Electronic Supplementary Information for

Catalytic intramolecular hydroamination of aminoallenes using titanium complexes of chiral, tridentate, dianionic imine-diol ligands

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Complete description of solid-state structures of ligands

Four of the five ligands were characterized by X-ray crystallography. L-H_2**L4**, L-H_2**L6**, L-H_2**L7**, and L-H_2**L8** each crystallized from 4:1 ether:isopropanol to give X-ray quality crystals. The molecular structure of L-H_2**L4** is shown in **Figure S1**. Rather than the expected imino-phenol tautomer, the crystal structure clearly showed the iminium-phenoxide tautomer, with the iminium N atom protonated and the phenol O atom deprotonated. There is an intramolecular hydrogen bond between N(1) and the phenoxide oxygen, O(1). Previously we have observed intramolecular hydrogen bonds between the aliphatic oxygen and the amine nitrogen in our bidentate amino alcohols.[66, 67] The atoms in the phenoxide aromatic ring, O(1), C(7), N(1) and H(1), are all essentially coplanar, with deviations from planarity of 0.131 Å for C(7) and 0.169Å for N1. The C(8) atom is displaced 0.544 Å, and the C(7)-N(1)-C(8)-C(9) dihedral angle is -86.7° which places the aliphatic alcohol oxygen atom 2.710 Å from the plane. There is a significant difference in the bond lengths from C(1)-O(1), at 1.2944(19) Å and C(9)-O(2), at 1.4240(18) Å, suggesting that a more accurate description of the structure is the keto-iminium ion with delocalization of charge along C(1)-C(6)-C(7)-N(1). The bonds between C(1)-C(2), C(1)-C(6), C(3)-C(4) and C(5)-C(6) are all long, at 1.410 – 1.440 Å, while the C(2)-C(3) and C(4)-C(5) bond lengths are both shorter at around 1.37 Å. In contrast, the C-C bond lengths in the aromatic ring on the benzyl side chain are typical aromatic bond distances ranging from 1.383 to 1.394 Å. There is residual electron density in the electron density map around C(6), suggesting a buildup of negative charge at that atom.

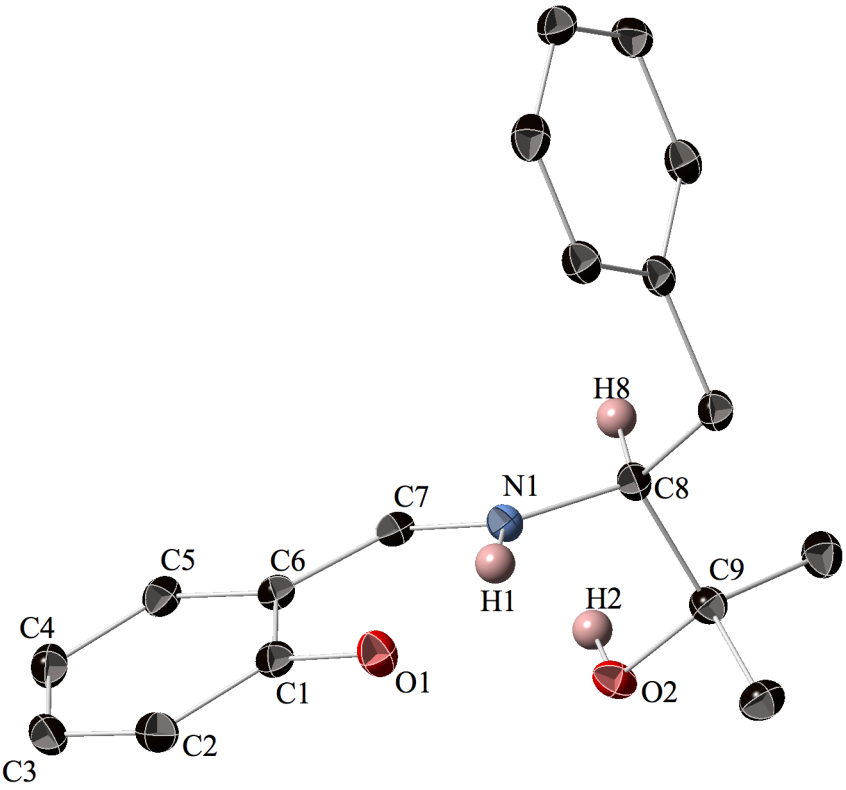

Figure S1. Thermal ellipsoid drawing of L-H_2**L4** (hydrogen atoms except H(1), H(2) and H(8) are omitted for clarity; ellipsoids shown at 50% probability). Selected bond distances (Å): C(1)-

C(2) 1.418(2), C(2)-C(3) 1.373(2), C(3)-C(4) 1.410(2), C(4)-C(5) 1.368(2), C(5)-C(6) 1.416(2), C(6)-C(1) 1.440(2), C(1)-O(1) 1.2944(19), C(9)-O(2) 1.4240(18).

The iminium phenoxide structure has been observed previously for imino phenols.[68] An interesting example by Salehi[69] has two similar structures exhibiting both possible tautomeric forms. One structure in that paper has the imino-phenol structure (HL^1), while another exhibits the iminium-phenoxide structure (HL^2). HL^2 has the deprotonated phenol oxygen engaged in both inter- and intramolecular H bonds to iminium hydrogens and has almost exactly the same C-C and C-O bond lengths as seen in L-H_2**L4**. Examining the intermolecular contacts of L-H_2**L4** shows that in addition to the intramolecular hydrogen bonding, there is a similar network of intermolecular hydrogen bonding of H(2) to O(1) of a neighboring molecule (Figure S2).

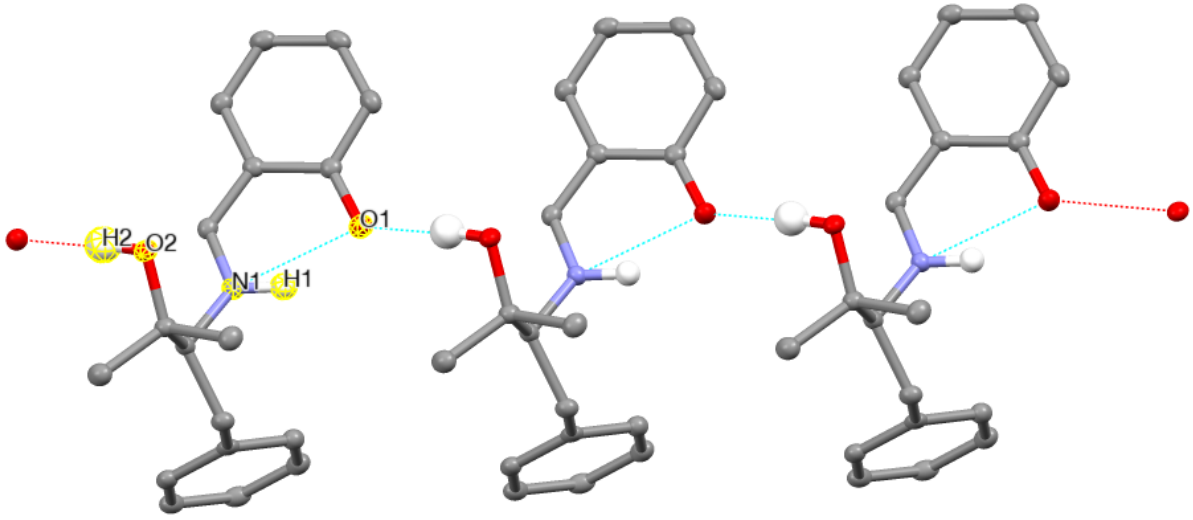

Figure S2. Hydrogen bonding network of l-H_2**L4** showing intramolecular contacts between H(1) and O(1), and intermolecular contacts between H(2) and O(1).

The molecular structure of L-H_2**L6** is shown in **Figure S2**. The structure has one disordered *tert*-butyl group on C(27) which was modeled with partial occupancies of 0.715 and 0.285. A diagram of the full structure is included in the ESI. The molecule crystallized with the expected imine-phenol tautomer structure, and contains an intramolecular hydrogen bond between N(1) and O(2). As with H_2**L4**, the benzyl carbon C(22) and N(1) are both almost within the plane described by the aromatic phenol ring, with a displacement of 0.041 Å for C(22) and 0.179 Å for N(1). The C(2) is displaced by 0.150 Å, while the C(22)-N(1)-C(2)-C(1) dihedral angle is -118.5°, which places O(1) 1.750 Å from the plane. The diphenyl substitution on the aliphatic alcohol group prevents intermolecular contacts involving O(1). Some of our bidentate amino alcohol ligands have exhibited intermolecular hydrogen bonding when the aliphatic oxygen is primary,[66] but tertiary alcohols have not exhibited this behavior.[66, 67] Aside from the intramolecular hydrogen bond between O(2)-H(2)-N(1), there are no additional contacts with the atoms H(2), O(1), O(2) or N(1) within 3Å. As seen in the structure of L-H_2**L4**, there is a significant difference in the bond lengths from C(24)-O(2), at 1.3570(18) Å, and C(1)-O(1), at 1.4323(19) Å. The bonds between C(24)-C(23), C(23)-C(28), C(27)-C(26) and C(24)-C(25) are all long, at 1.400 – 1.412 Å, while the C(28)-C(27) and C(26)-C(25) bonds are both shorter at around 1.39 Å. The differences in bond-lengths between the phenol aromatic ring and the side

chain aromatic ring are less pronounced than in the case with H_2**L4**, presumably due to the fact that the phenol is protonated and there is less disruption of the electronic structure of the aromatic ring.

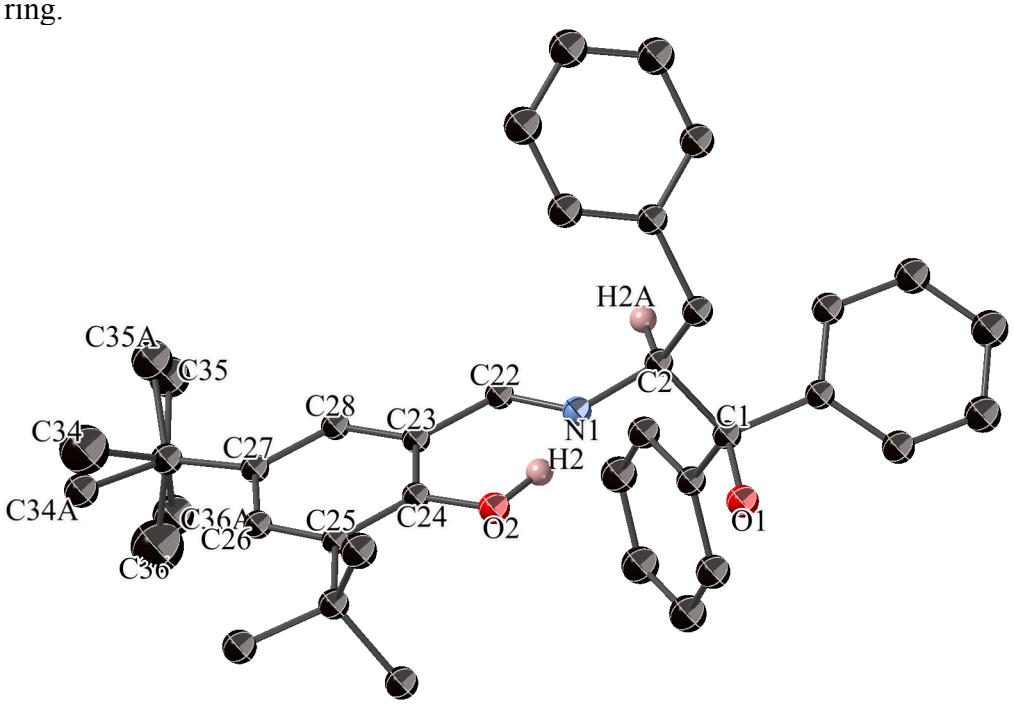

Figure S3. Complete thermal ellipsoid drawing of L-H_2**L6** showing the disordered *tert*-butyl group on C(27) (hydrogen atoms except H(2) and H(2A) are omitted for clarity; thermal ellipsoids are shown at 50% probability). C(34), C(35) and C(36) are modeled at 0.715 occupancy while C(34A), C(35A) and C(36A) are modeled at 0.285 occupancy. Selected bond distances (Å): C(24)-C(25) 1.405(2), C(25)-C(26) 1.393(2), C(26)-C(27) 1.402(2), C(27)-C(28) 1.385(2), C(23)-C(28) 1.400(2), C(24)-O(2) 1.3570(18), C(1)-O(1) 1.4323(19).

The molecular structure of L-H_2**L7** is shown in **Figure S4**. The structure is very similar to that of L-H_2**L6**, with the expected imine-phenol structure and an intramolecular hydrogen bond linking N(1) and O(2). The phenol aromatic ring is essentially coplanar with O(2), C(19) and N(1), though the deviations of those atoms are opposite in direction to the previous ligands, with C(19) 0.100 Å above the plane, N(1) 0.117 Å above the plane, and C(2) 0.156 Å above the plane. The C(19)-N(1)-C(2)-C(1) dihedral angle is -110.3 °, which places O(1) 1.389 Å below the plane. There are no observed intermolecular hydrogen bond contacts, as they are again blocked by the diphenyl substitution at C(1). The bond lengths from C(21)-O(2), at 1.349 Å, and C(1)-O(1), at 1.438 Å, are again different, intermediate between the previous two structures, but closer to that observed in L-H_2**L6**. Bond alternation in the phenol aromatic ring is again observed, with approximately the same magnitude as seen in L-H_2**L6**.

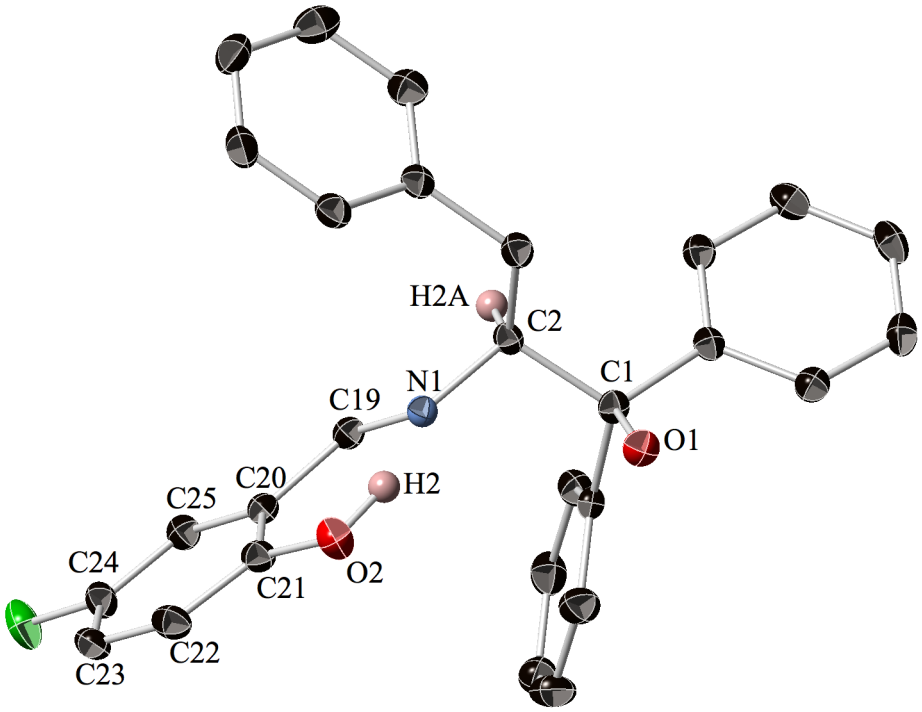

Figure S4. Thermal ellipsoid drawing of L-H_2**L7** (hydrogen atoms except H(2) and H(2A) are omitted for clarity; ellipsoids shown at 50% probability). Selected bond distances (Å): C(20)-C(21) 1.412(2), C(21)-C(22) 1.397(2), C(22)-C(23) 1.379(2), C(23)-C(24) 1.376(2), C(24)-C(25) 1.374(2), C(21)-O(2) 1.3492(19), C(1)-O(1) 1.4377(18).

The molecular structure of L-H_2**L8** is shown in **Figure S5**. The structure is similar to that of L-H_2**L7**, with the expected imine-phenol structure and an intramolecular hydrogen bond between N(1) and O(1). The phenol aromatic ring is again essentially co-planar with O(1), C(7) and N(1), and the deviations of those atoms are of the same sign as in L-H_2**L7**, with C(7) 0.080 Å above the plane, N(1) 0.142 Å above the plane, and C(8) 0.285 Å above the plane. The C(7)-N(1)-C(8)-C(12) dihedral angle is -122.6 °, which places O(2) 0.789 Å below the plane. The isopropyl group allows a different geometric placement of the aliphatic oxygen atom, allowing it to be much closer to the plane as compared to the previous ligands. There are no observed intermolecular hydrogen bond contacts, though there is a long range intermolecular contact between O(2) and F(1) in an adjacent molecule at 3.36 Å. The bond lengths from C(1)-O(1), at 1.353(2) Å, and C(12)-O(2), at 1.437 Å, are again different, but closer to L-H_2**L6** and L-H_2**L7** than the other tautomer exhibited by L-H_2**L4**. Bond alternation in the phenol aromatic ring is again observed, though this structure exhibits the least deviation from an aromatic structure of the four ligands. This structure is almost identical to that of the previously reported molecule lacking a fluorine.[60, 71]

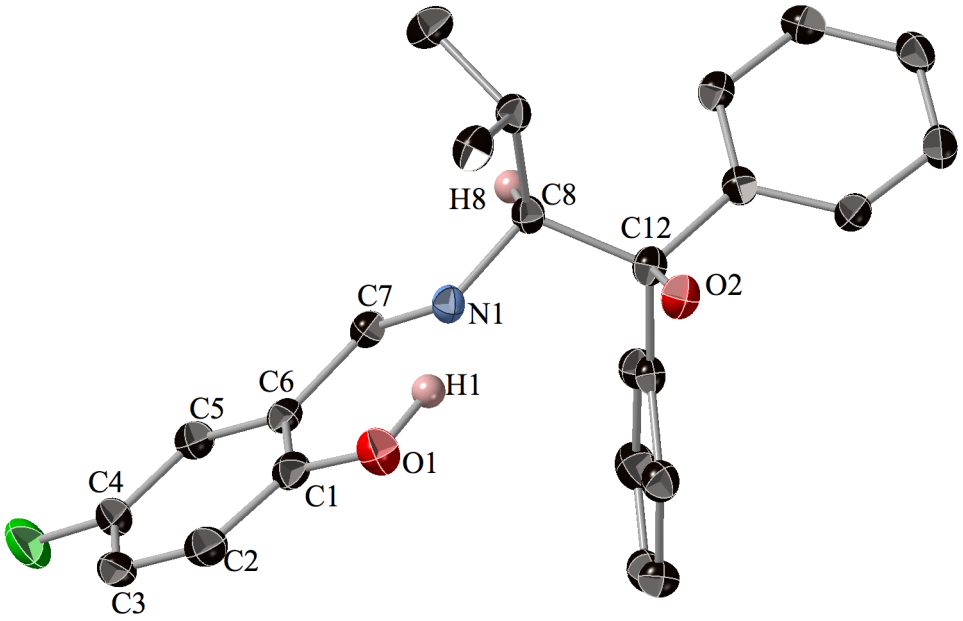

Figure S5. Thermal ellipsoid drawing of L-H_2**L8** (hydrogen atoms except H(2) and H(8) are omitted for clarity; ellipsoids shown at 50% probability). Selected bond distances (Å): C(1)-C(2) 1.398(3), C(2)-C(3) 1.380(3), C(3)-C(4) 1.380(3), C(4)-C(5) 1.374(3), C(5)-C(6) 1.400(3), C(6)-C(1) 1.406(3), C(1)-O(1) 1.353(2), C(12)-O(2) 1.437(2).

