	0.013563
22	6	0	2.660253	4.898360	-1.055708
23	8	0	0.614238	2.739386	1.603702
24	1	0	2.913388	4.446660	-2.018020
25	1	0	3.213925	5.826577	-0.933119
26	1	0	1.587636	5.102316	-1.028088
27	1	0	2.778218	2.080743	-0.781164
28	1	0	3.086194	0.009050	0.178721
29	1	0	3.958218	-2.117220	0.747481
30	1	0	4.003903	-4.559398	0.386902
31	1	0	2.114273	-5.669473	-0.761243
32	1	0	0.190242	-4.332047	-1.547136
33	1	0	0.121692	-1.908716	-1.152716
34	1	0	-0.769355	1.465177	-1.216541
35	1	0	-5.506931	1.296873	-1.763950
36	1	0	-3.108434	1.798297	-1.980813
37	1	0	-6.299836	-0.306935	-0.045961

38	1	0	-4.689483	-1.407183	1.457409
39	1	0	0.042922	-1.247231	1.987842
40	1	0	-2.361677	-1.731692	2.222730

(*Z*)-INTaa

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.151670	0.462990	0.256615
2	7	0	0.960357	0.935158	0.386185
3	6	0	-1.274813	0.436434	-0.372074
4	6	0	0.758808	2.429942	0.598855
5	6	0	2.562032	-0.890069	-0.092140
6	8	0	0.146369	2.742527	1.632066
7	6	0	1.261937	3.127929	-0.453812
8	6	0	-1.451181	-1.638945	1.495258
9	6	0	-2.461081	-0.331750	-0.308428
10	6	0	-0.232826	0.141378	0.456366
11	6	0	-0.313696	-0.891645	1.415322
12	6	0	-2.549815	-1.388819	0.634217
13	6	0	-3.561520	-0.073061	-1.162002
14	6	0	3.552604	-3.407752	-0.733409
15	6	0	3.864692	-1.251116	0.266363
16	6	0	1.767606	-1.795374	-0.806404
17	6	0	2.268941	-3.043133	-1.127997
18	6	0	4.351551	-2.511204	-0.037014
19	6	0	-4.694594	-0.832466	-1.080539
20	6	0	-4.783839	-1.885191	-0.141869
21	6	0	-3.738080	-2.155859	0.695625
22	8	0	1.176656	4.503211	-0.479636
23	6	0	-0.147404	4.976840	-0.675932
24	1	0	2.941352	1.188052	0.417231
25	1	0	1.711562	2.650498	-1.312761
26	1	0	-1.530961	-2.430526	2.228960
27	1	0	0.523890	-1.071621	2.075321
28	1	0	-3.488274	0.735960	-1.877432
29	1	0	3.933009	-4.389253	-0.981639
30	1	0	4.489098	-0.539196	0.790469
31	1	0	0.773920	-1.520201	-1.127745
32	1	0	1.658394	-3.735737	-1.690023
33	1	0	5.353948	-2.787898	0.257418
34	1	0	-5.531288	-0.629659	-1.735051
35	1	0	-5.688038	-2.476151	-0.088663
36	1	0	-3.803167	-2.959323	1.418238
37	1	0	-0.110605	6.063948	-0.645273
38	1	0	-0.805237	4.609193	0.113449
39	1	0	-0.530192	4.652867	-1.647660
40	1	0	-1.190055	1.252266	-1.079587

***trans*-TS2aa**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.515606	0.991605	0.326494
2	6	0	3.162326	0.591146	0.435512
3	6	0	2.729265	-0.572604	-0.251801
4	6	0	3.664709	-1.299873	-1.029559
5	6	0	4.964676	-0.887837	-1.116808
6	6	0	5.395827	0.270728	-0.431378
7	6	0	2.225970	1.310686	1.219670
8	6	0	0.929360	0.900970	1.315951
9	6	0	0.501696	-0.247775	0.609581
10	6	0	1.376567	-0.970361	-0.152725
11	7	0	-0.851028	-0.668144	0.723000
12	6	0	-1.216058	-2.053760	0.727143
13	6	0	-2.336384	-2.163787	-0.110690
14	8	0	-3.004075	-3.322669	-0.161955
15	6	0	-3.791753	-3.512293	-1.328939
16	6	0	-1.922358	0.125381	0.850697

17	6	0	-2.064059	1.417225	0.211723
18	6	0	-3.021022	2.308106	0.712735
19	6	0	-3.205435	3.545366	0.121055
20	6	0	-2.447011	3.904272	-0.987478
21	6	0	-1.508528	3.018043	-1.506672
22	6	0	-1.315652	1.782177	-0.915448
23	8	0	-0.630667	-2.908014	1.401094
24	1	0	-2.684578	-0.187781	1.546699
25	1	0	-2.535616	-1.427255	-0.877733
26	1	0	2.559316	2.188704	1.757885
27	1	0	0.220601	1.437394	1.932149
28	1	0	3.330900	-2.187980	-1.550901
29	1	0	-2.592272	4.869969	-1.452166
30	1	0	-3.612641	2.021061	1.572836
31	1	0	-0.595242	1.090642	-1.331700
32	1	0	-0.930464	3.291915	-2.378473
33	1	0	-3.941569	4.229595	0.519751
34	1	0	5.672272	-1.449387	-1.711613
35	1	0	6.428300	0.583246	-0.509115
36	1	0	4.840555	1.878695	0.855504
37	1	0	-4.300817	-4.464115	-1.216375
38	1	0	-3.157212	-3.534892	-2.216060
39	1	0	-4.527375	-2.711833	-1.425768
40	1	0	1.034515	-1.849979	-0.683405

trans-**3aa**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.574423	0.831598	-0.115930
2	6	0	1.093572	1.988342	0.394587
3	6	0	2.524217	1.557524	0.022670
4	6	0	1.855462	0.309007	-0.616481
5	8	0	0.578891	2.954078	0.900645
6	6	0	2.269404	-1.038088	-0.097671
7	6	0	1.865072	-1.477604	1.159916
8	6	0	2.290920	-2.707541	1.640869
9	6	0	3.125777	-3.507350	0.870289
10	6	0	3.529185	-3.074431	-0.385781
11	6	0	3.098190	-1.846272	-0.869008
12	6	0	-0.724278	0.332277	-0.242212
13	6	0	-1.786555	0.969668	0.349570
14	6	0	-3.093444	0.451220	0.202816
15	6	0	-4.214798	1.085217	0.796288
16	6	0	-5.469886	0.567009	0.643423
17	6	0	-5.672504	-0.611901	-0.110463
18	6	0	-4.610831	-1.244615	-0.693995
19	6	0	-3.298475	-0.731739	-0.553571
20	6	0	-2.177500	-1.360958	-1.147959
21	6	0	-0.922118	-0.848259	-1.001895
22	8	0	3.195171	2.361102	-0.889760
23	6	0	3.756556	3.515573	-0.284071
24	1	0	3.140304	1.317245	0.895369
25	1	0	1.919909	0.353300	-1.704762
26	1	0	1.208120	-0.860233	1.760647
27	1	0	1.967905	-3.043527	2.616929
28	1	0	3.455249	-4.466765	1.245385
29	1	0	4.174039	-3.695217	-0.992988
30	1	0	3.405497	-1.512587	-1.852627
31	1	0	-0.073102	-1.335920	-1.461631
32	1	0	-2.329728	-2.262429	-1.727826
33	1	0	-4.756912	-2.147562	-1.273765
34	1	0	-6.672099	-1.009239	-0.222775
35	1	0	-6.317835	1.059200	1.100534
36	1	0	-4.057493	1.988073	1.372837
37	1	0	-1.627041	1.871068	0.923976
38	1	0	4.266187	4.069252	-1.067412
39	1	0	2.979839	4.139989	0.160312
40	1	0	4.475906	3.230249	0.488305

TSRaa

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.576599	-3.202960	-0.005494
2	6	0	2.858258	-3.535893	1.140478
3	6	0	1.790439	-2.749411	1.561633
4	6	0	1.414482	-1.638729	0.829007
5	6	0	2.128122	-1.299163	-0.332611
6	6	0	3.224174	-2.082784	-0.730377
7	6	0	1.832896	-0.111850	-1.079501
8	7	0	0.732728	0.654625	-0.958979
9	6	0	1.316213	1.782600	-0.042586
10	6	0	2.011737	2.667424	-0.829113
11	8	0	2.731991	3.710984	-0.369409
12	6	0	3.371956	3.543177	0.889952
13	6	0	-1.482610	0.962353	-0.049702
14	6	0	-0.566961	0.186496	-0.714864
15	6	0	-0.966079	-1.056570	-1.277986
16	6	0	-2.249161	-1.491789	-1.144828
17	6	0	-3.217298	-0.719978	-0.452257
18	6	0	-2.821352	0.527188	0.094447
19	8	0	1.164744	1.625742	1.170617
20	1	0	2.583043	0.233288	-1.780291
21	1	0	1.880454	2.657642	-1.900252
22	1	0	-2.548465	-2.435432	-1.583420
23	6	0	-4.556800	-1.148390	-0.302902
24	1	0	-0.244397	-1.645057	-1.828561
25	1	0	3.138444	-4.409652	1.713344
26	1	0	3.785279	-1.799115	-1.611673
27	1	0	0.595201	-1.015028	1.156973
28	1	0	1.251991	-3.007481	2.462659
29	1	0	4.412505	-3.812499	-0.318339
30	1	0	2.645192	3.510755	1.699273
31	1	0	4.036085	4.394436	1.008277
32	1	0	3.948202	2.615936	0.894252
33	6	0	-5.466999	-0.373523	0.362643
34	1	0	-4.849093	-2.101612	-0.725922
35	1	0	-6.489505	-0.708089	0.473364
36	6	0	-5.074742	0.868658	0.909083
37	6	0	-3.786179	1.307886	0.779068
38	1	0	-5.802015	1.473877	1.433557
39	1	0	-3.483864	2.259505	1.197887
40	1	0	-1.182208	1.903899	0.387523

Cartesian coordinates (optimized at the M06-2X(PCM, solvent=CH_2Cl_2)/def-TZVPP level) of all the stationary points collected in the main text associated with the reaction of **1b** and **2b**.

1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.229615	-0.368363	0.000436
2	6	0	-2.134965	0.005392	-0.000154
3	6	0	-0.908945	0.473846	-0.000503
4	1	0	-0.725370	1.534839	0.000227
5	8	0	0.152191	-0.419863	-0.000413
6	8	0	1.576866	1.308265	0.000261
7	6	0	1.388884	0.123270	-0.000062
8	6	0	2.435927	-0.945574	0.000179
9	1	0	2.313160	-1.574790	-0.879753
10	1	0	2.312816	-1.574702	0.880129
11	1	0	3.418446	-0.487259	0.000364

(*E*)-2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.949793	-0.123966	0.133080
2	6	0	-3.161300	-1.227758	-0.162869
3	6	0	-3.326613	1.117584	0.233579
4	6	0	-1.959078	1.267733	0.051907
5	6	0	-1.186842	0.130816	-0.220507
6	6	0	-1.782602	-1.128438	-0.340708
7	7	0	0.197104	0.304008	-0.453372
8	6	0	1.019811	-0.184686	0.374669
9	6	0	2.478814	-0.087073	0.208368
10	6	0	3.305819	-0.658085	1.172239
11	6	0	4.686582	-0.585485	1.045530
12	6	0	5.245456	0.060669	-0.047739
13	6	0	4.423189	0.634157	-1.014615
14	6	0	3.047090	0.561276	-0.889266
15	1	0	0.678741	-0.708651	1.274724
16	1	0	2.863053	-1.160509	2.023707
17	1	0	5.323077	-1.031378	1.797517
18	1	0	6.320737	0.119378	-0.149914
19	1	0	4.861579	1.137417	-1.865778
20	1	0	2.396433	1.001620	-1.632421
21	1	0	-3.924378	1.996039	0.451592
22	1	0	-3.629168	-2.200358	-0.267915
23	6	0	-1.298494	2.612524	0.156084
24	1	0	-0.621475	2.653198	1.011118
25	1	0	-0.695809	2.815910	-0.730159
26	1	0	-2.040320	3.400673	0.268169
27	6	0	-0.971734	-2.347261	-0.693685
28	1	0	-0.371325	-2.695543	0.147812
29	1	0	-1.627223	-3.162798	-0.992816
30	1	0	-0.282255	-2.135969	-1.511663
31	6	0	-5.432891	-0.257161	0.347821
32	1	0	-5.978029	0.525812	-0.179364
33	1	0	-5.795772	-1.222440	-0.001269
34	1	0	-5.682065	-0.169533	1.406929

TSib

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.508485	0.000531	-0.419081
2	6	0	-1.317148	0.002706	-1.305222

3	7	0	-0.144822	0.003572	-0.906097
4	6	0	1.794584	-1.220086	-0.255636
5	6	0	-3.778137	-0.000379	-0.987199
6	6	0	-4.905460	-0.002473	-0.176539
7	6	0	-4.761961	-0.003657	1.204164
8	6	0	-3.492200	-0.002740	1.776268
9	6	0	-2.368770	-0.000645	0.967691
10	6	0	1.131438	0.004213	-0.481106
11	6	0	1.794435	1.224145	-0.252172
12	6	0	3.110404	1.189982	0.191348
13	6	0	3.793992	0.001059	0.419119
14	6	0	3.107473	-1.189057	0.186920
15	1	0	-1.553994	0.003449	-2.380770
16	1	0	-3.879738	0.000577	-2.065987
17	1	0	-5.891871	-0.003166	-0.619835
18	1	0	-5.638518	-0.005273	1.838024
19	1	0	-3.384801	-0.003648	2.852495
20	1	0	-1.373980	0.000129	1.396170
21	1	0	3.615892	2.134190	0.364737
22	6	0	1.059750	2.509801	-0.487828
23	1	0	0.743347	2.597964	-1.529698
24	1	0	0.152948	2.558473	0.120731
25	1	0	1.684555	3.366821	-0.244591
26	6	0	1.056935	-2.503081	-0.496039
27	1	0	1.680090	-3.362350	-0.256740
28	1	0	0.150461	-2.551749	0.112894
29	1	0	0.739675	-2.585664	-1.538038
30	6	0	5.215350	-0.009856	0.914832
31	1	0	5.640616	0.992816	0.902615
32	1	0	5.277172	-0.384809	1.938377
33	1	0	5.846097	-0.651162	0.297710
34	1	0	3.612600	-2.134379	0.357472

(*Z*)-2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.967680	-0.896514	-0.132608
2	6	0	-2.726522	0.199629	-0.955512
3	6	0	-2.159790	-1.061960	0.986995
4	6	0	-1.129220	-0.179212	1.293674
5	6	0	-0.908458	0.906076	0.439540
6	6	0	-1.715744	1.113248	-0.683744
7	7	0	0.080567	1.864574	0.748375
8	6	0	1.319909	1.668096	0.579076
9	6	0	2.047476	0.504797	0.021297
10	6	0	3.393406	0.387155	0.373505
11	6	0	4.158659	-0.675703	-0.081418
12	6	0	3.589126	-1.625201	-0.918487
13	6	0	2.257467	-1.503401	-1.298420
14	6	0	1.486102	-0.450085	-0.831977
15	1	0	1.977766	2.471355	0.914095
16	1	0	3.838827	1.136995	1.015892
17	1	0	5.196842	-0.757957	0.209777
18	1	0	4.182243	-2.453346	-1.282338
19	1	0	1.816732	-2.233242	-1.963838
20	1	0	0.455142	-0.369612	-1.143197
21	1	0	-2.332815	-1.906410	1.645269
22	1	0	-3.342821	0.350153	-1.835229
23	6	0	-0.264756	-0.389200	2.504743
24	1	0	-0.669430	-1.181251	3.131556
25	1	0	0.752749	-0.667911	2.221534
26	1	0	-0.192707	0.523766	3.097473
27	6	0	-1.447424	2.281097	-1.588504
28	1	0	-0.468737	2.191079	-2.065639
29	1	0	-2.202703	2.349937	-2.368742
30	1	0	-1.435934	3.214143	-1.023151
31	6	0	-4.093661	-1.850860	-0.424579
32	1	0	-3.887258	-2.839208	-0.015998
33	1	0	-5.027098	-1.499242	0.019424
34	1	0	-4.258121	-1.949049	-1.497007

(*E*)-TS1bb

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.434737	-0.155182	-0.258879
2	6	0	-3.568179	0.403979	-1.191819
3	6	0	-2.190342	0.225340	-1.120296
4	6	0	-1.686152	-0.552063	-0.075149
5	6	0	-2.523752	-1.136492	0.877165
6	6	0	-3.893300	-0.925390	0.764545
7	7	0	-0.279414	-0.719001	0.076519
8	6	0	0.306544	-1.661832	-0.535912
9	6	0	1.731355	-1.985952	-0.393440
10	6	0	2.370012	-2.644092	-1.442877
11	6	0	3.716369	-2.964300	-1.349870
12	6	0	4.420621	-2.653360	-0.194619
13	6	0	3.779232	-2.025506	0.868748
14	6	0	2.439983	-1.688993	0.771443
15	6	0	0.396073	0.920507	1.274858
16	8	0	-0.186731	0.843605	2.289711
17	6	0	1.231768	1.429298	0.376824
18	1	0	1.440887	0.994911	-0.580131
19	1	0	-0.264438	-2.293812	-1.222251
20	1	0	1.810129	-2.896203	-2.334919
21	1	0	4.211571	-3.462370	-2.171803
22	1	0	5.468095	-2.911193	-0.115362
23	1	0	4.325317	-1.803815	1.775286
24	1	0	1.932440	-1.215294	1.600229
25	1	0	-4.552792	-1.377800	1.496494
26	1	0	-3.973232	0.999207	-2.002330
27	6	0	-1.276473	0.850842	-2.137064
28	1	0	-0.611698	1.579444	-1.669893
29	1	0	-0.645630	0.104188	-2.621955
30	1	0	-1.855572	1.356191	-2.906993
31	6	0	-1.952681	-1.994745	1.971676
32	1	0	-1.557623	-2.929895	1.569399
33	1	0	-1.131048	-1.487175	2.476923
34	1	0	-2.718226	-2.239606	2.704859
35	6	0	-5.916544	0.090047	-0.338958
36	1	0	-6.190406	0.981373	0.228708
37	1	0	-6.234300	0.245730	-1.368910
38	1	0	-6.476920	-0.747612	0.073808
39	8	0	1.904422	2.596424	0.756201
40	6	0	1.922391	3.594284	-0.150236
41	8	0	1.397875	3.511442	-1.227692
42	6	0	2.693737	4.770365	0.365478
43	1	0	2.284437	5.085746	1.323515
44	1	0	2.644531	5.580927	-0.353073
45	1	0	3.730292	4.477776	0.527295

(*E*)-INTbb

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.653019	-2.026042	-0.156865
2	6	0	-3.186725	-1.603349	1.087230
3	6	0	-2.799048	-1.947171	-1.248118
4	6	0	-1.497014	-1.465555	-1.129883
5	6	0	-1.078091	-1.053692	0.132737
6	6	0	-1.905194	-1.102929	1.258025
7	7	0	0.262084	-0.541217	0.282535
8	6	0	0.444188	0.908110	0.701056
9	6	0	-0.382816	1.711024	-0.013722
10	6	0	1.250621	-1.357113	0.131021
11	6	0	2.663299	-1.063069	0.010542
12	6	0	3.534393	-2.145968	0.180323
13	6	0	4.899791	-1.977427	0.035767
14	6	0	5.401871	-0.732398	-0.321240
15	6	0	4.540190	0.339314	-0.533019
16	6	0	3.176663	0.186236	-0.360241

17	8	0	1.294772	1.122665	1.577667
18	1	0	-3.150450	-2.261246	-2.223528
19	1	0	-1.110671	1.382550	-0.732720
20	1	0	0.971851	-2.402410	0.037491
21	1	0	3.130901	-3.118209	0.433189
22	1	0	5.567885	-2.813353	0.187042
23	1	0	6.467807	-0.597395	-0.446211
24	1	0	4.936598	1.300259	-0.829518
25	1	0	2.515605	1.022507	-0.526743
26	8	0	-0.316243	3.071374	0.251295
27	6	0	-1.113488	3.893811	-0.440984
28	8	0	-1.881603	3.516420	-1.289906
29	6	0	-0.919978	5.317849	-0.014195
30	1	0	0.129195	5.591909	-0.109857
31	1	0	-1.194414	5.421286	1.034831
32	1	0	-1.536463	5.968206	-0.624965
33	1	0	-3.841679	-1.664302	1.948632
34	6	0	-1.421622	-0.639882	2.601727
35	1	0	-2.103290	-0.967469	3.383065
36	1	0	-0.424163	-1.020968	2.821492
37	1	0	-1.355982	0.449003	2.633221
38	6	0	-0.602208	-1.379401	-2.337452
39	1	0	0.095340	-2.217802	-2.380061
40	1	0	-1.199296	-1.402595	-3.246030
41	1	0	-0.014884	-0.460448	-2.335051
42	6	0	-5.056666	-2.543062	-0.302159
43	1	0	-5.241271	-2.906868	-1.310743
44	1	0	-5.243430	-3.357401	0.398227
45	1	0	-5.780053	-1.756108	-0.085255

cis-**TS2bb**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.601807	1.121623	0.076716
2	6	0	-1.897549	-0.084172	-0.027077
3	6	0	-2.560111	-1.313303	-0.148874
4	6	0	-3.948316	-1.300827	-0.188188
5	6	0	-4.681697	-0.121503	-0.111688
6	6	0	-3.990290	1.075504	0.025358
7	7	0	-0.471146	-0.043153	0.003640
8	6	0	0.265914	0.730151	-0.805369
9	6	0	1.357983	1.613478	-0.408600
10	6	0	1.697335	1.858078	0.930102
11	6	0	2.696885	2.760807	1.235808
12	6	0	3.378778	3.434115	0.223099
13	6	0	3.039938	3.206258	-1.101808
14	6	0	2.029391	2.308605	-1.416396
15	6	0	0.365460	-0.885438	0.796685
16	8	0	0.192118	-1.110147	1.992764
17	6	0	1.384668	-1.290192	-0.084722
18	1	0	1.214510	-1.467679	-1.132405
19	1	0	-0.167493	0.927726	-1.784525
20	1	0	1.174390	1.342574	1.725720
21	1	0	2.946139	2.948604	2.271360
22	1	0	4.161196	4.137720	0.471996
23	1	0	3.556713	3.730825	-1.893838
24	1	0	1.761176	2.136369	-2.451220
25	1	0	-4.544910	2.001914	0.115694
26	6	0	-1.910481	2.442979	0.291162
27	1	0	-1.453452	2.823469	-0.623529
28	1	0	-2.630499	3.183530	0.631761
29	1	0	-1.122223	2.360938	1.039171
30	6	0	-1.825444	-2.620247	-0.244750
31	1	0	-1.060051	-2.591629	-1.020380
32	1	0	-1.327152	-2.861814	0.695205
33	1	0	-2.522972	-3.421147	-0.478452
34	6	0	-6.181950	-0.144256	-0.190885
35	1	0	-6.586691	-1.035270	0.286748
36	1	0	-6.614475	0.733996	0.285062
37	1	0	-6.508274	-0.152595	-1.232566
38	1	0	-4.471996	-2.244599	-0.284705

39	8	0	2.503614	-1.839093	0.464857
40	6	0	3.326012	-2.573447	-0.331323
41	8	0	3.089593	-2.780582	-1.488333
42	6	0	4.520267	-3.045112	0.432952
43	1	0	4.195557	-3.598687	1.312341
44	1	0	5.089240	-2.182213	0.776984
45	1	0	5.136772	-3.670006	-0.203403

cis-3bb

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.692530	-0.361544	0.256023
2	6	0	-2.544188	0.135589	1.250010
3	6	0	-3.830875	0.513163	0.888985
4	6	0	-4.293353	0.395765	-0.417846
5	6	0	-3.429203	-0.118897	-1.374942
6	6	0	-2.125518	-0.498916	-1.067934
7	1	0	-4.496140	0.893612	1.655772
8	7	0	-0.367846	-0.748522	0.591472
9	6	0	0.279126	-1.940960	0.443290
10	8	0	-0.055948	-2.996502	-0.025284
11	6	0	1.490481	-1.427478	1.241445
12	1	0	1.524498	-1.889157	2.224704
13	6	0	0.741729	-0.057121	1.271067
14	6	0	1.385678	1.098288	0.558611
15	6	0	0.806028	1.714716	-0.543787
16	6	0	1.442888	2.782075	-1.163413
17	6	0	2.666093	3.238258	-0.691555
18	6	0	3.247700	2.628303	0.412880
19	6	0	2.606791	1.568259	1.038122
20	1	0	0.496436	0.233350	2.292038
21	1	0	3.061015	1.095836	1.901085
22	1	0	4.199579	2.978515	0.789060
23	1	0	3.163042	4.065657	-1.179628
24	1	0	0.982212	3.255054	-2.020264
25	1	0	-0.142408	1.361908	-0.924705
26	1	0	-3.771200	-0.222261	-2.398304
27	6	0	-2.103446	0.244881	2.682806
28	1	0	-1.462388	1.115033	2.837740
29	1	0	-2.967305	0.352731	3.335070
30	1	0	-1.545902	-0.639131	2.993521
31	6	0	-1.222696	-1.031818	-2.143417
32	1	0	-1.591262	-0.738607	-3.124450
33	1	0	-0.200782	-0.673763	-2.022261
34	1	0	-1.175111	-2.120566	-2.101234
35	6	0	-5.684754	0.834651	-0.781382
36	1	0	-6.396327	0.567766	-0.000739
37	1	0	-5.726181	1.918407	-0.904597
38	1	0	-6.009048	0.380623	-1.715974
39	8	0	2.800238	-1.499188	0.741677
40	6	0	3.007569	-1.312626	-0.580420
41	8	0	2.112954	-1.155011	-1.363335
42	6	0	4.469024	-1.325975	-0.897928
43	1	0	4.934255	-2.214731	-0.476699
44	1	0	4.932048	-0.453806	-0.435933
45	1	0	4.608672	-1.292881	-1.972666

(*Z*)-TS1bb

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.827747	3.491053	0.274145
2	6	0	1.015605	2.178914	-0.163779
3	6	0	2.268677	1.795409	-0.650798
4	6	0	3.310210	2.708811	-0.674723
5	6	0	3.120906	4.005251	-0.208844
6	6	0	1.876598	4.397440	0.264941
7	6	0	-0.157167	1.285556	-0.094258

8	7	0	-0.222048	0.021113	-0.073705
9	6	0	0.890357	-0.846848	-0.033206
10	6	0	1.623028	-0.992713	1.147521
11	6	0	2.669375	-1.909945	1.158972
12	6	0	2.991901	-2.676891	0.045259
13	6	0	2.223938	-2.520951	-1.105504
14	6	0	1.163548	-1.626369	-1.161123
15	6	0	-2.112491	-1.220883	0.510501
16	6	0	-2.941011	-0.464832	-0.191565
17	8	0	-1.625243	-2.041313	1.176796
18	1	0	-2.627792	0.335016	-0.831577
19	1	0	-1.113842	1.808147	-0.033592
20	1	0	-0.148478	3.796445	0.629934
21	1	0	1.721187	5.407354	0.618447
22	1	0	3.941163	4.710120	-0.224901
23	1	0	4.274948	2.408431	-1.059973
24	1	0	2.429784	0.793867	-1.022033
25	1	0	3.246391	-2.028064	2.069310
26	8	0	-4.299573	-0.779553	-0.095275
27	6	0	-5.154238	0.263209	-0.078699
28	8	0	-4.793313	1.406727	-0.145283
29	6	0	-6.572309	-0.211607	0.003301
30	1	0	-6.692806	-0.861644	0.867937
31	1	0	-6.808539	-0.794291	-0.886022
32	1	0	-7.237033	0.642048	0.075159
33	6	0	0.335066	-1.457467	-2.401724
34	1	0	0.446876	-0.452857	-2.815630
35	1	0	0.625872	-2.177030	-3.163997
36	1	0	-0.725598	-1.589158	-2.177699
37	6	0	1.292810	-0.179501	2.366997
38	1	0	1.829691	-0.557991	3.234258
39	1	0	1.566434	0.869252	2.231557
40	1	0	0.223007	-0.211467	2.577921
41	6	0	4.111206	-3.680582	0.092955
42	1	0	4.845509	-3.415352	0.852009
43	1	0	3.729285	-4.674333	0.334619
44	1	0	4.617867	-3.750084	-0.868918
45	1	0	2.452913	-3.115420	-1.982980

(*Z*)-INTbb

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.106937	1.336669	0.355787
2	7	0	-0.320179	0.067925	0.364293
3	6	0	0.753408	-1.588239	-1.066474
4	6	0	-1.678922	-0.485127	0.783652
5	6	0	1.095822	2.078789	0.010072
6	8	0	-1.638060	-1.346014	1.673663
7	6	0	-2.673075	0.083339	0.057433
8	6	0	2.605904	-2.107434	0.954832
9	6	0	1.770472	-2.518304	-1.249087
10	6	0	0.708563	-0.921277	0.154764
11	6	0	1.612305	-1.163327	1.185832
12	6	0	2.702258	-2.791610	-0.252719
13	6	0	3.275669	3.730166	-0.519620
14	6	0	1.081543	3.426717	0.392040
15	6	0	2.216120	1.571124	-0.664721
16	6	0	3.291673	2.399907	-0.926877
17	6	0	2.168451	4.245154	0.139721
18	1	0	-0.957150	1.931059	0.671749
19	1	0	-2.541993	0.762646	-0.763903
20	1	0	3.321581	-2.313939	1.741754
21	1	0	4.126032	4.366031	-0.725261
22	1	0	0.210653	3.826407	0.895328
23	1	0	2.249607	0.544968	-0.995894
24	1	0	4.149702	2.006661	-1.453645
25	1	0	2.148437	5.280410	0.449053
26	8	0	-3.973926	-0.310379	0.358018
27	6	0	-4.972343	0.189779	-0.373783
28	8	0	-4.808468	0.966772	-1.282508
29	6	0	-6.298979	-0.334607	0.089009
30	1	0	-6.472967	-0.022484	1.117956