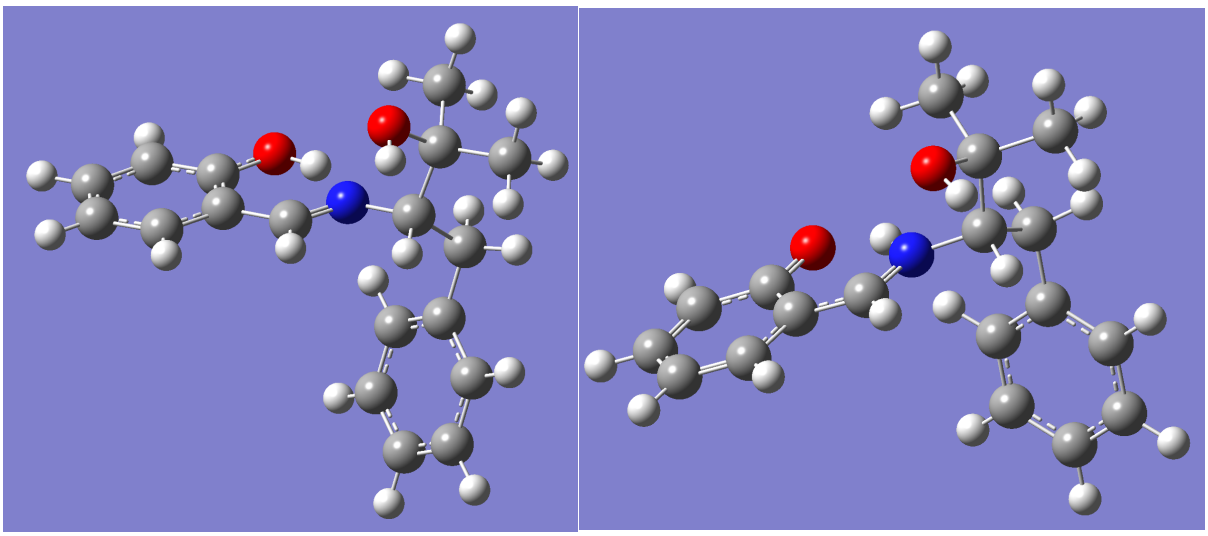

Figure S6. Calculated structures of imine phenol (left) and iminium phenoxide tautomers of L-H_2**L4** (Gaussian B3LYP 6-31G(d,p)). Energies: iminium phenoxide, -903.79254086 au, imine phenol, -903.79907612 au, energy difference: 0.00653 au = 4.1 kcal/mol.

XYZ files output from Gaussian

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C       4.567000   -0.745000   -1.249000
C       3.335000   -0.228000   -1.556000
C       2.336000   -0.066000   -0.554000
C       1.077000    0.466000   -0.886000
C      -1.186000    1.198000   -0.202000
C      -1.137000    2.756000   -0.020000
C      -2.504000    3.393000   -0.307000
C      -0.613000    3.166000    1.357000
C      -2.207000    0.460000    0.697000
C      -2.398000   -0.998000    0.326000
C      -3.439000   -1.373000   -0.534000
C      -3.622000   -2.706000   -0.901000
C      -2.761000   -3.689000   -0.410000
C      -1.721000   -3.328000    0.448000
C      -1.540000   -1.994000    0.815000
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H      -0.583000    3.251000   -1.837000
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C       4.456000   -0.770000   -1.340000
C       3.160000   -0.343000   -1.589000
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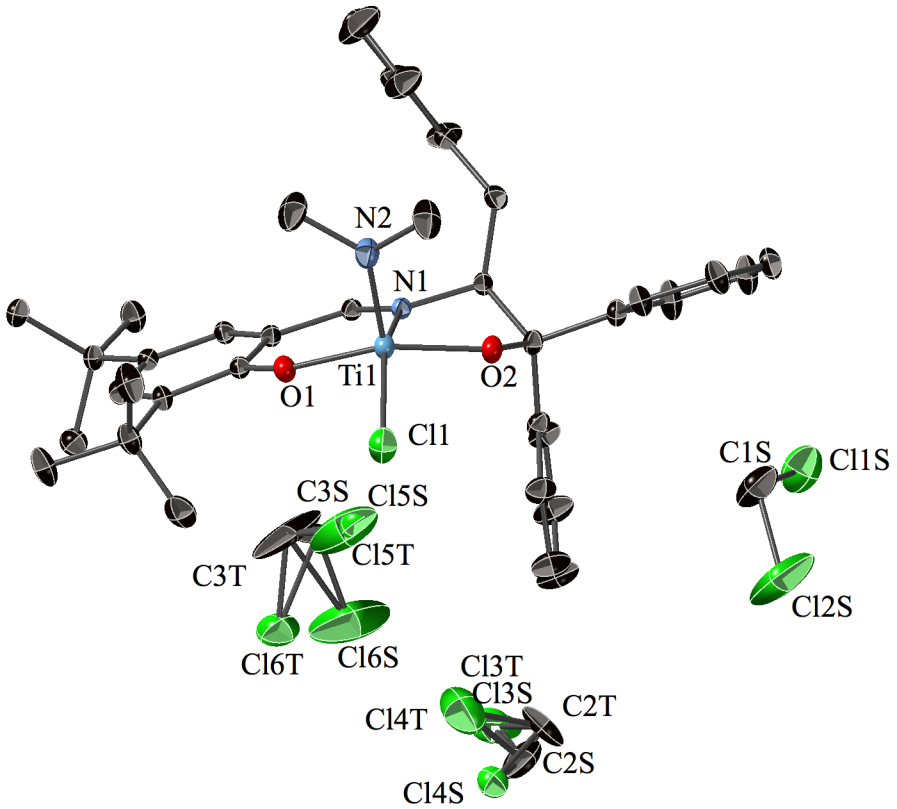
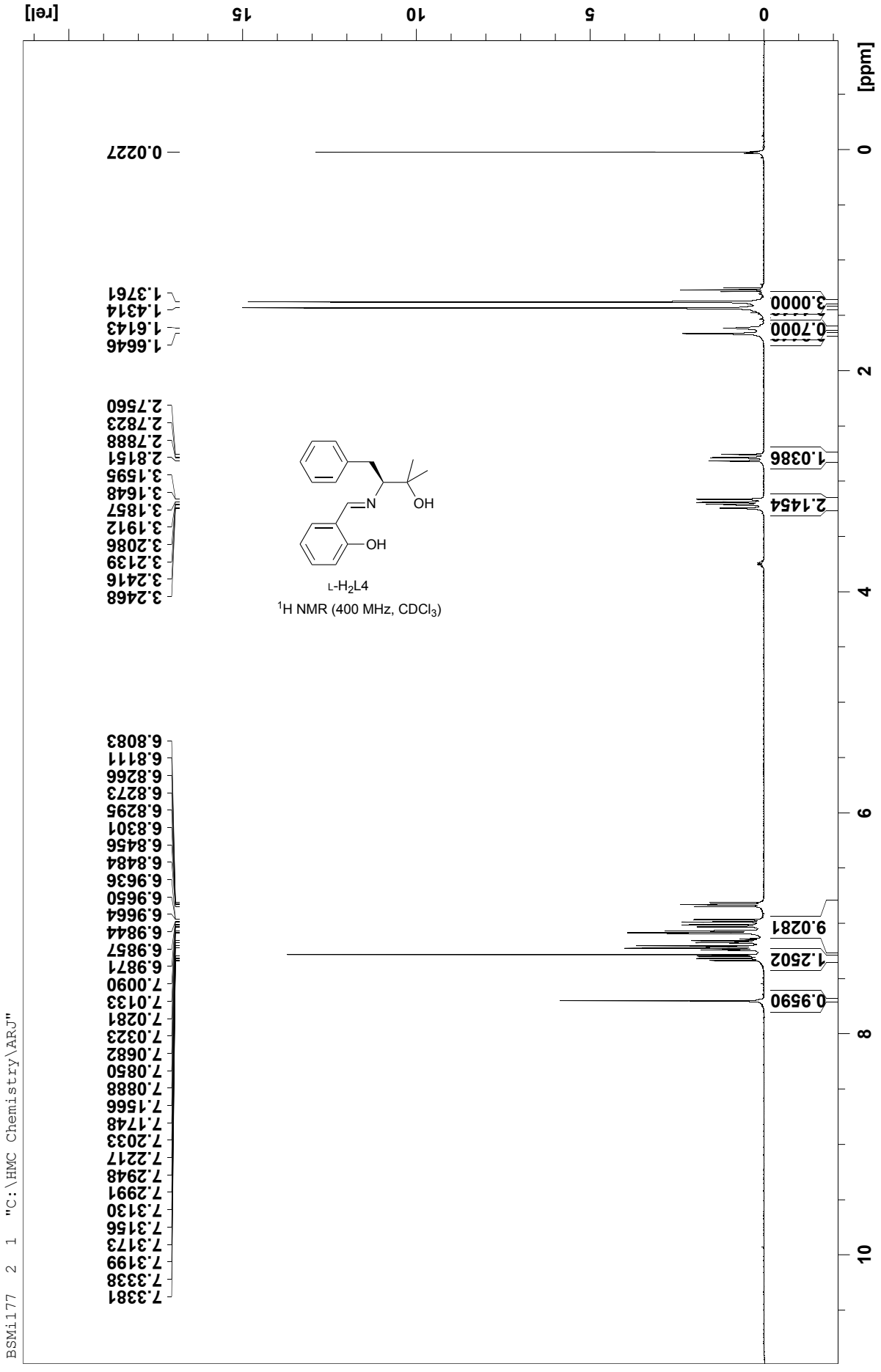


Figure S7. Thermal ellipsoid drawing of complex **14** showing three solvent molecules (two disordered) of CH_2Cl_2 (hydrogen atoms are omitted for clarity; thermal ellipsoids are shown at 50% probability). C(3S), Cl(5S), Cl(6S), C(2S), Cl(3S) and Cl(4S) are modeled at 0.519 occupancy; C(3T), Cl(5T), Cl(6T), C(2T), Cl(3T) and Cl(4T) are modeled at 0.481 occupancy.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L-H_2L4