31	1	0	-6.291724	-1.423020	0.070406
32	1	0	-7.085791	0.047322	-0.552302
33	1	0	1.836435	-3.038923	-2.197025
34	6	0	-0.230948	-1.286778	-2.160350
35	1	0	-0.269944	-0.216665	-2.373915
36	1	0	0.045912	-1.808416	-3.073386
37	1	0	-1.238028	-1.591346	-1.874546
38	6	0	1.530245	-0.421191	2.488895
39	1	0	2.177671	-0.884978	3.229335
40	1	0	1.848341	0.617379	2.369972
41	1	0	0.507135	-0.421647	2.863597
42	6	0	3.769309	-3.828665	-0.464323
43	1	0	4.047773	-3.897675	-1.514577
44	1	0	4.659707	-3.601813	0.119560
45	1	0	3.410273	-4.811005	-0.152189

trans-**TS2bb**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.681807	1.960653	-1.023078
2	6	0	-0.036237	2.030949	0.217805
3	6	0	0.100315	3.271876	0.850721
4	6	0	-0.420362	4.414939	0.269773
5	6	0	-1.072540	4.332554	-0.955056
6	6	0	-1.196927	3.106572	-1.601547
7	6	0	0.531005	0.865107	0.861790
8	7	0	0.154001	-0.396955	0.584991
9	6	0	1.268858	-1.275258	0.703073
10	6	0	2.352118	-0.543198	0.179389
11	8	0	3.606880	-1.038191	0.412059
12	6	0	4.627431	-0.611296	-0.370928
13	6	0	5.919154	-1.233907	0.053274
14	6	0	-1.171408	-0.837681	0.281906
15	6	0	-2.218787	-0.473576	1.132897
16	6	0	-3.500886	-0.912943	0.814255
17	6	0	-3.754471	-1.701003	-0.299484
18	6	0	-2.682212	-2.056116	-1.113262
19	6	0	-1.385514	-1.641989	-0.845386
20	6	0	-2.006467	0.351338	2.372430
21	6	0	-0.264558	-2.040455	-1.762832
22	6	0	-5.141890	-2.188294	-0.609457
23	8	0	1.211985	-2.394139	1.209586
24	8	0	4.475628	0.171673	-1.267736
25	1	0	2.245361	0.128351	-0.655244
26	1	0	1.158257	1.022425	1.725106
27	1	0	0.612920	3.327283	1.802909
28	1	0	-0.316531	5.369305	0.766877
29	1	0	-1.477446	5.225406	-1.411737
30	1	0	-1.691590	3.048881	-2.561143
31	1	0	-0.767017	1.011299	-1.534483
32	1	0	-4.320279	-0.637686	1.467654
33	1	0	0.406142	-2.748851	-1.273932
34	1	0	-0.663867	-2.508033	-2.659840
35	1	0	0.336668	-1.179772	-2.059708
36	1	0	-2.852440	0.231876	3.045658
37	1	0	-1.101662	0.052949	2.901417
38	1	0	-1.916458	1.413510	2.136247
39	1	0	-5.356497	-2.104161	-1.674383
40	1	0	-5.247238	-3.240065	-0.337865
41	1	0	-5.891003	-1.623037	-0.058384
42	1	0	-2.861552	-2.669700	-1.988509
43	1	0	6.711707	-0.922457	-0.617889
44	1	0	5.821338	-2.318112	0.050774
45	1	0	6.148336	-0.925099	1.072564

trans-**3bb**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	7	0	-0.137137	-0.888322	-0.066791
2	6	0	0.584133	-1.852486	-0.706628
3	6	0	1.869555	-1.035176	-0.581265
4	6	0	1.036858	-0.063098	0.299446
5	8	0	0.297738	-2.931169	-1.157581
6	6	0	0.964678	1.388439	-0.063319
7	6	0	0.256882	1.821948	-1.180234
8	6	0	0.223693	3.170101	-1.510074
9	6	0	0.895734	4.096337	-0.723932
10	6	0	1.598579	3.670316	0.396182
11	6	0	1.628141	2.323343	0.725939
12	6	0	-1.525634	-0.686454	0.124282
13	6	0	-2.401357	-0.843046	-0.956330
14	6	0	-3.759809	-0.624486	-0.736429
15	6	0	-4.257435	-0.243808	0.500862
16	6	0	-3.356469	-0.090766	1.550905
17	6	0	-1.996477	-0.310465	1.390201
18	1	0	2.197395	-0.580060	-1.515298
19	1	0	1.316329	-0.183156	1.345948
20	1	0	-0.278292	1.106894	-1.791336
21	1	0	-0.331396	3.496733	-2.379010
22	1	0	0.867587	5.146882	-0.979737
23	1	0	2.120534	4.387689	1.014891
24	1	0	2.176278	1.989454	1.598423
25	1	0	-3.725380	0.194212	2.529570
26	1	0	-4.443416	-0.746190	-1.568540
27	6	0	-1.930752	-1.232814	-2.328546
28	1	0	-2.681220	-0.968959	-3.070575
29	1	0	-0.995083	-0.740734	-2.595725
30	1	0	-1.742989	-2.304906	-2.387293
31	6	0	-1.067354	-0.165513	2.562958
32	1	0	-0.444112	0.726844	2.470521
33	1	0	-1.637556	-0.077004	3.484882
34	1	0	-0.404583	-1.027029	2.649876
35	6	0	-5.723232	0.018510	0.707426
36	1	0	-5.914869	1.089914	0.787498
37	1	0	-6.313539	-0.367094	-0.121623
38	1	0	-6.076628	-0.444395	1.628554
39	8	0	2.909038	-1.755923	0.036669
40	6	0	4.019712	-1.044879	0.322120
41	8	0	4.095712	0.133741	0.103196
42	6	0	5.082531	-1.907664	0.924335
43	1	0	5.364821	-2.680004	0.210285
44	1	0	4.690679	-2.403619	1.810673
45	1	0	5.943615	-1.300435	1.179885

TSRbb

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.597574	-1.085070	0.304884
2	6	0	1.810724	0.056197	0.039153
3	6	0	2.431657	1.321150	0.009334
4	6	0	3.822840	1.379709	0.048813
5	6	0	4.626425	0.256293	0.162771
6	6	0	3.981870	-0.959340	0.334202
7	7	0	0.394750	-0.116490	-0.080972
8	6	0	-0.401822	0.952443	-0.673060
9	6	0	-1.476262	1.397441	0.158446
10	8	0	-2.319891	2.287963	-0.365523
11	6	0	-3.359085	2.751841	0.426421
12	6	0	-4.185949	3.728813	-0.334761
13	6	0	1.705179	2.645665	0.028437
14	6	0	6.125967	0.356046	0.146248
15	6	0	2.021368	-2.428643	0.693254
16	6	0	-0.033348	-1.295015	-0.748305
17	6	0	-1.184447	-2.021009	-0.364101
18	6	0	-1.828998	-1.827503	0.877258
19	6	0	-2.942456	-2.572032	1.216157
20	6	0	-3.446216	-3.532515	0.341982
21	6	0	-2.809268	-3.752004	-0.878378

22	6	0	-1.696209	-3.014574	-1.228350
23	8	0	-0.195654	1.371528	-1.793972
24	8	0	-3.507797	2.377433	1.547278
25	1	0	-1.614642	1.093350	1.181906
26	1	0	0.527529	-1.589499	-1.628735
27	1	0	-1.418411	-1.113830	1.578007
28	1	0	-3.419127	-2.412900	2.174357
29	1	0	-4.318971	-4.110517	0.612458
30	1	0	-3.188720	-4.503719	-1.557615
31	1	0	-1.207238	-3.184241	-2.179548
32	1	0	4.289462	2.357601	0.011309
33	1	0	4.571121	-1.847338	0.534228
34	1	0	2.761810	-2.969273	1.280761
35	1	0	1.125044	-2.315948	1.303065
36	1	0	1.759470	-3.052663	-0.160716
37	1	0	1.338035	2.941569	-0.952661
38	1	0	0.854175	2.634066	0.710334
39	1	0	2.388293	3.414819	0.382162
40	1	0	6.460270	1.327939	0.506922
41	1	0	6.578467	-0.417110	0.766148
42	1	0	6.511135	0.230852	-0.867652
43	1	0	-4.993989	4.086905	0.292665
44	1	0	-3.556837	4.557040	-0.657831
45	1	0	-4.580652	3.245583	-1.227451

Cartesian coordinates (optimized at the M06-2X(PCM, solvent=CH_2Cl_2)/def-TZVPP level) of all the stationary points collected in the main text associated with the reaction of **1b** and **2c**.

1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.229615	-0.368363	0.000436
2	6	0	-2.134965	0.005392	-0.000154
3	6	0	-0.908945	0.473846	-0.000503
4	1	0	-0.725370	1.534839	0.000227
5	8	0	0.152191	-0.419863	-0.000413
6	8	0	1.576866	1.308265	0.000261
7	6	0	1.388884	0.123270	-0.000062
8	6	0	2.435927	-0.945574	0.000179
9	1	0	2.313160	-1.574790	-0.879753
10	1	0	2.312816	-1.574702	0.880129
11	1	0	3.418446	-0.487259	0.000364

(*E*)-2c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.061006	-1.623918	-0.005991
2	7	0	-3.421323	-0.661078	0.027828
3	8	0	4.998957	0.620029	0.439099
4	8	0	-2.674310	-2.835962	0.067008
5	6	0	-1.118573	-0.932242	0.006033
6	6	0	1.210327	-1.021035	0.077912
7	6	0	2.160018	-1.294215	-0.896268
8	1	0	1.894332	-1.932564	-1.727982
9	6	0	3.434871	-0.744806	-0.822538
10	1	0	4.145388	-0.957620	-1.606752
11	6	0	3.780629	0.051559	0.264746
12	6	0	2.840879	0.292694	1.269284
13	1	0	3.130856	0.896210	2.118565
14	6	0	1.569221	-0.232858	1.174268
15	1	0	0.842459	-0.043469	1.953803
16	6	0	5.981524	0.384185	-0.551167
17	1	0	5.658298	0.763352	-1.522617
18	1	0	6.206622	-0.680772	-0.634259
19	1	0	6.870403	0.918620	-0.231046
20	6	0	-2.474072	-1.645454	0.032800
21	6	0	-2.831268	0.604427	-0.042308
22	6	0	-1.430413	0.508101	-0.047421
23	6	0	-0.666850	1.658137	-0.173377
24	1	0	0.411577	1.609049	-0.199727
25	6	0	-1.311594	2.889283	-0.265340
26	1	0	-0.726613	3.792947	-0.359921
27	6	0	-2.697995	2.964048	-0.232029
28	1	0	-3.182121	3.929082	-0.297396
29	6	0	-3.483779	1.817951	-0.124733
30	1	0	-4.562854	1.878489	-0.115475
31	6	0	-4.845770	-0.894196	0.043184
32	1	0	-5.006687	-1.966886	0.095954
33	1	0	-5.306078	-0.502079	-0.863814
34	1	0	-5.299397	-0.415404	0.910664

TSic

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.178791	-0.303891	-0.003677
2	7	0	-3.203566	-1.262557	0.028826

3	8	0	5.675573	-0.177365	-0.031708
4	8	0	-1.465490	-2.774513	0.046660
5	6	0	-1.060820	-0.339005	0.003124
6	6	0	1.530949	-0.241934	-0.010963
7	6	0	2.205925	0.982767	0.075806
8	1	0	1.622611	1.890712	0.146898
9	6	0	3.588671	1.047354	0.079030
10	1	0	4.076943	2.006945	0.153675
11	6	0	4.329609	-0.131484	-0.020148
12	6	0	3.674381	-1.365368	-0.115073
13	1	0	4.271924	-2.263347	-0.190553
14	6	0	2.300913	-1.418329	-0.103937
15	1	0	1.782093	-2.364980	-0.169603
16	6	0	6.387420	1.044690	0.064787
17	1	0	6.159779	1.554665	1.002031
18	1	0	6.151893	1.699903	-0.775192
19	1	0	7.440191	0.783257	0.038693
20	6	0	-1.888213	-1.639175	0.028539
21	6	0	-3.329091	0.132871	0.003747
22	6	0	-2.068090	0.739671	-0.011036
23	6	0	-1.954369	2.114461	-0.037633
24	1	0	-0.976654	2.579314	-0.050155
25	6	0	-3.117309	2.883443	-0.048705
26	1	0	-3.052766	3.962252	-0.069488
27	6	0	-4.363001	2.267432	-0.033131
28	1	0	-5.257177	2.876147	-0.041925
29	6	0	-4.491775	0.877199	-0.006630
30	1	0	-5.465562	0.407633	0.005059
31	6	0	-4.321889	-2.174089	0.048142
32	1	0	-3.926910	-3.185735	0.067704
33	1	0	-4.937721	-2.042397	-0.841843
34	1	0	-4.935751	-2.007240	0.933527

(*Z*)-2c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.033797	-1.090698	-0.029688
2	7	0	2.393291	1.500744	0.179551
3	8	0	-5.367296	0.402031	-0.361069
4	8	0	0.156376	1.997518	0.300554
5	6	0	0.974322	-0.326164	-0.014538
6	6	0	-1.367951	-0.654206	-0.088731
7	6	0	-2.297890	-1.298154	0.718502
8	1	0	-1.956557	-2.068489	1.396926
9	6	0	-3.643595	-0.955811	0.679006
10	1	0	-4.335964	-1.457462	1.337723
11	6	0	-4.077758	0.009074	-0.224421
12	6	0	-3.155479	0.623195	-1.076119
13	1	0	-3.514161	1.353487	-1.788546
14	6	0	-1.817872	0.302623	-1.003945
15	1	0	-1.111556	0.779600	-1.668642
16	6	0	-6.332312	-0.206790	0.475417
17	1	0	-6.113592	-0.017662	1.528100
18	1	0	-6.377827	-1.283702	0.302323
19	1	0	-7.285956	0.242572	0.216858
20	6	0	1.057363	1.204056	0.154877
21	6	0	3.180966	0.350086	0.057513
22	6	0	2.367153	-0.780159	-0.050388
23	6	0	2.922448	-2.036867	-0.182183
24	1	0	2.285182	-2.906750	-0.269208
25	6	0	4.311128	-2.150623	-0.197472
26	1	0	4.771977	-3.123156	-0.296521
27	6	0	5.109455	-1.017933	-0.086325
28	1	0	6.185861	-1.123543	-0.100197
29	6	0	4.557948	0.257844	0.042646
30	1	0	5.186941	1.132713	0.128428
31	6	0	2.925264	2.829973	0.364834
32	1	0	2.088265	3.516959	0.445784
33	1	0	3.546370	3.111312	-0.485326
34	1	0	3.522769	2.876536	1.275339

(*E*)-TS1bc

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.083299	0.317096	0.432946
2	7	0	3.299099	1.689195	0.166326
3	8	0	-1.285079	1.608906	2.288746
4	8	0	-2.306181	-4.687741	0.457871
5	8	0	1.456164	2.841353	0.919458
6	8	0	-2.676143	3.124471	-0.038189
7	8	0	-3.695818	2.039537	-1.715336
8	6	0	1.324526	0.482171	0.237278
9	6	0	-1.644140	2.177856	-0.063406
10	1	0	-1.196693	1.926001	-1.003935
11	6	0	-1.248301	1.706522	1.116729
12	6	0	-0.519554	-0.964163	0.392890
13	6	0	-1.587294	-1.205753	-0.458894
14	1	0	-1.938329	-0.421369	-1.115196
15	6	0	-2.200884	-2.452045	-0.477288
16	1	0	-3.017394	-2.623824	-1.161697
17	6	0	-1.767413	-3.449914	0.391694
18	6	0	-0.717189	-3.190558	1.276386
19	1	0	-0.407638	-3.968890	1.959937
20	6	0	-0.097430	-1.959692	1.275292
21	1	0	0.715149	-1.755888	1.960410
22	6	0	-3.383237	-4.987736	-0.411591
23	1	0	-3.078804	-4.898811	-1.455938
24	1	0	-4.233138	-4.329845	-0.222351
25	1	0	-3.664696	-6.014569	-0.201533
26	6	0	1.983423	1.847113	0.490157
27	6	0	3.556361	0.392119	-0.284758
28	6	0	2.394681	-0.395946	-0.245623
29	6	0	2.432009	-1.703105	-0.709537
30	1	0	1.546674	-2.321343	-0.705693
31	6	0	3.637646	-2.211841	-1.181042
32	1	0	3.684035	-3.229361	-1.541143
33	6	0	4.782178	-1.423391	-1.187123
34	1	0	5.712402	-1.838772	-1.550374
35	6	0	4.759984	-0.102917	-0.742876
36	1	0	5.649559	0.510246	-0.764709
37	6	0	4.295232	2.730368	0.269186
38	1	0	3.806405	3.621950	0.650130
39	1	0	4.725339	2.941074	-0.709518
40	1	0	5.087531	2.428963	0.953632
41	6	0	-3.670526	2.946624	-0.926232
42	6	0	-4.696649	4.032292	-0.806690
43	1	0	-5.518313	3.833720	-1.485958
44	1	0	-4.237149	4.989873	-1.048043
45	1	0	-5.055809	4.086561	0.219373

(*E*)-INTbc

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.211129	-0.774875	0.014120
2	6	0	-2.226846	-1.421240	-0.004018
3	1	0	-2.496827	-0.596204	0.628628
4	6	0	-0.998007	-1.633590	-0.559913
5	6	0	-0.522817	0.817376	-0.139241
6	6	0	-1.176972	1.341508	-1.251552
7	1	0	-1.332594	0.722680	-2.124320
8	6	0	-1.596694	2.653350	-1.233101
9	1	0	-2.094465	3.091128	-2.086577
10	6	0	-1.390462	3.443832	-0.097112
11	6	0	-0.756748	2.904625	1.023575
12	1	0	-0.607893	3.489712	1.917683
13	6	0	-0.321923	1.589176	0.992953
14	1	0	0.169661	1.157800	1.854975
15	6	0	-1.660685	5.551632	0.955010
16	1	0	-2.180869	5.152815	1.826940

17	1	0	-2.087321	6.511571	0.683972
18	1	0	-0.600573	5.672706	1.182779
19	6	0	1.731498	-2.144953	0.436990
20	6	0	3.486284	-0.748019	0.067487
21	6	0	2.363347	0.084714	-0.118379
22	6	0	2.545584	1.415180	-0.492774
23	1	0	1.703096	2.073040	-0.648252
24	6	0	3.837528	1.891677	-0.655040
25	1	0	3.994773	2.921873	-0.939506
26	6	0	4.933382	1.058040	-0.442591
27	1	0	5.932532	1.454166	-0.562780
28	6	0	4.775311	-0.276720	-0.082503
29	1	0	5.629086	-0.921880	0.067105
30	6	0	4.003224	-3.100803	0.773164
31	1	0	4.569955	-2.813384	1.658714
32	1	0	4.692229	-3.321525	-0.040842
33	1	0	3.409503	-3.982598	0.994052
34	6	0	-4.439335	-2.148855	0.199047
35	6	0	-5.357186	-3.266342	-0.190014
36	1	0	-6.357032	-3.060295	0.175724
37	1	0	-4.988913	-4.200071	0.232907
38	1	0	-5.364856	-3.374603	-1.273282
39	7	0	-0.053582	-0.530828	-0.154798
40	7	0	3.097567	-2.043127	0.387163
41	8	0	-0.552173	-2.514498	-1.301952
42	8	0	-1.842502	4.708701	-0.171150
43	8	0	1.092971	-3.074540	0.854817
44	8	0	-3.201080	-2.353448	-0.284186
45	8	0	-4.739100	-1.187906	0.858579

cis-TS2bc

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.156427	-0.447384	-0.572332
2	7	0	2.332443	2.075817	-0.890721
3	8	0	0.188745	-2.535403	-1.585809
4	8	0	-5.672927	-0.322377	-0.098726
5	8	0	2.268934	0.205978	-2.232002
6	6	0	0.602490	0.627240	-0.465495
7	6	0	0.555227	-1.695131	-0.766998
8	6	0	-1.571955	-0.436192	-0.441642
9	6	0	-2.204827	-1.447191	0.263433
10	1	0	-1.615813	-2.234441	0.714768
11	6	0	-3.583994	-1.444579	0.398741
12	1	0	-4.060487	-2.237680	0.953673
13	6	0	-4.330973	-0.417025	-0.177110
14	6	0	-3.686350	0.594987	-0.895449
15	1	0	-4.284445	1.372418	-1.349375
16	6	0	-2.316326	0.581215	-1.034164
17	1	0	-1.816180	1.350805	-1.606919
18	6	0	-6.373219	-1.339380	0.597811
19	1	0	-6.069003	-1.375110	1.645046
20	1	0	-6.207326	-2.313171	0.134642
21	1	0	-7.424702	-1.079626	0.533201
22	6	0	1.845824	0.859328	-1.307232
23	6	0	1.497139	2.651879	0.058325
24	6	0	0.394052	1.815616	0.317654
25	6	0	-0.553675	2.182479	1.268822
26	1	0	-1.400736	1.544575	1.480554
27	6	0	-0.394584	3.390268	1.931674
28	1	0	-1.122250	3.698306	2.668405
29	6	0	0.694776	4.213419	1.650354
30	1	0	0.795791	5.154502	2.173751
31	6	0	1.661624	3.856183	0.713886
32	1	0	2.508203	4.496520	0.511422
33	6	0	3.499034	2.716483	-1.452687
34	1	0	3.221057	3.643911	-1.953283
35	1	0	3.937244	2.034414	-2.175002
36	1	0	4.224806	2.933113	-0.669667
37	6	0	1.594575	-1.710654	0.161675
38	1	0	1.662000	-1.054346	1.011738
39	8	0	2.448695	-2.766657	0.109700

40	8	0	3.318584	-2.251271	2.114965
41	6	0	3.301943	-2.962867	1.150187
42	6	0	4.177372	-4.147409	0.899338
43	1	0	4.764115	-3.977248	-0.002330
44	1	0	3.558680	-5.027156	0.729355
45	1	0	4.831774	-4.303000	1.749622

cis-3bc

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.873330	-0.248365	-0.288064
2	6	0	-1.741233	-1.375425	-0.947578
3	6	0	-0.425834	-2.146223	-1.075875
4	6	0	1.643192	-0.882629	-0.294989
5	6	0	2.596136	-1.815203	-0.712539
6	1	0	2.280541	-2.709792	-1.228526
7	6	0	3.931413	-1.586945	-0.456391
8	1	0	4.681931	-2.299057	-0.770781
9	6	0	4.342529	-0.432803	0.213778
10	6	0	3.392907	0.493598	0.628763
11	1	0	3.679533	1.393925	1.150104
12	6	0	2.045732	0.263331	0.373120
13	1	0	1.316851	0.993260	0.700906
14	6	0	6.128183	0.853413	1.093951
15	1	0	5.861335	1.759753	0.546887
16	1	0	7.208806	0.769673	1.151242
17	1	0	5.712379	0.902253	2.102217
18	6	0	-1.173297	0.015318	1.202139
19	6	0	-1.261090	2.021926	0.118021
20	6	0	-0.910192	1.121535	-0.887347
21	6	0	-0.682080	1.558306	-2.172542
22	1	0	-0.396022	0.863476	-2.952417
23	6	0	-0.821592	2.920263	-2.447225
24	1	0	-0.646837	3.287340	-3.448541
25	6	0	-1.183871	3.804956	-1.441156
26	1	0	-1.291260	4.856464	-1.670207
27	6	0	-1.409848	3.370762	-0.133998
28	1	0	-1.687299	4.065861	0.646039
29	6	0	-1.786785	1.986943	2.577166
30	1	0	-2.778533	2.428404	2.478949
31	1	0	-1.071414	2.764676	2.842983
32	1	0	-1.802000	1.227627	3.353326
33	6	0	-3.720129	-1.328812	0.280234
34	6	0	-4.646552	-2.142936	1.121937
35	1	0	-5.521377	-1.554775	1.375426
36	1	0	-4.119056	-2.439192	2.028431
37	1	0	-4.932178	-3.048560	0.590775
38	7	0	0.280845	-1.104914	-0.547995
39	7	0	-1.399451	1.351488	1.339750
40	8	0	-0.108858	-3.233422	-1.477777
41	8	0	5.676547	-0.302099	0.413794
42	8	0	-1.207950	-0.821783	2.074892
43	8	0	-2.672991	-2.061078	-0.154662
44	8	0	-3.830347	-0.162250	0.011384
45	1	0	-2.181926	-1.048371	-1.888574

(*Z*)-TS1bc

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.103031	-0.149849	0.317751
2	7	0	2.774780	-2.223148	-0.742196
3	8	0	-0.382742	1.662265	2.259506
4	8	0	-4.840240	-2.661084	0.407055
5	8	0	0.583870	-2.851591	-1.011686
6	8	0	-0.295951	3.832405	-0.015528
7	8	0	-1.952432	3.581440	-1.509697
8	6	0	1.212952	-0.708698	0.064499

9	6	0	-0.079823	2.450561	-0.045374
10	1	0	0.160852	1.980402	-0.978410
11	6	0	-0.206880	1.806709	1.110205
12	6	0	-1.144003	-0.813862	0.282733
13	6	0	-2.208422	-0.227936	-0.388798
14	1	0	-2.057468	0.699276	-0.925506
15	6	0	-3.459893	-0.830949	-0.388198
16	1	0	-4.265756	-0.367705	-0.936548
17	6	0	-3.658666	-2.006956	0.329080
18	6	0	-2.596915	-2.573090	1.040143
19	1	0	-2.774357	-3.474911	1.609552
20	6	0	-1.352610	-1.985127	1.013574
21	1	0	-0.532564	-2.420747	1.568303
22	6	0	-5.945284	-2.112733	-0.287456
23	1	0	-5.748756	-2.065399	-1.360022
24	1	0	-6.183727	-1.114172	0.083063
25	1	0	-6.781701	-2.778714	-0.100711
26	6	0	1.423951	-2.083946	-0.610514
27	6	0	3.457490	-1.114381	-0.232947
28	6	0	2.555827	-0.159065	0.252983
29	6	0	3.025841	1.005700	0.835492
30	1	0	2.341654	1.742764	1.229151
31	6	0	4.400678	1.211015	0.900918
32	1	0	4.786665	2.116242	1.346999
33	6	0	5.280214	0.259957	0.397165
34	1	0	6.345586	0.437401	0.454723
35	6	0	4.822902	-0.925816	-0.176158
36	1	0	5.512150	-1.666190	-0.556497
37	6	0	3.417135	-3.356327	-1.367170
38	1	0	2.642024	-4.049696	-1.679106
39	1	0	4.084266	-3.849189	-0.660594
40	1	0	3.989031	-3.034223	-2.237059
41	6	0	-1.282475	4.295657	-0.816085
42	6	0	-1.388135	5.786446	-0.721627
43	1	0	-0.455884	6.235445	-1.061367
44	1	0	-1.536764	6.076932	0.316888
45	1	0	-2.213289	6.133035	-1.333739

(*Z*)-INTbc

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.342176	-0.313345	0.290853
2	6	0	-0.166085	2.665544	0.305640
3	1	0	-0.234559	3.714672	0.541590
4	6	0	0.389515	1.772515	1.151823
5	6	0	-1.050916	-0.209168	0.575184
6	6	0	-1.874014	0.001380	1.678331
7	1	0	-1.481525	0.505295	2.551380
8	6	0	-3.176337	-0.445899	1.648145
9	1	0	-3.832160	-0.307010	2.495714
10	6	0	-3.678559	-1.071509	0.503798
11	6	0	-2.858582	-1.247129	-0.611563
12	1	0	-3.232269	-1.705705	-1.513909
13	6	0	-1.543126	-0.815486	-0.566712
14	1	0	-0.905219	-0.932475	-1.432435
15	6	0	-5.525740	-2.086321	-0.581968
16	1	0	-5.504521	-1.416010	-1.442876
17	1	0	-6.554688	-2.317490	-0.326685
18	1	0	-4.992129	-3.007451	-0.821584
19	6	0	1.425186	-1.836953	0.053530
20	6	0	3.476042	-0.898637	-0.258604
21	6	0	2.684873	0.197567	0.128477
22	6	0	3.251086	1.464654	0.229914
23	1	0	2.663860	2.309799	0.553452
24	6	0	4.599545	1.610377	-0.069142
25	1	0	5.060876	2.584074	0.007273
26	6	0	5.363685	0.513348	-0.452187
27	1	0	6.413785	0.649578	-0.672710
28	6	0	4.814813	-0.764278	-0.553249
29	1	0	5.416175	-1.611718	-0.848810
30	6	0	3.260459	-3.384609	-0.570532
31	1	0	4.032385	-3.636374	0.155808

32	1	0	3.684112	-3.410284	-1.573525
33	1	0	2.448395	-4.101608	-0.500034
34	6	0	-1.993216	2.374567	-1.143580
35	6	0	-2.361628	1.965989	-2.538376
36	1	0	-3.411288	1.691389	-2.569392
37	1	0	-1.736121	1.146356	-2.881620
38	1	0	-2.198191	2.818043	-3.199472
39	7	0	0.273345	0.322966	0.607416
40	7	0	2.720775	-2.072485	-0.291332
41	8	0	0.977461	1.858506	2.238657
42	8	0	-4.967607	-1.460152	0.560198
43	8	0	0.553701	-2.654666	0.197147
44	8	0	-0.664503	2.256177	-0.935729
45	8	0	-2.757904	2.789872	-0.316953

trans-**TS2bc**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.491162	0.574608	-0.498984
2	6	0	1.751647	-0.557414	-0.199439
3	6	0	2.394468	-1.751290	0.126542
4	6	0	3.768441	-1.795859	0.165630
5	6	0	4.521116	-0.649203	-0.114420
6	6	0	3.877076	0.540030	-0.446907
7	7	0	0.337545	-0.513409	-0.238667
8	6	0	-0.460500	-1.604214	-0.692789
9	6	0	-1.538737	-1.677403	0.213434
10	8	0	-2.572766	-2.472514	-0.120259
11	6	0	-3.485445	-2.802421	0.851848
12	6	0	-4.569852	-3.653326	0.281833
13	8	0	5.860574	-0.792702	-0.046394
14	6	0	6.664805	0.341282	-0.320208
15	6	0	-0.406691	0.547628	0.092490
16	6	0	-0.058089	1.441938	1.258383
17	7	0	-0.885691	2.524448	1.152097
18	6	0	-1.707992	2.422118	0.025975
19	6	0	-1.463140	1.214519	-0.646997
20	6	0	-2.631756	3.338962	-0.434514
21	6	0	-3.311024	3.031900	-1.611658
22	6	0	-3.065581	1.846802	-2.300743
23	6	0	-2.143839	0.925072	-1.821044
24	6	0	-0.920205	3.619269	2.092952
25	8	0	0.745662	1.221901	2.139488
26	8	0	-0.207846	-2.286104	-1.681976
27	8	0	-3.375855	-2.425018	1.980188
28	1	0	-1.483167	-1.323766	1.229474
29	1	0	1.809059	-2.631247	0.356619
30	1	0	4.289144	-2.708209	0.420220
31	1	0	4.436328	1.431967	-0.682948
32	1	0	1.985727	1.486688	-0.789590
33	1	0	6.505257	0.695121	-1.340117
34	1	0	7.693805	0.016786	-0.204813
35	1	0	6.453929	1.147743	0.383955
36	1	0	-1.970692	-0.007166	-2.343666
37	1	0	-3.605531	1.636515	-3.213011
38	1	0	-4.041829	3.730248	-1.995643
39	1	0	-2.816800	4.263993	0.093374
40	1	0	-1.911092	3.704239	2.538227
41	1	0	-0.669252	4.555578	1.594891
42	1	0	-0.189762	3.415209	2.870162
43	1	0	-5.270366	-3.921626	1.064416
44	1	0	-4.132830	-4.546564	-0.161926
45	1	0	-5.078229	-3.105266	-0.510331

trans-**3bc**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.763791	-0.385752	0.450075
2	6	0	-1.591326	-1.707355	0.582315
3	1	0	-1.924258	-1.889167	1.603048
4	6	0	-0.288302	-2.418661	0.213868
5	6	0	1.743038	-0.887910	0.028462
6	6	0	2.701900	-1.877601	-0.201456
7	1	0	2.402036	-2.913904	-0.249566
8	6	0	4.023784	-1.520954	-0.363491
9	1	0	4.779372	-2.273830	-0.540922
10	6	0	4.414858	-0.181792	-0.301196
11	6	0	3.459062	0.801424	-0.073735
12	1	0	3.730222	1.844672	-0.021523
13	6	0	2.125532	0.443160	0.089103
14	1	0	1.390120	1.219117	0.259250
15	6	0	6.168864	1.408153	-0.414839
16	1	0	5.695817	2.006421	-1.196010
17	1	0	7.242574	1.389982	-0.572553
18	1	0	5.951143	1.847322	0.560654
19	6	0	-0.725645	0.436345	1.750403
20	6	0	-1.420655	1.824033	0.078727
21	6	0	-1.173209	0.617937	-0.579017
22	6	0	-1.356856	0.509381	-1.939236
23	1	0	-1.160907	-0.424343	-2.450846
24	6	0	-1.800842	1.631797	-2.642416
25	1	0	-1.950564	1.571750	-3.711034
26	6	0	-2.050463	2.823027	-1.976109
27	1	0	-2.396474	3.682520	-2.533991
28	6	0	-1.862551	2.942328	-0.597792
29	1	0	-2.057512	3.874028	-0.085600
30	6	0	-1.308141	2.757755	2.412951
31	1	0	-2.347029	3.084665	2.445964
32	1	0	-0.672699	3.603783	2.152355
33	1	0	-1.017662	2.371611	3.385440
34	6	0	-3.723249	-1.143461	-0.133627
35	6	0	-4.754539	-1.369831	-1.189758
36	1	0	-5.659906	-0.829380	-0.937332
37	1	0	-4.956305	-2.434389	-1.289371
38	1	0	-4.361007	-1.013353	-2.141859
39	7	0	0.394990	-1.235786	0.201094
40	7	0	-1.149233	1.695254	1.447258
41	8	0	0.040426	-3.557541	0.017961
42	8	0	5.736706	0.062288	-0.473869
43	8	0	-0.396560	0.015899	2.835767
44	8	0	-2.619059	-1.898782	-0.349543
45	8	0	-3.800523	-0.390104	0.797941

TSRbc

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.008997	0.041852	-0.572313
2	6	0	-0.104656	1.450837	-0.866424
3	6	0	-1.162974	-0.515676	-0.042872
4	6	0	1.255076	-0.587738	-0.492172
5	6	0	2.404884	0.069527	-0.944357
6	6	0	3.636451	-0.553339	-0.901569
7	6	0	3.757195	-1.857049	-0.427804
8	6	0	2.613067	-2.533689	-0.019125
9	6	0	1.377161	-1.902719	-0.057116
10	8	0	-0.741159	1.873986	-1.809417
11	6	0	0.551454	2.277038	0.099166
12	1	0	1.034747	1.895387	0.985534
13	6	0	-2.441517	-0.589231	-0.628317
14	6	0	-3.308168	-1.141014	0.356467
15	7	0	-2.601608	-1.369637	1.516847
16	6	0	-1.281231	-0.978242	1.356560
17	8	0	-0.431874	-0.986993	2.232115
18	6	0	-2.944414	-0.296140	-1.905206
19	6	0	-4.278044	-0.544415	-2.165434
20	6	0	-5.115519	-1.079270	-1.178177
21	6	0	-4.642099	-1.389298	0.093425
22	6	0	-3.154225	-1.893564	2.742769
23	8	0	5.008138	-2.384590	-0.419900

24	6	0	5.154457	-3.710259	0.050138
25	8	0	0.568598	3.589537	-0.133877
26	8	0	1.713219	3.973598	1.768466
27	6	0	1.196366	4.413380	0.790609
28	6	0	1.103708	5.834422	0.355633
29	1	0	2.347428	1.066728	-1.358565
30	1	0	4.521832	-0.038912	-1.248941
31	1	0	2.662515	-3.554663	0.328040
32	1	0	0.504235	-2.456562	0.253222
33	1	0	-2.290441	0.118554	-2.657841
34	1	0	-4.684017	-0.326402	-3.143195
35	1	0	-6.156382	-1.260909	-1.409357
36	1	0	-5.294809	-1.809488	0.845964
37	1	0	-2.348925	-1.951907	3.469402
38	1	0	-3.936177	-1.236508	3.123526
39	1	0	-3.569695	-2.888389	2.582898
40	1	0	6.213421	-3.940544	-0.012894
41	1	0	4.823342	-3.798063	1.086860
42	1	0	4.592147	-4.411424	-0.569847
43	1	0	1.554443	5.940005	-0.630016
44	1	0	0.054485	6.114139	0.271547
45	1	0	1.608875	6.467775	1.075664

Cartesian coordinates (optimized at the M06-2X(PCM, solvent=toluene)/def-TZVPP level) of all the stationary points collected in the main text associated with the reaction of **1b** and **2c**.

1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.229898	-0.366951	0.000189
2	6	0	-2.135110	0.005367	-0.000074
3	6	0	-0.908454	0.472588	-0.000206
4	1	0	-0.719557	1.532730	0.000127
5	8	0	0.151770	-0.422517	-0.000186
6	8	0	1.575618	1.307946	0.000107
7	6	0	1.388480	0.124825	-0.000027
8	6	0	2.436955	-0.944277	0.000080
9	1	0	2.315019	-1.574129	-0.879550
10	1	0	2.315020	-1.573915	0.879867
11	1	0	3.418367	-0.483525	0.000038

(*E*)-2c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.058281	-1.620411	-0.005015
2	7	0	-3.422538	-0.660346	0.032400
3	8	0	5.001426	0.622767	0.436984
4	8	0	-2.676097	-2.835750	0.065882
5	6	0	-1.117813	-0.932978	0.005670
6	6	0	1.211013	-1.016972	0.078016
7	6	0	2.161746	-1.295262	-0.893324
8	1	0	1.895436	-1.939962	-1.719729
9	6	0	3.436664	-0.746168	-0.820696
10	1	0	4.148313	-0.964298	-1.602478
11	6	0	3.782334	0.054533	0.262878
12	6	0	2.842182	0.300655	1.265265
13	1	0	3.134422	0.906017	2.112320
14	6	0	1.570542	-0.224393	1.171148
15	1	0	0.843281	-0.033315	1.949774
16	6	0	5.985344	0.376836	-0.545622
17	1	0	5.668608	0.749955	-1.522094
18	1	0	6.208124	-0.689666	-0.620955
19	1	0	6.875149	0.910428	-0.225988
20	6	0	-2.471370	-1.649901	0.033548
21	6	0	-2.834474	0.602963	-0.040499
22	6	0	-1.432956	0.507823	-0.048877
23	6	0	-0.671346	1.658215	-0.178469
24	1	0	0.407001	1.608365	-0.208492
25	6	0	-1.316295	2.889302	-0.270040
26	1	0	-0.731661	3.792918	-0.367300
27	6	0	-2.702131	2.963630	-0.233229
28	1	0	-3.186789	3.928498	-0.298468
29	6	0	-3.486604	1.817382	-0.122833
30	1	0	-4.565816	1.877331	-0.111300
31	6	0	-4.844240	-0.900072	0.045620
32	1	0	-4.997336	-1.974216	0.099763
33	1	0	-5.307322	-0.512974	-0.862790
34	1	0	-5.303887	-0.423477	0.911776

TSic

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.178868	-0.319481	-0.003308
2	7	0	-3.209810	-1.257299	0.026550

3	8	0	5.674749	-0.174820	-0.028289
4	8	0	-1.478689	-2.778042	0.038375
5	6	0	-1.060358	-0.345103	0.002146
6	6	0	1.529986	-0.247912	-0.009489
7	6	0	2.201266	0.978498	0.067926
8	1	0	1.614938	1.885016	0.131792
9	6	0	3.584132	1.046177	0.070609
10	1	0	4.070502	2.007408	0.137080
11	6	0	4.327362	-0.131462	-0.017848
12	6	0	3.675583	-1.367179	-0.101963
13	1	0	4.276844	-2.263263	-0.168492
14	6	0	2.302371	-1.423213	-0.091828
15	1	0	1.781453	-2.369343	-0.148628
16	6	0	6.382451	1.046843	0.058163
17	1	0	6.154125	1.565840	0.990942
18	1	0	6.147447	1.695922	-0.787443
19	1	0	7.436211	0.788057	0.035205
20	6	0	-1.891680	-1.642918	0.024371
21	6	0	-3.327846	0.136565	0.004134
22	6	0	-2.063508	0.737905	-0.010363
23	6	0	-1.944384	2.111693	-0.035167
24	1	0	-0.963949	2.570757	-0.048059
25	6	0	-3.102748	2.887163	-0.044527
26	1	0	-3.032769	3.965649	-0.064034
27	6	0	-4.350963	2.277493	-0.029006
28	1	0	-5.242130	2.890727	-0.036416
29	6	0	-4.486214	0.888237	-0.004476
30	1	0	-5.462430	0.423505	0.006981
31	6	0	-4.327784	-2.166764	0.044200
32	1	0	-3.930942	-3.178116	0.061494
33	1	0	-4.944892	-2.034727	-0.845468
34	1	0	-4.942293	-2.003211	0.930367

(*Z*)-2c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.044514	-1.046998	-0.053710
2	7	0	2.436126	1.495965	0.182345
3	8	0	-5.388415	0.410883	-0.312552
4	8	0	0.212243	2.051391	0.264889
5	6	0	0.973560	-0.295112	-0.036527
6	6	0	-1.377976	-0.615780	-0.102143
7	6	0	-2.305207	-1.332745	0.645666
8	1	0	-1.954135	-2.150840	1.259983
9	6	0	-3.653945	-1.004960	0.627016
10	1	0	-4.343458	-1.565303	1.239811
11	6	0	-4.095316	0.022802	-0.200358
12	6	0	-3.177473	0.711959	-0.996858
13	1	0	-3.544086	1.491391	-1.650409
14	6	0	-1.836706	0.404298	-0.942540
15	1	0	-1.135491	0.942295	-1.563186
16	6	0	-6.348501	-0.269043	0.468459
17	1	0	-6.136425	-0.160919	1.534325
18	1	0	-6.383937	-1.330179	0.212441
19	1	0	-7.305929	0.189869	0.241728
20	6	0	1.089295	1.231758	0.136177
21	6	0	3.197274	0.329442	0.061325
22	6	0	2.357075	-0.779540	-0.063826
23	6	0	2.883018	-2.048081	-0.196841
24	1	0	2.222929	-2.899409	-0.295960
25	6	0	4.268541	-2.196305	-0.197572
26	1	0	4.706198	-3.179414	-0.297839
27	6	0	5.093396	-1.085174	-0.070259
28	1	0	6.166999	-1.217479	-0.072836
29	6	0	4.571767	0.202674	0.061152
30	1	0	5.220925	1.061440	0.160377
31	6	0	2.991442	2.812319	0.378279
32	1	0	2.165424	3.512998	0.459377
33	1	0	3.622661	3.089725	-0.466443
34	1	0	3.584951	2.843793	1.292584

(*E*)-TS1bc

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.068891	0.325256	0.451540
2	7	0	3.358608	1.536619	0.190377
3	8	0	-1.212377	1.591185	2.253572
4	8	0	-2.510316	-4.581343	0.451650
5	8	0	1.589115	2.786563	0.960767
6	8	0	-2.463110	3.213759	-0.033017
7	8	0	-3.519048	2.248078	-1.761498
8	6	0	1.315861	0.444629	0.248103
9	6	0	-1.479206	2.220123	-0.085146
10	1	0	-1.048948	1.982559	-1.038181
11	6	0	-1.102949	1.677064	1.076993
12	6	0	-0.587901	-0.931825	0.407212
13	6	0	-1.667407	-1.121750	-0.441368
14	1	0	-1.993885	-0.315014	-1.083405
15	6	0	-2.326724	-2.343966	-0.465494
16	1	0	-3.154826	-2.477957	-1.144262
17	6	0	-1.926270	-3.364615	0.392586
18	6	0	-0.863152	-3.153238	1.275025
19	1	0	-0.585372	-3.947834	1.953205
20	6	0	-0.198662	-1.946748	1.281209
21	1	0	0.620320	-1.774911	1.967251
22	6	0	-3.608587	-4.829867	-0.404181
23	1	0	-3.315584	-4.744880	-1.452557
24	1	0	-4.429199	-4.140025	-0.198595
25	1	0	-3.928627	-5.846353	-0.198444
26	6	0	2.048963	1.770464	0.519144
27	6	0	3.538768	0.237640	-0.281136
28	6	0	2.333008	-0.483101	-0.252208
29	6	0	2.293668	-1.781850	-0.740297
30	1	0	1.373426	-2.346666	-0.745290
31	6	0	3.466051	-2.351577	-1.223819
32	1	0	3.451929	-3.363205	-1.602613
33	6	0	4.654834	-1.631868	-1.217654
34	1	0	5.558767	-2.094991	-1.589617
35	6	0	4.710564	-0.320958	-0.750594
36	1	0	5.634794	0.238985	-0.763079
37	6	0	4.407518	2.521881	0.303800
38	1	0	3.967720	3.427613	0.711049
39	1	0	4.837920	2.734995	-0.674823
40	1	0	5.191259	2.166082	0.972294
41	6	0	-3.454260	3.116874	-0.932383
42	6	0	-4.432067	4.244093	-0.774408
43	1	0	-5.263328	4.102810	-1.456538
44	1	0	-3.931122	5.187351	-0.988604
45	1	0	-4.784144	4.283960	0.254690

(*E*)-INTbc

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.225546	-0.774465	0.057294
2	6	0	-2.230915	-1.441698	-0.001400
3	1	0	-2.535165	-0.584194	0.570108
4	6	0	-0.965694	-1.688237	-0.474451
5	6	0	-0.537927	0.781047	-0.084264
6	6	0	-1.189429	1.292899	-1.203493
7	1	0	-1.336883	0.663791	-2.070150
8	6	0	-1.616920	2.603217	-1.199009
9	1	0	-2.115908	3.031078	-2.056724
10	6	0	-1.418324	3.405373	-0.071322
11	6	0	-0.784166	2.880429	1.055753
12	1	0	-0.641351	3.475170	1.944567
13	6	0	-0.343515	1.566570	1.039349
14	1	0	0.148120	1.144521	1.905952
15	6	0	-1.712666	5.518202	0.960817
16	1	0	-2.235921	5.120704	1.832132

17	1	0	-2.146369	6.472716	0.681099
18	1	0	-0.655567	5.652608	1.197806
19	6	0	1.784442	-2.113468	0.501873
20	6	0	3.502005	-0.699491	0.024472
21	6	0	2.353334	0.106021	-0.137001
22	6	0	2.495728	1.432820	-0.539857
23	1	0	1.633960	2.069824	-0.676916
24	6	0	3.770789	1.934567	-0.755441
25	1	0	3.894597	2.962793	-1.063185
26	6	0	4.891721	1.129480	-0.568655
27	1	0	5.877154	1.544514	-0.731724
28	6	0	4.774403	-0.200971	-0.179872
29	1	0	5.646692	-0.825497	-0.049301
30	6	0	4.085794	-3.024927	0.762510
31	1	0	4.691280	-2.705062	1.611405
32	1	0	4.739391	-3.271392	-0.073771
33	1	0	3.509506	-3.902483	1.040976
34	6	0	-4.454857	-2.139732	0.105126
35	6	0	-5.348876	-3.282204	-0.267680
36	1	0	-6.369739	-3.051236	0.015980
37	1	0	-5.011665	-4.185023	0.239740
38	1	0	-5.282979	-3.463708	-1.339156
39	7	0	-0.053327	-0.561157	-0.085651
40	7	0	3.153156	-1.991236	0.383579
41	8	0	-0.487501	-2.613288	-1.124949
42	8	0	-1.876795	4.668454	-0.159335
43	8	0	1.190928	-3.035252	0.990884
44	8	0	-3.184838	-2.383790	-0.279599
45	8	0	-4.790644	-1.135495	0.671397

cis-TS2bc

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.126044	-0.419329	-0.611786
2	7	0	2.359877	2.122742	-0.849380
3	8	0	0.204598	-2.493478	-1.654935
4	8	0	-5.640735	-0.309297	-0.093307
5	8	0	2.332992	0.272997	-2.220512
6	6	0	0.638366	0.650161	-0.471741
7	6	0	0.573829	-1.670560	-0.831862
8	6	0	-1.540989	-0.410911	-0.478765
9	6	0	-2.166782	-1.434377	0.213614
10	1	0	-1.571581	-2.229696	0.641906
11	6	0	-3.544303	-1.436073	0.362333
12	1	0	-4.013827	-2.240301	0.907107
13	6	0	-4.298146	-0.400889	-0.188569
14	6	0	-3.662022	0.622456	-0.896984
15	1	0	-4.267132	1.404628	-1.332982
16	6	0	-2.292777	0.613277	-1.048276
17	1	0	-1.797928	1.392528	-1.612453
18	6	0	-6.327592	-1.336617	0.595863
19	1	0	-6.010297	-1.387750	1.639230
20	1	0	-6.165553	-2.304280	0.117609
21	1	0	-7.381019	-1.080140	0.549336
22	6	0	1.885492	0.903431	-1.294934
23	6	0	1.510440	2.677164	0.095573
24	6	0	0.415199	1.823355	0.333801
25	6	0	-0.549318	2.173372	1.273516
26	1	0	-1.391946	1.524113	1.467722
27	6	0	-0.416461	3.379521	1.946674
28	1	0	-1.160010	3.672908	2.673604
29	6	0	0.665018	4.218646	1.687668
30	1	0	0.745493	5.157984	2.217897
31	6	0	1.649050	3.879046	0.762871
32	1	0	2.489622	4.532070	0.575328
33	6	0	3.532425	2.772399	-1.383205
34	1	0	3.263830	3.710341	-1.870401
35	1	0	3.977583	2.102847	-2.113470
36	1	0	4.250457	2.973619	-0.588116
37	6	0	1.601262	-1.716084	0.119499
38	1	0	1.656951	-1.080438	0.986476
39	8	0	2.415264	-2.798635	0.078318

40	8	0	3.191478	-2.392988	2.147998
41	6	0	3.189564	-3.074161	1.163330
42	6	0	3.996715	-4.310622	0.928490
43	1	0	4.623398	-4.173881	0.048556
44	1	0	3.325944	-5.144617	0.726270
45	1	0	4.606579	-4.517821	1.800666

cis-3bc

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.870855	-0.244490	-0.292871
2	6	0	-1.734188	-1.365282	-0.970380
3	6	0	-0.411289	-2.121058	-1.128908
4	6	0	1.646375	-0.869734	-0.297355
5	6	0	2.601128	-1.804692	-0.706163
6	1	0	2.285741	-2.700109	-1.221075
7	6	0	3.934267	-1.577687	-0.440387
8	1	0	4.687327	-2.290658	-0.746263
9	6	0	4.341979	-0.423827	0.231533
10	6	0	3.391027	0.504049	0.638182
11	1	0	3.675564	1.404209	1.161067
12	6	0	2.045350	0.275973	0.372289
13	1	0	1.313629	1.006314	0.692783
14	6	0	6.123205	0.854110	1.127314
15	1	0	5.864957	1.763910	0.580719
16	1	0	7.203260	0.767596	1.194893
17	1	0	5.698782	0.903058	2.132604
18	6	0	-1.186794	0.009766	1.195722
19	6	0	-1.281985	2.022686	0.118353
20	6	0	-0.912142	1.128603	-0.885902
21	6	0	-0.672139	1.571785	-2.166138
22	1	0	-0.368407	0.881253	-2.943396
23	6	0	-0.821341	2.932706	-2.439943
24	1	0	-0.637904	3.304076	-3.438099
25	6	0	-1.204806	3.810580	-1.436518
26	1	0	-1.321054	4.861412	-1.664569
27	6	0	-1.441189	3.370498	-0.133445
28	1	0	-1.736281	4.060802	0.644476
29	6	0	-1.858617	1.965157	2.564424
30	1	0	-2.863585	2.371866	2.446783
31	1	0	-1.177008	2.766328	2.850303
32	1	0	-1.863788	1.201390	3.336796
33	6	0	-3.686794	-1.364989	0.298987
34	6	0	-4.569518	-2.203904	1.164366
35	1	0	-5.454697	-1.640074	1.437014
36	1	0	-4.008274	-2.477329	2.057909
37	1	0	-4.839318	-3.121434	0.645709
38	7	0	0.286712	-1.091930	-0.559854
39	7	0	-1.423182	1.348297	1.335499
40	8	0	-0.084381	-3.184483	-1.576211
41	8	0	5.675555	-0.295993	0.441751
42	8	0	-1.232857	-0.826185	2.065418
43	8	0	-2.645356	-2.077729	-0.178055
44	8	0	-3.825447	-0.197812	0.049603
45	1	0	-2.193813	-1.021065	-1.896189

(*Z*)-TS1bc

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.090084	-0.153565	0.330721
2	7	0	2.752495	-2.218212	-0.773585
3	8	0	-0.213024	1.703571	2.236545
4	8	0	-4.875550	-2.615583	0.407749
5	8	0	0.560452	-2.845270	-1.030696
6	8	0	-0.219775	3.797191	-0.092775
7	8	0	-1.992013	3.552813	-1.451105
8	6	0	1.197623	-0.720845	0.079313

9	6	0	-0.040422	2.409817	-0.103999
10	1	0	0.106447	1.914937	-1.043591
11	6	0	-0.114594	1.788954	1.071077
12	6	0	-1.164974	-0.799768	0.295236
13	6	0	-2.239409	-0.165812	-0.315380
14	1	0	-2.094941	0.789132	-0.802615
15	6	0	-3.495736	-0.756750	-0.316949
16	1	0	-4.309255	-0.254818	-0.817707
17	6	0	-3.689817	-1.969308	0.337270
18	6	0	-2.618116	-2.584693	0.989927
19	1	0	-2.793688	-3.514674	1.512223
20	6	0	-1.369837	-2.008468	0.964774
21	1	0	-0.543216	-2.481052	1.477272
22	6	0	-5.988854	-2.022108	-0.229372
23	1	0	-5.817137	-1.918340	-1.302647
24	1	0	-6.210116	-1.042521	0.199065
25	1	0	-6.827463	-2.690121	-0.059360
26	6	0	1.399013	-2.083505	-0.622203
27	6	0	3.440781	-1.126572	-0.239802
28	6	0	2.544427	-0.182137	0.277847
29	6	0	3.024015	0.960253	0.896516
30	1	0	2.347829	1.684980	1.324461
31	6	0	4.400076	1.156902	0.961098
32	1	0	4.791435	2.045155	1.435669
33	6	0	5.273217	0.220262	0.422175
34	1	0	6.339641	0.391808	0.479633
35	6	0	4.807375	-0.945031	-0.184445
36	1	0	5.490894	-1.676993	-0.590814
37	6	0	3.382417	-3.338181	-1.430813
38	1	0	2.599028	-4.017705	-1.753500
39	1	0	4.052421	-3.854551	-0.743182
40	1	0	3.949836	-2.999441	-2.297845
41	6	0	-1.257310	4.262907	-0.823810
42	6	0	-1.331029	5.758087	-0.746909
43	1	0	-0.407094	6.187050	-1.131704
44	1	0	-1.428932	6.063607	0.293534
45	1	0	-2.177540	6.110179	-1.325902

(*Z*)-INTbc

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.362496	-0.313217	0.238589
2	6	0	-0.261573	2.655313	0.347728
3	1	0	-0.353081	3.690182	0.631460
4	6	0	0.393650	1.759687	1.119905
5	6	0	-1.029465	-0.245147	0.511358
6	6	0	-1.883835	0.022978	1.579214
7	1	0	-1.524445	0.598747	2.421252
8	6	0	-3.172450	-0.462694	1.556936
9	1	0	-3.851507	-0.278358	2.376856
10	6	0	-3.630188	-1.192479	0.457697
11	6	0	-2.781362	-1.427726	-0.625007
12	1	0	-3.121890	-1.967915	-1.494844
13	6	0	-1.482732	-0.949837	-0.590603
14	1	0	-0.826494	-1.108556	-1.435405
15	6	0	-5.418502	-2.356636	-0.571914
16	1	0	-5.405001	-1.760628	-1.486582
17	1	0	-6.443768	-2.604207	-0.316337
18	1	0	-4.848237	-3.274762	-0.725343
19	6	0	1.488001	-1.838348	0.057074
20	6	0	3.522651	-0.858549	-0.259458
21	6	0	2.693397	0.228169	0.070276
22	6	0	3.219550	1.514711	0.118347
23	1	0	2.604120	2.355517	0.396758
24	6	0	4.567633	1.687597	-0.172926
25	1	0	4.997322	2.677992	-0.135486
26	6	0	5.370578	0.599798	-0.492653
27	1	0	6.419644	0.758049	-0.703833
28	6	0	4.860839	-0.697599	-0.541914
29	1	0	5.491362	-1.539552	-0.789135
30	6	0	3.375600	-3.360336	-0.463945
31	1	0	4.141876	-3.561354	0.284581

32	1	0	3.817102	-3.424012	-1.458181
33	1	0	2.579183	-4.092808	-0.371749
34	6	0	-2.172599	2.550535	-1.002231
35	6	0	-2.663358	2.098659	-2.346179
36	1	0	-3.725492	2.301150	-2.431363
37	1	0	-2.470641	1.033241	-2.463748
38	1	0	-2.117440	2.625449	-3.127730
39	7	0	0.280073	0.312251	0.539056
40	7	0	2.800326	-2.052536	-0.253874
41	8	0	1.070636	1.834506	2.147351
42	8	0	-4.907342	-1.618821	0.520981
43	8	0	0.642681	-2.679951	0.212305
44	8	0	-0.861902	2.263403	-0.850414
45	8	0	-2.828497	3.108933	-0.168874

trans-**TS2bc**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.496901	0.611303	-0.471412
2	6	0	1.751779	-0.527602	-0.217418
3	6	0	2.390129	-1.734829	0.065391
4	6	0	3.763106	-1.784863	0.111569
5	6	0	4.520421	-0.631180	-0.119145
6	6	0	3.881960	0.570724	-0.412008
7	7	0	0.339067	-0.478882	-0.263054
8	6	0	-0.457353	-1.578107	-0.724440
9	6	0	-1.514688	-1.682359	0.203544
10	8	0	-2.523879	-2.519851	-0.105767
11	6	0	-3.406037	-2.872514	0.883430
12	6	0	-4.462728	-3.776414	0.338755
13	8	0	5.859894	-0.781407	-0.046833
14	6	0	6.667015	0.358784	-0.265386
15	6	0	-0.404023	0.578891	0.071385
16	6	0	-0.065045	1.473539	1.238835
17	7	0	-0.925072	2.537868	1.145521
18	6	0	-1.753581	2.421428	0.027210
19	6	0	-1.482378	1.224306	-0.655151
20	6	0	-2.704538	3.316336	-0.421494
21	6	0	-3.382939	3.000126	-1.596429
22	6	0	-3.109077	1.827764	-2.295857
23	6	0	-2.160463	0.927278	-1.828965
24	6	0	-0.980501	3.617891	2.099969
25	8	0	0.749479	1.275148	2.111506
26	8	0	-0.209072	-2.239262	-1.723045
27	8	0	-3.300828	-2.477735	2.005504
28	1	0	-1.457651	-1.317089	1.215355
29	1	0	1.800598	-2.621847	0.252852
30	1	0	4.281114	-2.707241	0.332712
31	1	0	4.445422	1.469031	-0.610984
32	1	0	1.995437	1.534366	-0.732012
33	1	0	6.519619	0.755695	-1.271779
34	1	0	7.694737	0.028381	-0.153148
35	1	0	6.451128	1.137328	0.468866
36	1	0	-1.963125	0.004620	-2.360102
37	1	0	-3.647349	1.610571	-3.207526
38	1	0	-4.134544	3.681384	-1.970993
39	1	0	-2.910612	4.232338	0.114602
40	1	0	-1.968183	3.669786	2.558465
41	1	0	-0.761422	4.568951	1.613873
42	1	0	-0.235649	3.422431	2.866160
43	1	0	-5.138642	-4.064592	1.135908
44	1	0	-3.995181	-4.654940	-0.103204
45	1	0	-5.006189	-3.260221	-0.451520

trans-**3bc**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.756877	-0.390331	0.448295
2	6	0	-1.579144	-1.715585	0.575124
3	1	0	-1.907036	-1.900480	1.597038
4	6	0	-0.273619	-2.421779	0.201181
5	6	0	1.751796	-0.879572	0.032003
6	6	0	2.714089	-1.866187	-0.197698
7	1	0	2.415345	-2.902883	-0.246906
8	6	0	4.034714	-1.505289	-0.356468
9	1	0	4.794315	-2.254172	-0.532974
10	6	0	4.421688	-0.165467	-0.291091
11	6	0	3.463005	0.814177	-0.063994
12	1	0	3.731845	1.857925	-0.009061
13	6	0	2.130020	0.451998	0.095582
14	1	0	1.390475	1.223932	0.266269
15	6	0	6.172714	1.425503	-0.394911
16	1	0	5.701920	2.027725	-1.175233
17	1	0	7.247234	1.410620	-0.549041
18	1	0	5.951556	1.861785	0.581740
19	6	0	-0.737785	0.430332	1.749960
20	6	0	-1.437639	1.813294	0.072866
21	6	0	-1.168925	0.610342	-0.583084
22	6	0	-1.336803	0.500485	-1.944678
23	1	0	-1.121482	-0.431073	-2.452726
24	6	0	-1.788446	1.616614	-2.653102
25	1	0	-1.924585	1.555447	-3.723528
26	6	0	-2.061496	2.803585	-1.989208
27	1	0	-2.413937	3.658330	-2.550510
28	6	0	-1.888587	2.924878	-0.609342
29	1	0	-2.102554	3.853449	-0.098847
30	6	0	-1.376355	2.737142	2.411380
31	1	0	-2.425235	3.033121	2.435609
32	1	0	-0.763023	3.604849	2.167520
33	1	0	-1.086062	2.349706	3.383785
34	6	0	-3.711308	-1.142724	-0.127264
35	6	0	-4.748160	-1.359782	-1.181756
36	1	0	-5.660516	-0.842774	-0.905996
37	1	0	-4.930201	-2.424209	-1.313735
38	1	0	-4.368914	-0.965243	-2.124777
39	7	0	0.405629	-1.233040	0.200561
40	7	0	-1.174819	1.688611	1.440907
41	8	0	0.059266	-3.554980	-0.004946
42	8	0	5.744175	0.082017	-0.460786
43	8	0	-0.417595	0.018032	2.837489
44	8	0	-2.612377	-1.902752	-0.352099
45	8	0	-3.783731	-0.391674	0.805132