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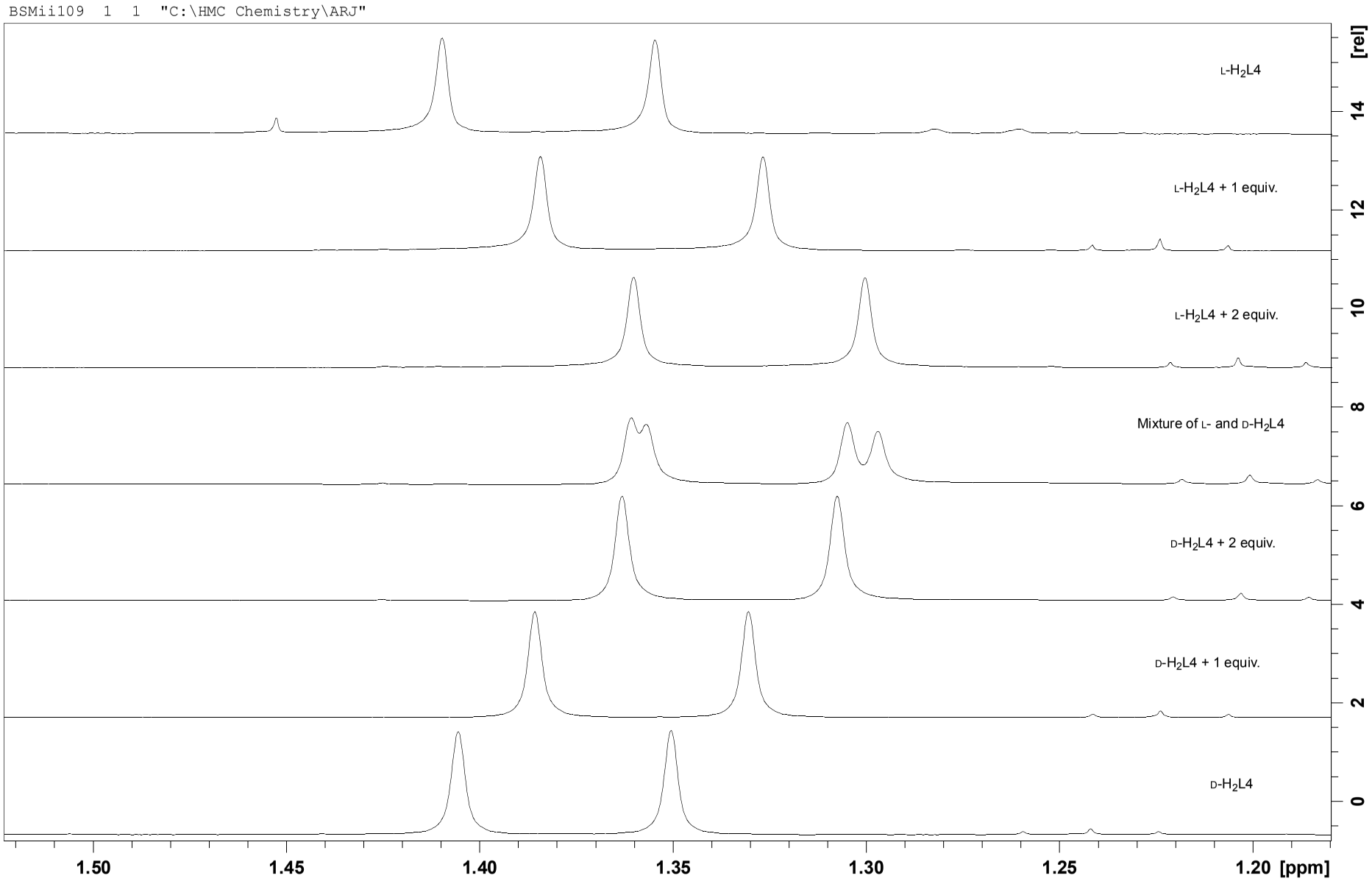
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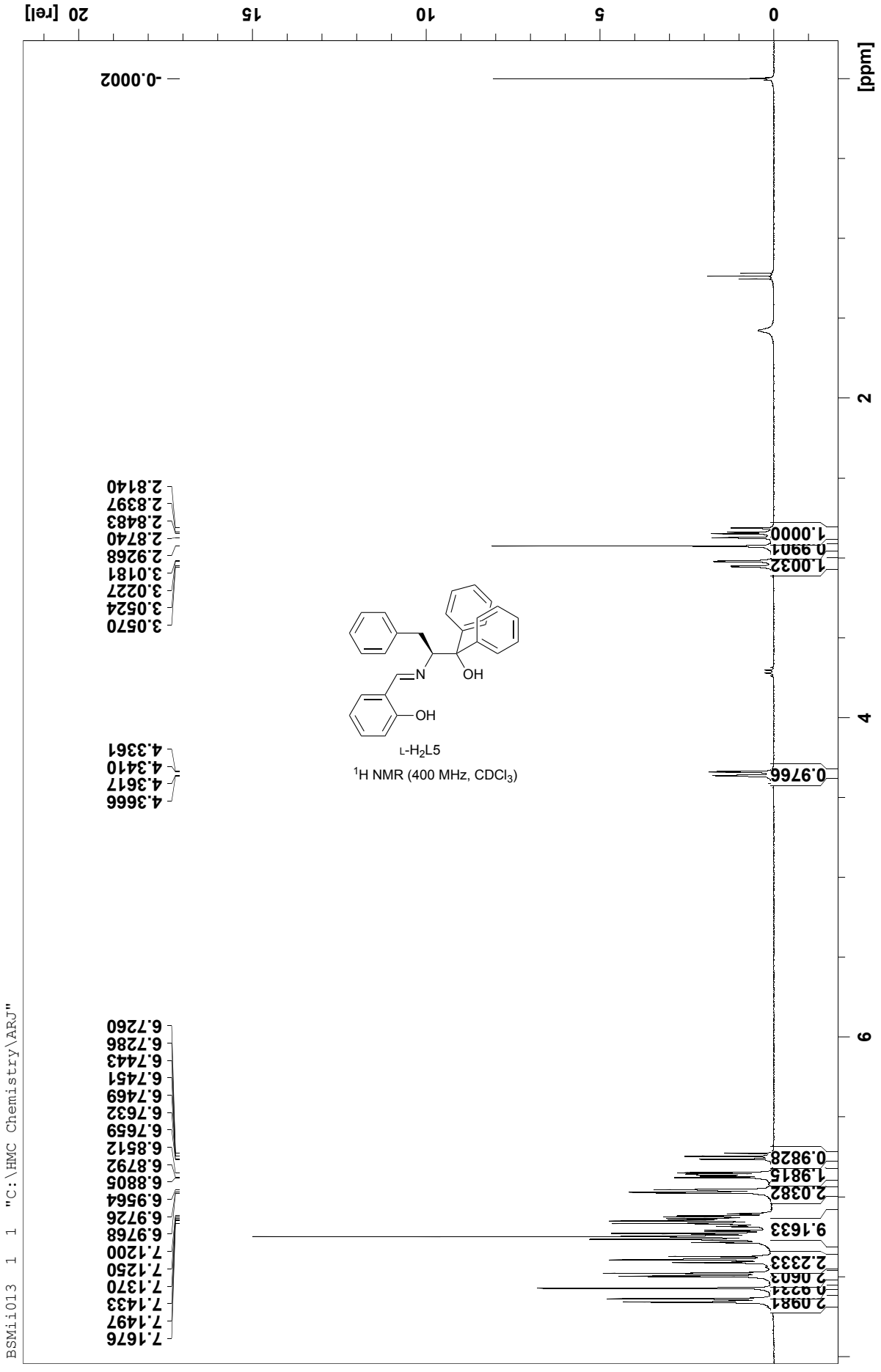
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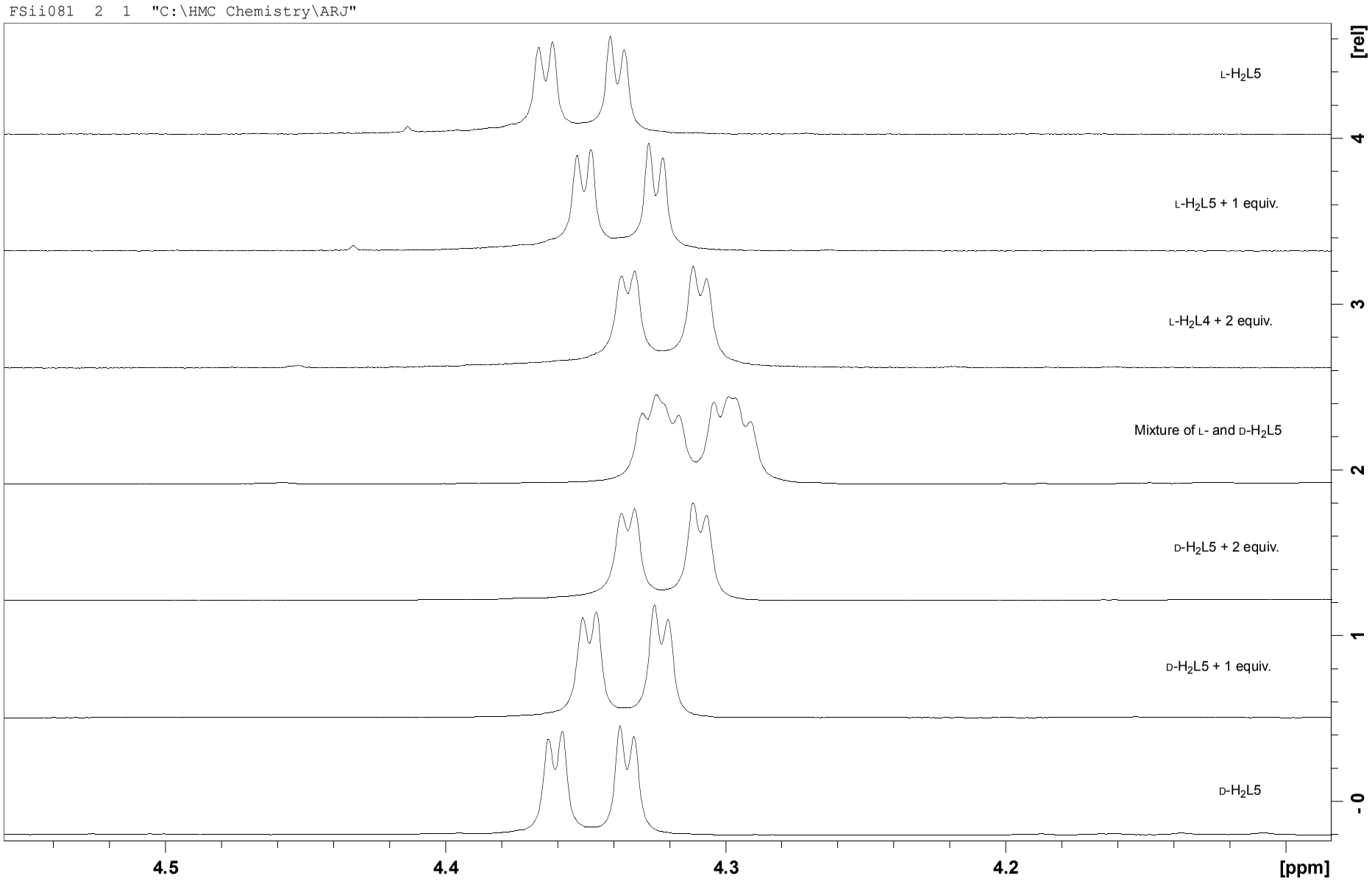
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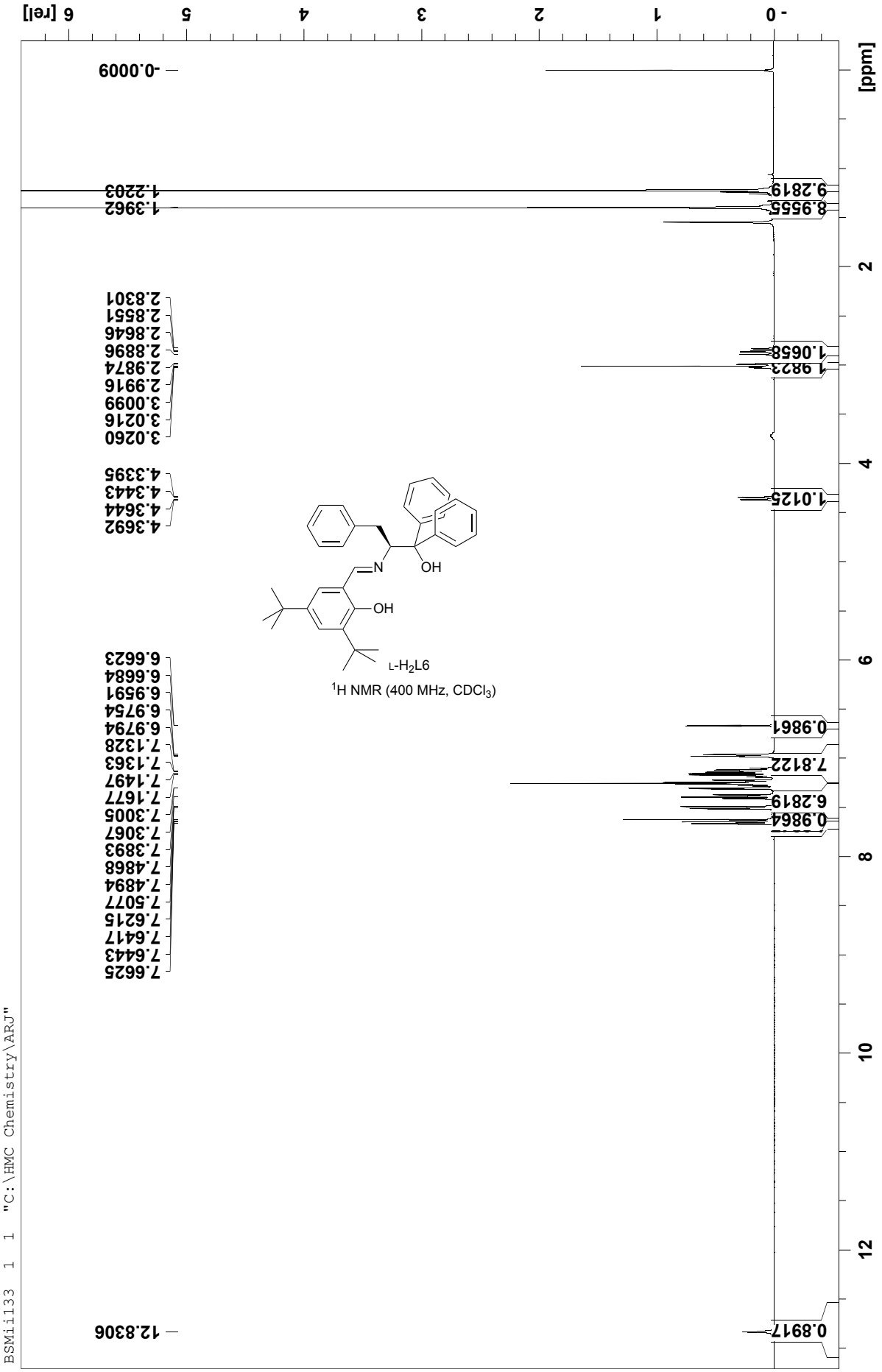
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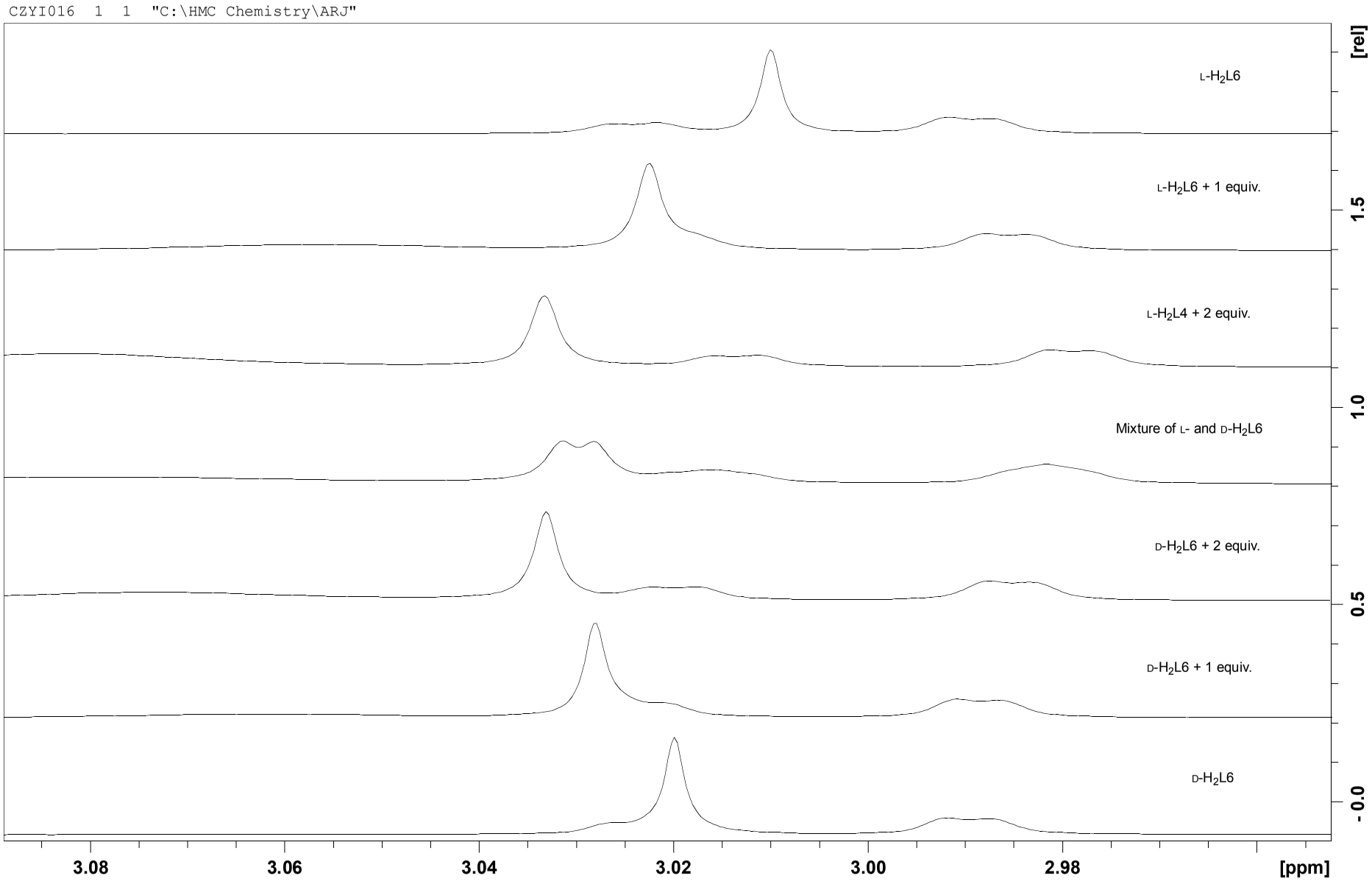
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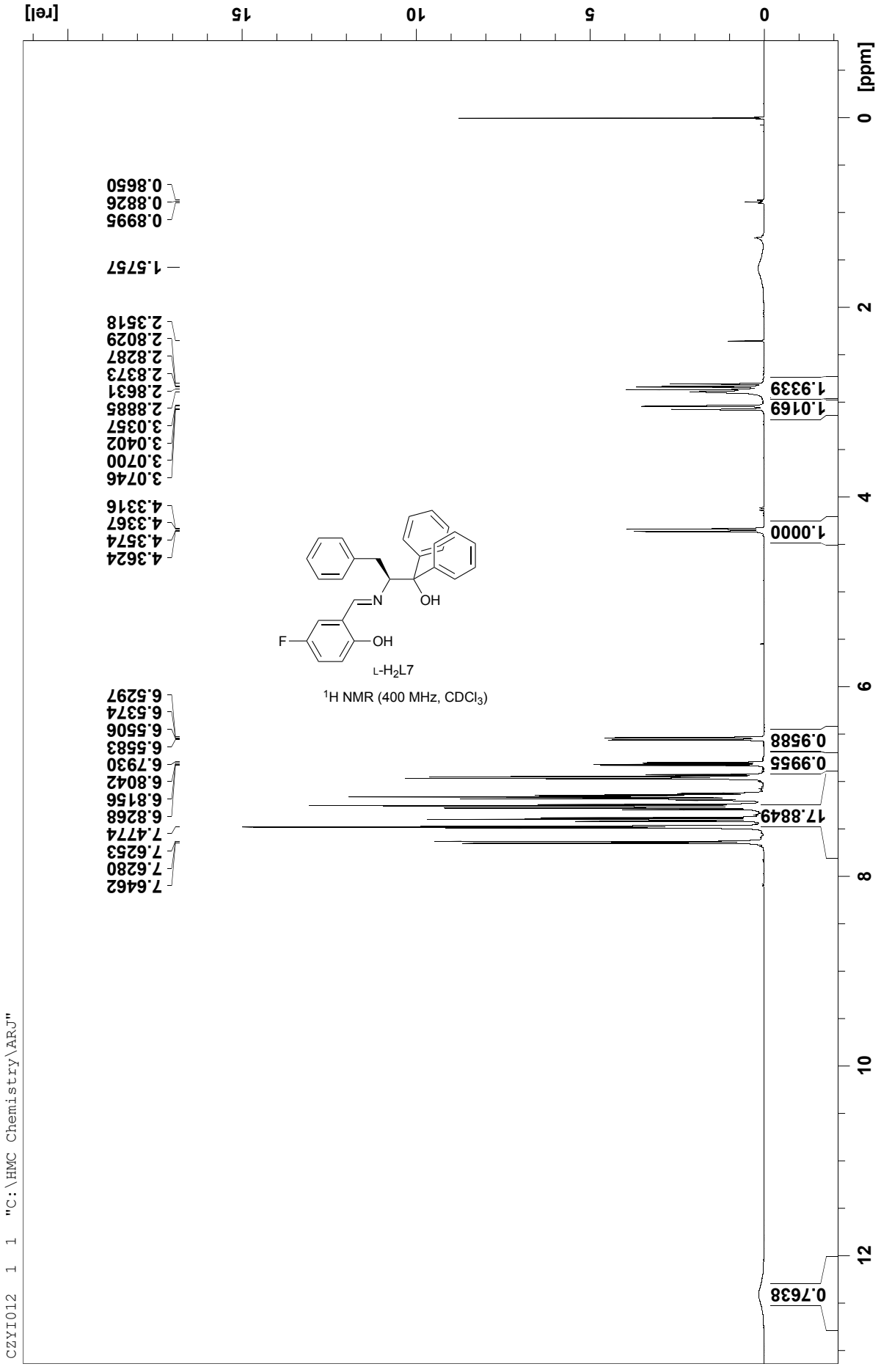
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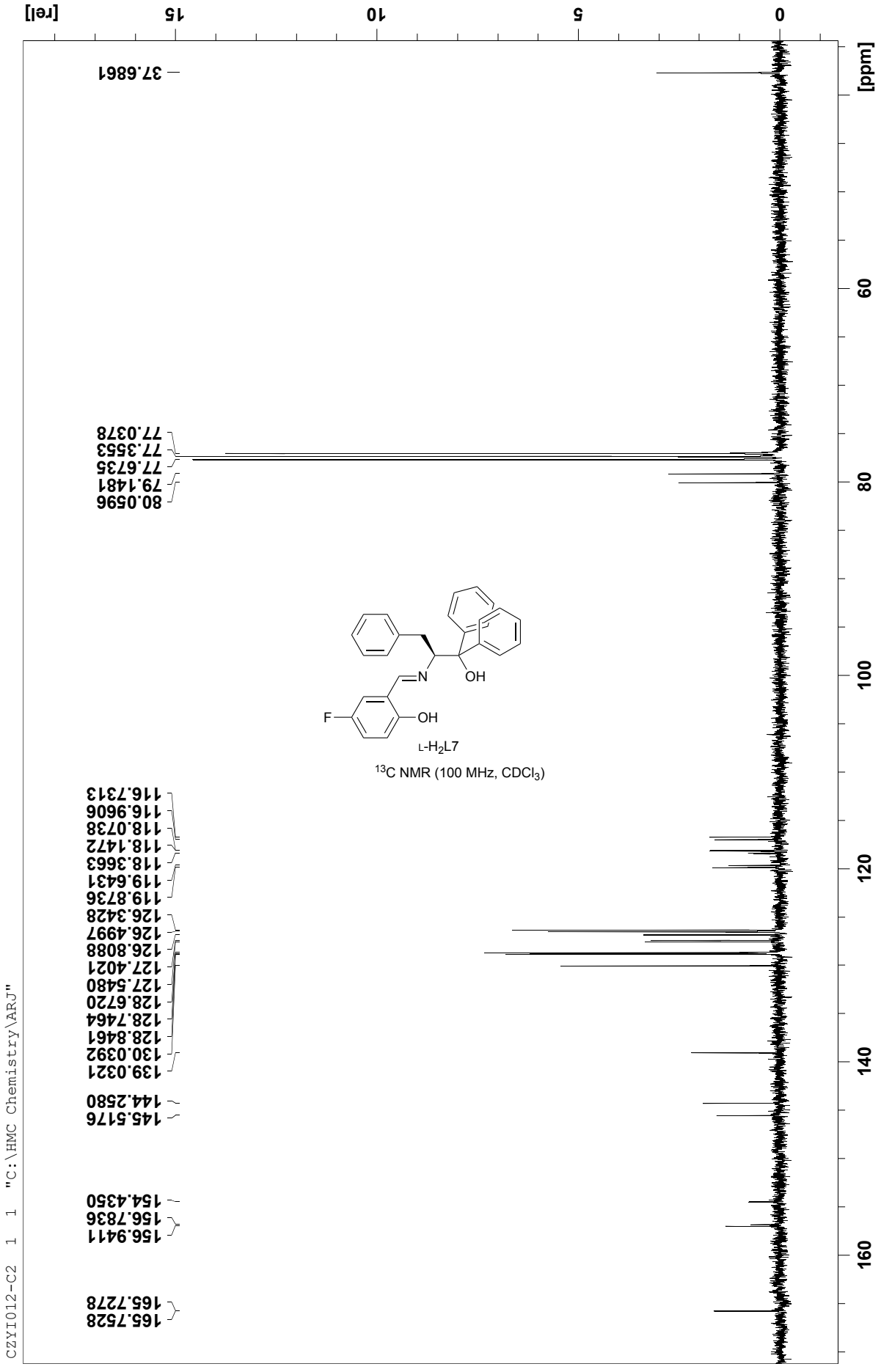
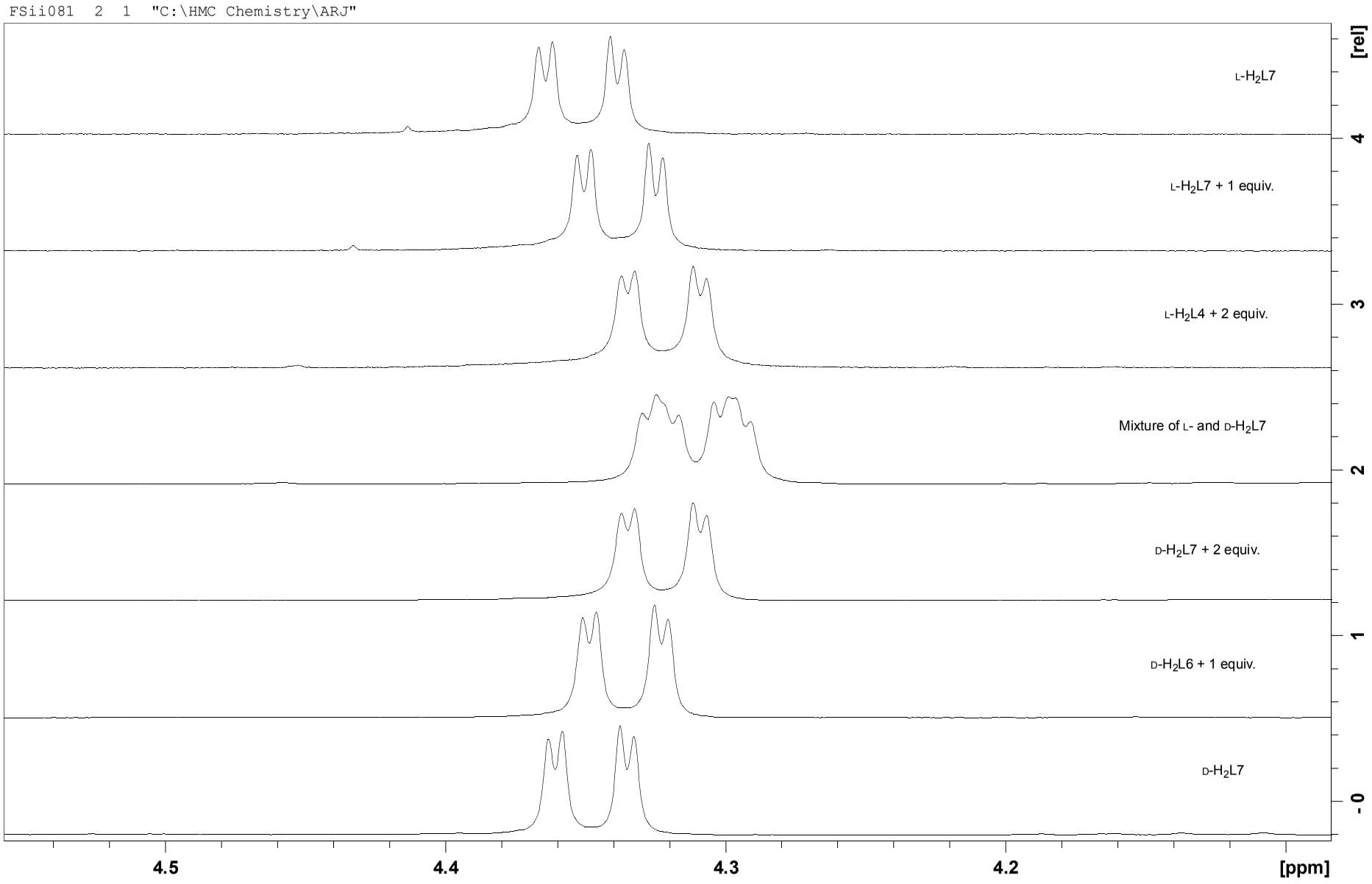
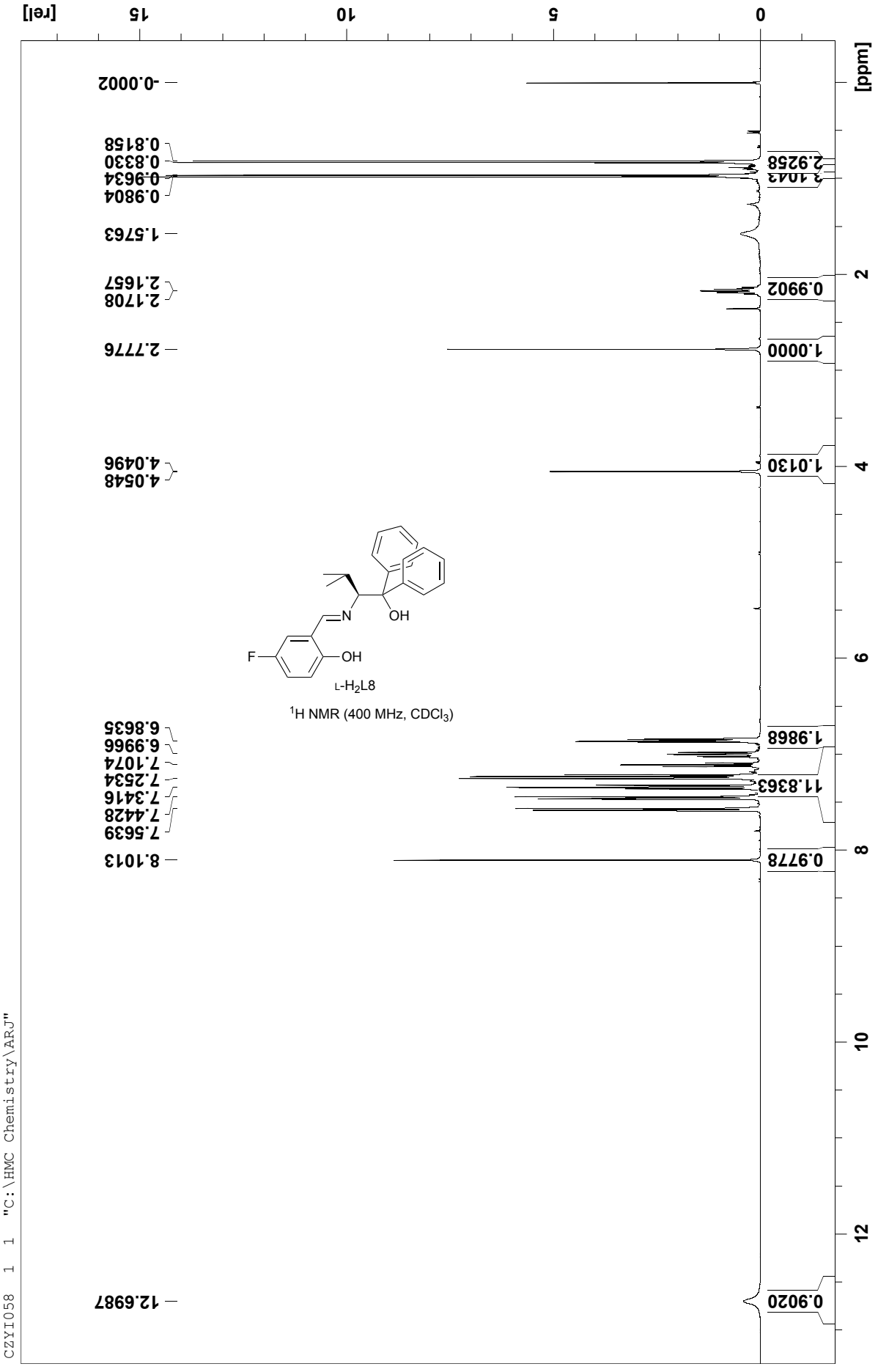
2.8885
3.0357
3.0402
3.0700
3.0746
4.3316
4.3367
4.3574
4.3624
6.5297
6.5374
6.5506
6.5583
6.7930
6.8042
6.8156
6.8268
7.4774
7.6253
7.6280
7.6462
0.7638
17.8849
0.9588
0.9955
1.0169
1.9339
1.0000
N
OH
F
OH
L-H2L7
1H NMR (400 MHz, CDCl3)
CZYI012 1 1 "C:\HMC Chemistry\ARJ"