TSRbc

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.010756	0.032345	-0.557884
2	6	0	-0.105034	1.442068	-0.853193
3	6	0	-1.166360	-0.530142	-0.040878
4	6	0	1.256615	-0.590228	-0.486353
5	6	0	2.391974	0.067991	-0.973258
6	6	0	3.629854	-0.541628	-0.942468
7	6	0	3.771618	-1.833709	-0.444610
8	6	0	2.641952	-2.511850	-0.000812
9	6	0	1.399371	-1.894593	-0.027696
10	8	0	-0.736575	1.868561	-1.795658
11	6	0	0.552884	2.263747	0.116917
12	1	0	1.037855	1.880109	1.001765
13	6	0	-2.447006	-0.580218	-0.628280
14	6	0	-3.318556	-1.146894	0.343387
15	7	0	-2.615388	-1.404648	1.498941
16	6	0	-1.288618	-1.019626	1.348877
17	8	0	-0.445625	-1.051872	2.227000
18	6	0	-2.946700	-0.257224	-1.898464
19	6	0	-4.281843	-0.491555	-2.165331
20	6	0	-5.123699	-1.041839	-1.191975
21	6	0	-4.653346	-1.381595	0.073039
22	6	0	-3.168223	-1.945415	2.715394
23	8	0	5.027658	-2.349044	-0.450011

24	6	0	5.196466	-3.659703	0.045991
25	8	0	0.566006	3.579197	-0.111286
26	8	0	1.713836	3.964520	1.790369
27	6	0	1.189831	4.399892	0.815232
28	6	0	1.084651	5.823925	0.385822
29	1	0	2.314101	1.055329	-1.407367
30	1	0	4.504299	-0.029190	-1.318799
31	1	0	2.708538	-3.523798	0.369129
32	1	0	0.539369	-2.448587	0.314705
33	1	0	-2.289476	0.171253	-2.640312
34	1	0	-4.684534	-0.248929	-3.138616
35	1	0	-6.165489	-1.211871	-1.428033
36	1	0	-5.309116	-1.814024	0.816032
37	1	0	-2.366381	-1.996932	3.446890
38	1	0	-3.961945	-1.302103	3.096489
39	1	0	-3.569214	-2.945263	2.546501
40	1	0	6.256535	-3.881249	-0.031638
41	1	0	4.886111	-3.728330	1.091016
42	1	0	4.630438	-4.381704	-0.547020
43	1	0	1.543262	5.939681	-0.595134
44	1	0	0.033902	6.094409	0.291694
45	1	0	1.577386	6.458015	1.113955

Standard States

Inclusion of solvent effects in the calculations involves, aside the computation of the solvation free energies, the conversion from the gas phase standard state (P=1 atm) to the solution standard state (1 M). It is found (See rf. 13 of the main text) that the relation between Gibbs free energies of activation in solution at 298.15 K and under both standard states is given by:

$$\Delta Ga_s^* = \Delta Ga_s^0 - 1.9\Delta n \qquad (1)$$

Where ΔGa_s^* and ΔGa_s^0 are the activation Gibbs energies in solution (in kcal/mol) at the 1 M and 1 atm standard states, respectively, and Δn is an stechiometric term given by

$$\Delta n = 1 - \sum_i^{reac\,tan\,ts} n_i \qquad (2)$$

Similarly, the Gibbs energies of reaction in solution at the computed temperature under both standard states can be converted as follows:

$$\Delta Grxn_s^* = \Delta Grxn_s^0 - 1.9\Delta n \qquad (3)$$

In this latter case, the stechiometric term is given by

$$\Delta n = \sum_i^{products} n_i - \sum_j^{reac\,tan\,ts} n_j \qquad (4)$$

Table S2. Calculated kinetic constants[a] (kn) associated with the reaction of ketenes **1a,b** and imines **2a,b,c**.

k_n	**1a+2a→3aa** (195.15 K)	**1b+2b→3bb** (195.15 K)	**1b+2b→3bb** (298.15 K)	**1b+2c→3bc** (298.15 K)	**1b+2c→3bc** (384.15 K)
k_i	7.3178 x 10^{-10}	4.5706 x 10^{-08}	6.9492 x 10^{-08}	4.6187 x 10^{-01}	8.7620 x 10^{+02}
k_{-i}	2.2730 x 10^{-04}	6.2862 x 10^{-05}	8.3841 x 10^{-08}	2.5002 x 10^{+00}	1.4801 x 10^{+03}
k_1^E	1.8657 x 10^{-01}	7.0964 x 10^{+01}	1.1929 x 10^{+00}	5.2261 x 10^{+01}	5.5887 x 10^{+01}
k_{-1}^E	2.1930 x 10^{+07}	1.2381 x 10^{+04}	1.8568 x 10^{+01}	2.7940 x 10^{+10}	3.1985 x 10^{+12}
k_2^c	1.6603 x 10^{+06}	1.0968 x 10^{-02}	5.0726 x 10^{-05}	4.4318 x 10^{+12}	6.1595 x 10^{+12}
k_1^Z	6.6450 x 10^{-02}	3.4067 x 10^{+03}	1.8568 x 10^{+01}	5.2261 x 10^{+01}	2.6936 x 10^{+02}
k_{-1}^Z	1.6603 x 10^{+06}	1.6027 x 10^{+04}	5.3198 x 10^{+02}	3.9167 x 10^{+10}	1.4835 x 10^{+10}
k_2^t	1.0528 x 10^{+09}	4.3216 x 10^{+02}	2.5191 x 10^{+01}	1.4218 x 10^{+10}	6.6363 x 10^{+11}
k_R	7.1793 x 10^{-18}	1.2364 x 10^{-28}	1.9449 x 10^{-15}	3.4049 x 10^{+05}	2.8207 x 10^{+08}
k_{-R}	8.4883 x 10^{-19}	3.3154 x 10^{-29}	5.9634 x 10^{-16}	4.7731 x 10^{+05}	6.9396 x 10^{+07}

Full reference 28 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

Supplementary Figures.

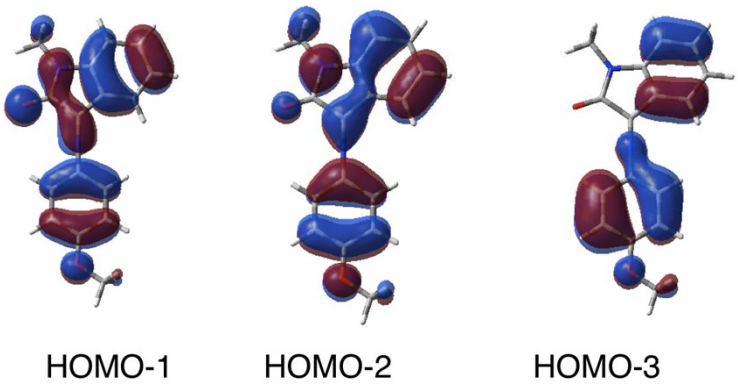
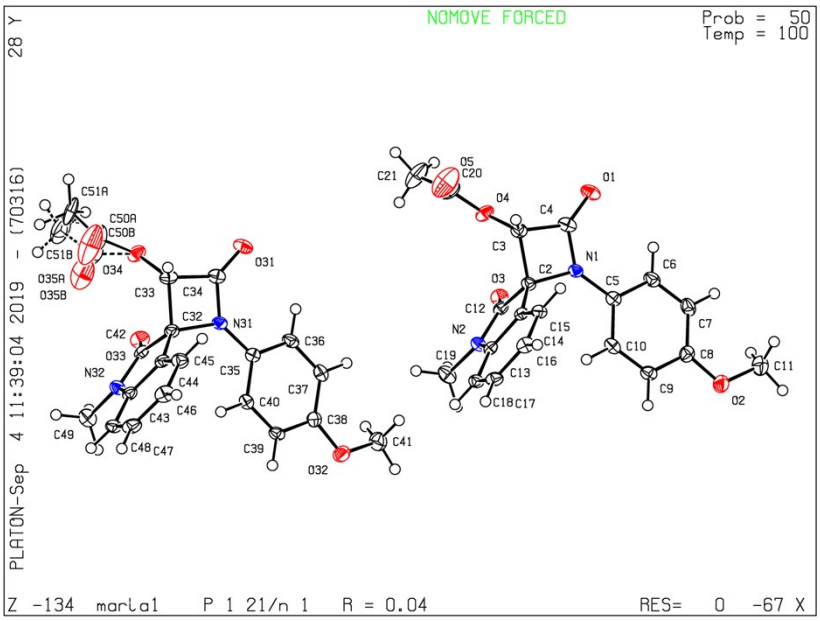


Figure S1. Relevant Kohn–Sham MOs of TSic.

X-ray structure of compounds cis–3bc and trans-3bc

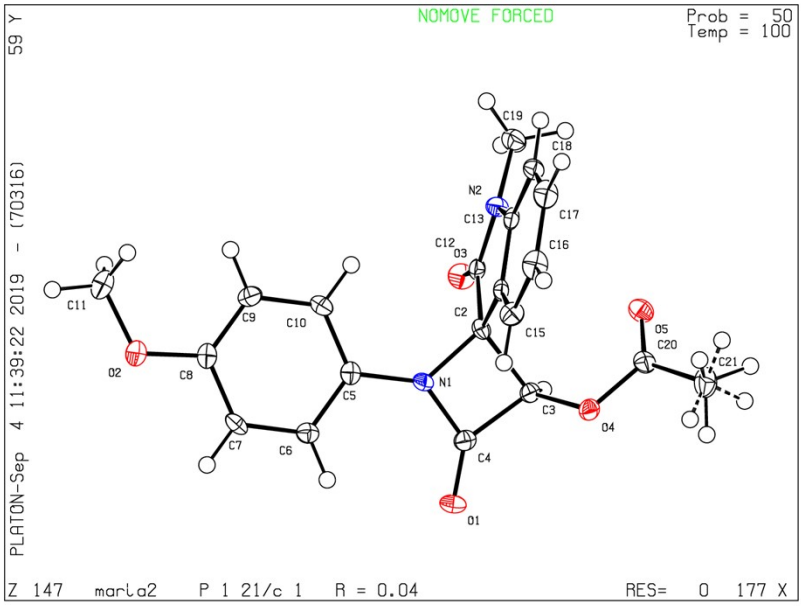
cis–3bc

```
Bond precision:                          C-C = 0.0027 A                                                    Wavelength=0.71073
Cell:              a=20.945(4)        b=8.7506(13)          c=21.976(4)
                   alpha=90           beta=116.49(2)        gamma=90
Temperature:       100 K
                                  Calculated                    Reported
 Volume                           3604.9(13)                    3604.9(11)
 Space group                      P 21/n                        P 1 21/n 1
 Hall group                       -P 2yn                        -P 2yn
 Moiety formula                   C20 H18 N2 O5                 C20 H18 N2 O5
 Sum formula                      C20 H18 N2 O5                 C20 H18 N2 O5
 Mr                               366.36                        366.36
 Dx,g cm-3                        1.350                         1.350
 Z                                8                             8
 Mu (mm-1)                        0.098                         0.098
 F000                             1536.0                        1536.0
 F000'                            1536.80
 h,k,lmax                         24,10,26                      24,10,26
 Nref                             6345                          6336
 Tmin,Tmax                        0.969,0.993                   0.922,1.000
 Tmin'                            0.966
Correction method= # Reported T Limits: Tmin=0.922 Tmax=1.000 AbsCorr = MULTI-SCAN
Data completeness= 0.999                                        Theta(max)= 25.000
R(reflections)= 0.0384( 3782)                                   wR2(reflections)= 0.0764( 6336)
S = 0.829                                  Npar= 520
```



trans–**3bc**

```
Bond precision:                                C-C = 0.0024 A                  Wavelength=0.71073
Cell:              a=10.9199(12)       b=20.1342(16)          c=8.5465(9)
                   alpha=90            beta=107.303(12)       gamma=90
Temperature:       100 K
                                 Calculated                      Reported
Volume                           1794.0(3)                       1794.0(3)
Space group                      P 21/c                          P 1 21/c 1
Hall group                       -P 2ybc                         -P 2ybc
Moiety formula                   C20 H18 N2 O5                   C20 H18 N2 O5
Sum formula                      C20 H18 N2 O5                   C20 H18 N2 O5
Mr                               366.36                          366.36
Dx,g cm-3                        1.357                           1.357
Z                                4                               4
Mu (mm-1)                        0.099                           0.099
F000                             768.0                           768.0
F000'                            768.40
h,k,lmax                         13,25,10                        13,25,10
Nref                             3674                            3671
Tmin,Tmax                        0.980,0.993                     0.659,1.000
Tmin'                            0.956
Correction method= # Reported T Limits: Tmin=0.659 Tmax=1.000 AbsCorr = MULTI-SCAN
Data completeness= 0.999                                         Theta(max)= 26.370
R(reflections)= 0.0421( 2256)                                    wR2(reflections)= 0.0906( 3671)
S = 0.834                                  Npar= 248
```



NMR approximate determination of the (E)–/(Z)–2c equilibrium barrier

The (*E*)–/(*Z*)–**2c** dynamic equilibrium was analyzed experimentally. For that ^{1}H-NMR spectra of a 3:1 (*E*)–/(*Z*)–**2c** mixture was recorded at different temperatures. The effect of the temperature increase was clearly shown on the evolution of the signals of the methyl groups. The N–methyl group signals (initial difference of 46.4 Hz between (*E*)–**2c** and (*Z*)–**2c** signals) coalesce at 393 K, whereas the methoxy moiety signals (initial difference of 46.4 Hz between (*E*)–**2c** and (*Z*)–**2c** signals) coalesce at 373 K.

At this temperature, the kinetic constant to the exchange process can be approximated to :

$$k_{exch} = \frac{\pi \Delta \nu_0}{\sqrt{2}} \qquad (5)$$

Combination of the results obtained with eq .5 and Eyring equation (eq 6 in the main manuscript) at the adequate temperature, lead to an experimental value of 19.1–19.6 kcal/mol activation barrier for the (*E*)–/(*Z*)–**2c** isomerization process.

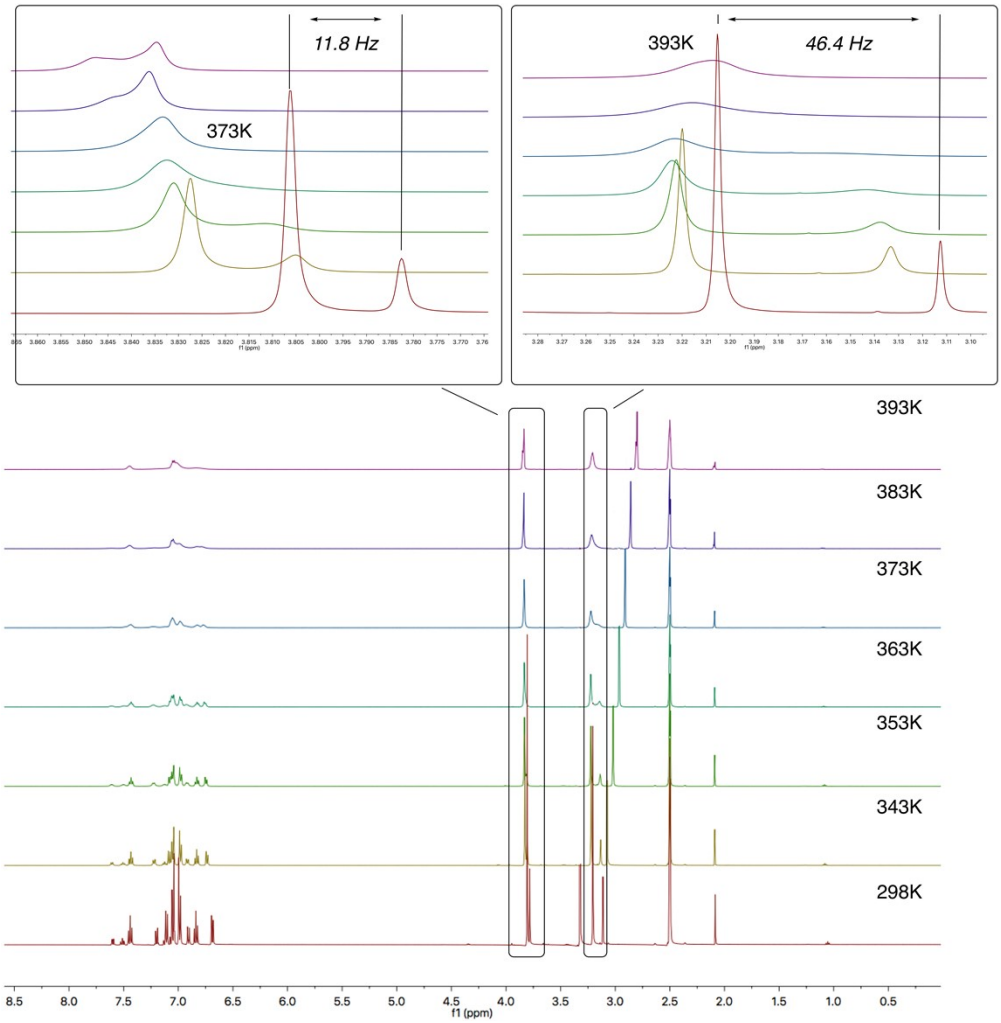
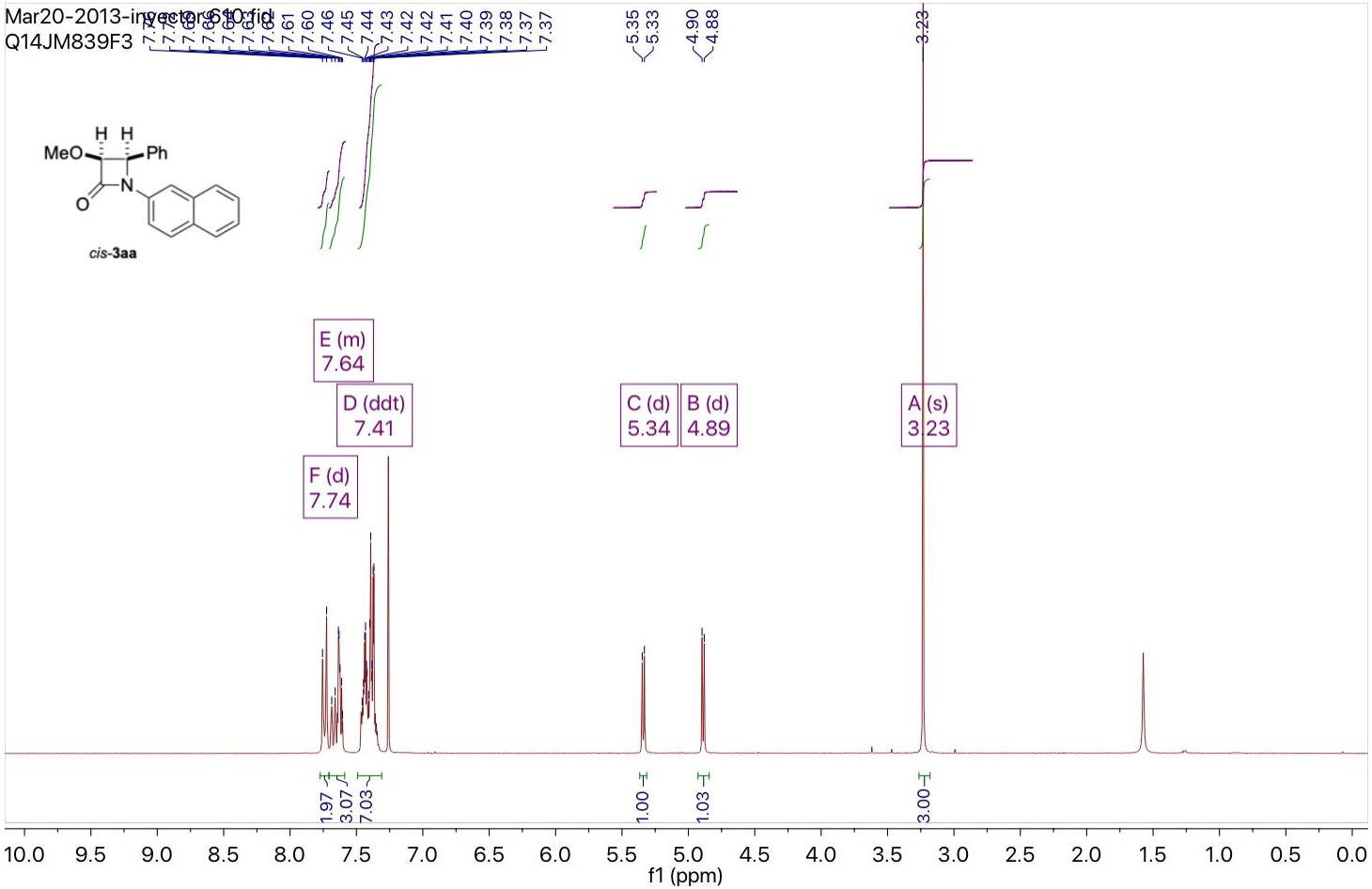


Figure S2. ^{1}H-NMR (DMSO) spectra of (*E*)–/(*Z*)–**2c** recorded at different temperatures. Coalescence of the signals corresponding to the methyl groups are highligthed.

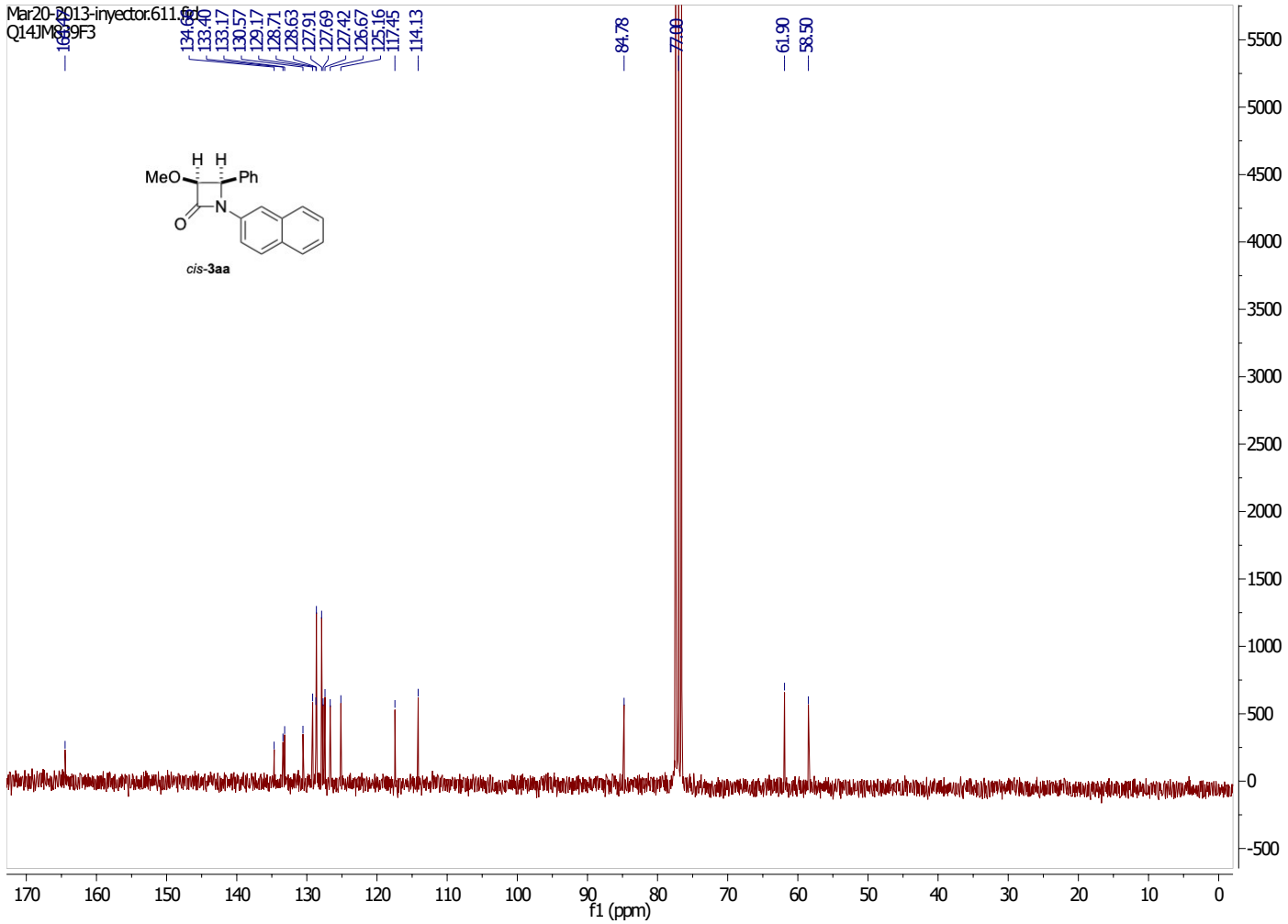
NMR and IR spectra

^{1}H NMR ($CDCl_3$) cis-3aa

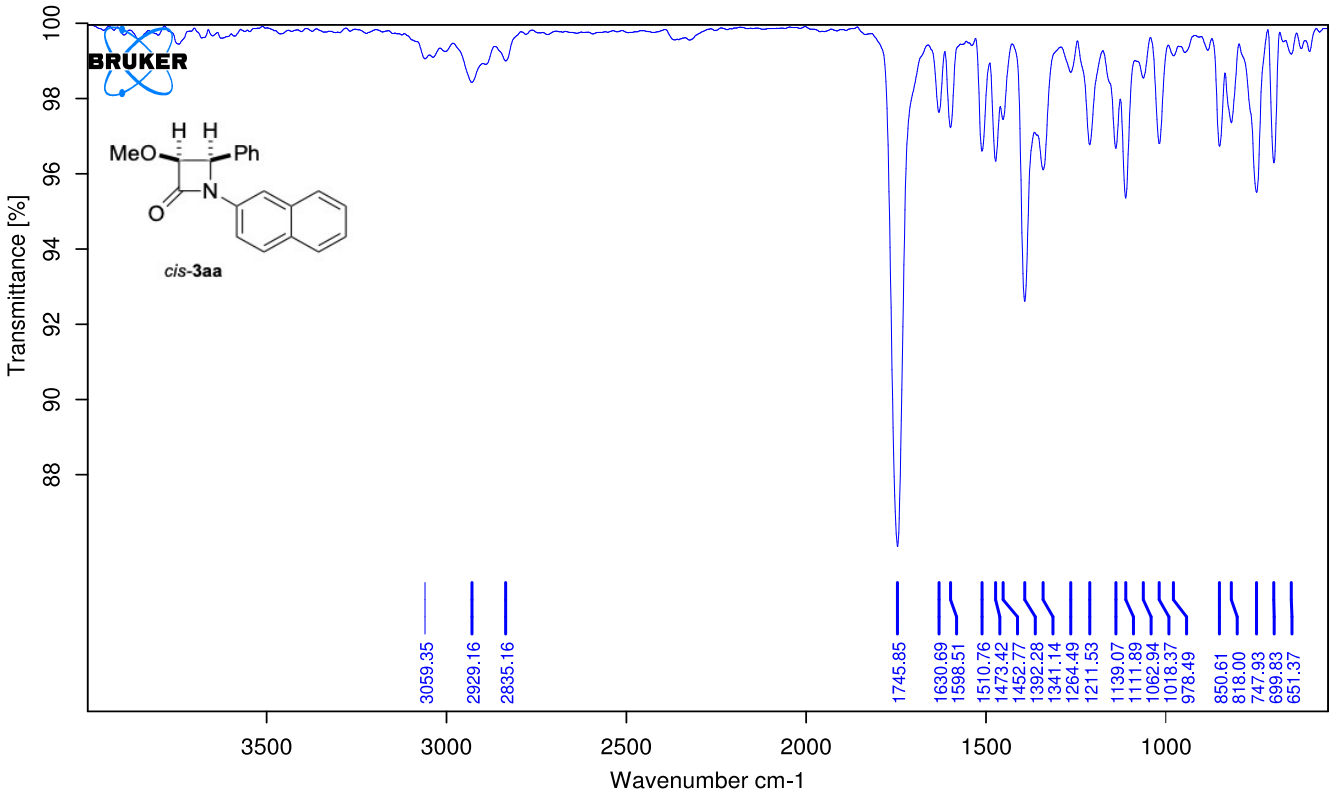


^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.74 (d, *J* = 9.3 Hz, 2H), 7.70 – 7.58 (m, 4H), 7.41 (ddt, *J* = 15.5, 4.5, 2.2 Hz, 10H), 5.34 (d, *J* = 4.9 Hz, 1H), 4.89 (d, *J* = 4.9 Hz, 1H), 3.23 (s, 3H).

^{13}C NMR ($CDCl_3$) cis-3aa



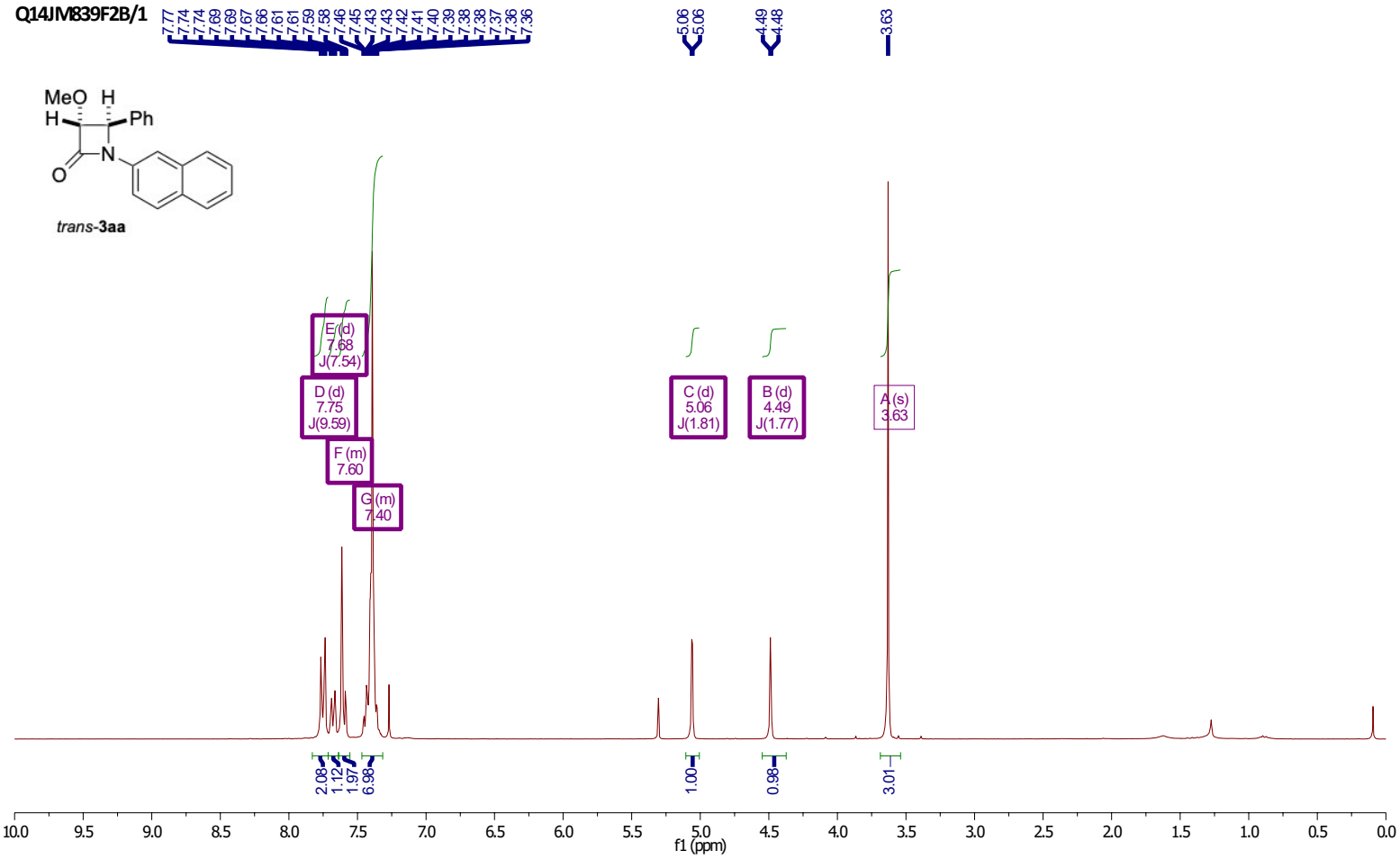
IR cis-**3aa**



F:\ESPECTROS\GRUPO-14 MAS\JM-839F3.0	JM-839F3	Instrument type and / or accessory	20/12/2013

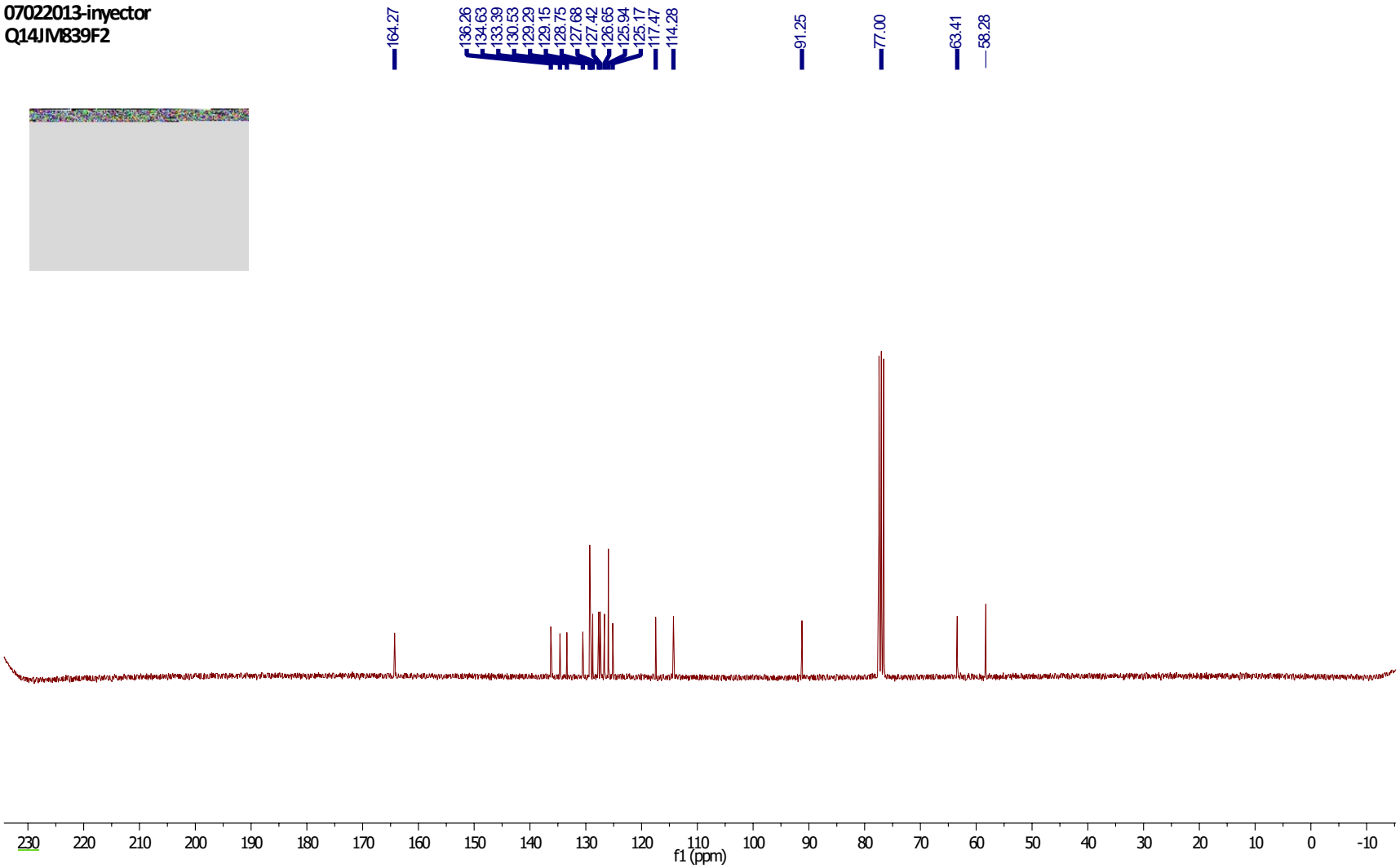
Page 1 of 1

^{1}H NMR ($CDCl_3$) trans-**3aa**



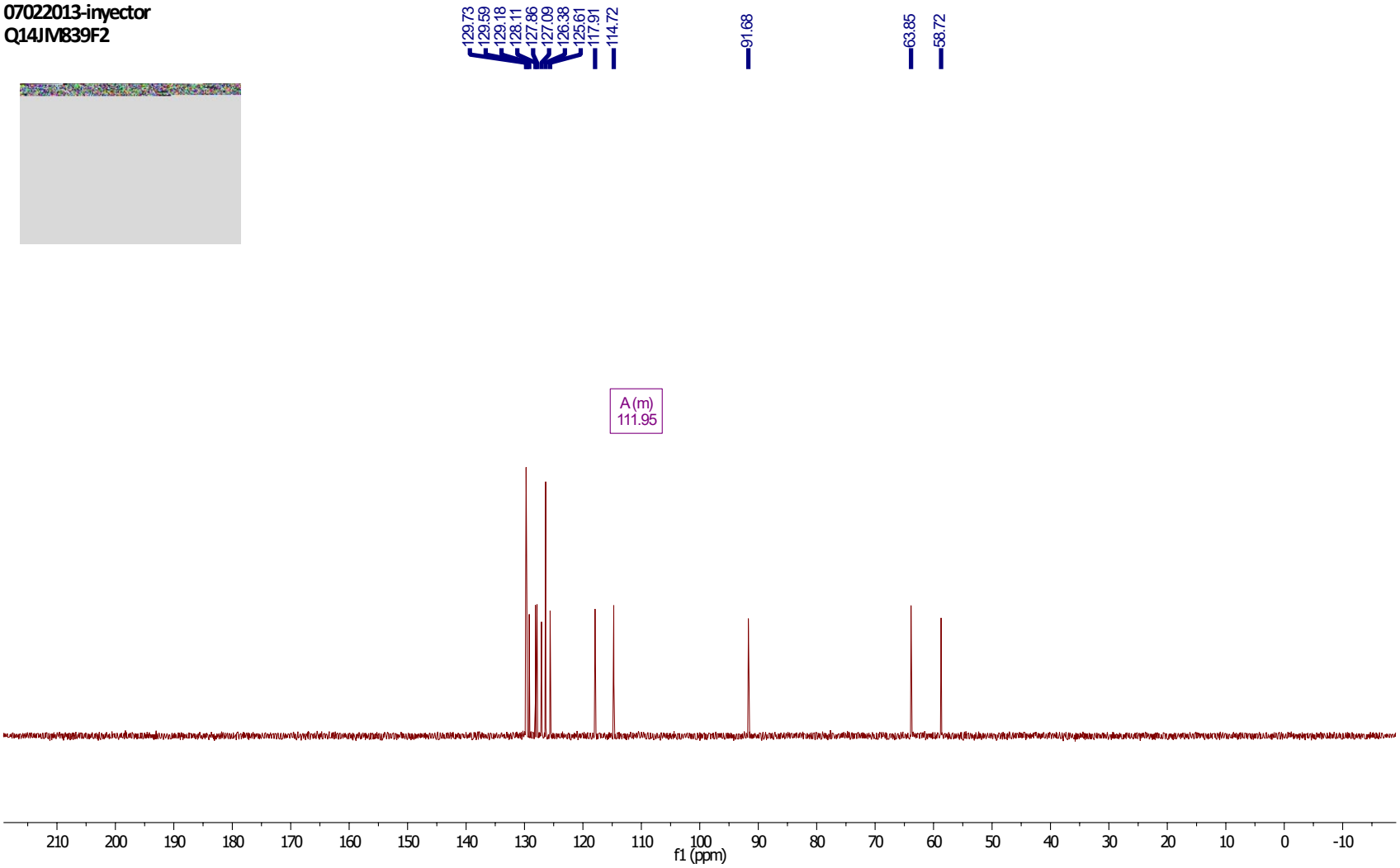
^{1}H NMR(Chloroform-d, 300 MHz): δ = 7.75 (d, 2H, *J*=9.6 Hz), 7.68 (d, 1H, *J*=7.5 Hz), 7.63 – 7.55 (m, 2H), 7.49 – 7.32 (m, 7H), 5.06 (d, 1H, *J*=1.8 Hz), 4.49 (d, 1H, *J*=1.8 Hz), 3.63 (s, 3H) ppm

^{13}C NMR ($CDCl_3$) trans-**3aa**

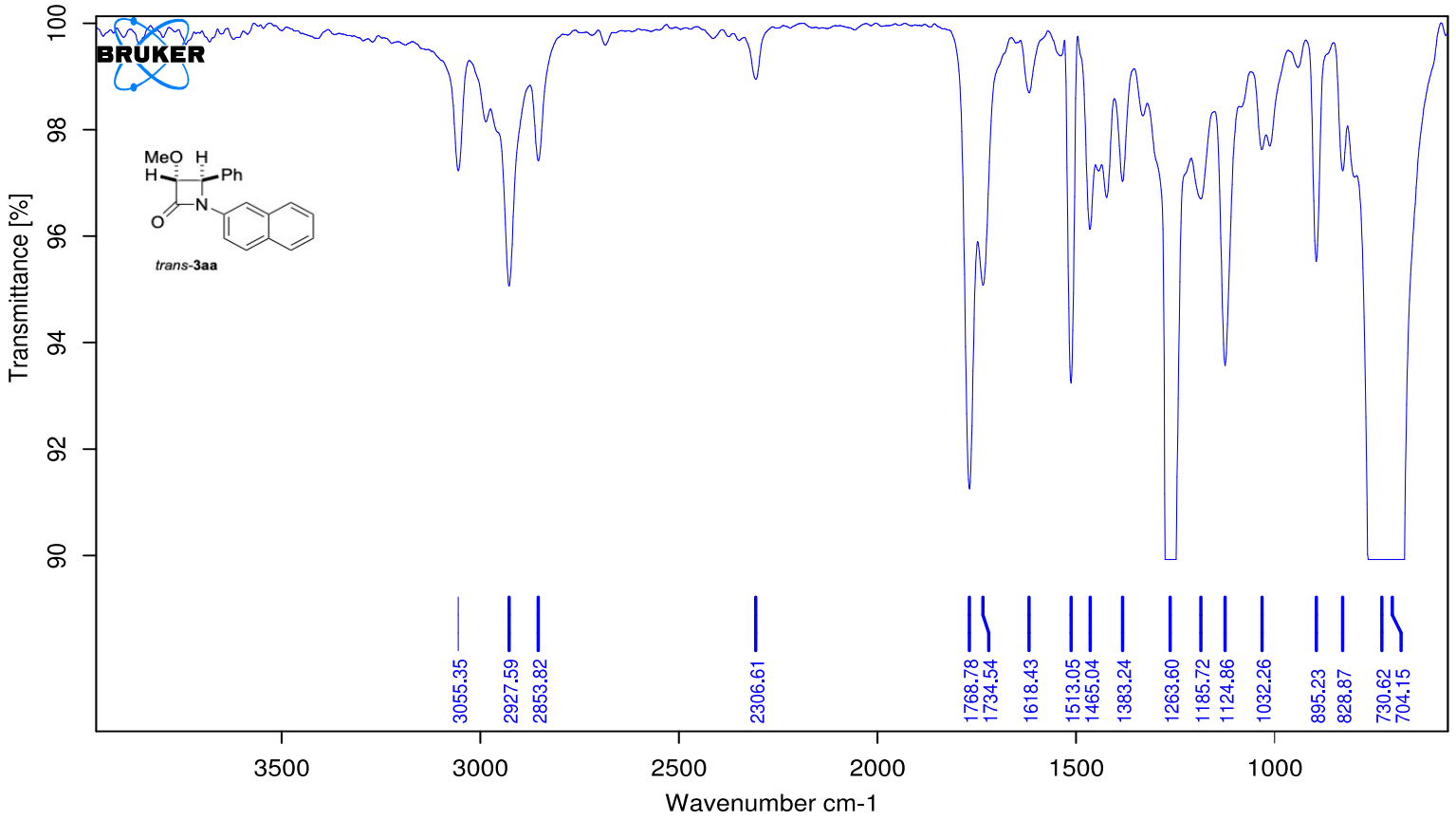


^{13}C NMR($CDCl_3$, 75 MHz): δ = 164.3, 136.3, 134.6, 133.4, 130.5, 129.3, 129.2, 128.7, 127.7, 127.4, 126.6, 125.9, 125.2, 117.5, 114.3, 91.2, 63.4, 58.3.

^{13}C-DEPT NMR ($CDCl_3$) trans-**3aa**



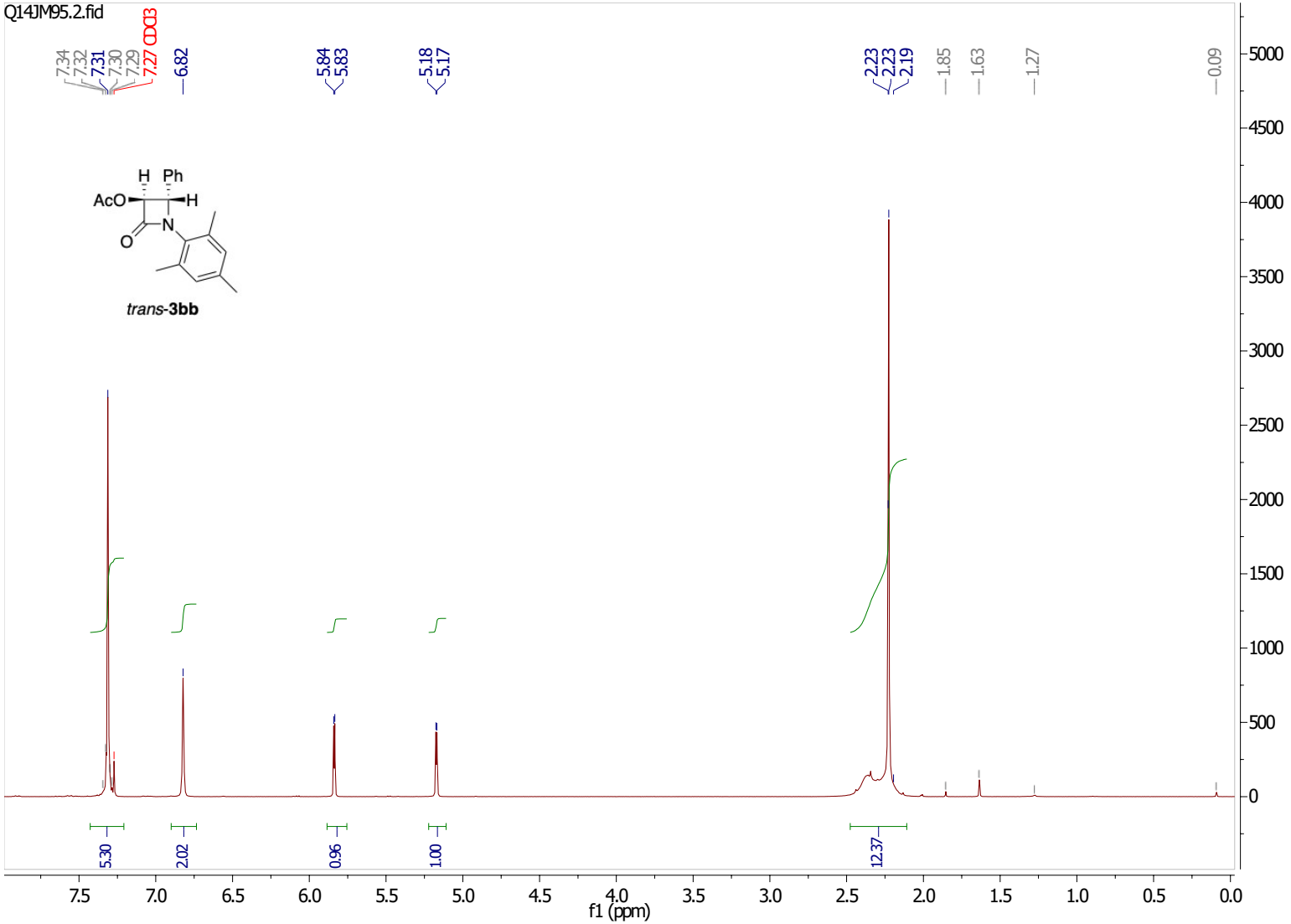
IR trans-**3aa**



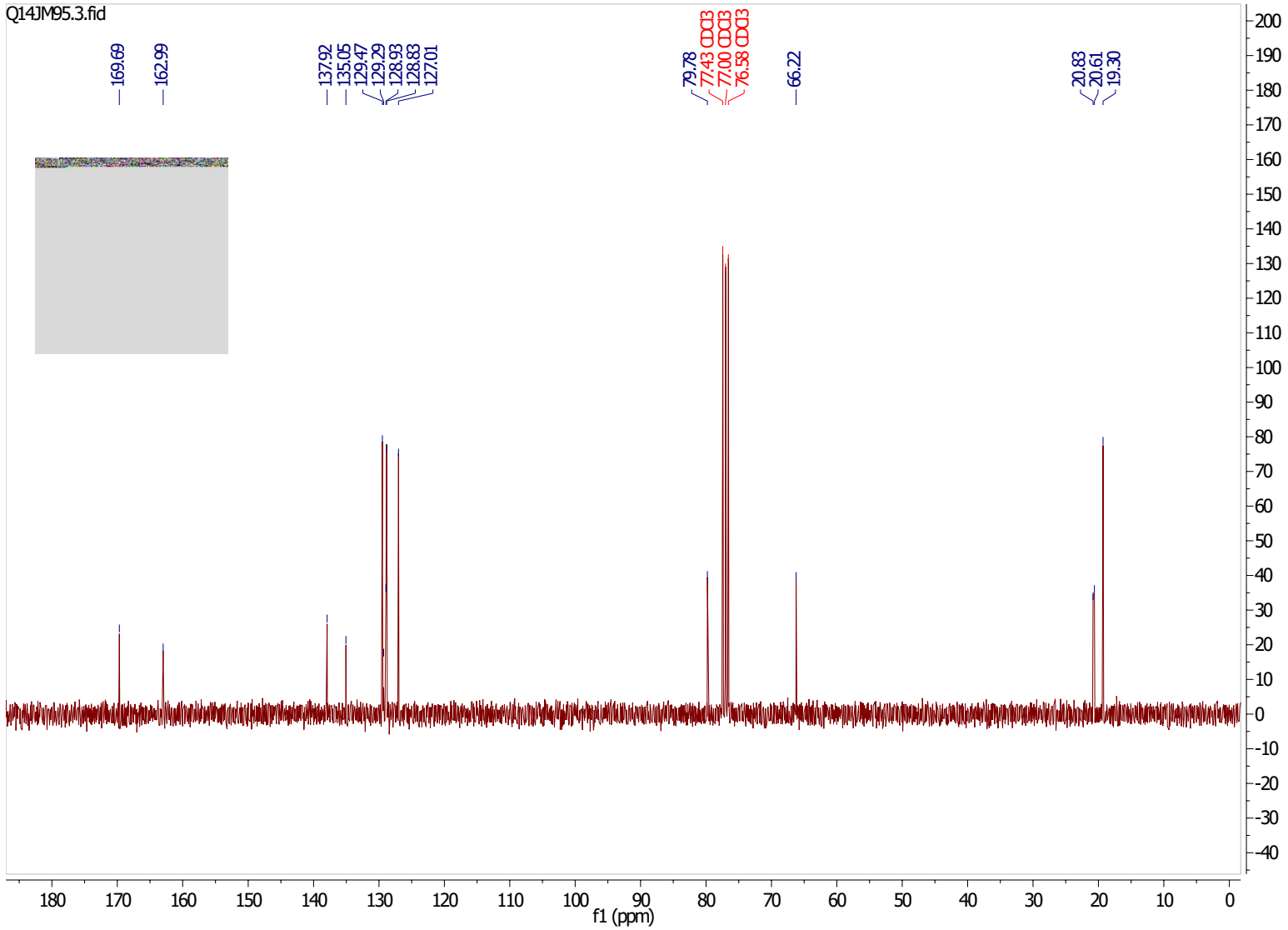
F:\ESPECTROS\GRUPO-14 MAS\JM-839F2.1	JM-839F2	Instrument type and / or accessory	20/12/2013

Page 1 of 1

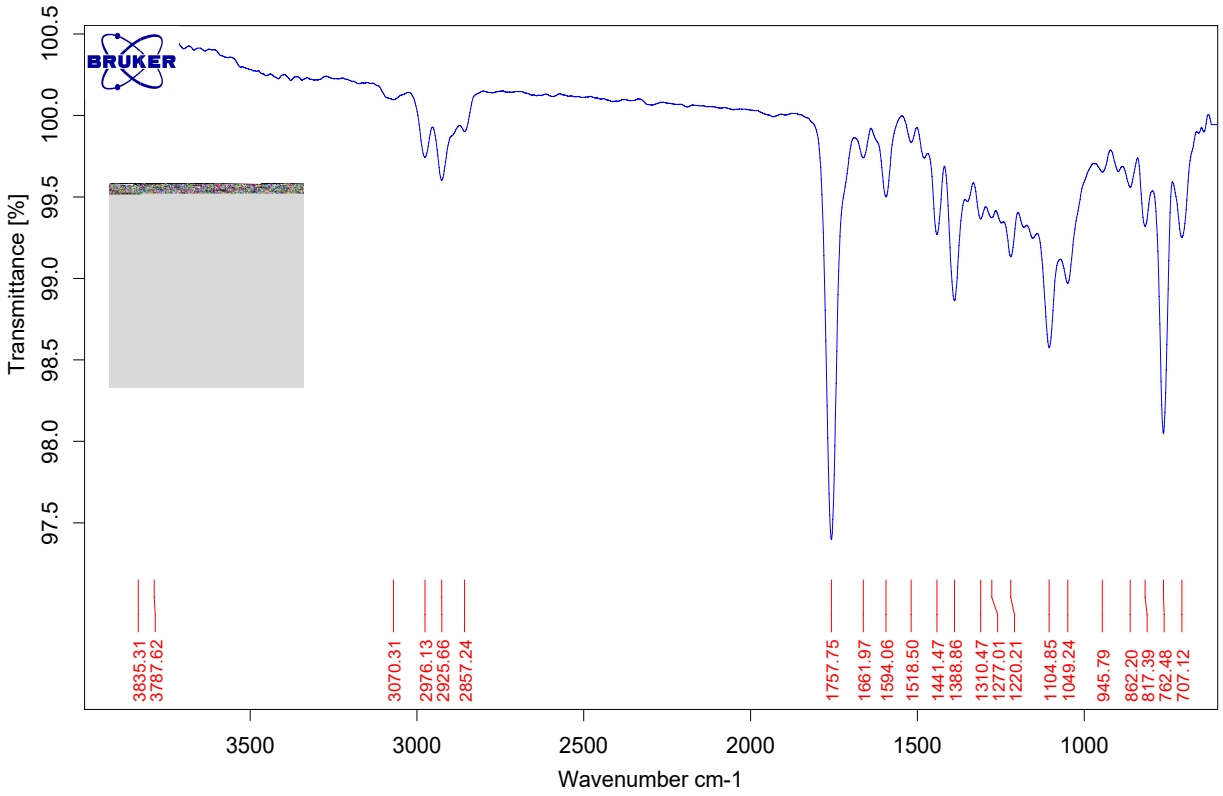
^{1}H NMR ($CDCl_3$) trans-**3bb**



^{13}C NMR ($CDCl_3$) trans-**3bb**



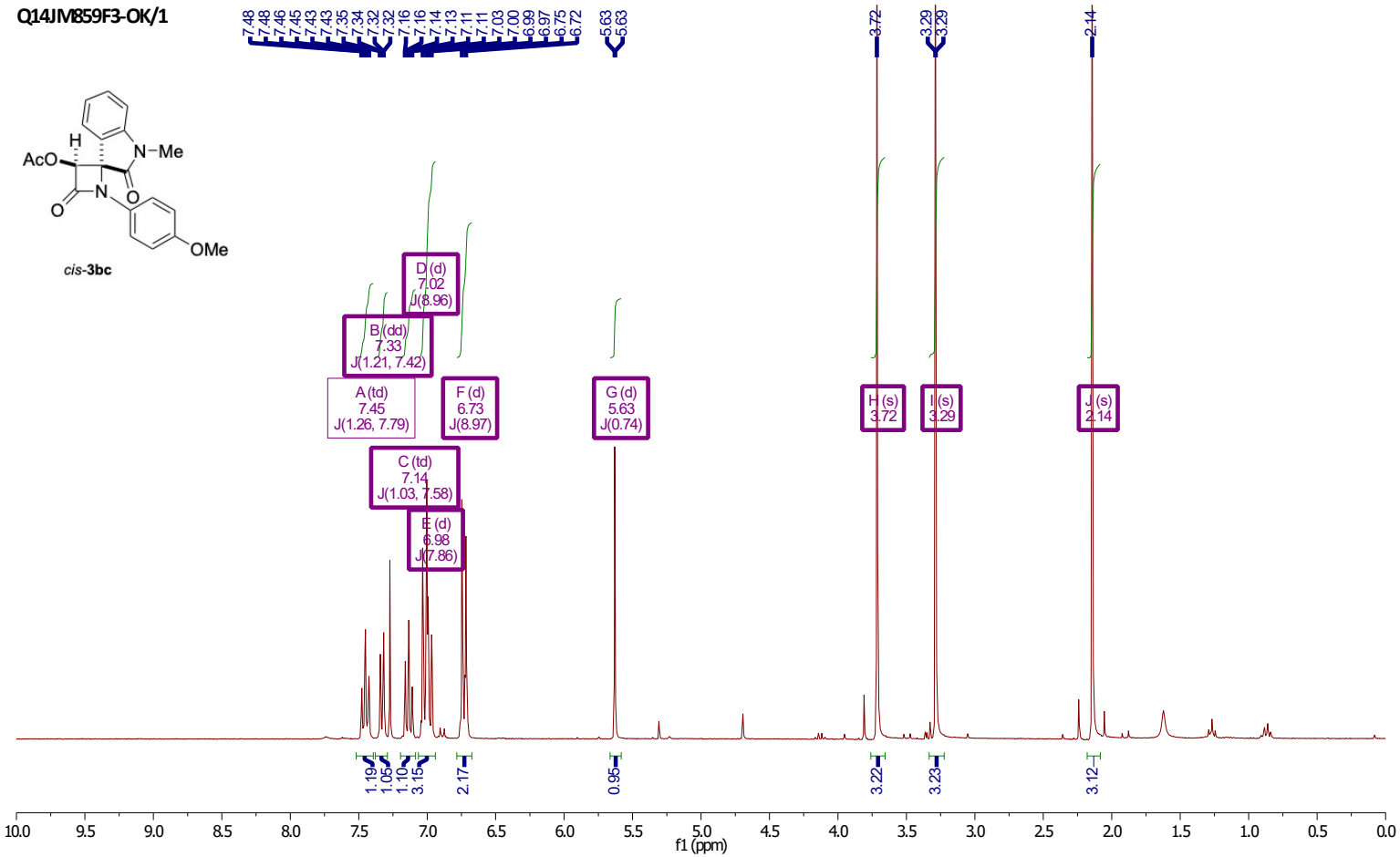
IR trans-**3bb**



C:\QCA ORGÁNICA\Espectros\GRUPO-14 MAS\JM-15F3.0	JM-15F3	Instrument type and / or accessory	07/10/2009