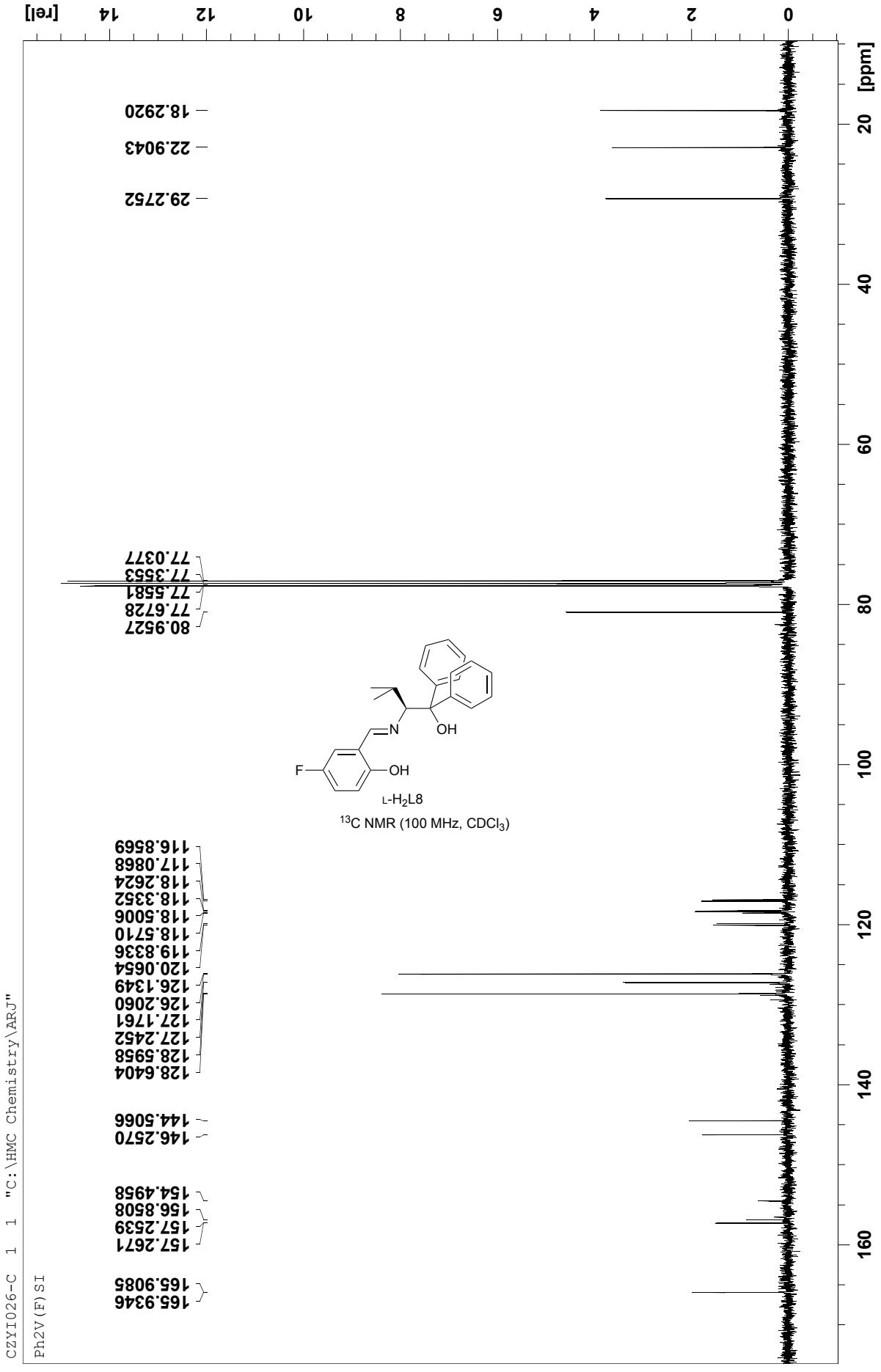


L-H_2L7

^{13}C NMR (100 MHz, $CDCl_3$)

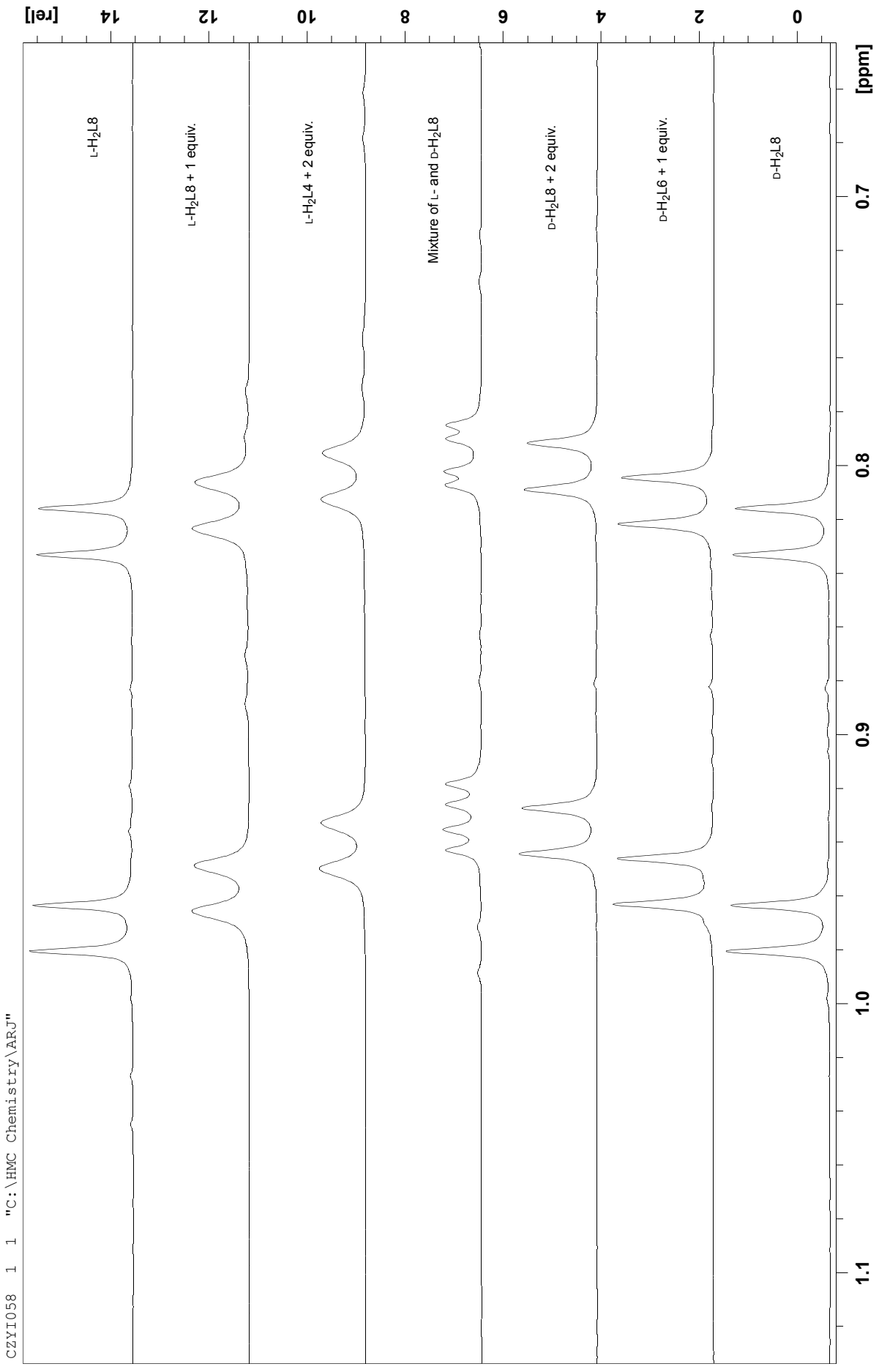

FSii081 2 1 "C:\HMC Chemistry\ARJ"
L-H2L7
L-H2L7 + 1 equiv.
L-H2L4 + 2 equiv.
Mixture of L- and D-H2L7
D-H2L7 + 2 equiv.
D-H2L6 + 1 equiv.
D-H2L7
[rel]
4
3
2
1
0
4.5
4.4
4.3
4.2
[ppm]

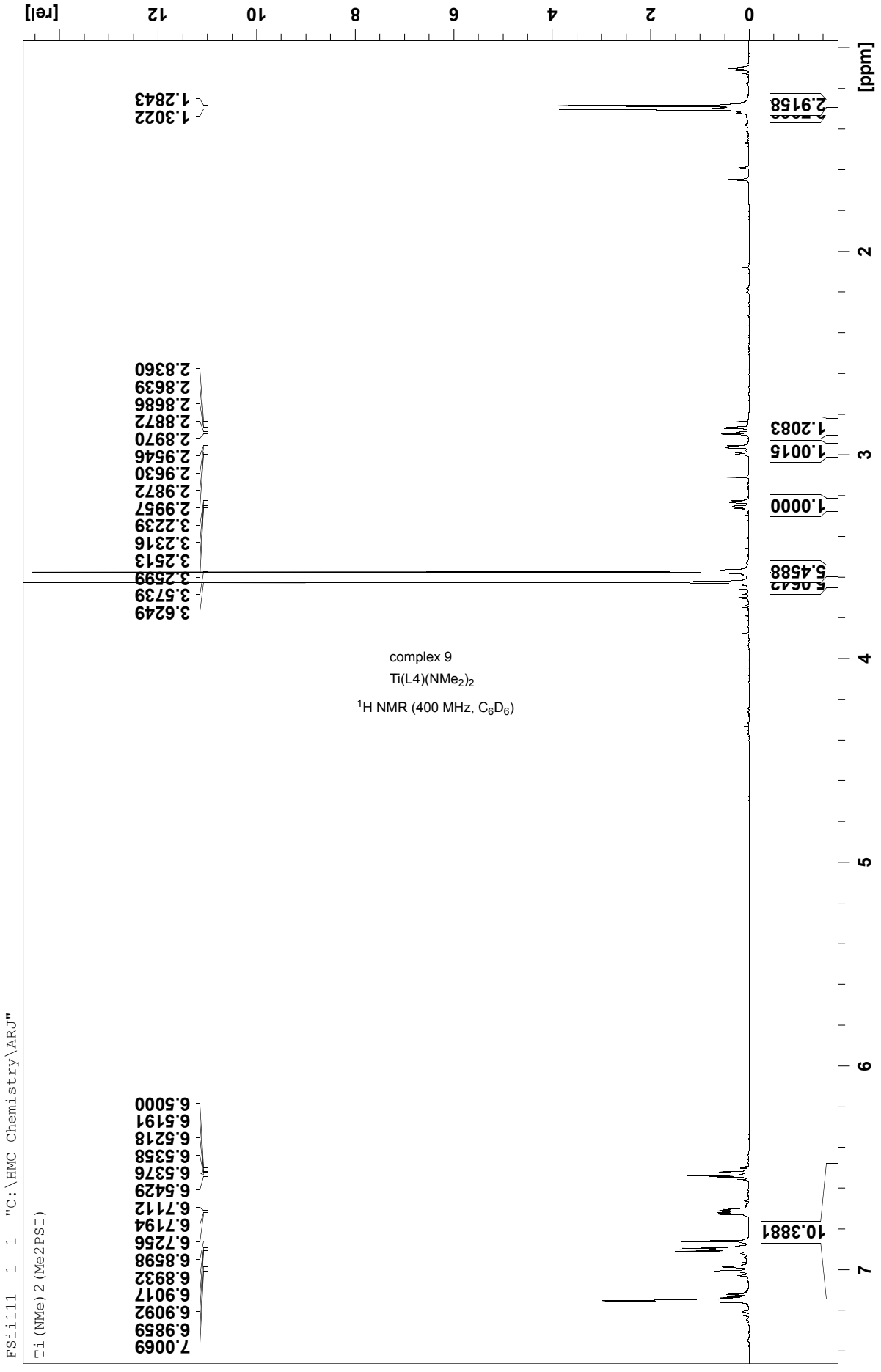

[rel]
15
10
5
0
[ppm]
-0.0002
0.8158
0.8330
0.9634
0.9804
1.5763
2.1657
2.1708
2.7776
4.0496
4.0548
6.8635
6.9966
7.1074
7.2534
7.3416
7.4428
7.5639
8.1013
12.6987
2.9258
2.1042
0.9902
1.0000
1.0130
1.9868
11.8363
0.9778
0.9020
N
OH
F
OH
L-H2L8
1H NMR (400 MHz, CDCl3)
CZYI058 1 1 "C:\HMC Chemistry\ARJ"