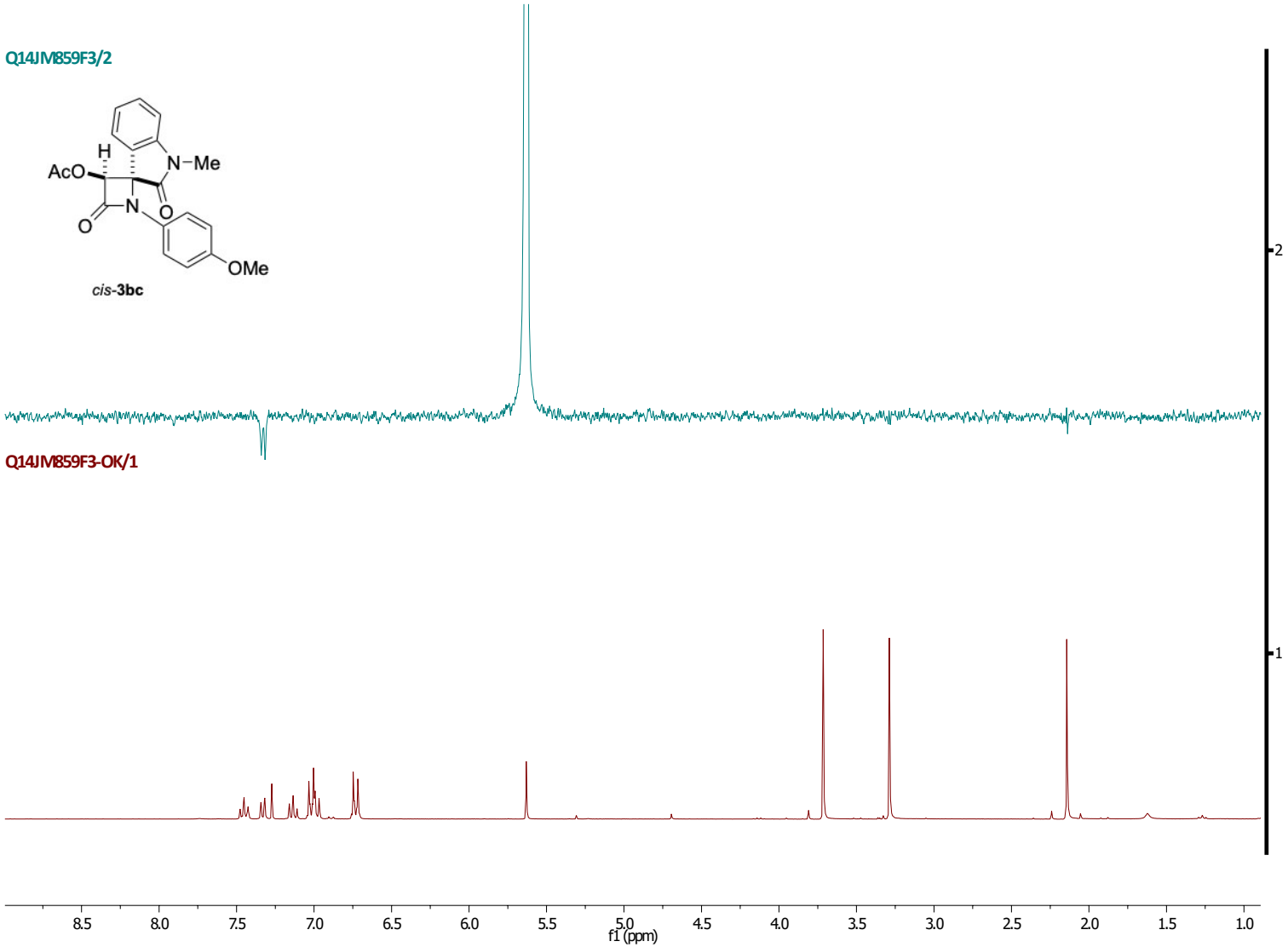
Page 1/1

^{1}H NMR ($CDCl_3$) cis-**3bc**

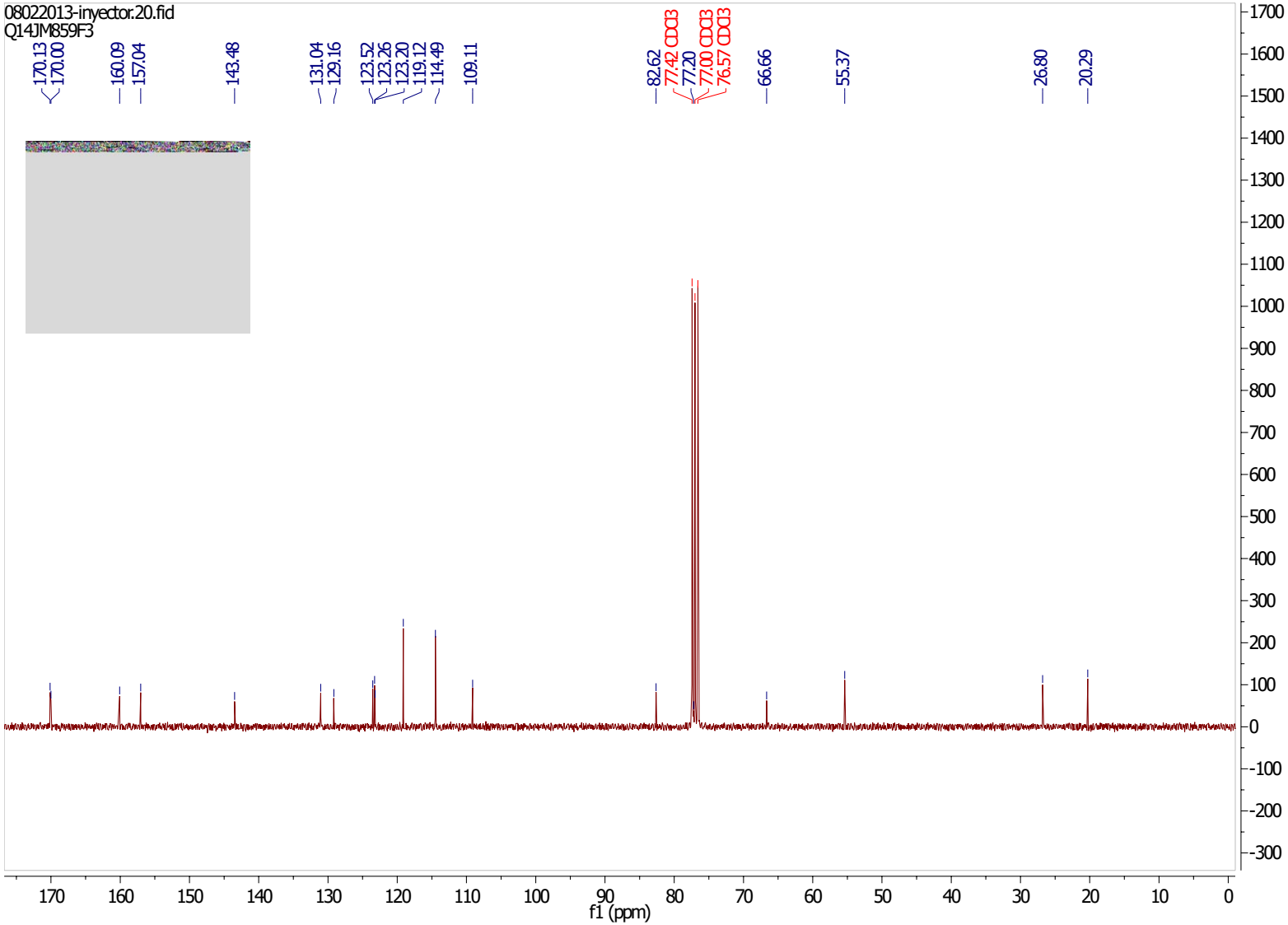


^{1}H NMR(Chloroform-d, 300 MHz): δ = 7.45 (td, 1H, *J*=7.8, 1.3 Hz), 7.33 (dd, 1H, *J*=7.4, 1.2 Hz), 7.14 (td, 1H, *J*=7.6, 1.0 Hz), 7.02 (d, 2H, *J*=9.0 Hz), 6.98 (d, 1H, *J*=7.9 Hz), 6.73 (d, 2H, *J*=9.0 Hz), 5.63 (d, 1H, *J*=0.7 Hz), 3.72 (s, 3H), 3.29 (s, 3H), 2.14 (s, 3H) ppm

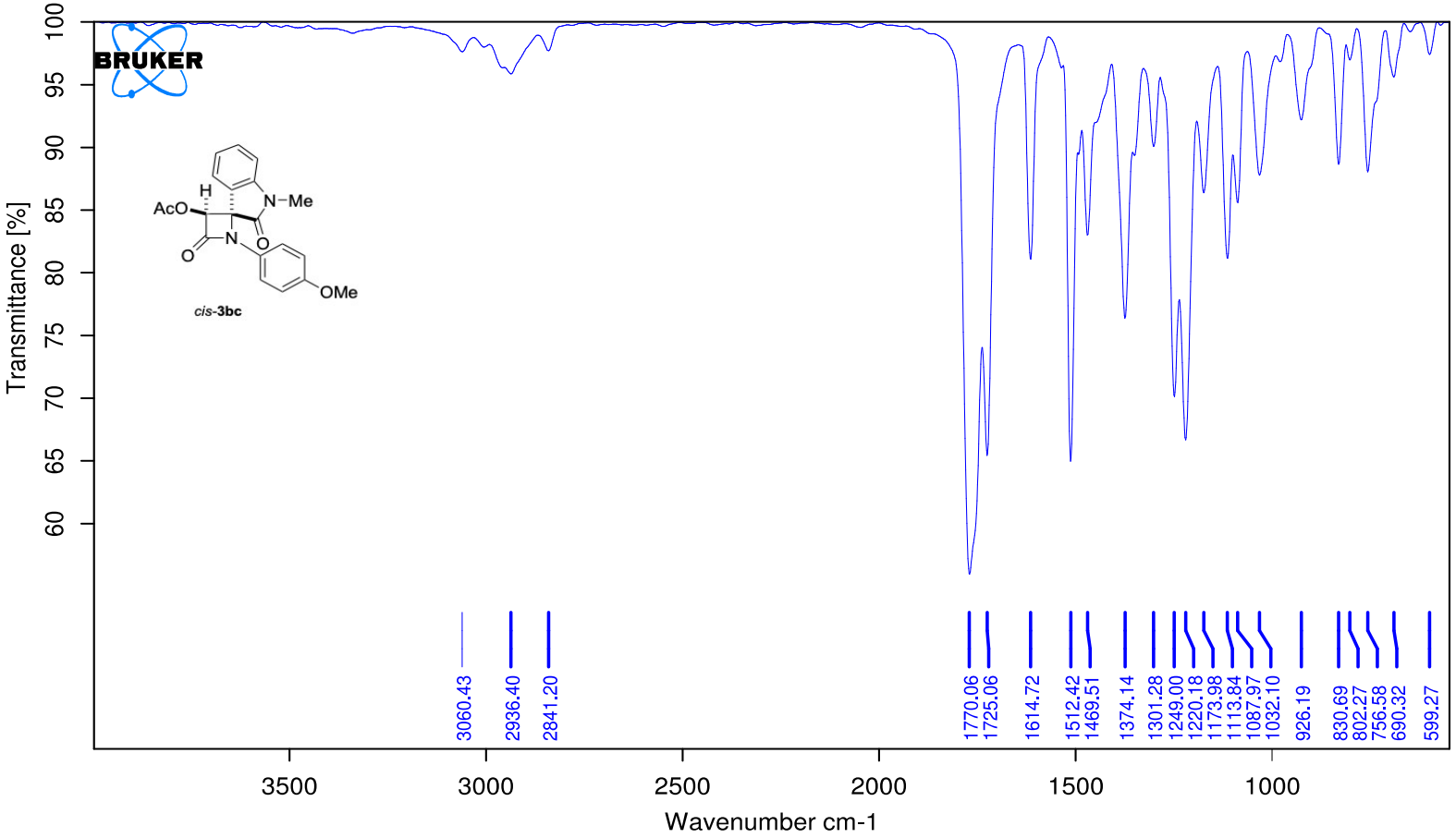
^{1}H NMR and nOe ($CDCl_3$) cis-**3bc**



^{13}C NMR ($CDCl_3$) cis-**3bc**



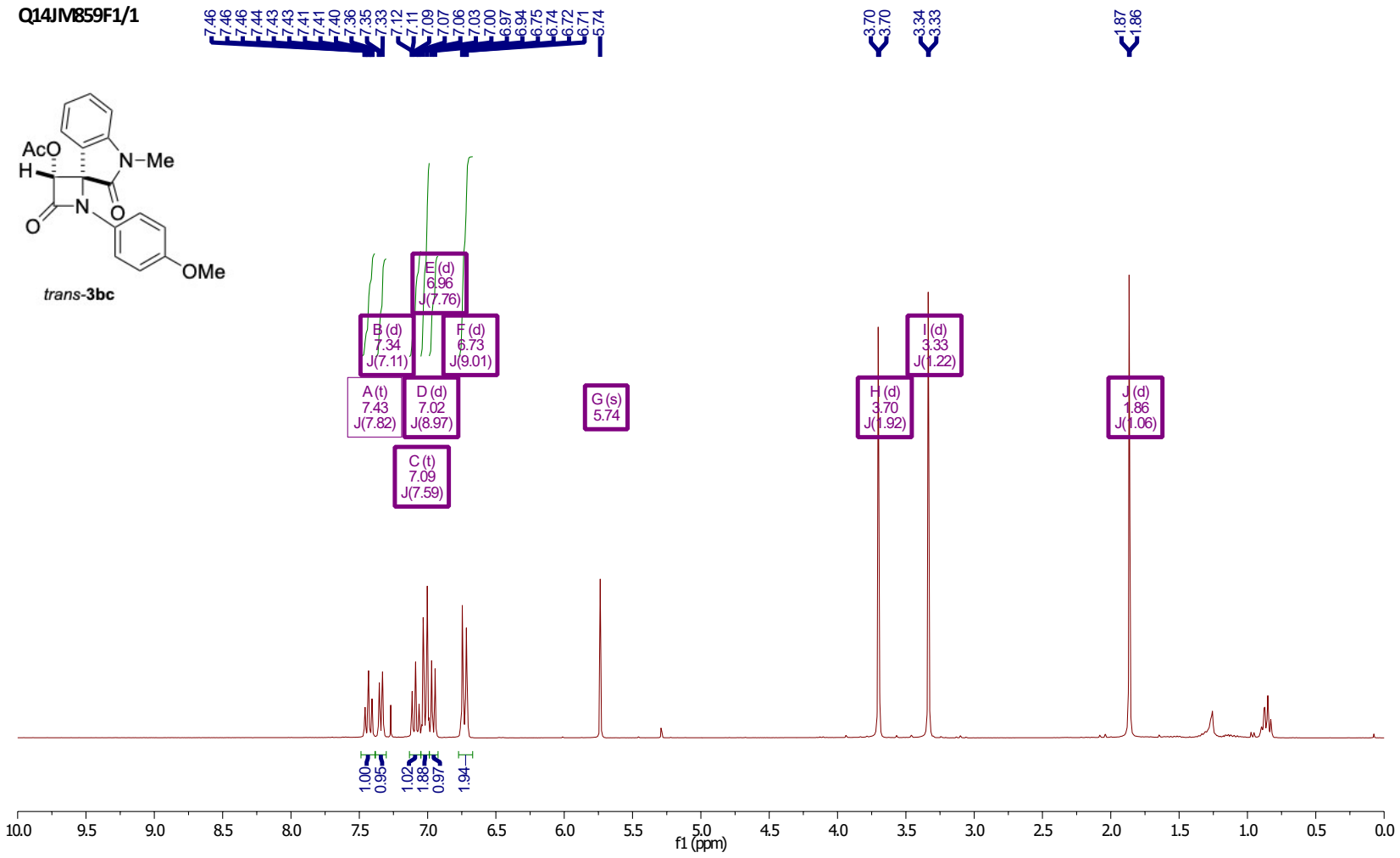
IR cis-**3bc**



F:\ESPECTROS\GRUPO-14 MAS\JM-859F3.1	JM-859F3	Instrument type and / or accessory	20/12/2013

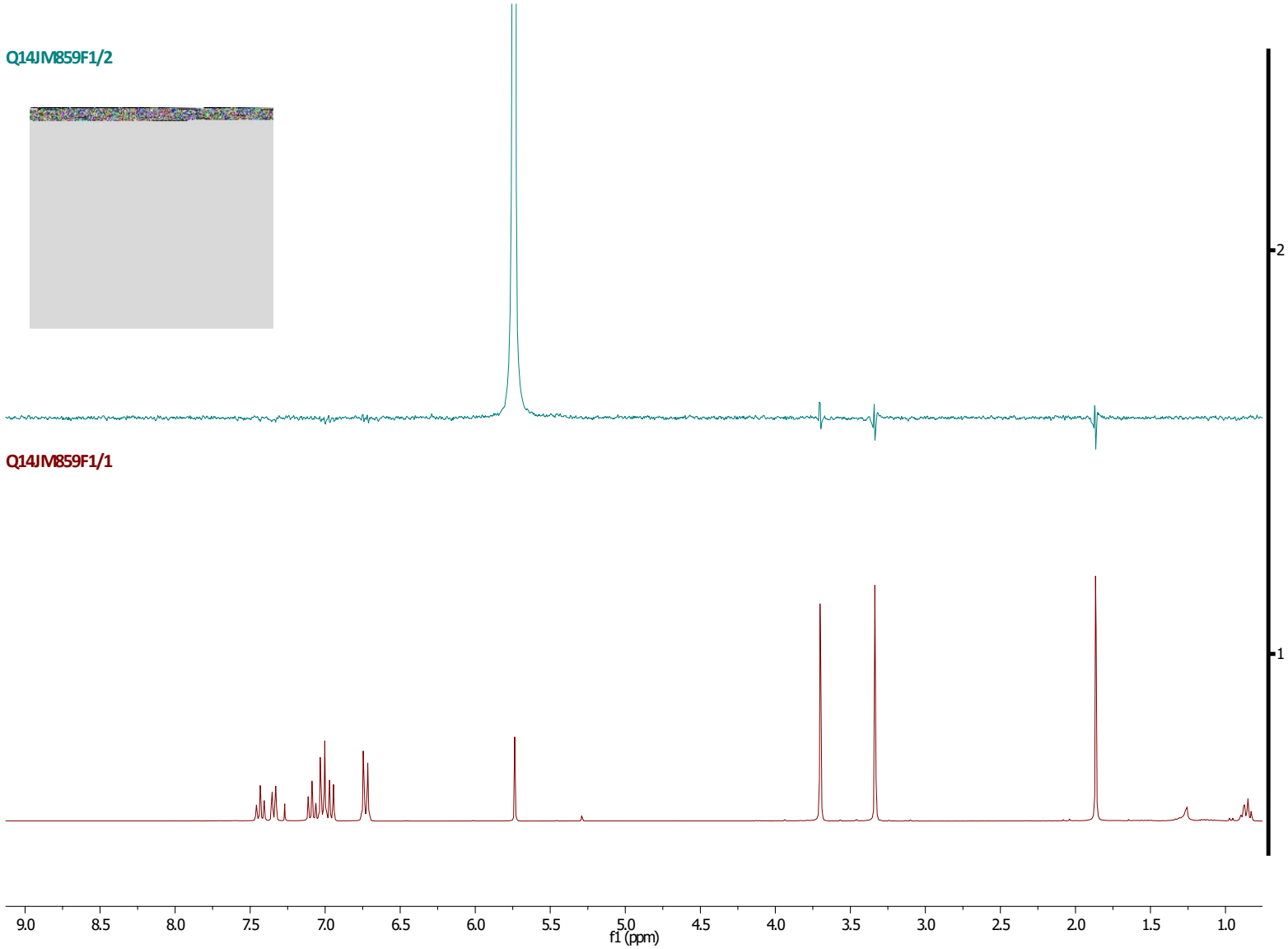
Page 1 of 1

^{1}H NMR ($CDCl_3$) trans-**3bc**

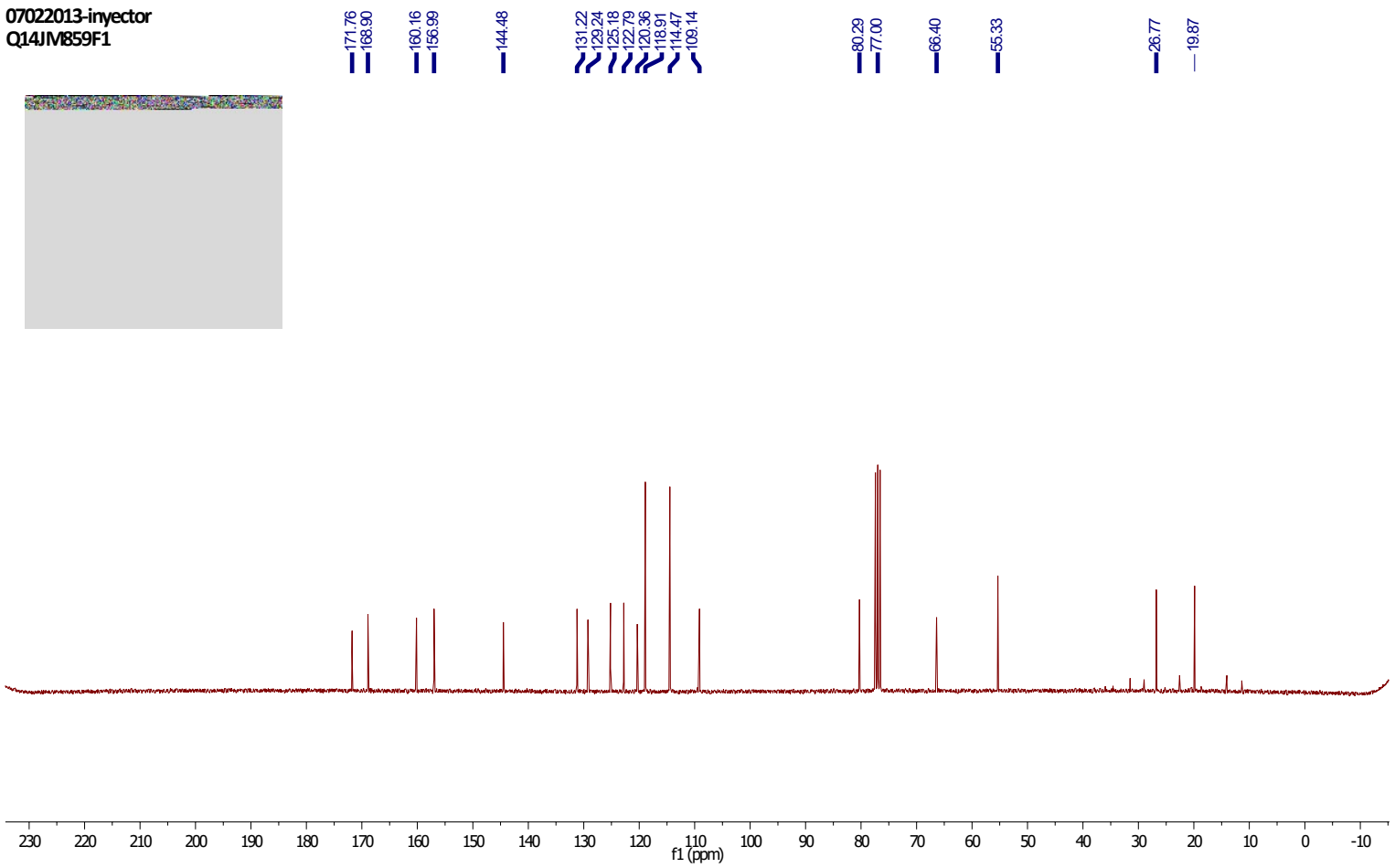


^{1}H NMR(Chloroform-d, 300 MHz): δ = 7.43 (t, 1H, *J*=7.8 Hz), 7.34 (d, 1H, *J*=7.1 Hz), 7.09 (t, 1H, *J*=7.6 Hz), 7.02 (d, 2H, *J*=9.0 Hz), 6.96 (d, 1H, *J*=7.8 Hz), 6.73 (d, 2H, *J*=9.0 Hz), 5.74 (s, 1H), 3.70 (s, 3H), 3.33 (s, 3H), 1.86 (s, 3H) ppm

^{1}H NMR and nOe ($CDCl_3$) trans-**3bc**

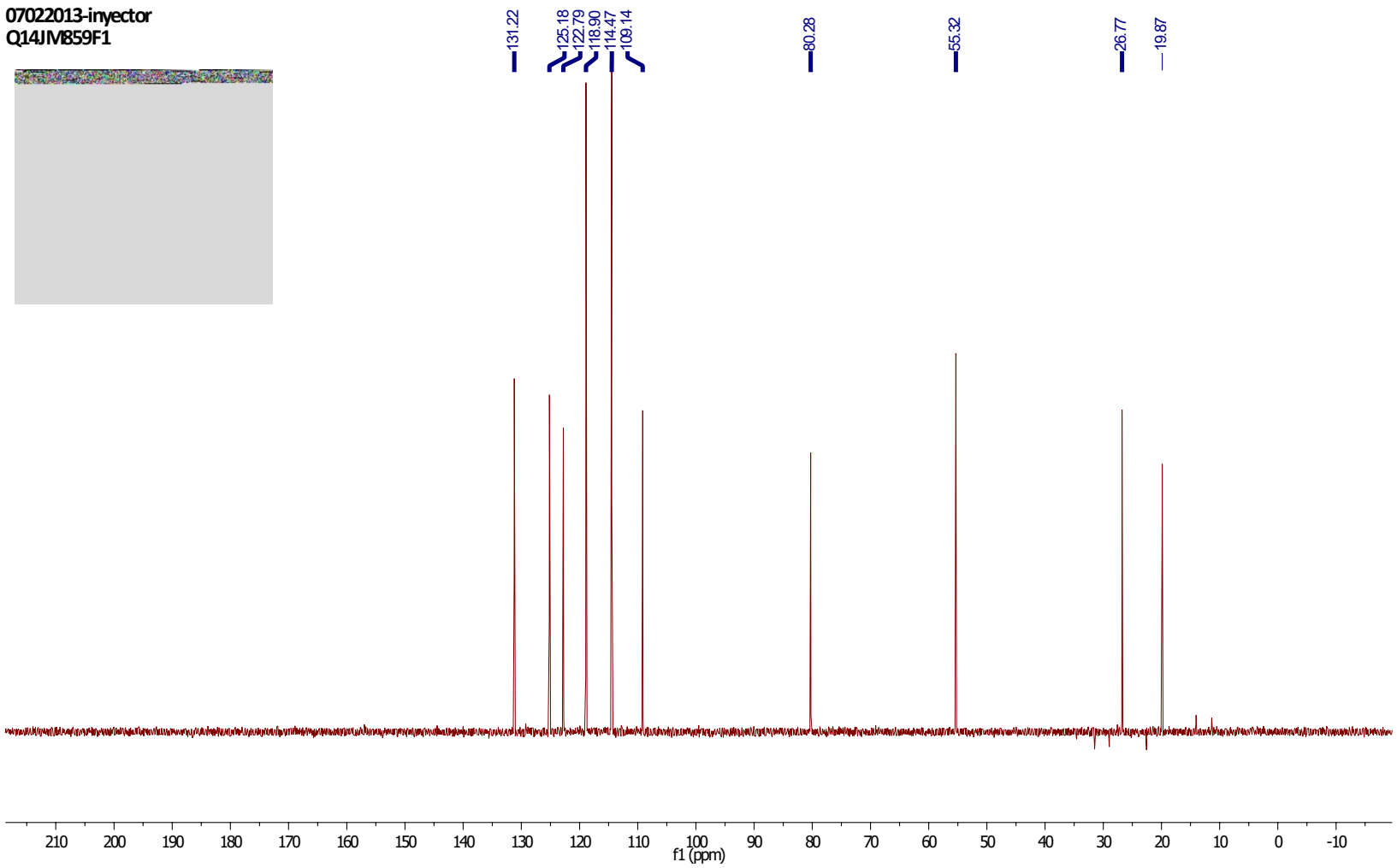


^{13}C NMR ($CDCl_3$) trans-**3bc**

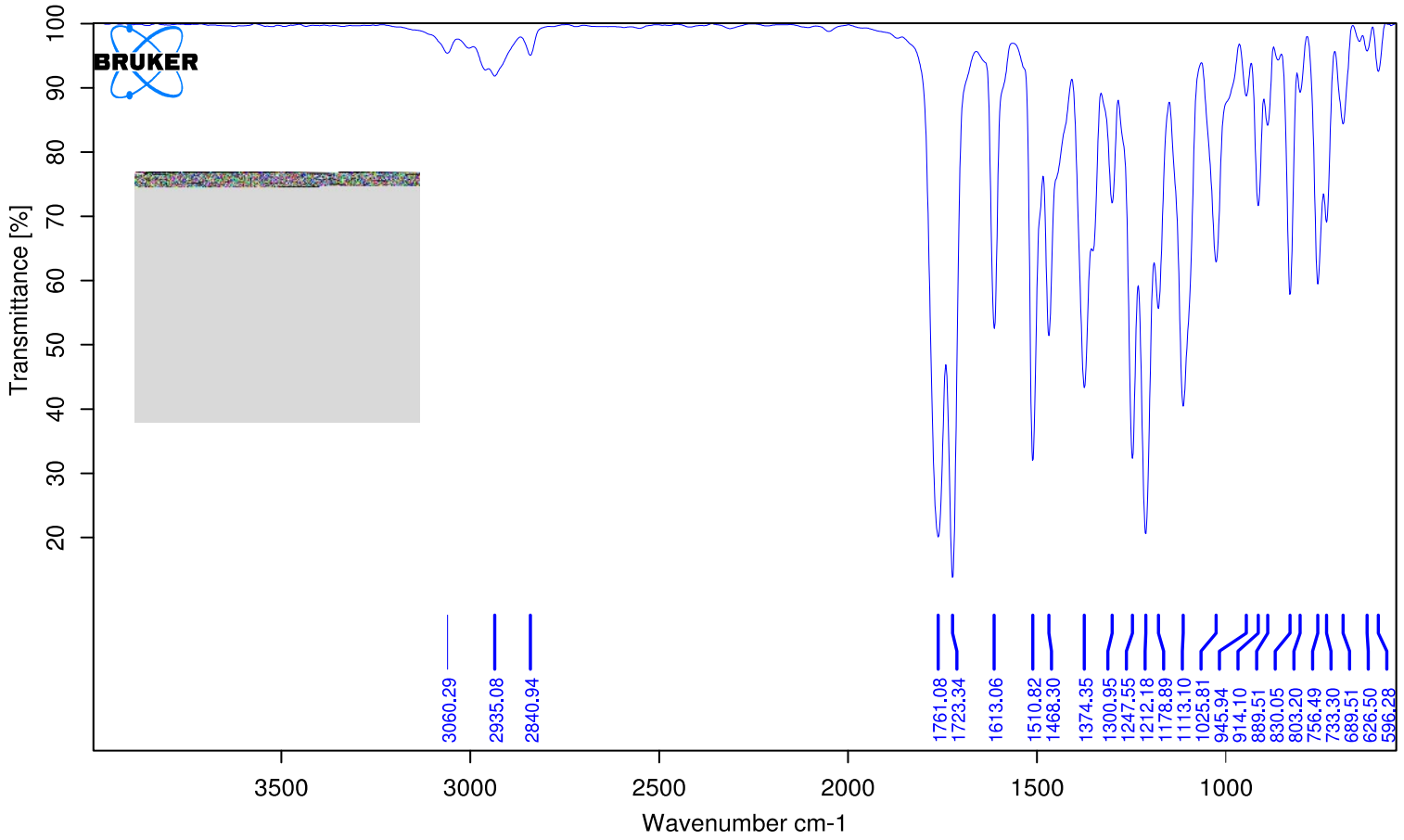


^{13}C NMR($CDCl_3$, 75 MHz): δ = 171.8, 168.9, 160.2, 157.0, 144.5, 131.2, 129.2, 125.2, 122.8, 120.4, 118.9, 114.5, 109.1, 80.3, 66.4, 55.3, 26.8, 19.9.

^{13}C-DEPT NMR ($CDCl_3$) trans-**3bc**



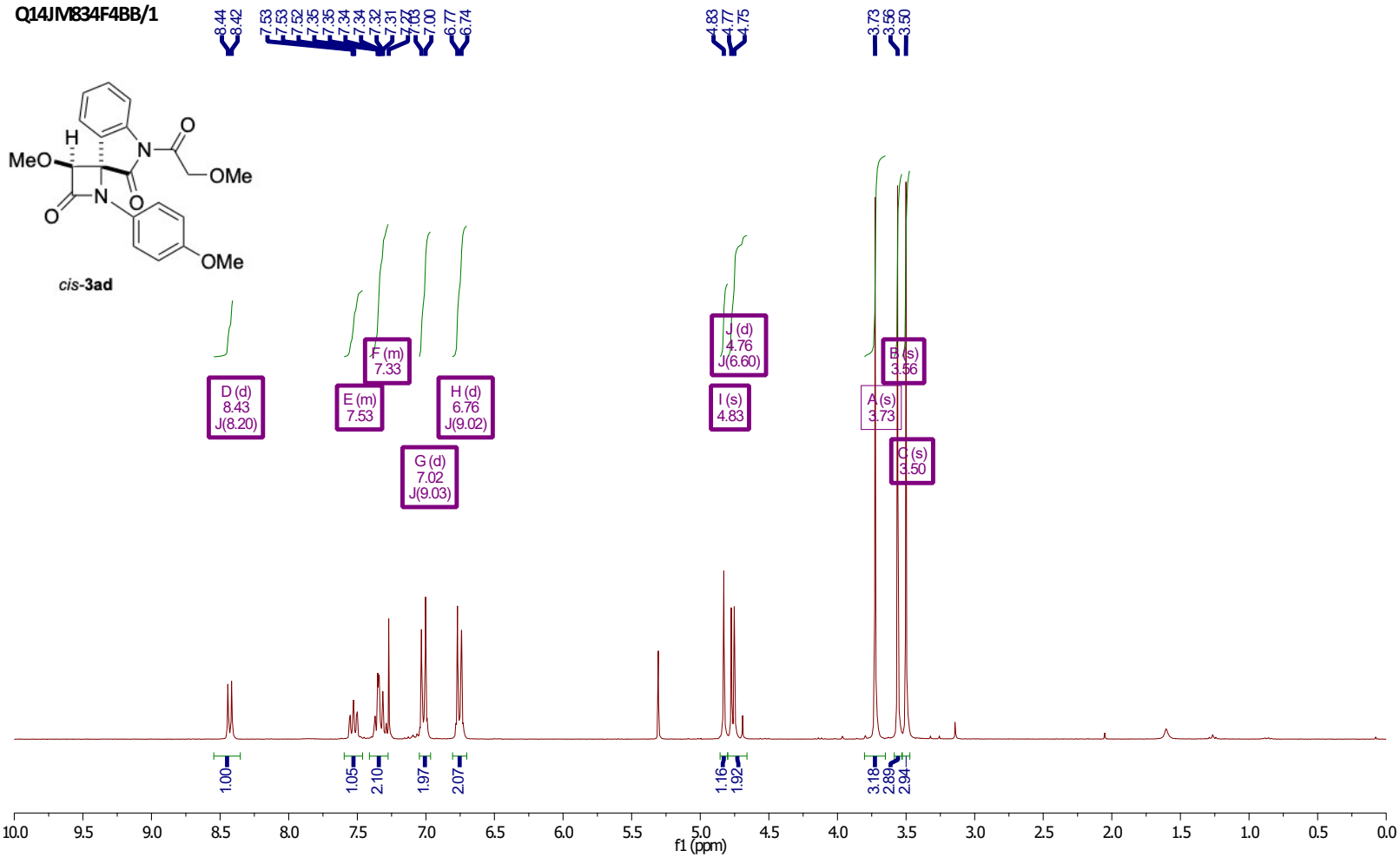
IR trans-**3bc**



F:\ESPECTROS\GRUPO-14 MAS\JM-859F1.1	JM-859F1	Instrument type and / or accessory	20/12/2013

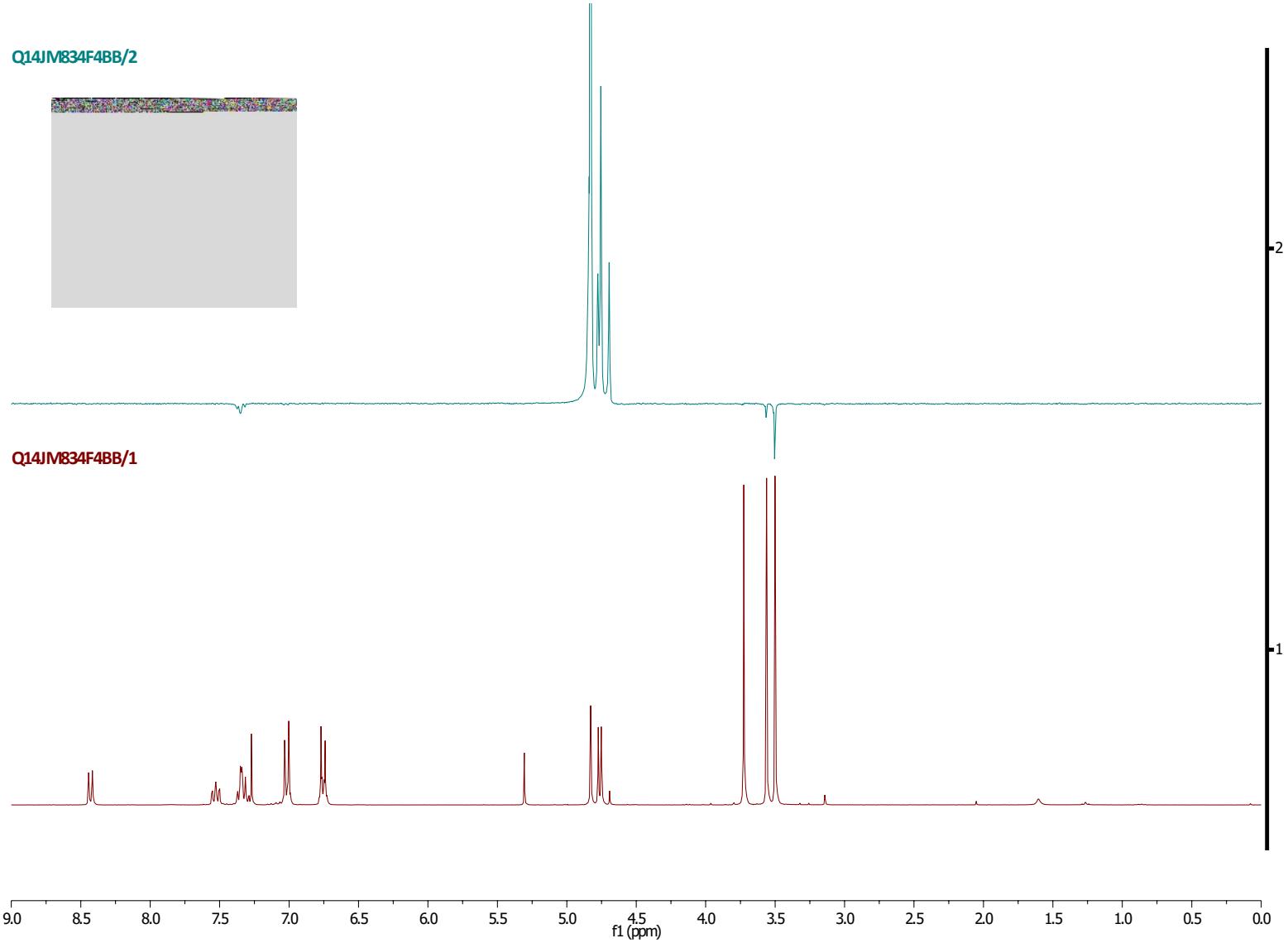
Page 1 of 1

^{1}H NMR ($CDCl_3$) cis-**3ad**

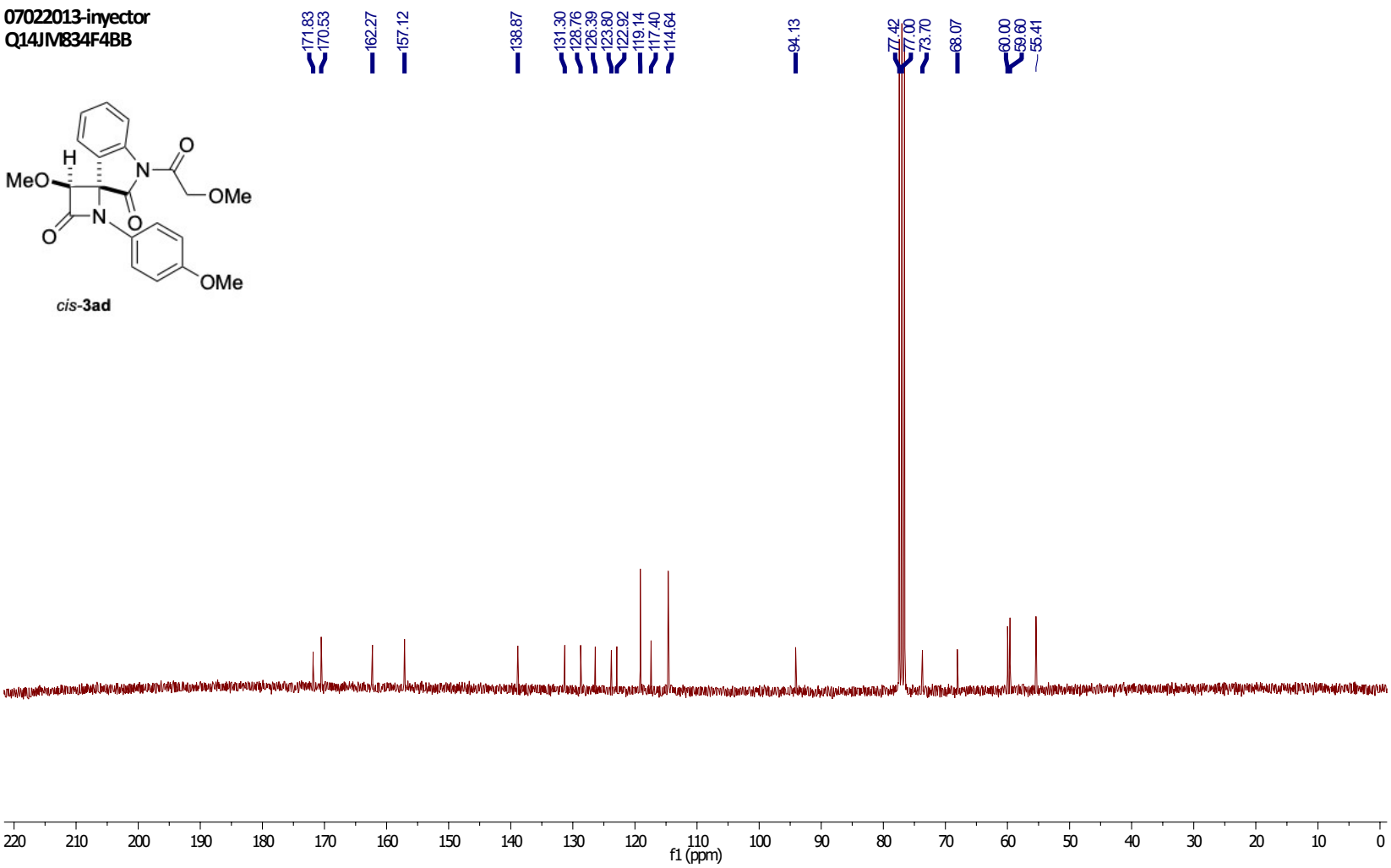


^{1}H NMR(Chloroform-d, 300 MHz): δ = 8.43 (d, 1H, *J*=8.2 Hz), 7.58 – 7.46 (m, 1H), 7.41 – 7.26 (m, 2H), 7.02 (d, 2H, *J*=9.0 Hz), 6.76 (d, 2H, *J*=9.0 Hz), 4.83 (s, 1H), 4.76 (d, 2H, *J*=6.6 Hz), 3.73 (s, 3H), 3.56 (s, 3H), 3.50 (s, 3H) ppm

^{1}H NMR and nOe ($CDCl_3$) cis-3ad

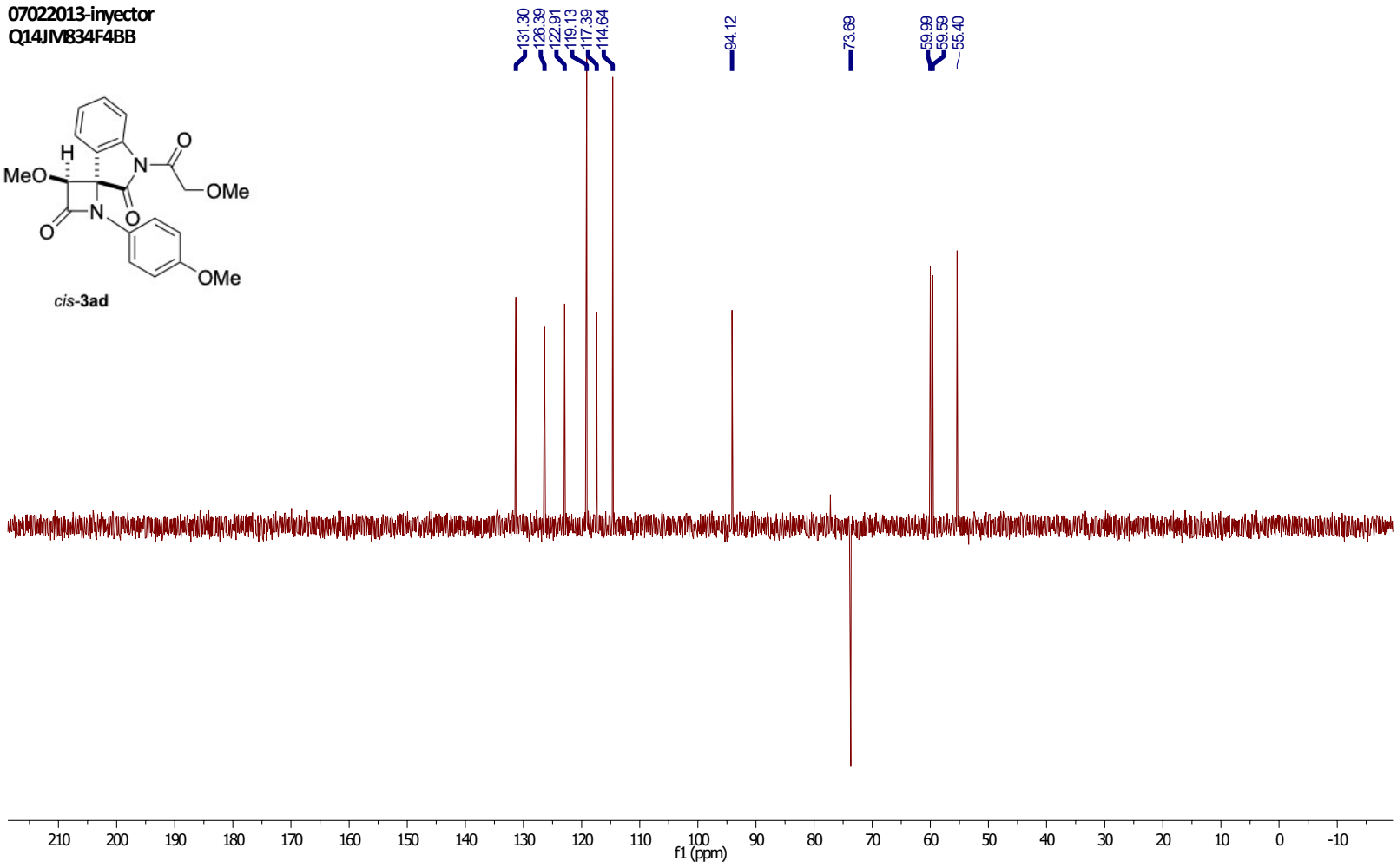


^{13}C NMR ($CDCl_3$) cis-**3ad**

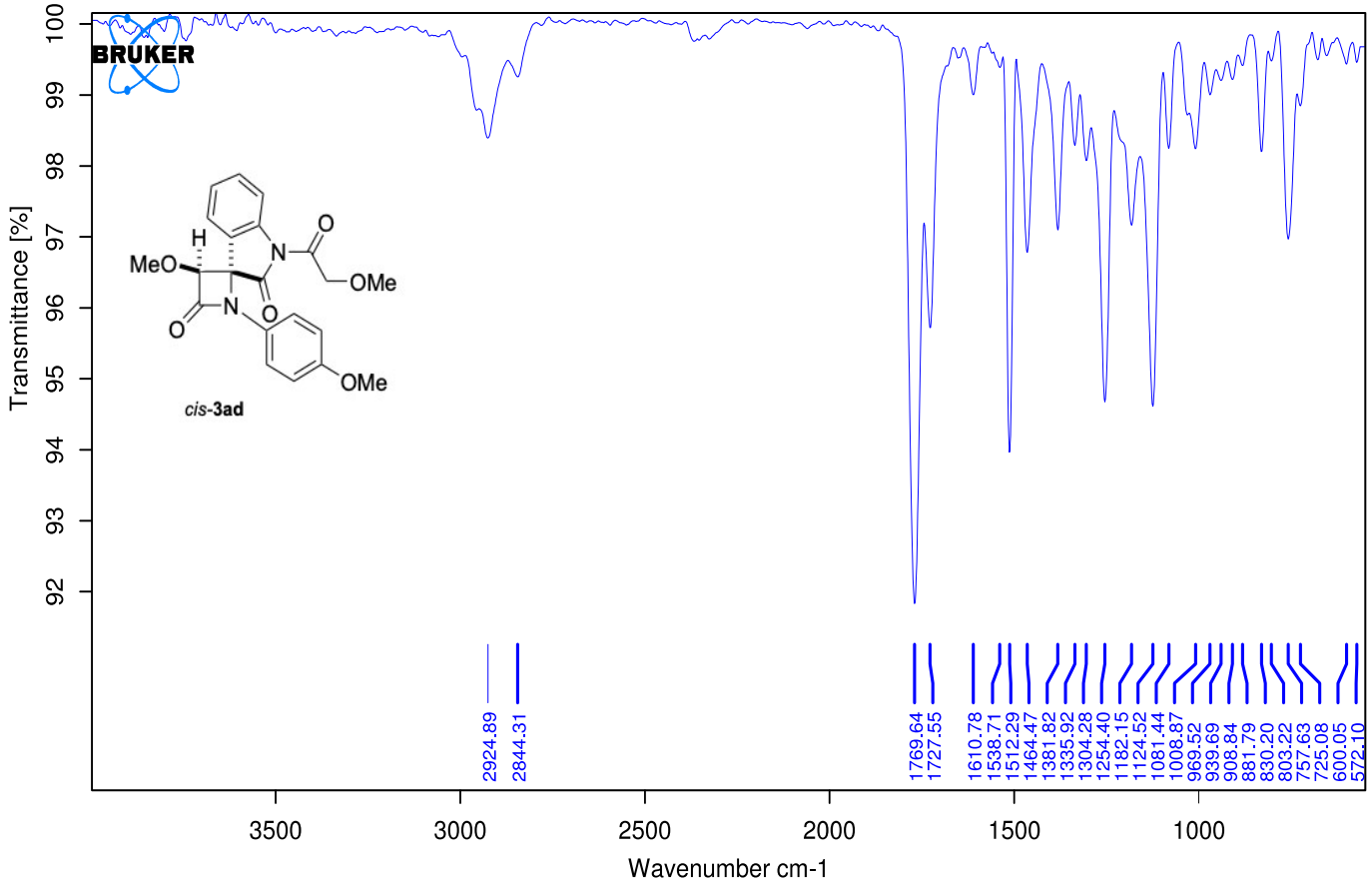


^{13}C NMR($CDCl_3$, 75 MHz): δ = 171.8, 170.5, 162.3, 157.1, 138.9, 131.3, 128.8, 126.4, 123.8, 122.9, 119.1, 117.4, 114.6, 94.1, 73.7, 68.1, 60.0, 59.6, 55.4.

^{13}C-DEPT NMR ($CDCl_3$) cis-**3ad**



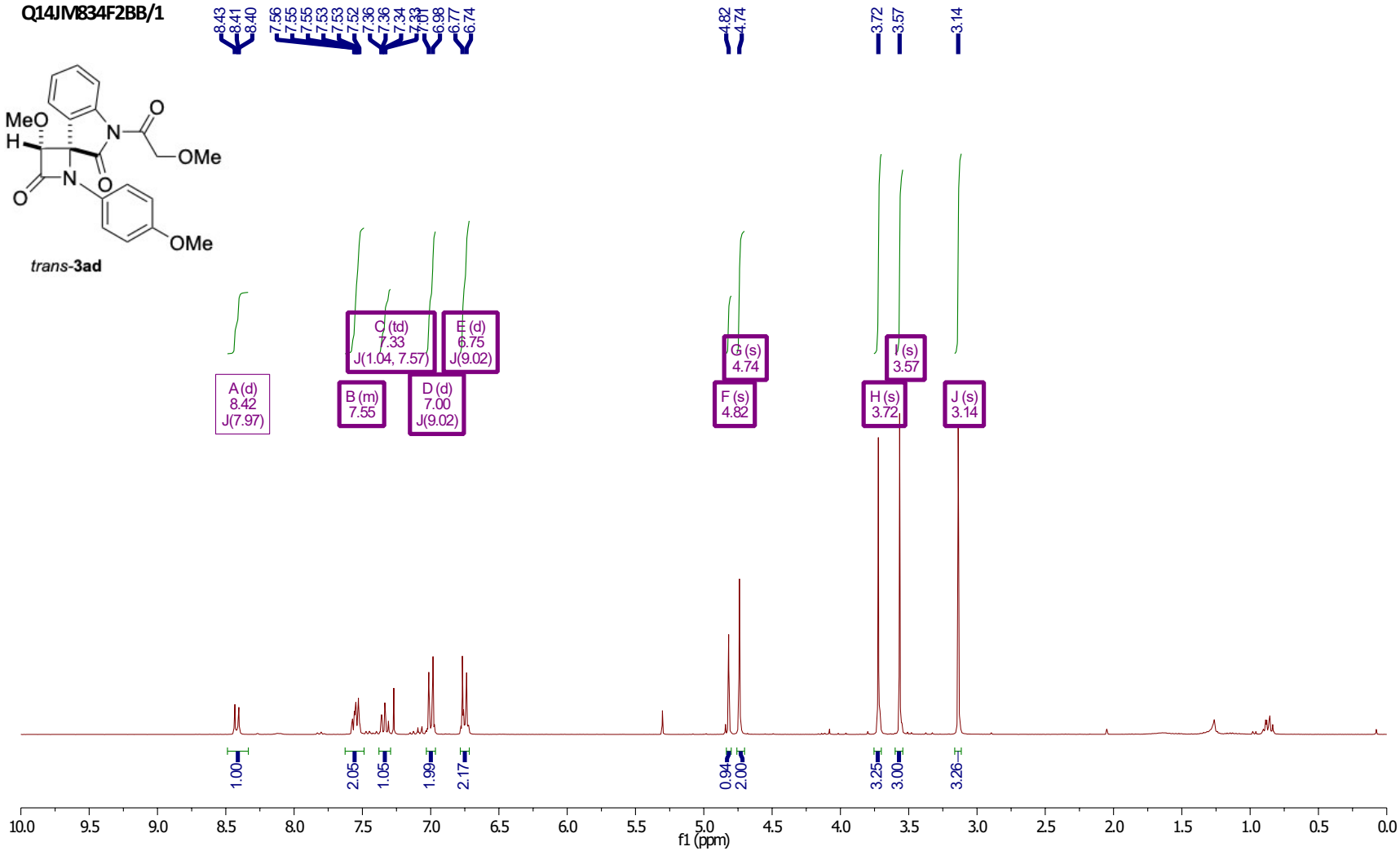
IR cis-**3ad**



F:\ESPECTROS\GRUPO-14 MAS\JM-834F4.1	JM-834F4	Instrument type and / or accessory	20/12/2013

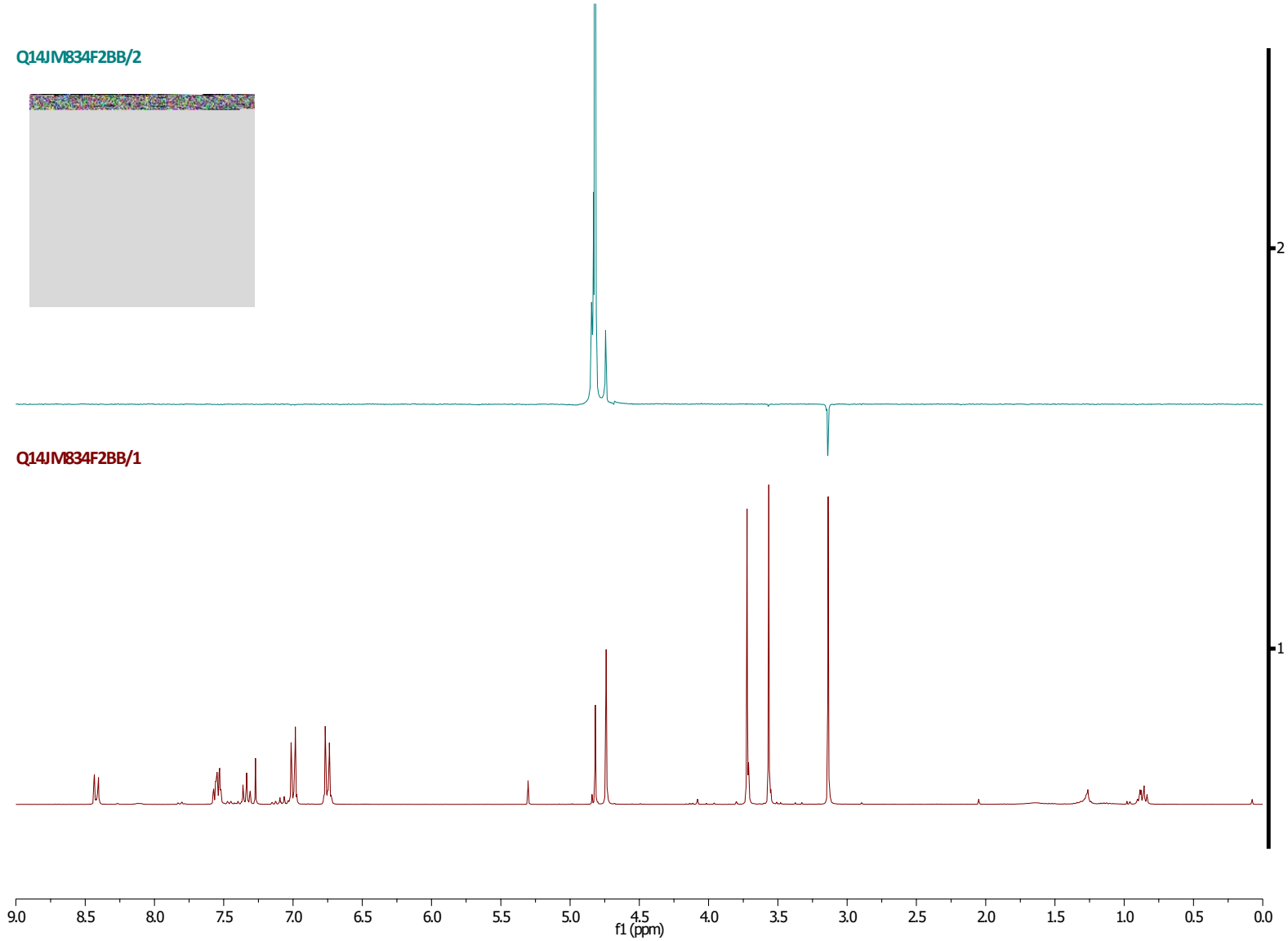
Page 1 of 1

^{1}H NMR ($CDCl_3$) trans-**3ad**

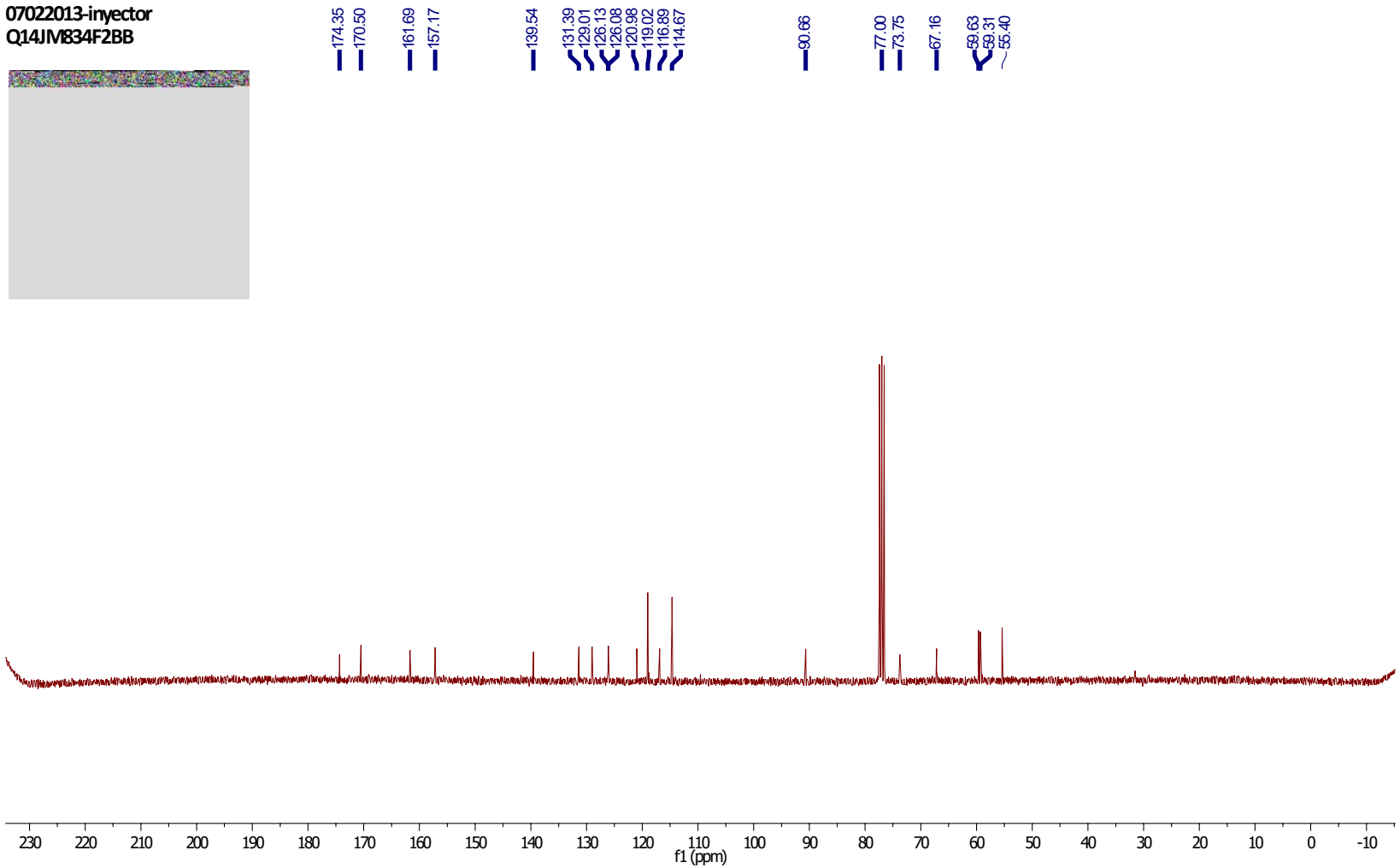


^{1}H NMR(Chloroform-d, 300 MHz): δ = 8.42 (d, 1H, *J*=8.0 Hz), 7.62 – 7.47 (m, 2H), 7.33 (td, 1H, *J*=7.6, 1.0 Hz), 7.00 (d, 2H, *J*=9.0 Hz), 6.75 (d, 2H, *J*=9.0 Hz), 4.82 (s, 1H), 4.74 (s, 2H), 3.72 (s, 3H), 3.57 (s, 3H), 3.14 (s, 3H) ppm