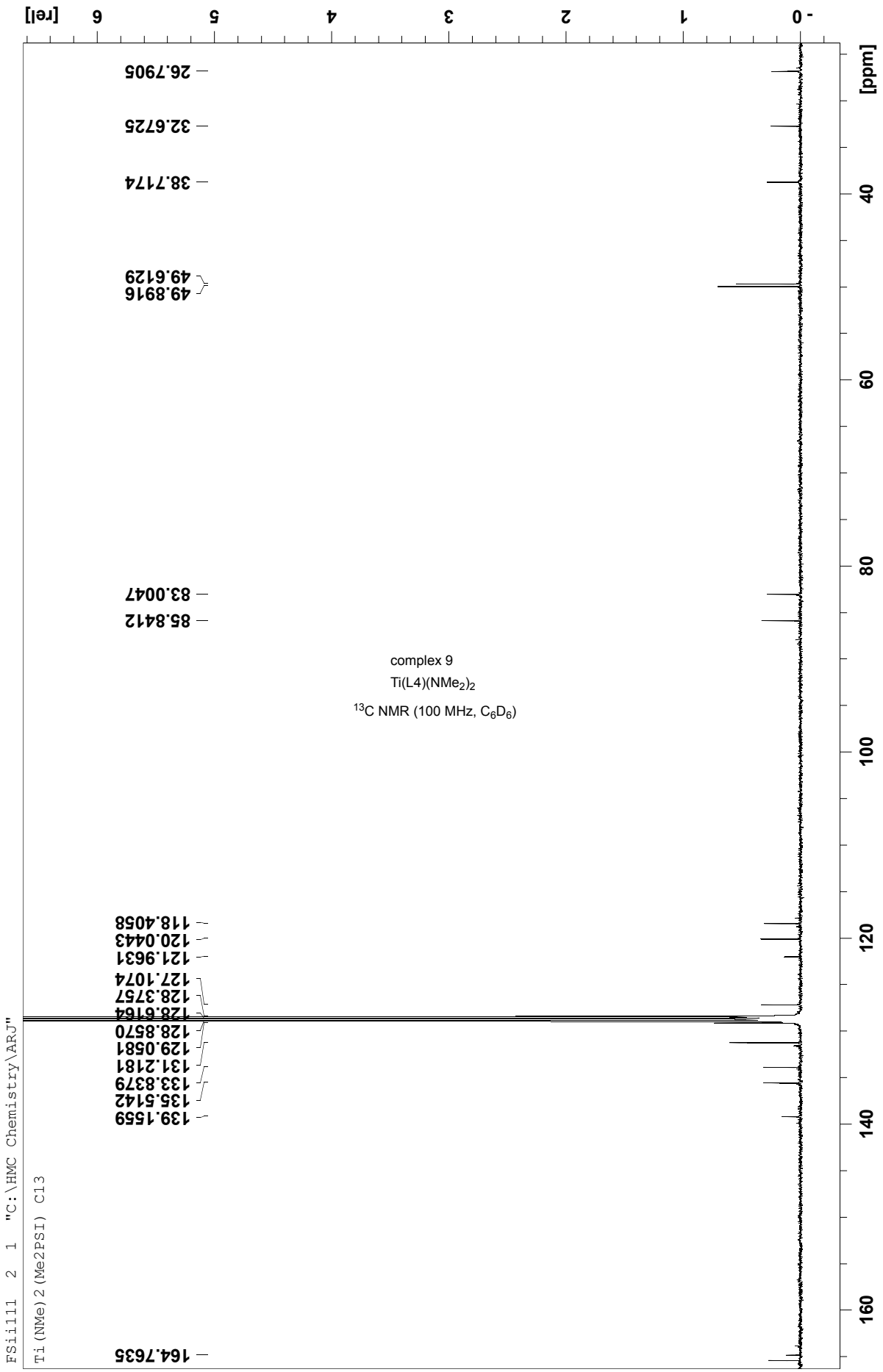


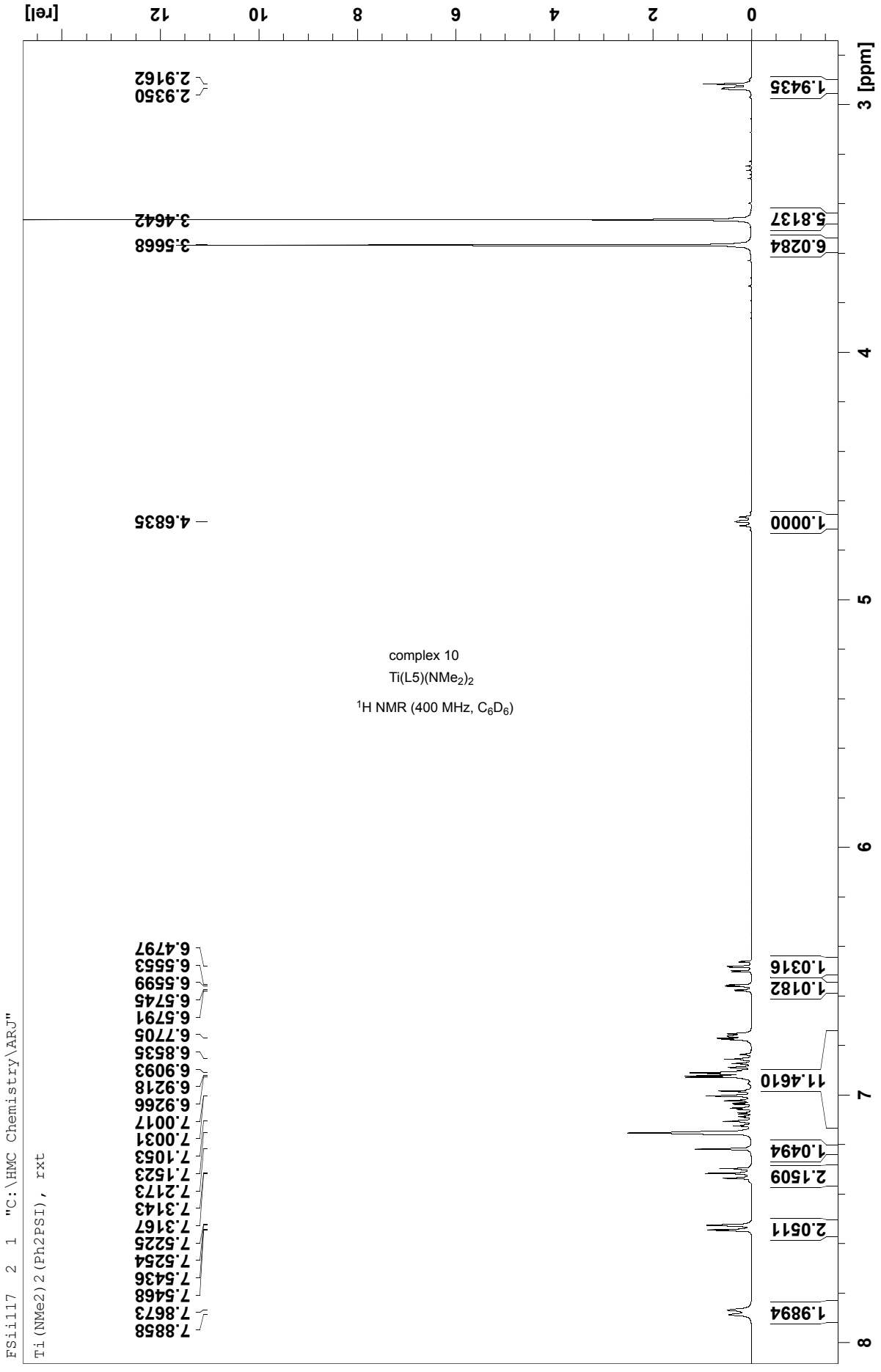
L-H_2L8

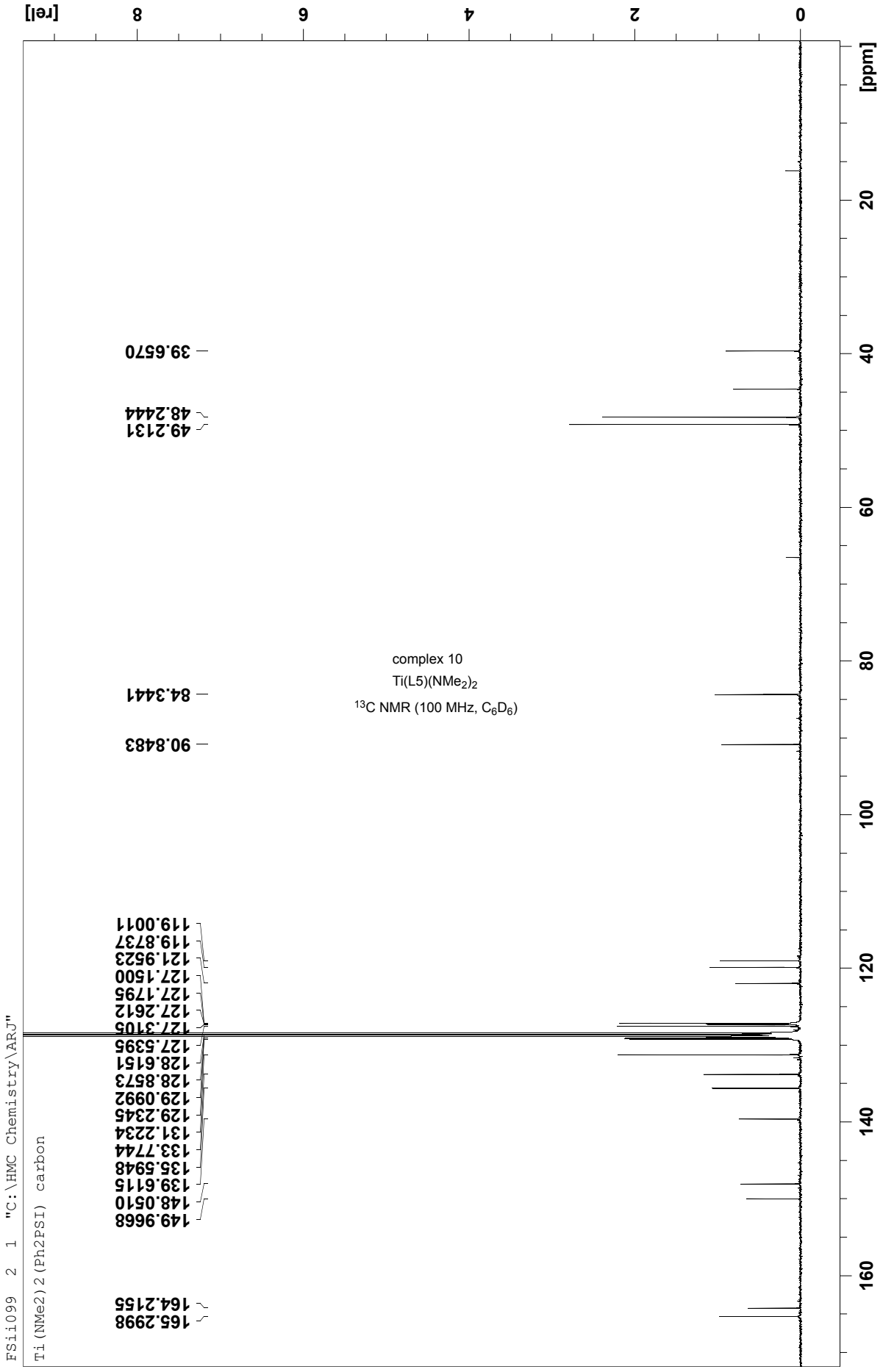
^{13}C NMR (100 MHz, $CDCl_3$)

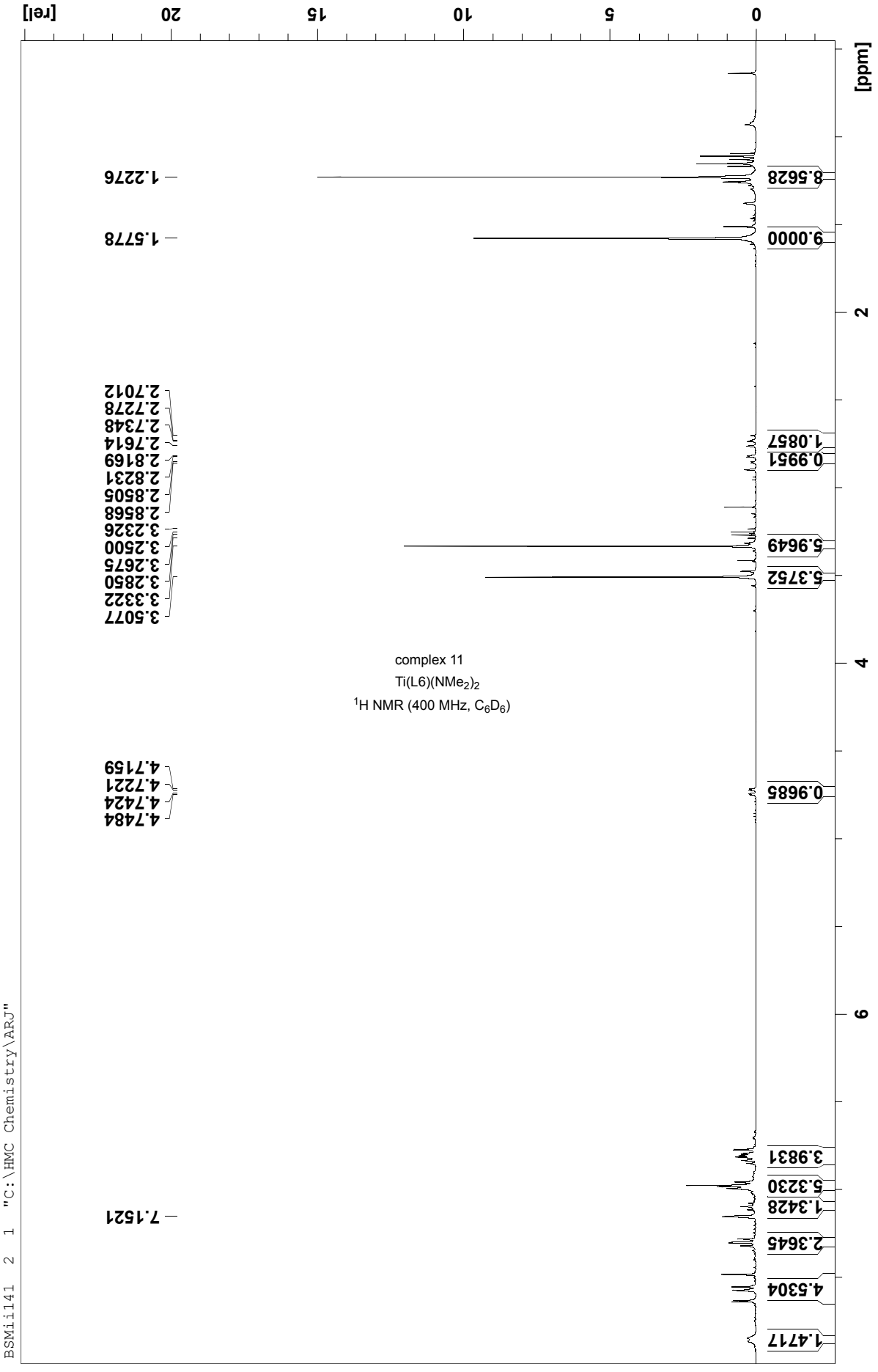

CZYI058 1 1 "C:\HMC Chemistry\ARJ"
[rel]
14
12
10
8
6
4
2
0
[ppm]
0.7
0.8
0.9
1.0
1.1
L-H2L8
L-H2L8 + 1 equiv.
L-H2L4 + 2 equiv.
Mixture of L- and D-H2L8
D-H2L8 + 2 equiv.
D-H2L6 + 1 equiv.
D-H2L8

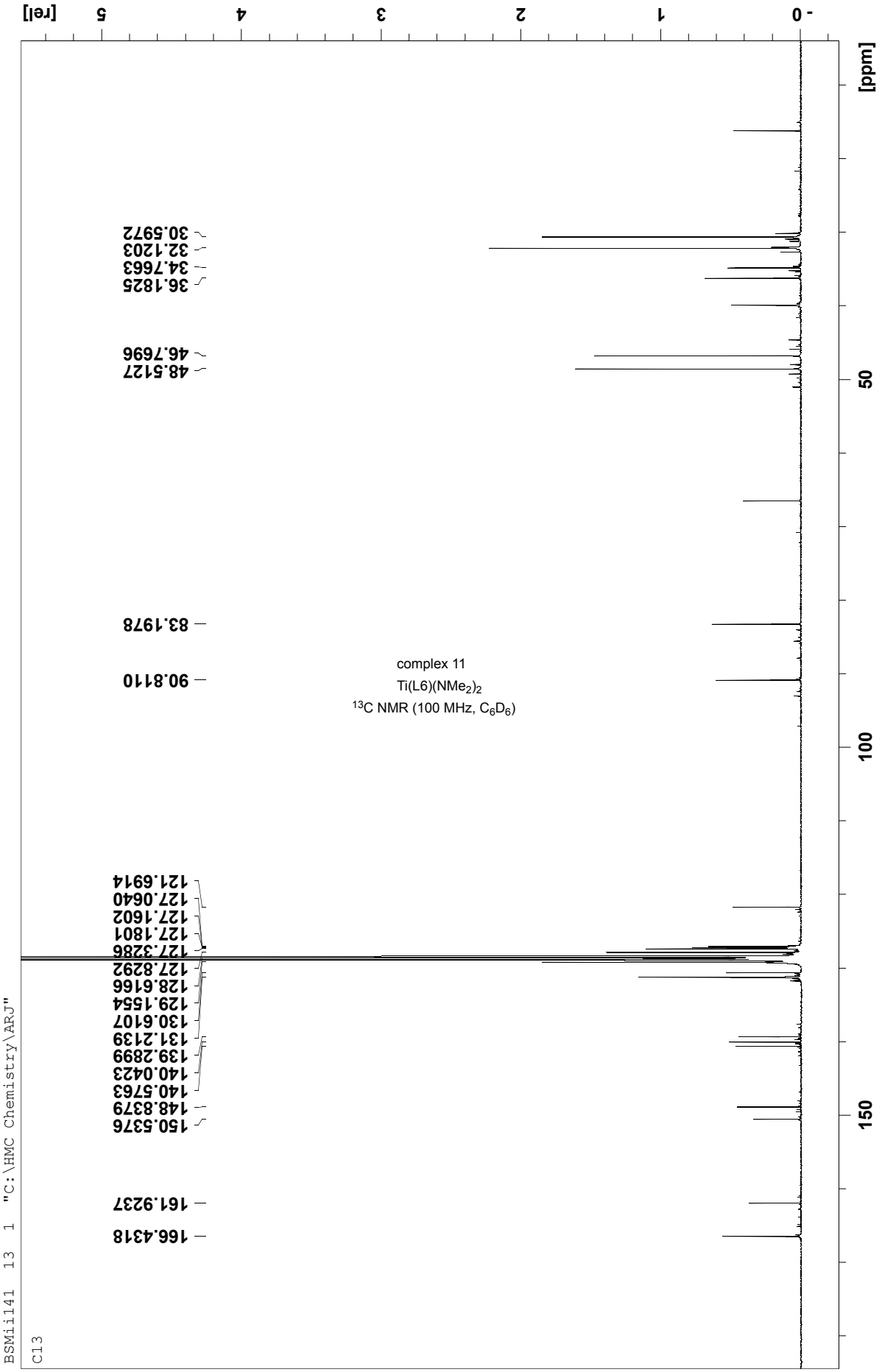

complex 9
Ti(L4)(NMe2)2
1H NMR (400 MHz, C6D6)
FSi111 1 1 "C:\HMC Chemistry\ARJ"
Ti(NMe)2(Me2PSI)
[rel]
[ppm]
10.3881
2.9158
1.2083
1.0015
1.0000
5.4588
3.6249
3.5739
3.2599
3.2513
3.2316
3.2239
2.9957
2.9872
2.9630
2.9546
2.8970
2.8872
2.8686
2.8639
2.8360
1.3022
1.2843
7.0069
6.9859
6.9092
6.9017
6.8932
6.8598
6.7256
6.7194
6.7112
6.5429
6.5376
6.5358
6.5218
6.5191
6.5000

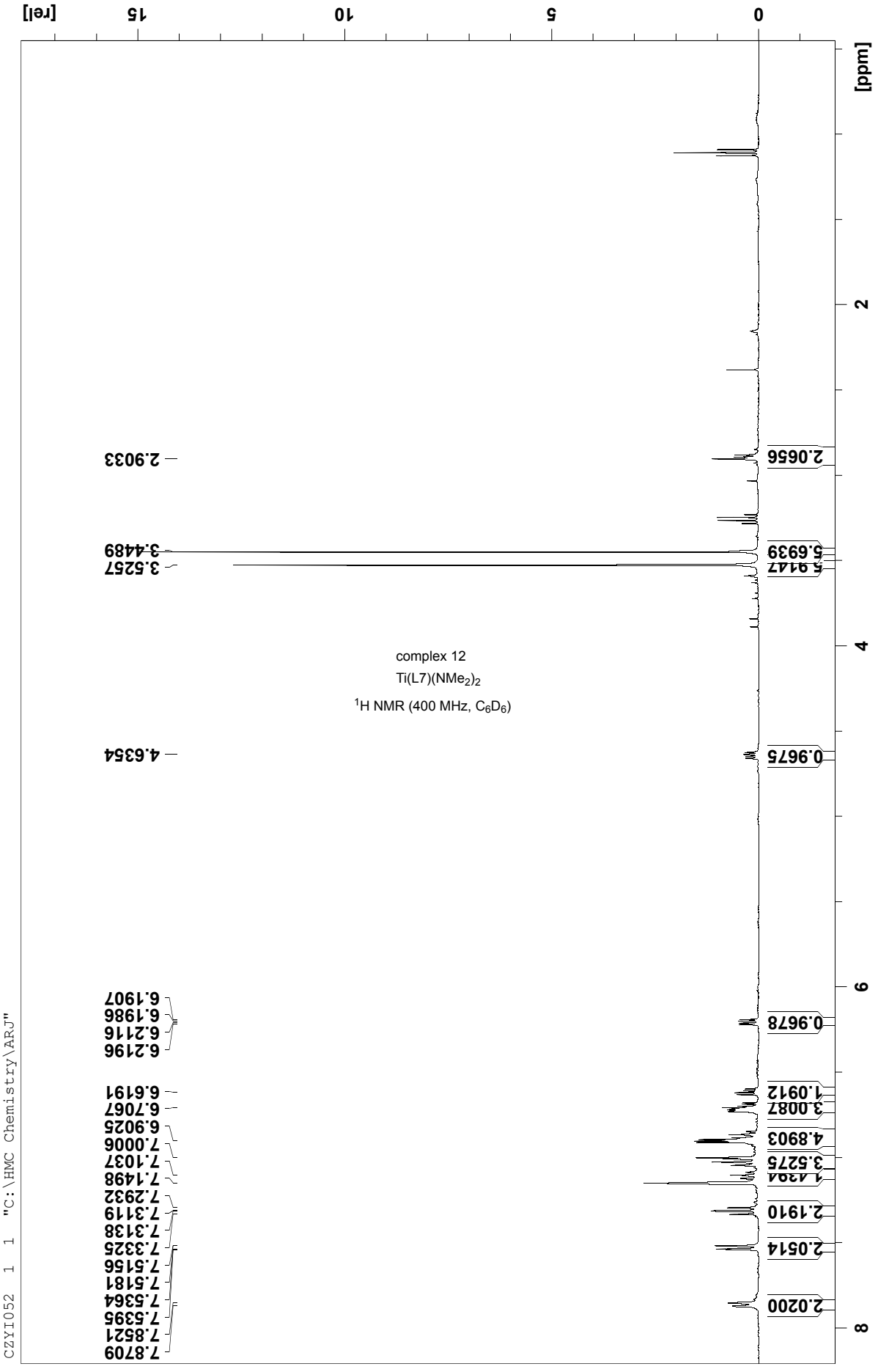

FSi1111 2 1 "C:\HMC Chemistry\ARJ"
Ti(NMe)2(Me2PSI) C13
complex 9
Ti(L4)(NMe2)2
13C NMR (100 MHz, C6D6)
164.7635
139.1559
135.5142
133.8379
131.2181
129.0581
128.8570
128.6164
128.3757
127.1074
121.9631
120.0443
118.4058
85.8412
83.0047
49.8916
49.6129
38.7174
32.6725
26.7905
[rel]
[ppm]

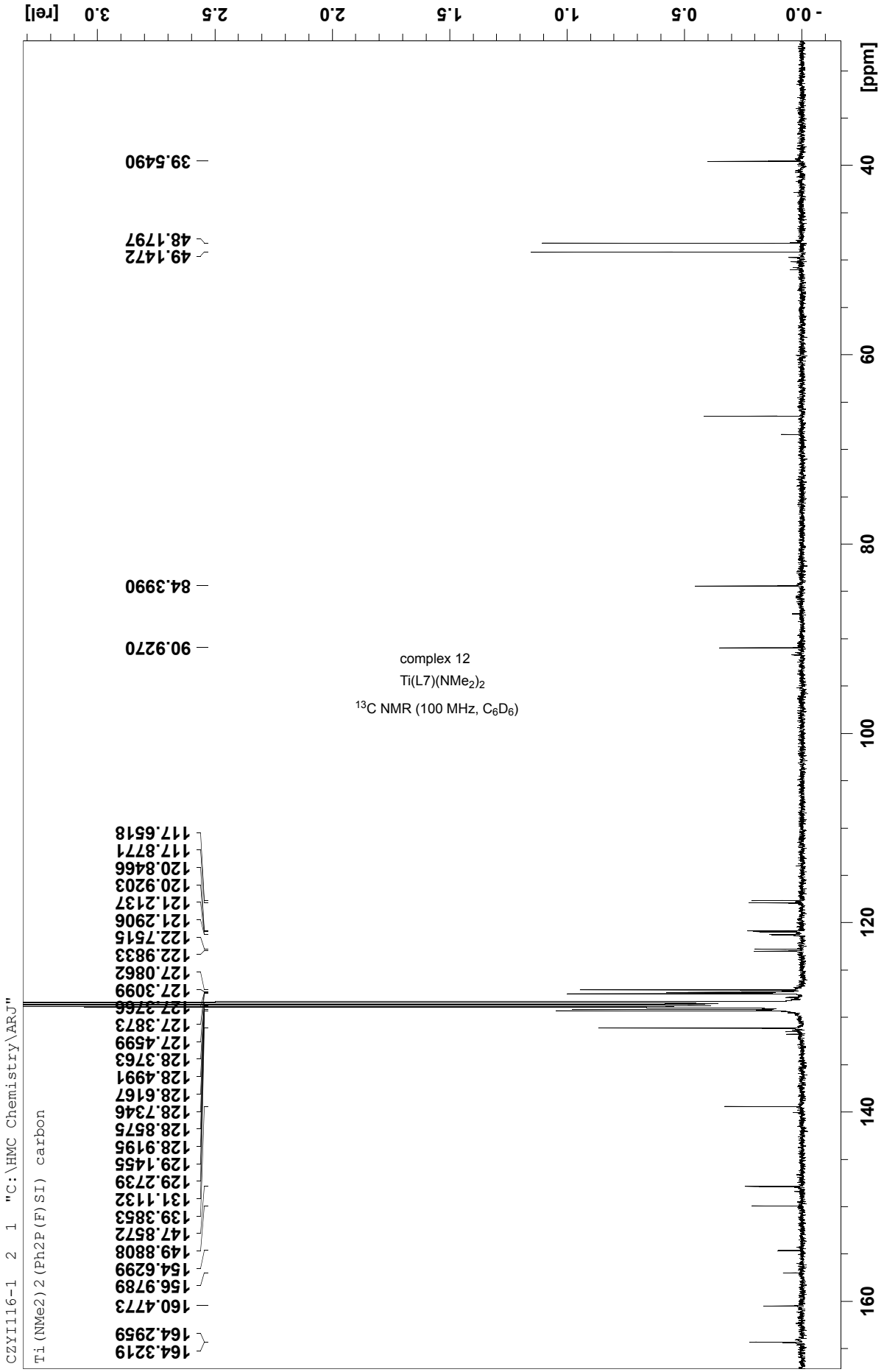

FSi117 2 1 "C:\HMC Chemistry\ARJ"
Ti(NMe2)2(Ph2PSI), rxt
complex 10
Ti(L5)(NMe2)2
1H NMR (400 MHz, C6D6)
[rel]
[ppm]
7.8858
7.8673
7.5468
7.5436
7.5254
7.5225
7.3167
7.3143
7.2173
7.1523
7.1053
7.0031
7.0017
6.9266
6.9218
6.9093
6.8535
6.7705
6.5791
6.5745
6.5599
6.5553
6.4797
4.6835
3.5668
3.4642
2.9350
2.9162
1.9894
2.0511
2.1509
1.0494
11.4610
1.0316
1.0182
1.0000
6.0284
5.8137
1.9435