^{1}H NMR and nOe ($CDCl_3$) trans-**3ad**

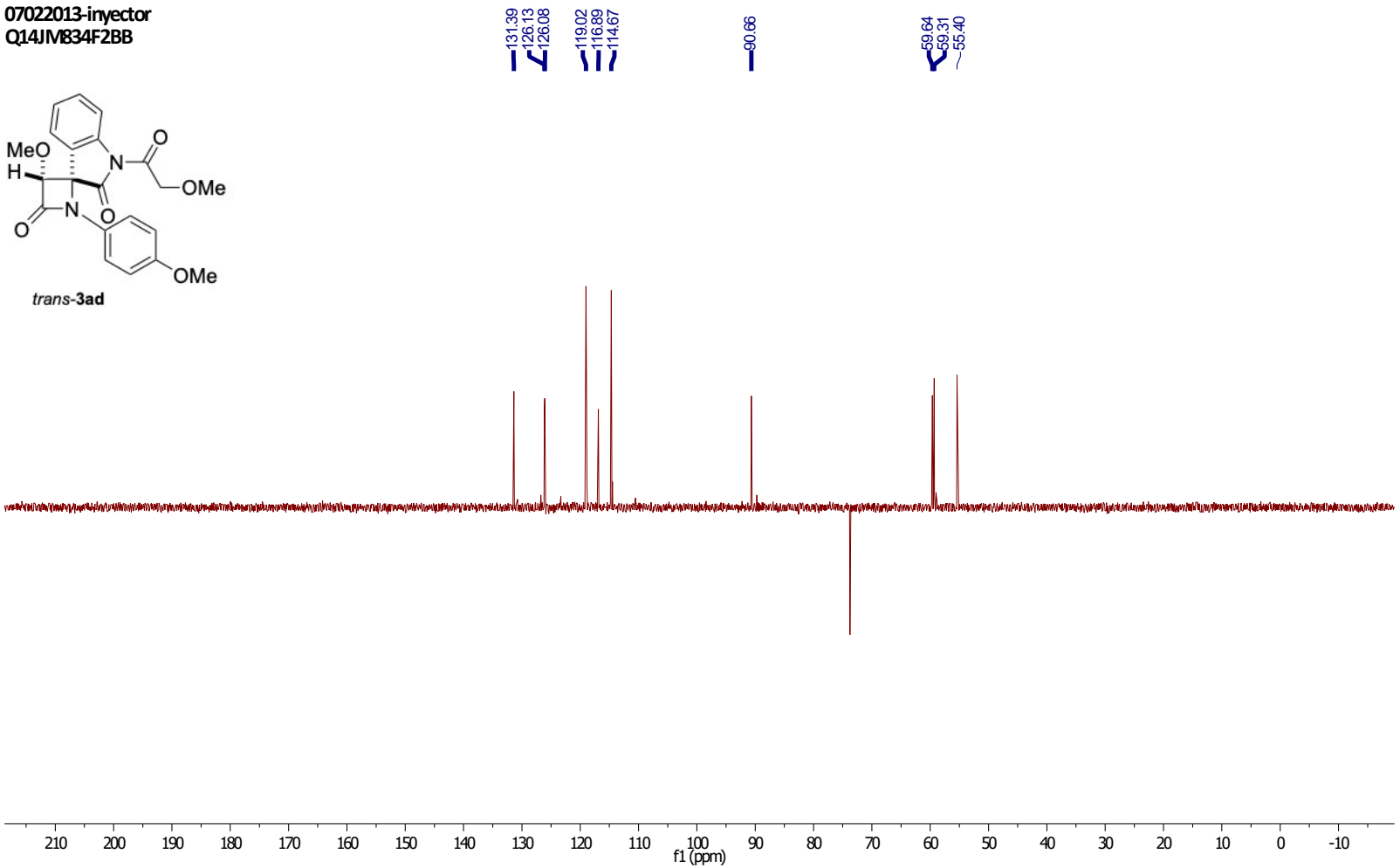


^{13}C NMR ($CDCl_3$) trans-**3ad**

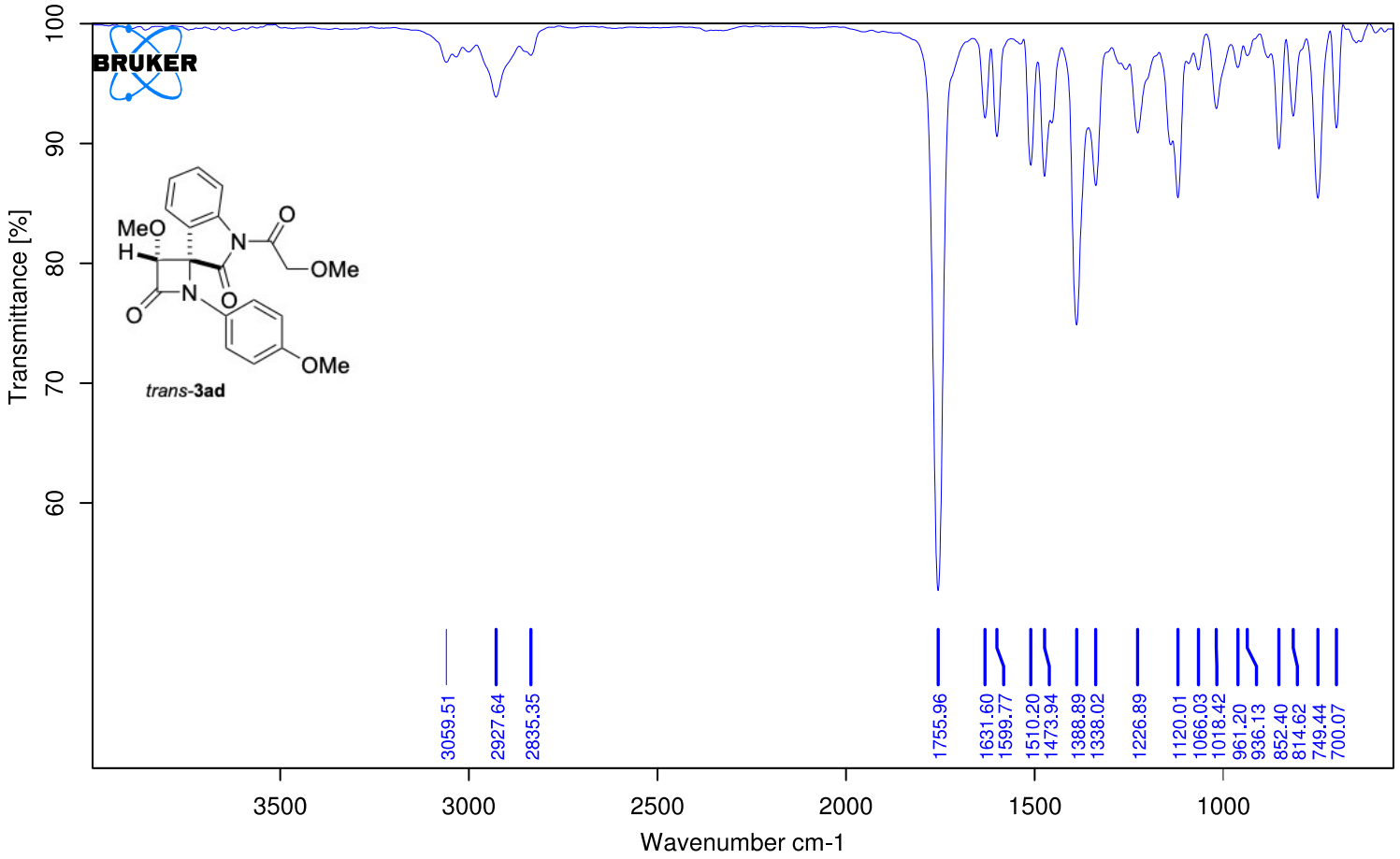


^{13}C NMR($CDCl_3$, 75 MHz): δ = 174.3, 170.5, 161.7, 157.2, 139.5, 131.4, 129.0, 126.1, 126.1, 121.0, 119.0, 116.9, 114.7, 90.7, 73.8, 67.2, 59.6, 59.3, 55.4.

^{13}C-DEPT NMR ($CDCl_3$) trans-**3ad**



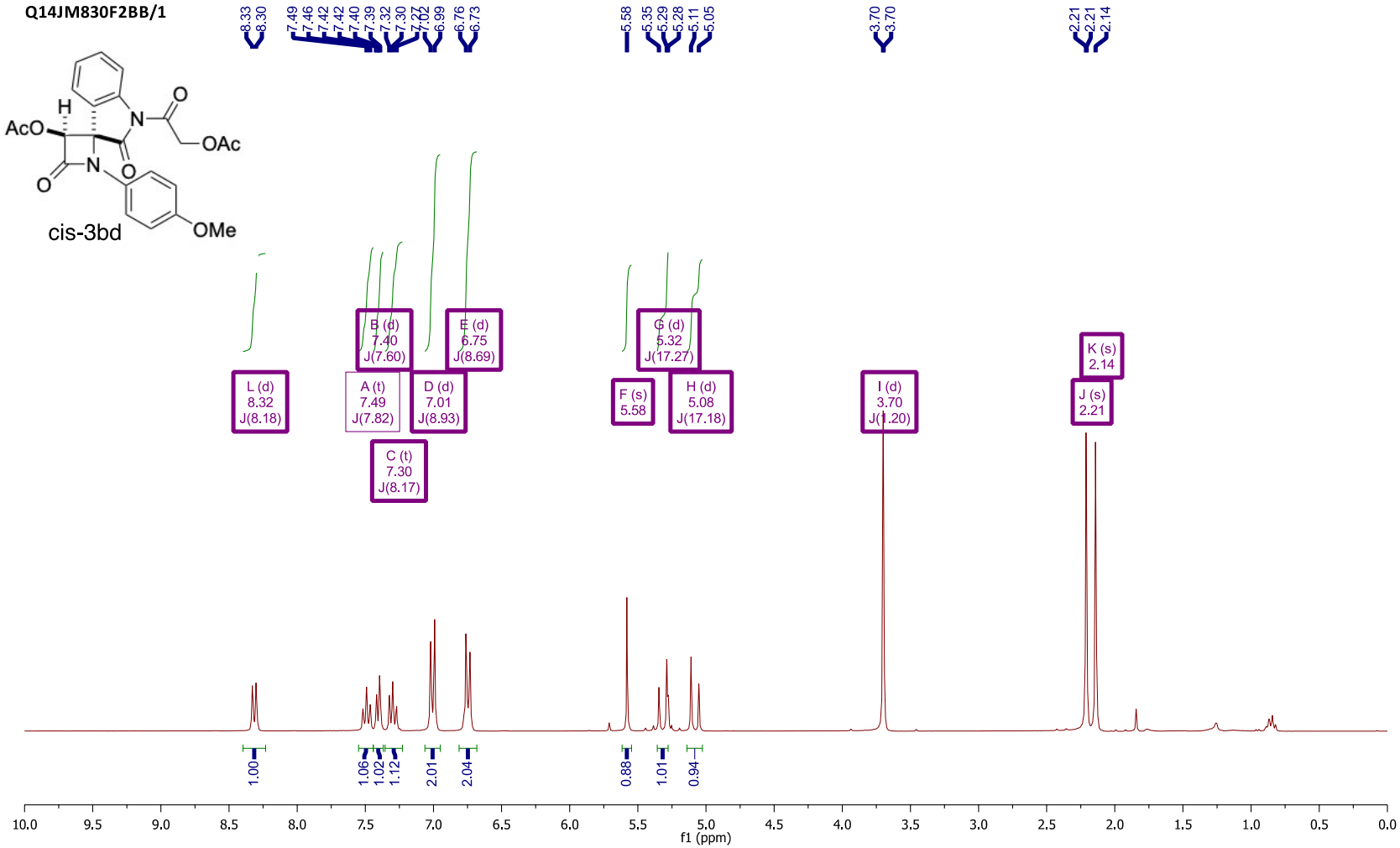
IR trans-**3ad**



F:\ESPECTROS\GRUPO-14 MAS\JM-839F2.2	JM-839F2	Instrument type and / or accessory	20/12/2013

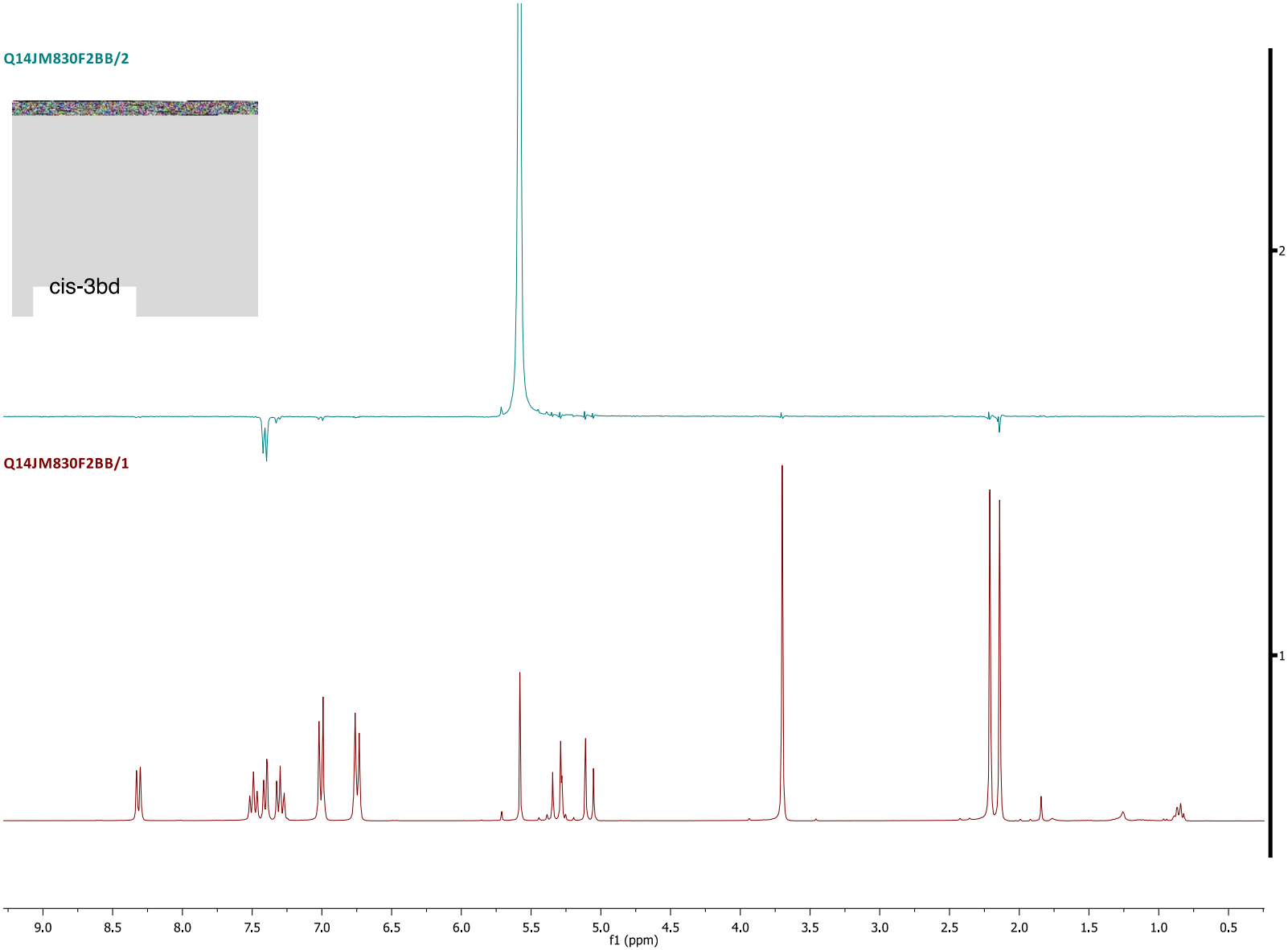
Page 1 of 1

^{1}H NMR ($CDCl_3$) cis-**3bd**

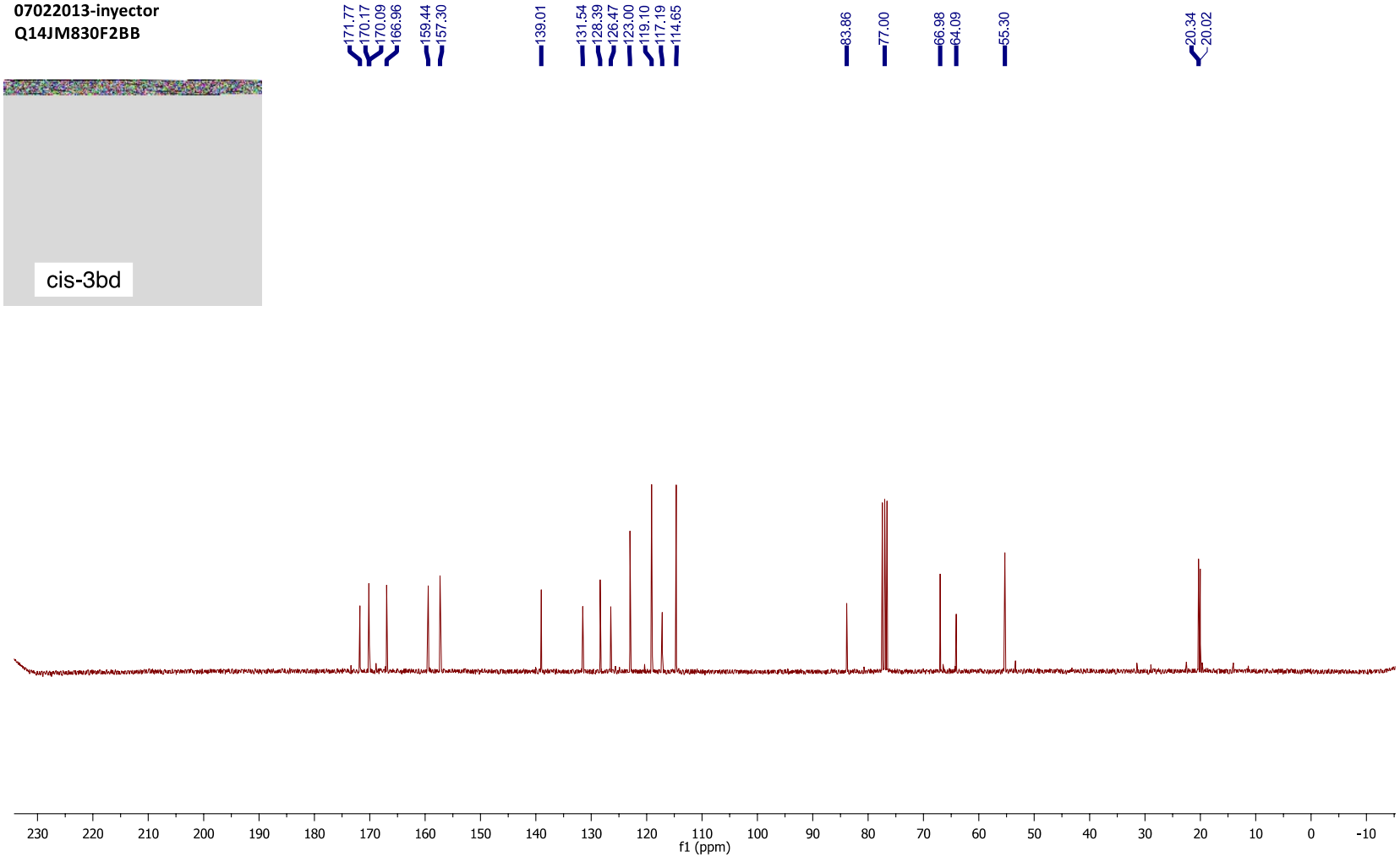


^{1}H NMR(Chloroform-d, 300 MHz): δ = 8.32 (d, 1H, *J*=8.2 Hz), 7.49 (t, 1H, *J*=7.8 Hz), 7.40 (d, 1H, *J*=7.6 Hz), 7.30 (t, 1H, *J*=8.2 Hz), 7.01 (d, 2H, *J*=8.9 Hz), 6.75 (d, 2H, *J*=8.7 Hz), 5.58 (s, 1H), 5.32 (d, 1H, *J*=17.3 Hz), 5.08 (d, 1H, *J*=17.2 Hz), 3.70 (d, 3H, *J*=1.2 Hz), 2.21 (s, 2H), 2.14 (s, 3H) ppm

^{1}H NMR and nOe ($CDCl_3$) cis-**3bd**

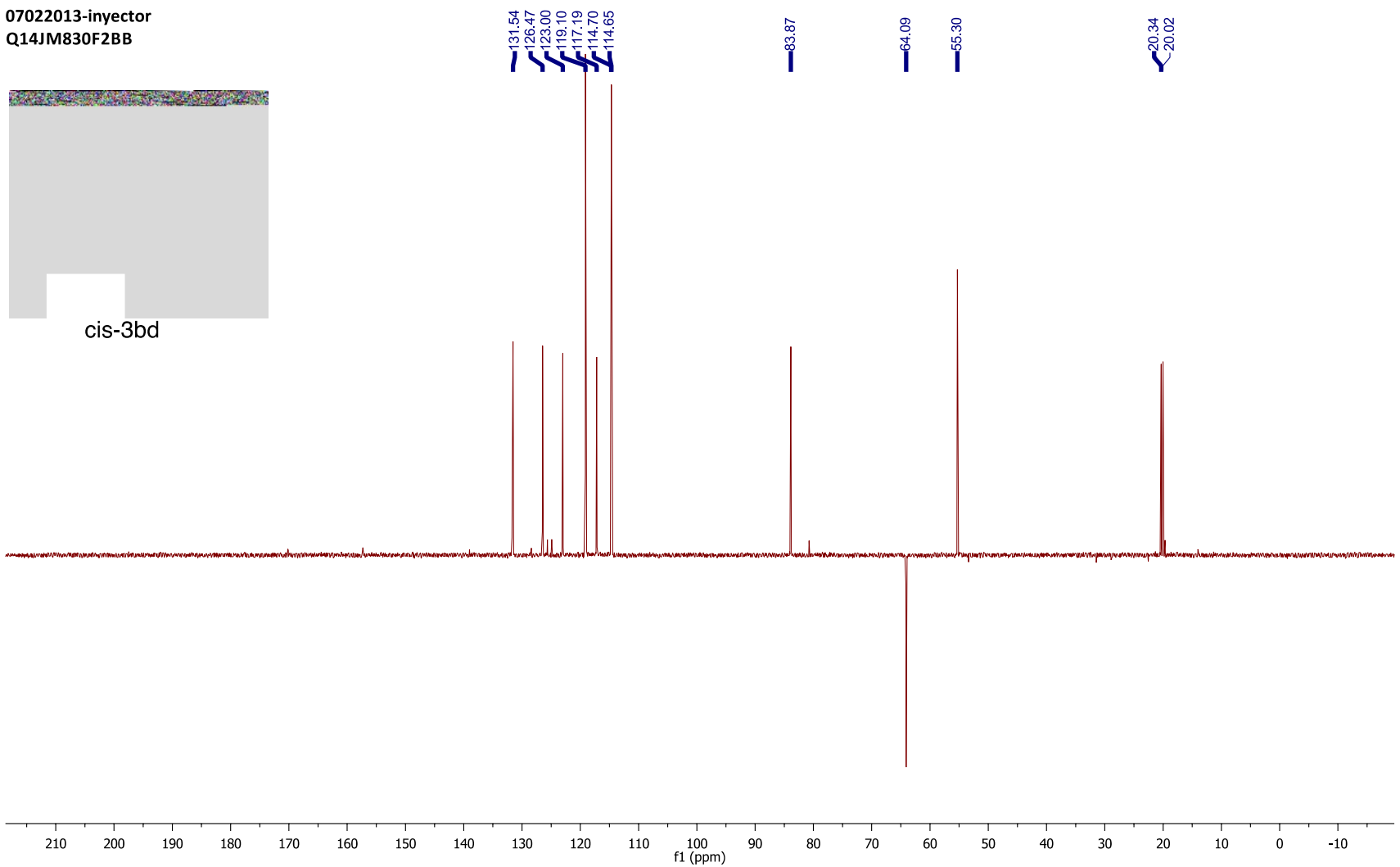


^{13}C NMR ($CDCl_3$) cis-**3bd**

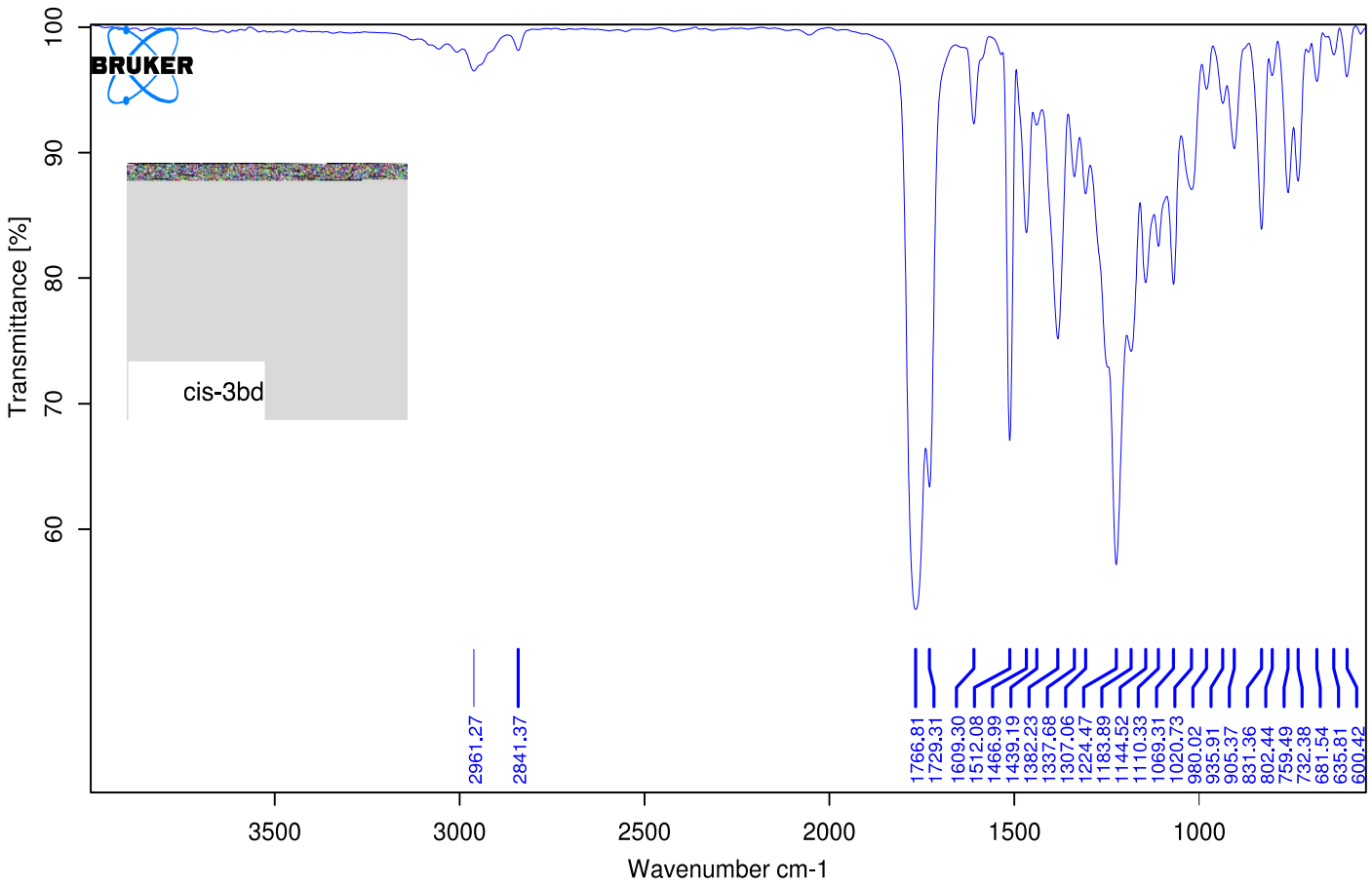


^{13}C NMR($CDCl_3$, 75 MHz): δ = 171.8, 170.2, 170.1, 167.0, 159.4, 157.3, 139.0, 131.5, 128.4, 126.5, 123.0, 119.1, 117.2, 114.7, 83.9, 67.0, 64.1, 55.3, 20.3, 20.0.

^{13}C-DEPT NMR ($CDCl_3$) cis-**3bd**



IR cis-**3bd**



F:\ESPECTROS\GRUPO-14 MAS\JM-830F2B.1	JM-830F2B	Instrument type and / or accessory	20/12/2013

Page 1 of 1