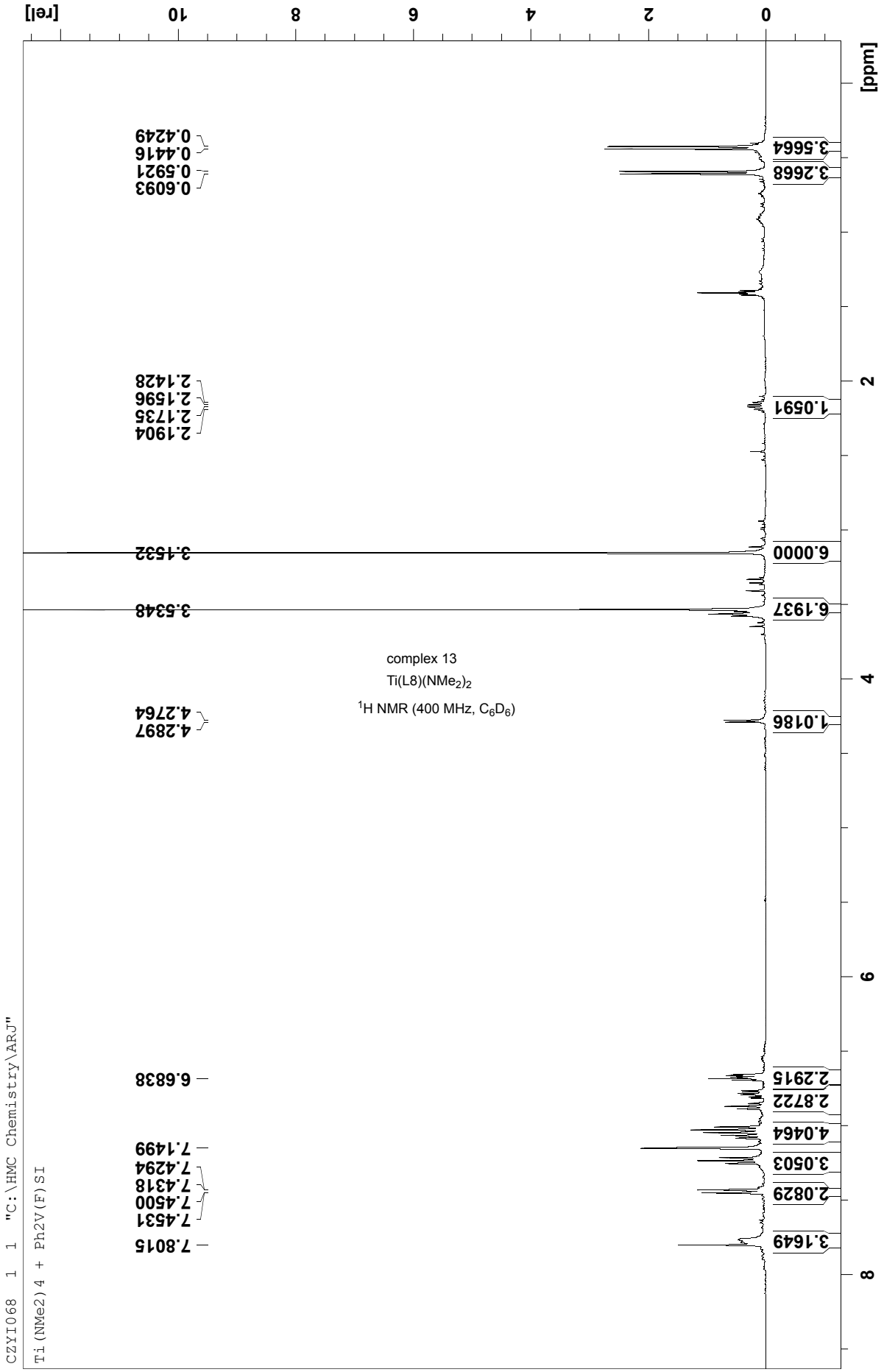

complex 10
Ti(L5)(NMe2)2
13C NMR (100 MHz, C6D6)
FSi1099 2 1 "C:\HMC Chemistry\ARJ"
Ti(NMe2)2(Ph2PSI) carbon
[rel]
[ppm]
39.6570
48.2444
49.2131
84.3441
90.8483
119.0011
119.8737
121.9523
127.1500
127.1795
127.2612
127.3105
127.5395
128.6151
128.8573
129.0992
129.2345
131.2234
133.7744
135.5948
139.6115
148.0510
149.9668
164.2155
165.2998

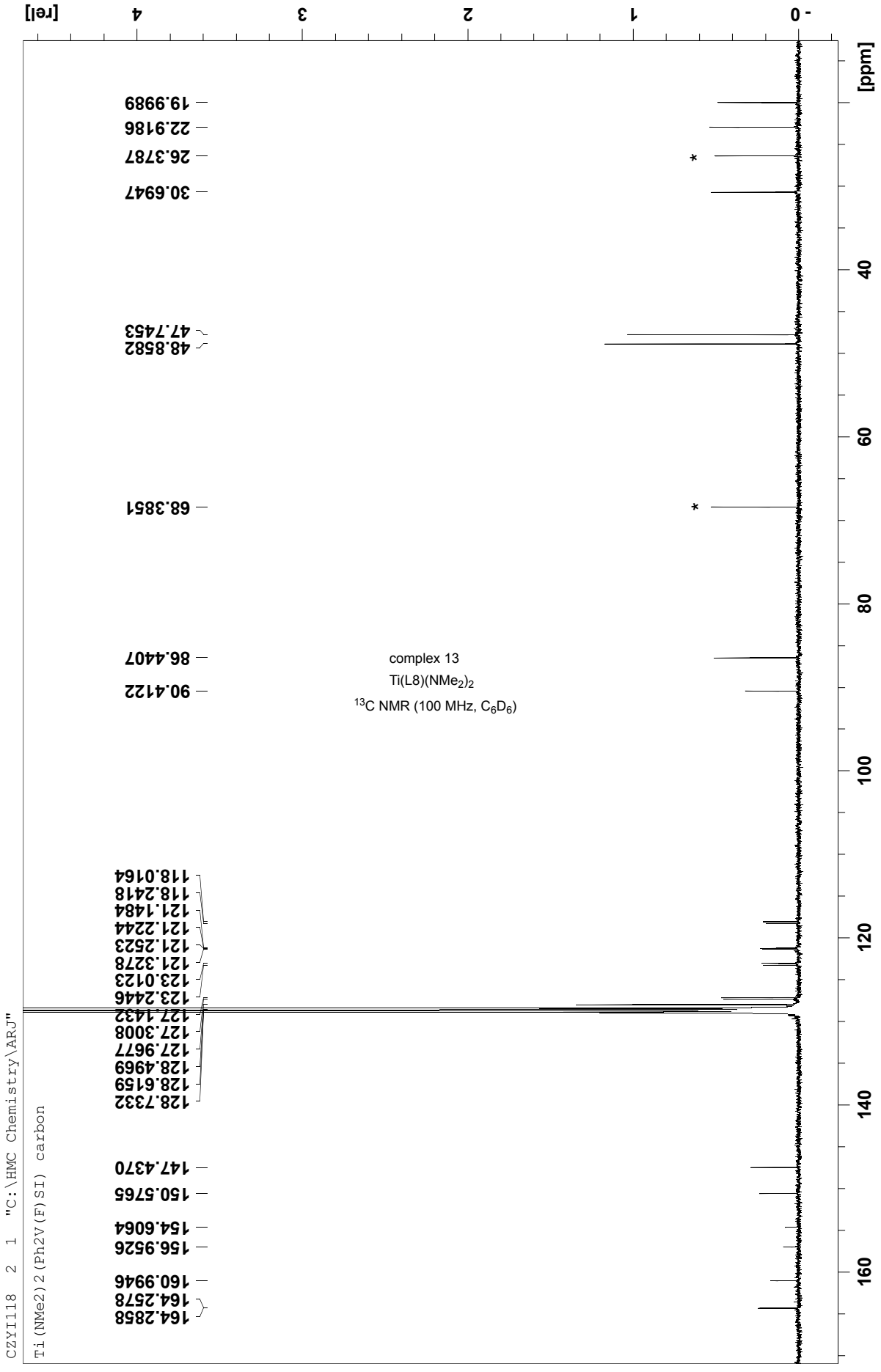

complex 11
Ti(L6)(NMe2)2
1H NMR (400 MHz, C6D6)
[ppm]
[rel]
BSMi1141 2 1 "C:\HMC Chemistry\ARJ"

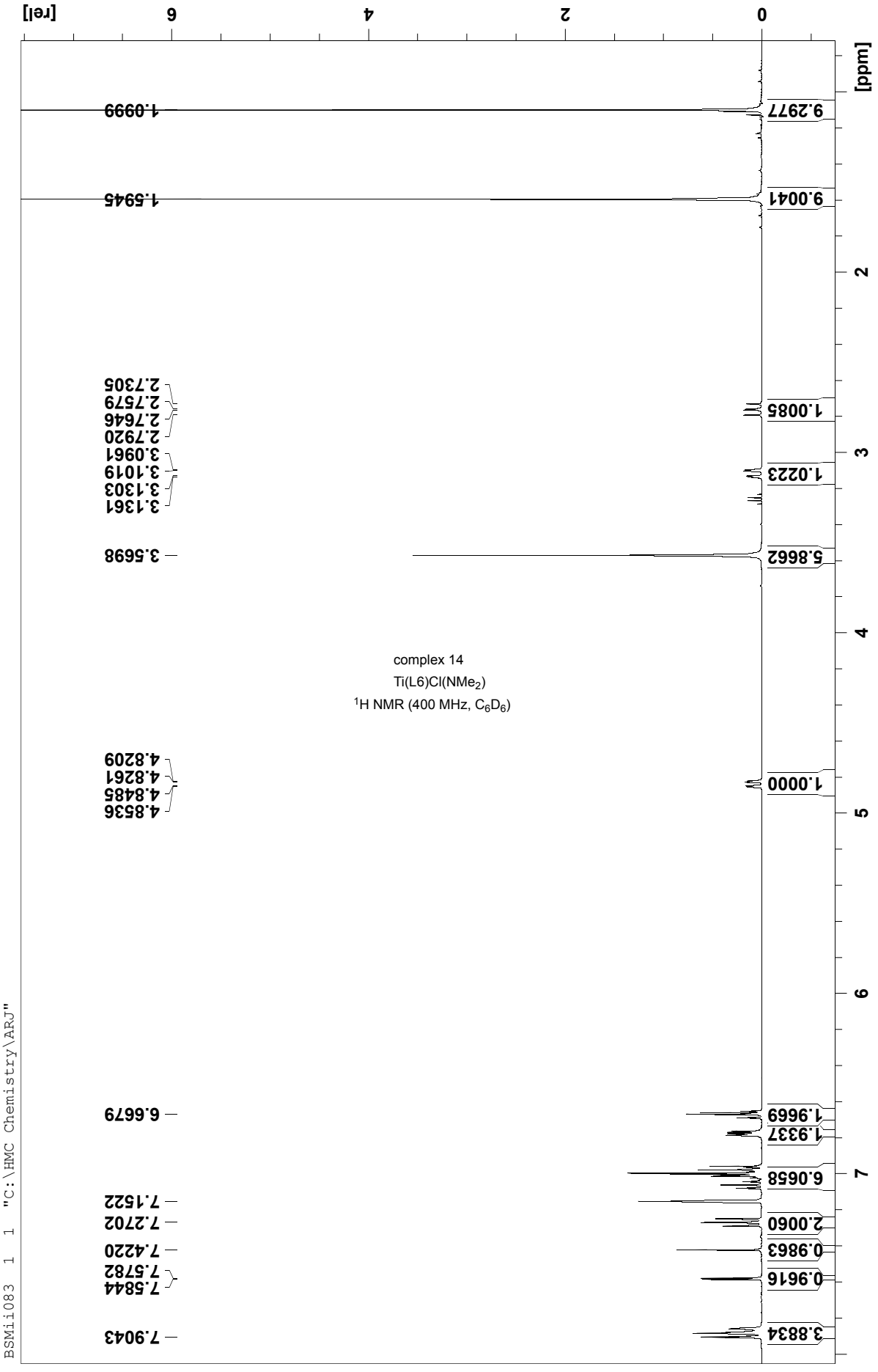

complex 11
Ti(L6)(NMe2)2
13C NMR (100 MHz, C6D6)
BSMi1141 13 1 "C:\HMC Chemistry\ARJ"
C13
[rel]
[ppm]
166.4318
161.9237
150.5376
148.8379
140.5763
140.0423
139.2899
131.2139
130.6107
129.1554
128.6166
127.8292
127.3286
127.1801
127.1602
127.0640
121.6914
90.8110
83.1978
48.5127
46.7696
36.1825
34.7663
32.1203
30.5972

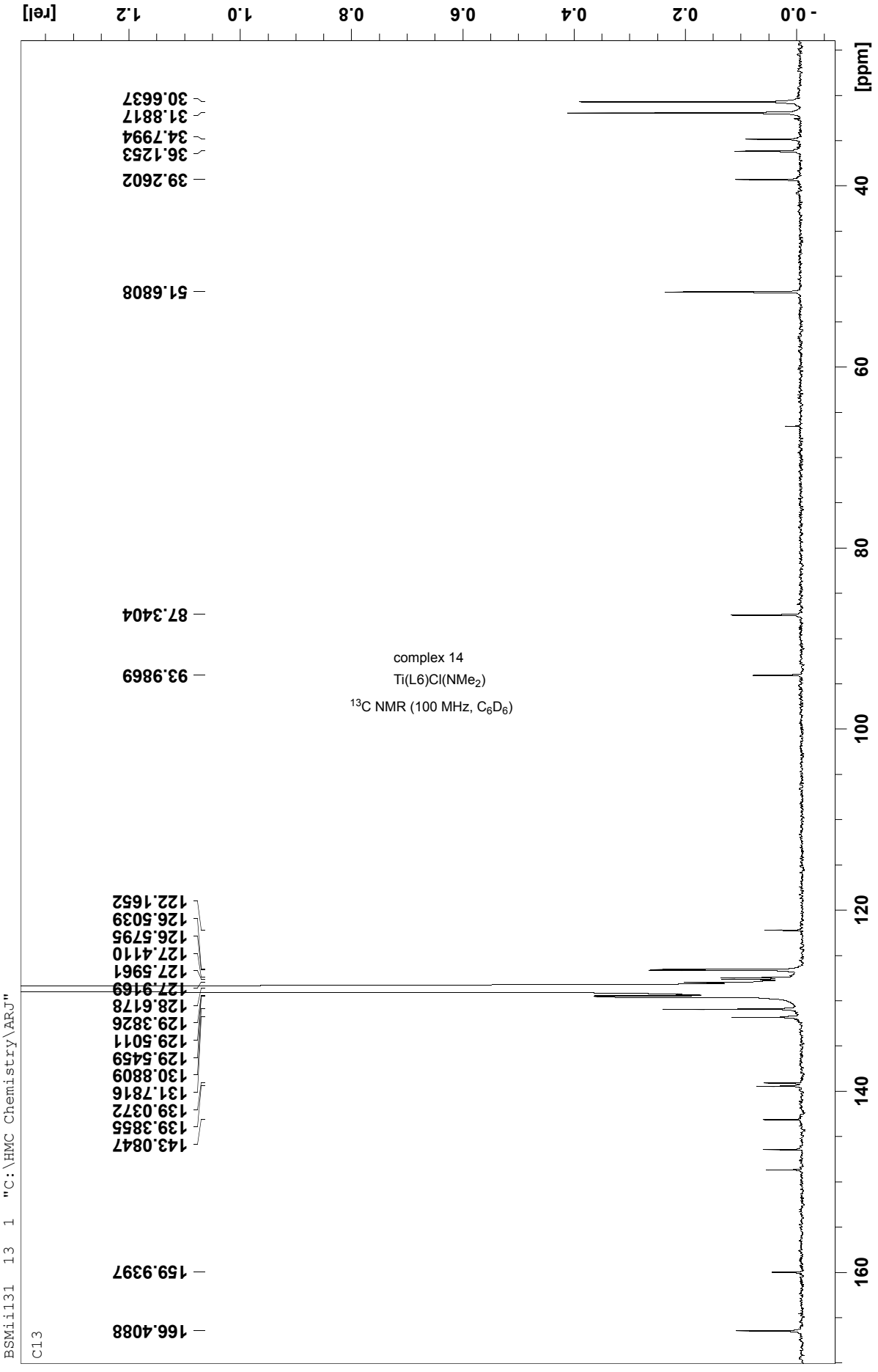

complex 12
Ti(L7)(NMe2)2
1H NMR (400 MHz, C6D6)
[rel]
15
10
5
0
[ppm]
8
6
4
2
7.8709
7.8521
7.5395
7.5364
7.5181
7.5156
7.3325
7.3138
7.3119
7.2932
7.1498
7.1037
7.0006
6.9025
6.7067
6.6191
6.2196
6.2116
6.1986
6.1907
4.6354
3.5257
3.4489
2.9033
2.0200
2.0514
2.1910
1.4294
3.5275
4.8903
3.0087
1.0912
0.9678
0.9675
5.9147
5.6939
2.0656
CZYI052 1 1 "C:\HMC Chemistry\ARJ"


CZYI116-1 2 1 "C:\HMC Chemistry\ARJ"
Ti(NMe2)2(Ph2P(F)SI) carbon
complex 12
Ti(L7)(NMe2)2
13C NMR (100 MHz, C6D6)
[rel]
[ppm]
39.5490
48.1797
49.1472
84.3990
90.9270
117.6518
117.8771
120.8466
120.9203
121.2137
121.2906
122.7515
122.9833
127.0862
127.3099
127.3766
127.3873
127.4599
128.3763
128.4991
128.6167
128.7346
128.8575
128.9195
129.1455
129.2739
131.1132
139.3853
147.8572
149.8808
154.6299
156.9789
160.4773
164.2959
164.3219

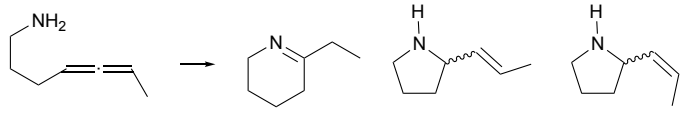

CZYI068 1 1 "C:\HMC Chemistry\ARJ"
Ti(NMe2)4 + Ph2V(F)SI
complex 13
Ti(L8)(NMe2)2
1H NMR (400 MHz, C6D6)
[rel]
[ppm]
0
2
4
6
8
10
0.4249
0.4416
0.5921
0.6093
2.1904
2.1735
2.1596
2.1428
3.1532
3.5348
4.2897
4.2764
6.6838
7.1499
7.4531
7.4500
7.4318
7.4294
7.8015
3.5664
3.2668
1.0591
6.0000
6.1937
1.0186
2.2915
2.8722
4.0464
3.0503
2.0829
3.1649


complex 13
Ti(L8)(NMe2)2
13C NMR (100 MHz, C6D6)
CZYI118 2 1 "C:\HMC Chemistry\ARJ"
Ti(NMe2)2(Ph2V(F)SI) carbon
[rel]
[ppm]
19.9989
22.9186
26.3787
30.6947
47.7453
48.8582
68.3851
86.4407
90.4122
118.0164
118.2418
121.1484
121.2244
121.2523
121.3278
123.0123
123.2446
127.1432
127.3008
127.9677
128.4969
128.6159
128.7332
147.4370
150.5765
154.6064
156.9526
160.9946
164.2578
164.2858

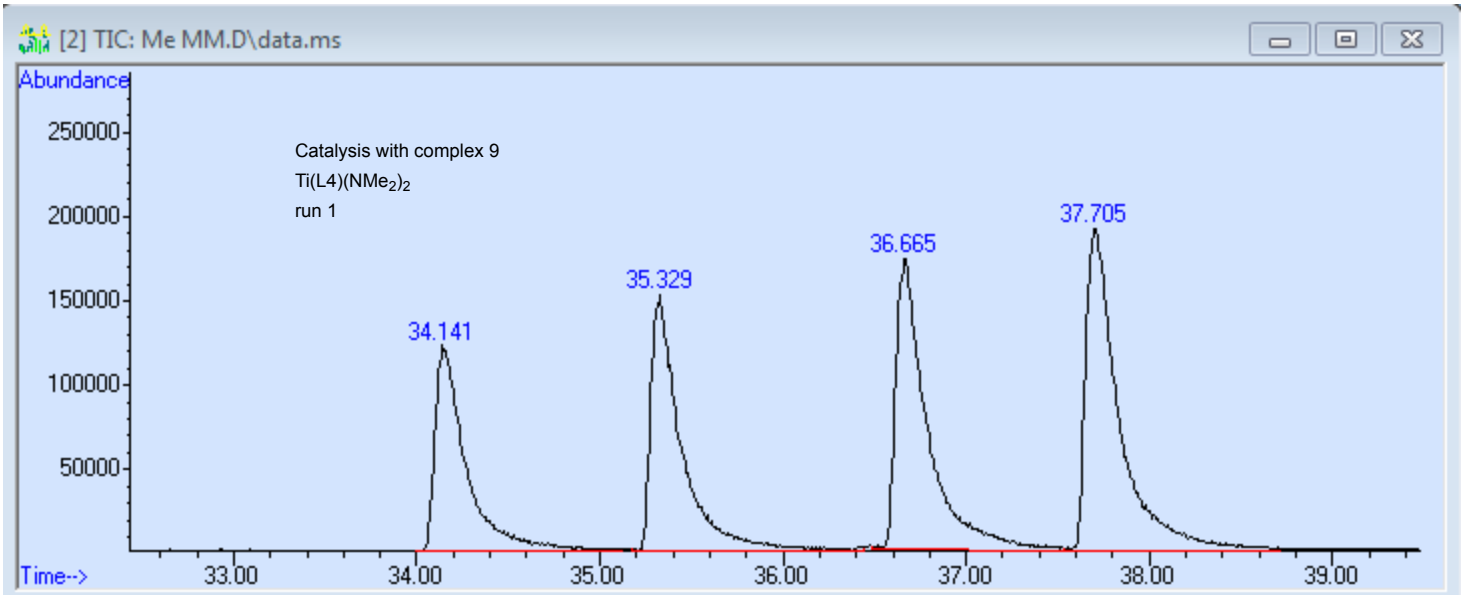

complex 14
Ti(L6)Cl(NMe2)
1H NMR (400 MHz, C6D6)
BSMi1083 1 1 "C:\HMC Chemistry\ARJ"
[rel]
[ppm]
9.2977
9.0041
1.0085
1.0223
5.8662
1.0000
1.9669
1.9337
6.0658
2.0060
0.9863
0.9616
3.8834
1.0999
1.5945
2.7305
2.7579
2.7646
2.7920
3.0961
3.1019
3.1303
3.1361
3.5698
4.8209
4.8261
4.8485
4.8536
6.6679
7.1522
7.2702
7.4220
7.5782
7.5844
7.9043

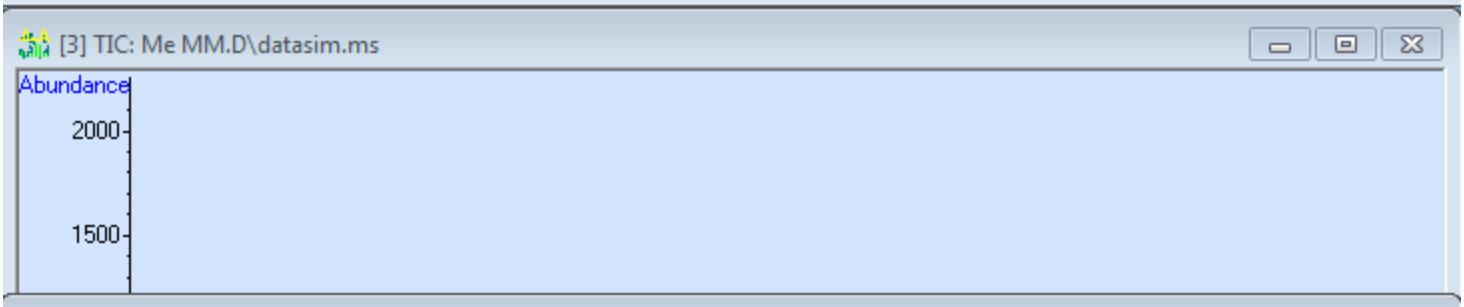

complex 14
Ti(L6)Cl(NMe2)
13C NMR (100 MHz, C6D6)
BSMi1131 13 1 "C:\HMC Chemistry\ARJ"
C13
[rel]
[ppm]
166.4088
159.9397
143.0847
139.3855
139.0372
131.7816
130.8809
129.5459
129.5011
129.3826
128.6178
127.9169
127.5961
127.4110
126.5795
126.5039
122.1652
93.9869
87.3404
51.6808
39.2602
36.1253
34.7994
31.8817
30.6637

Hydroamination of hepta-4,5-dienylamine at 135 °C with *in situ* catalysts (5 mol% catalyst) to give tetrahydropyridine **2a**, *Z*- or *E*-α-vinylpyrrolidines *Z*- and *E*-**3a**



1a **2a** ***E*-3a** **34.2, 35.4 min** ***Z*-3a** **36.6, 37.7 min**





D:\MassHunter\GCMS\1\data\Johnson Lab\Me MM.D\rteres.txt

Area Percent Report

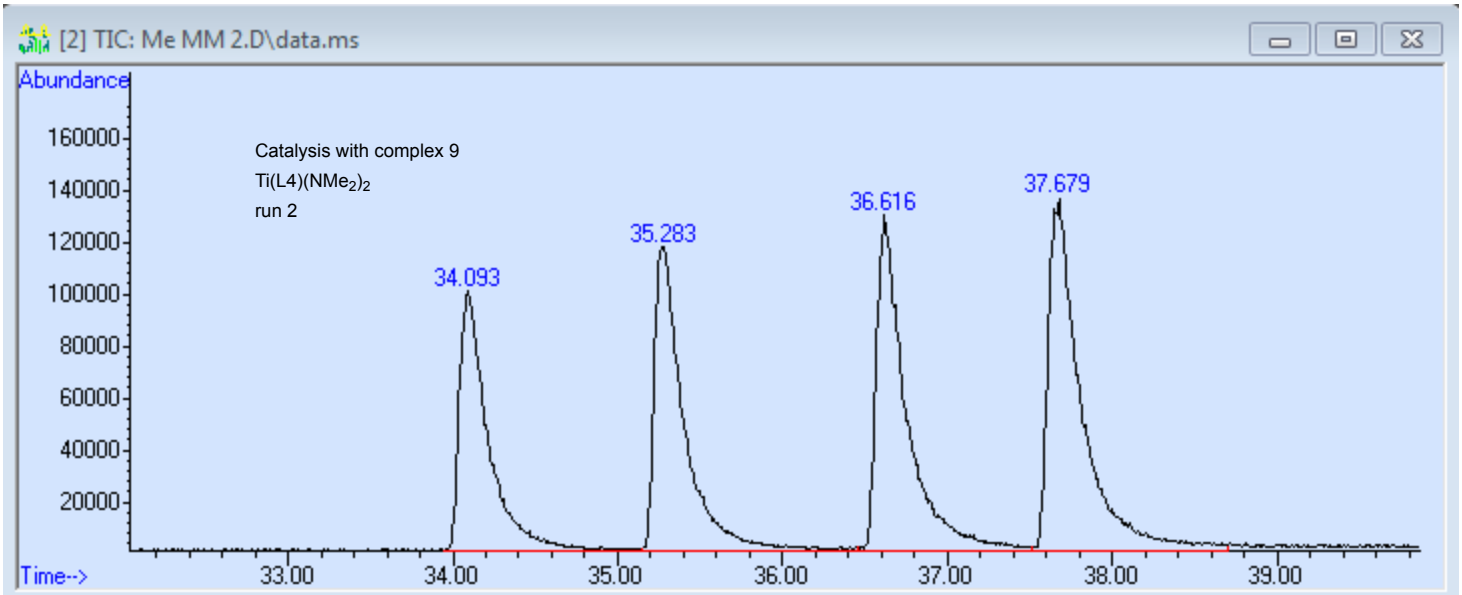
Data Path : D:\MassHunter\GCMS\1\data\Johnson Lab\
Data File : Me MM.D
Acq On : 16 Jul 2018 11:25
Operator : arj
Sample :
Misc :
ALS Vial : 1 Sample Multiplier: 1

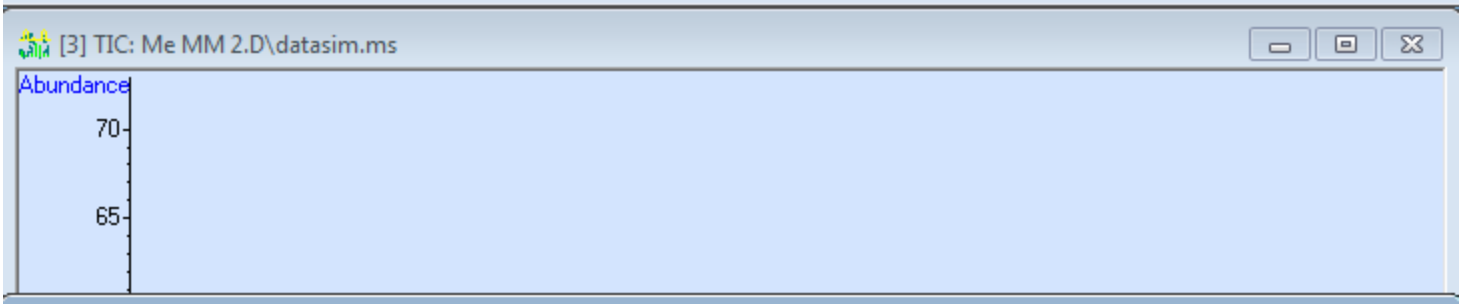
Integration Parameters: autoint1.e
Integrator: ChemStation

Method : D:\MassHunter\GCMS\1\data\Johnson Lab\ph3 Ti.D\chiraldexbDM_400split.M
Title :

Signal : TIC: Me MM.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	34.141	3864	3883	4015	M2	121735	14511910	59.00%	18.730%
2	35.329	4021	4042	4191	M2	152115	17580769	71.47%	22.691%
3	36.665	4196	4220	4337	M2	173016	20789132	84.52%	26.832%
4	37.705	4337	4359	4494	M3	191367	24597733	100.00%	31.747%





D:\MassHunter\GCMS\1\data\Johnson Lab\Me MM 2.D\rteres.txt

Area Percent Report

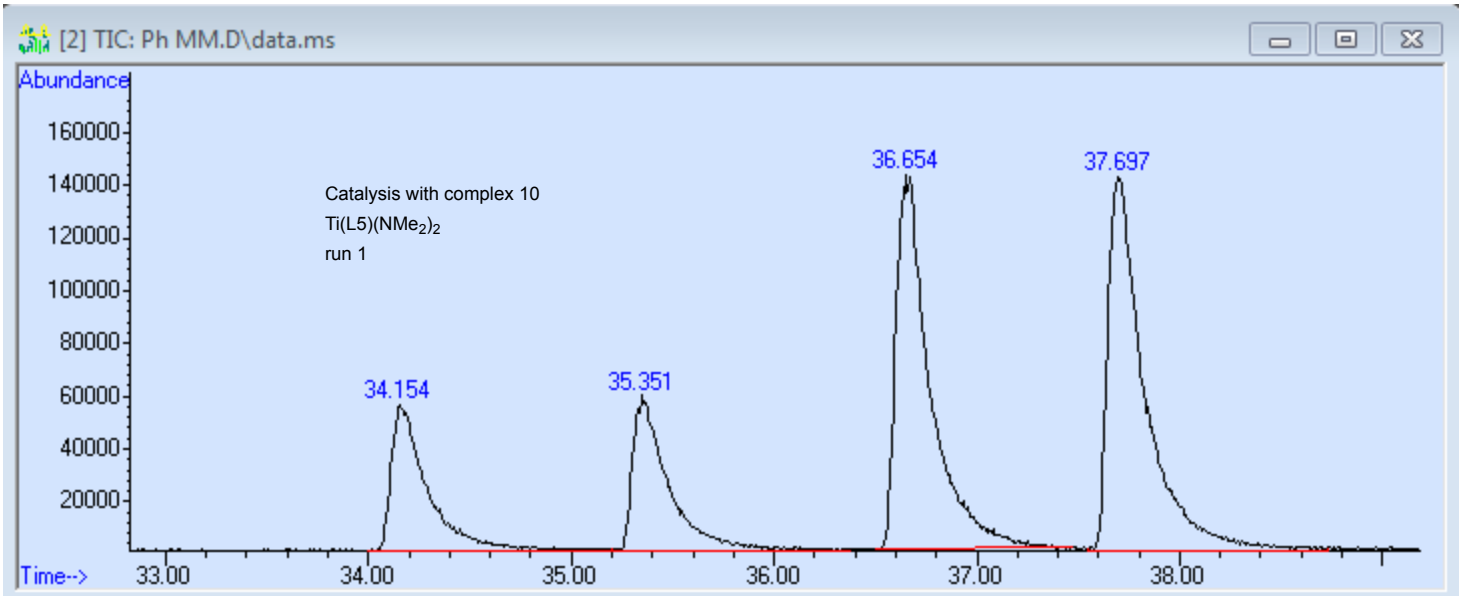
Data Path : D:\MassHunter\GCMS\1\data\Johnson Lab\
Data File : Me MM 2.D
Acq On : 23 Jul 2018 16:56
Operator : arj
Sample :
Misc :
ALS Vial : 4 Sample Multiplier: 1

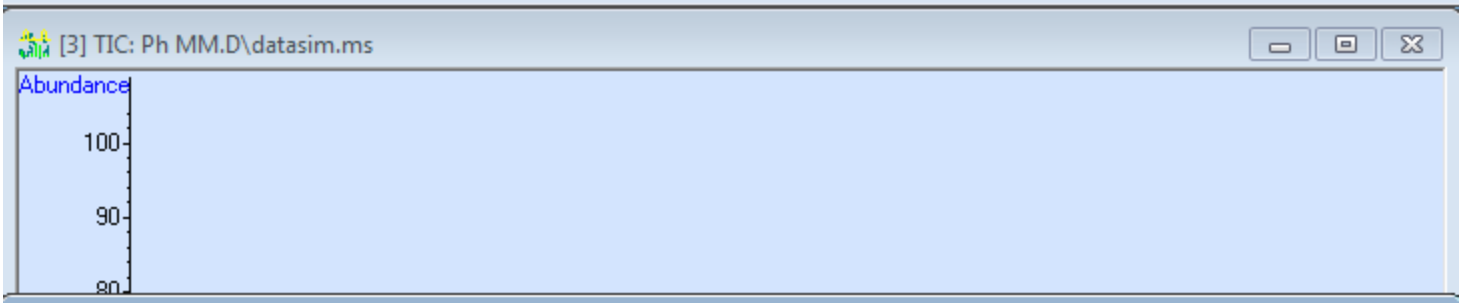
Integration Parameters: autoint1.e
Integrator: ChemStation

Method : D:\MassHunter\GCMS\1\data\Johnson Lab\ph3 Ti.D\chiraldexbDM_400split.M
Title :

Signal : TIC: Me MM 2.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	34.093	3857	3877	4018	M2	100025	12250849	63.98%	19.622%
2	35.283	4018	4036	4193	M3	117006	14761112	77.09%	23.642%
3	36.616	4193	4214	4334	M2	129356	16274659	84.99%	26.066%
4	37.679	4334	4356	4493	M3	135628	19148771	100.00%	30.670%





D:\MassHunter\GCMS\1\data\Johnson Lab\Ph MM.D\rteres.txt

Area Percent Report

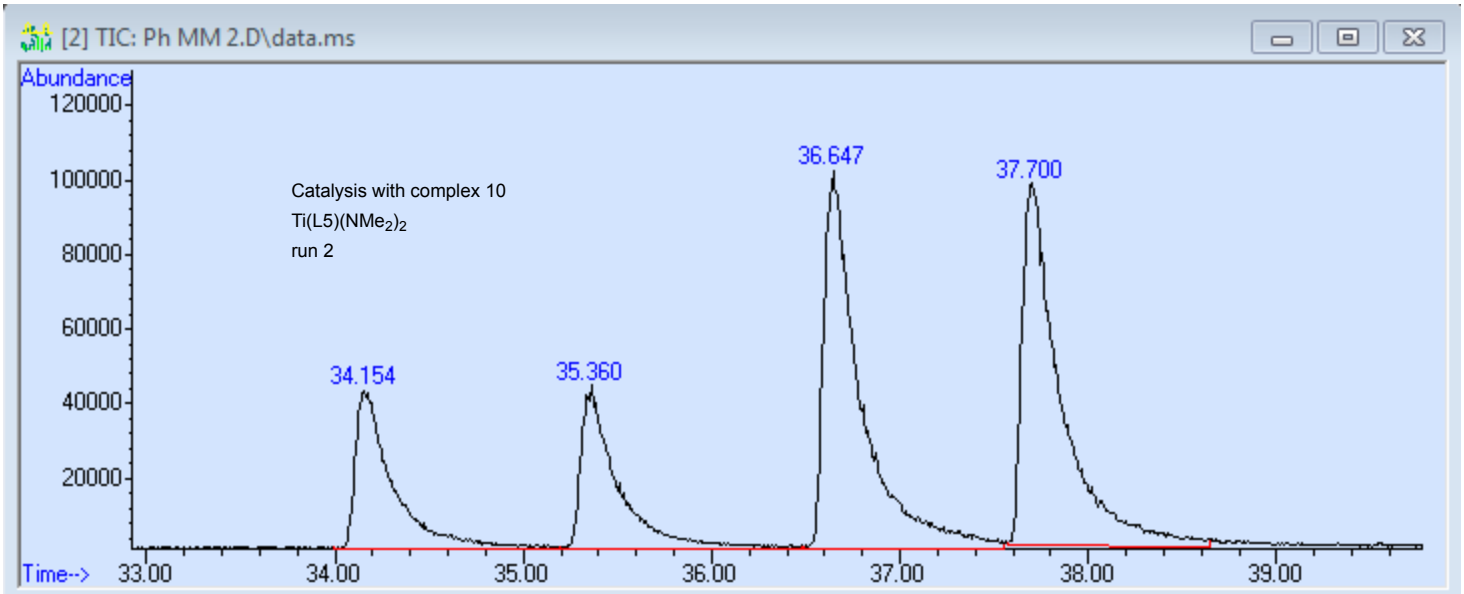
Data Path : D:\MassHunter\GCMS\1\data\Johnson Lab\
Data File : Ph MM.D
Acq On : 16 Jul 2018 13:49
Operator : arj
Sample :
Misc :
ALS Vial : 2 Sample Multiplier: 1

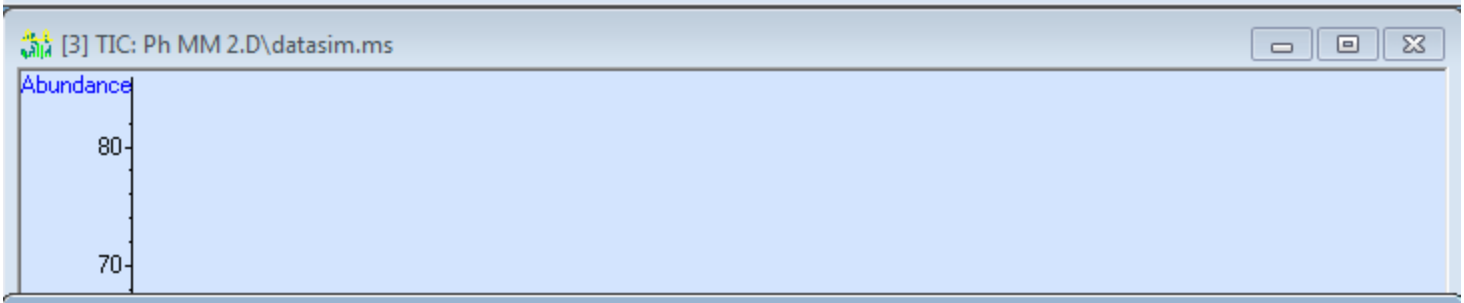
Integration Parameters: autoint1.e
Integrator: ChemStation

Method : D:\MassHunter\GCMS\1\data\Johnson Lab\ph3 Ti.D\chiraldexbDM_400split.M
Title :

Signal : TIC: Ph MM.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	34.154	3864	3885	4025	M3	55491	6962772	38.27%	14.209%
2	35.351	4025	4045	4181	M3	58959	7289794	40.07%	14.876%
3	36.654	4199	4219	4329	M2	141911	16556669	91.00%	33.787%
4	37.697	4338	4358	4496	M2	142562	18193615	100.00%	37.128%





D:\MassHunter\GCMS\1\data\Johnson Lab\Ph MM 2.D\rteres.txt

Area Percent Report

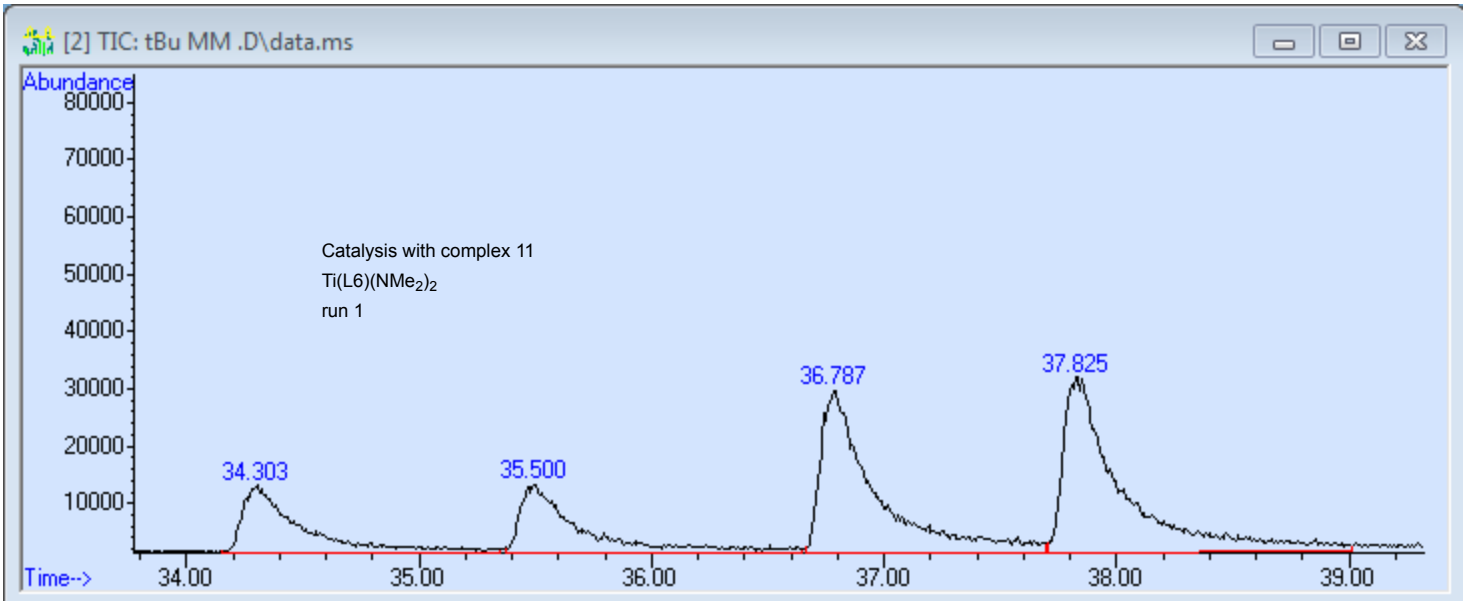
Data Path : D:\MassHunter\GCMS\1\data\Johnson Lab\
Data File : Ph MM 2.D
Acq On : 23 Jul 2018 18:06
Operator : arj
Sample :
Misc :
ALS Vial : 5 Sample Multiplier: 1

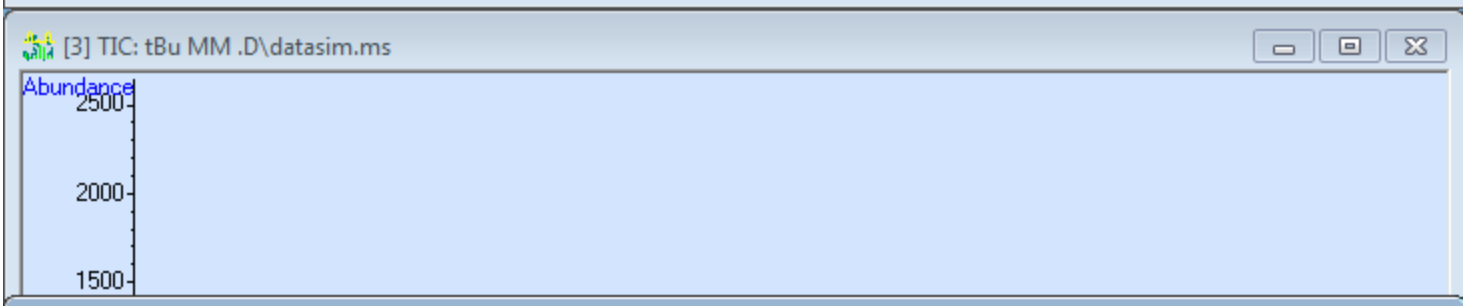
Integration Parameters: autoint1.e
Integrator: ChemStation

Method : D:\MassHunter\GCMS\1\data\Johnson Lab\ph3 Ti.D\chiraldexbDM_400split.M
Title :

Signal : TIC: Ph MM 2.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	34.154	3864	3885	4024	M4	42508	5971319	42.72%	14.975%
2	35.360	4024	4046	4196	M3	43809	5984491	42.82%	15.008%
3	36.647	4197	4218	4339	M3	101667	13976273	100.00%	35.050%
4	37.700	4342	4359	4485	M3	97042	13943629	99.77%	34.968%





D:\MassHunter\GCMS\1\data\Johnson Lab\tBu MM .D\rteres.txt

Area Percent Report

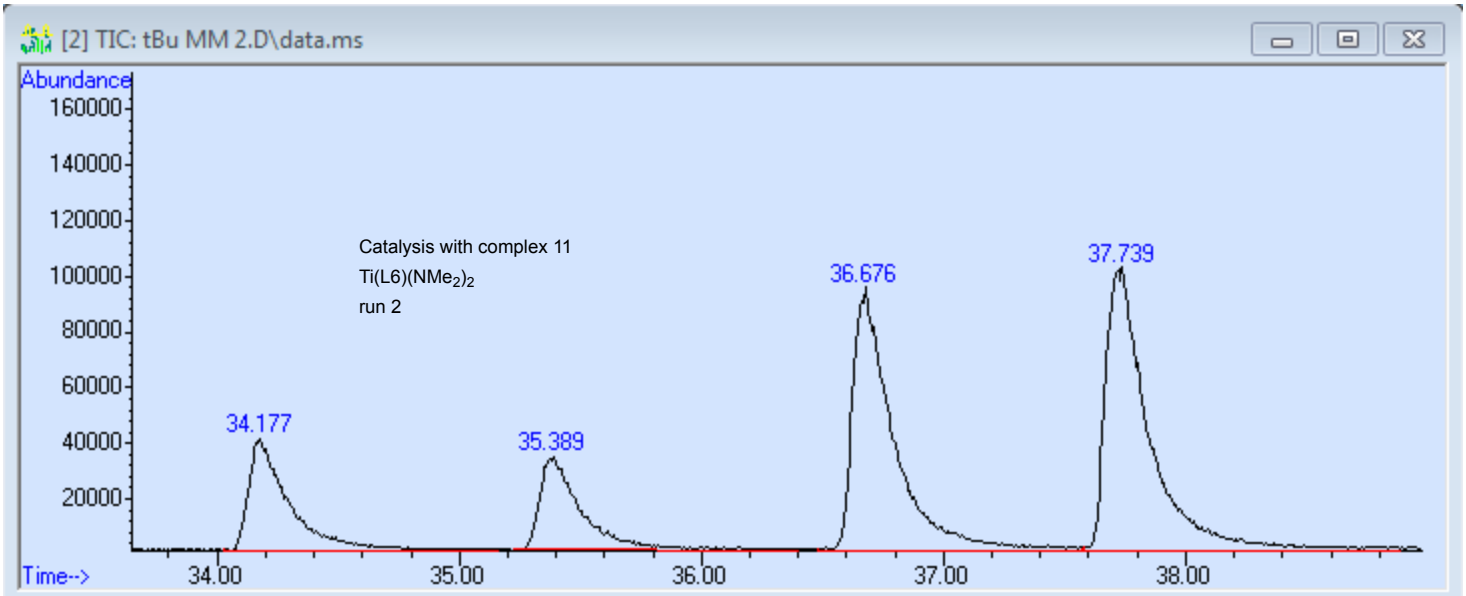
Data Path : D:\MassHunter\GCMS\1\data\Johnson Lab\
Data File : tBu MM .D
Acq On : 10 Jul 2018 10:07
Operator : arj
Sample :
Misc :
ALS Vial : 1 Sample Multiplier: 1

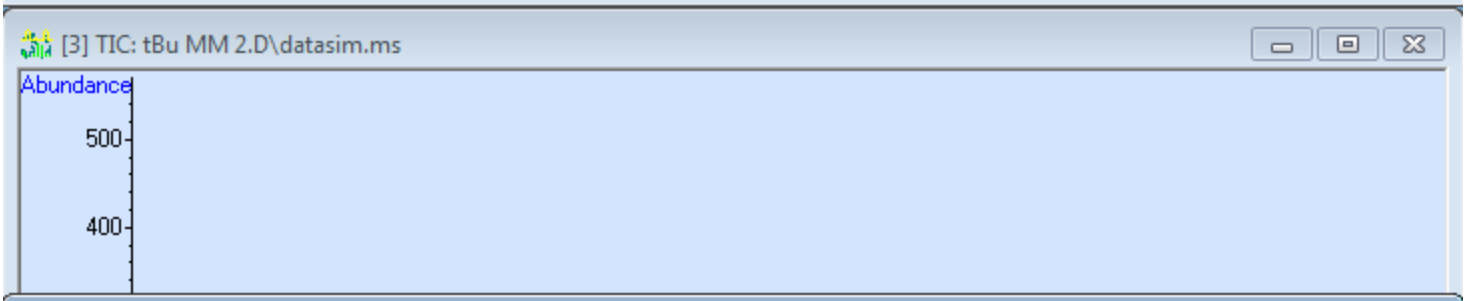
Integration Parameters: autoint1.e
Integrator: ChemStation

Method : D:\MassHunter\GCMS\1\data\Johnson Lab\ph3 Ti.D\chiraldexbDM_400split.M
Title :

Signal : TIC: tBu MM .D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	34.303	3885	3905	4044	M8	11785	2088591	38.73%	14.595%
2	35.500	4048	4065	4218	M9	12136	2169338	40.23%	15.159%
3	36.787	4220	4237	4358	M3	28520	4660185	86.43%	32.565%
4	37.825	4359	4375	4534	M6	30847	5392155	100.00%	37.680%





D:\MassHunter\GCMS\1\data\Johnson Lab\tBu MM 2.D\rteres.txt

Area Percent Report

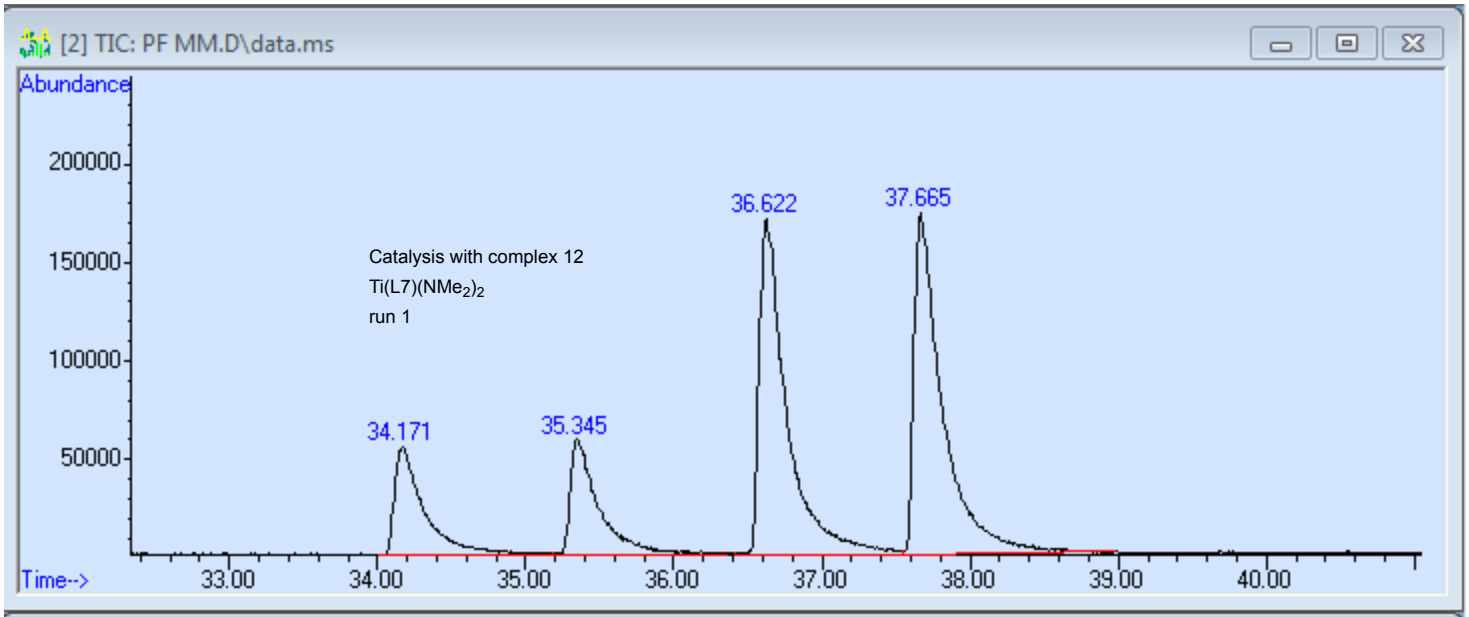
Data Path : D:\MassHunter\GCMS\1\data\Johnson Lab\
Data File : tBu MM 2.D
Acq On : 23 Jul 2018 10:05
Operator : arj
Sample :
Misc :
ALS Vial : 1 Sample Multiplier: 1

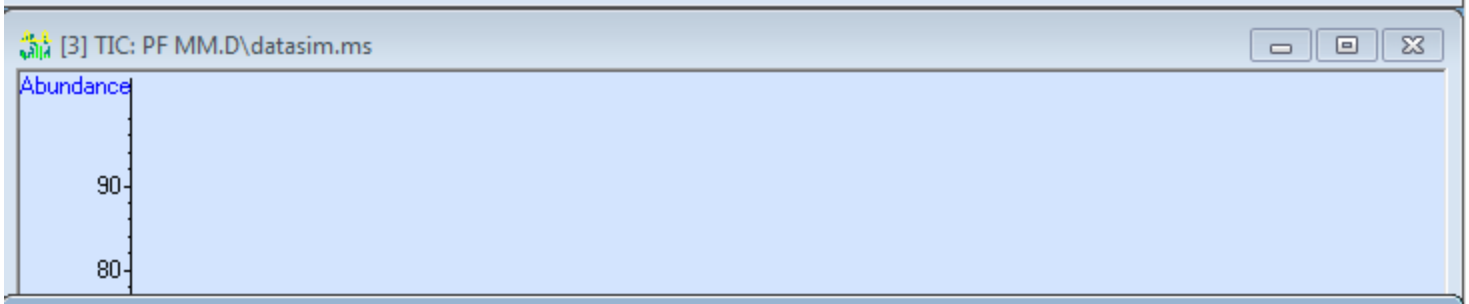
Integration Parameters: autoint1.e
Integrator: ChemStation

Method : D:\MassHunter\GCMS\1\data\Johnson Lab\ph3 Ti.D\chiraldexbDM_400split.M
Title :

Signal : TIC: tBu MM 2.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	34.177	3868	3888	4019	M3	40461	4823931	37.37%	14.647%
2	35.389	4028	4050	4185	M4	33297	4046220	31.35%	12.285%
3	36.676	4196	4222	4342	M3	94578	11156584	86.43%	33.874%
4	37.739	4343	4364	4517	M4	101982	12908496	100.00%	39.194%





D:\MassHunter\GCMS\1\data\Johnson Lab\PF MM.D\rteres.txt

Area Percent Report

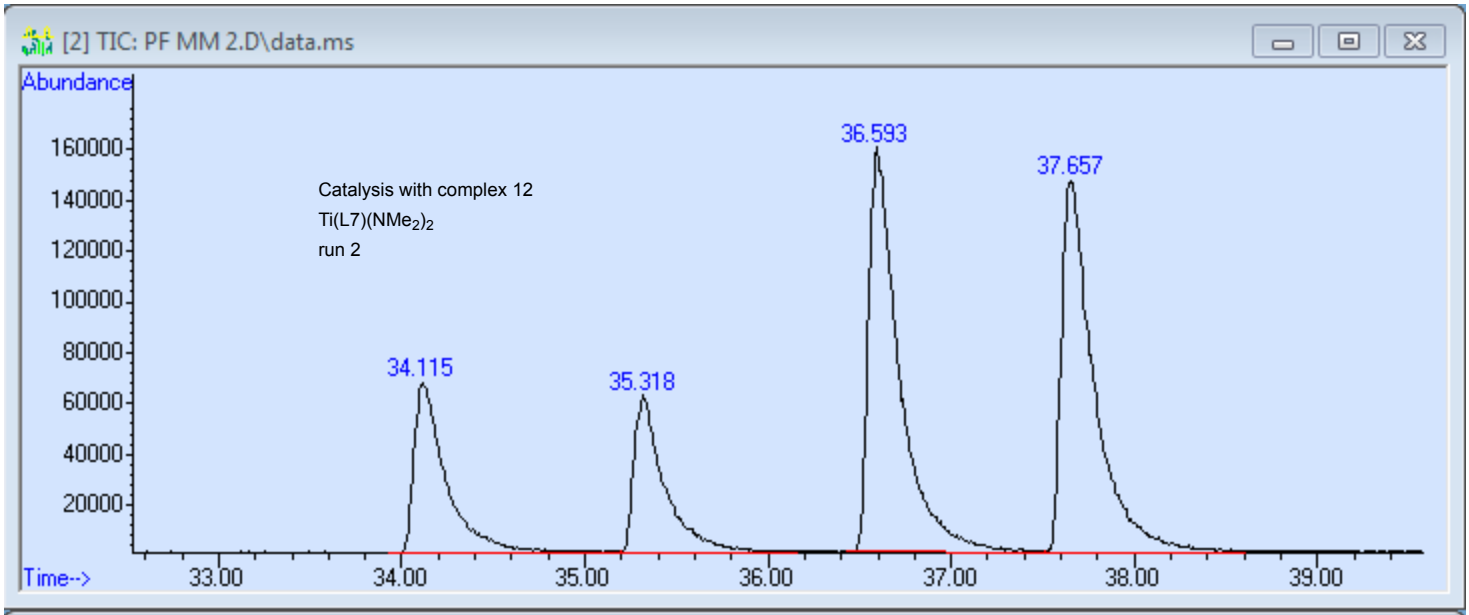
Data Path : D:\MassHunter\GCMS\1\data\Johnson Lab\
Data File : PF MM.D
Acq On : 10 Jul 2018 12:28
Operator : arj
Sample :
Misc :
ALS Vial : 3 Sample Multiplier: 1

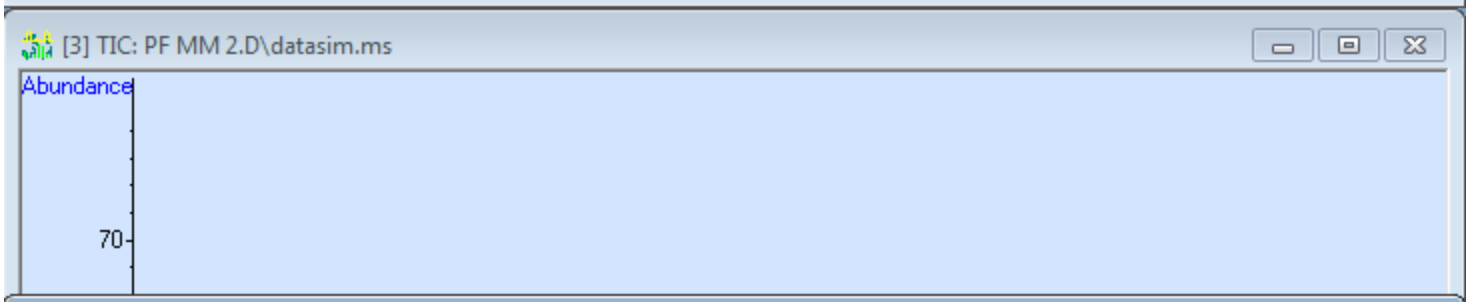
Integration Parameters: autoint1.e
Integrator: ChemStation

Method : D:\MassHunter\GCMS\1\data\Johnson Lab\ph3 Ti.D\chiraldexbDM_400split.M
Title :

Signal : TIC: PF MM.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	34.171	3866	3887	4022	M3	55113	7785962	33.67%	12.696%
2	35.345	4022	4044	4179	M3	58887	8051720	34.82%	13.129%
3	36.622	4187	4215	4338	M3	171267	22363458	96.71%	36.467%
4	37.665	4338	4354	4531	M2	173764	23124477	100.00%	37.708%





D:\MassHunter\GCMS\1\data\Johnson Lab\PF MM 2.D\rteres.txt

Area Percent Report

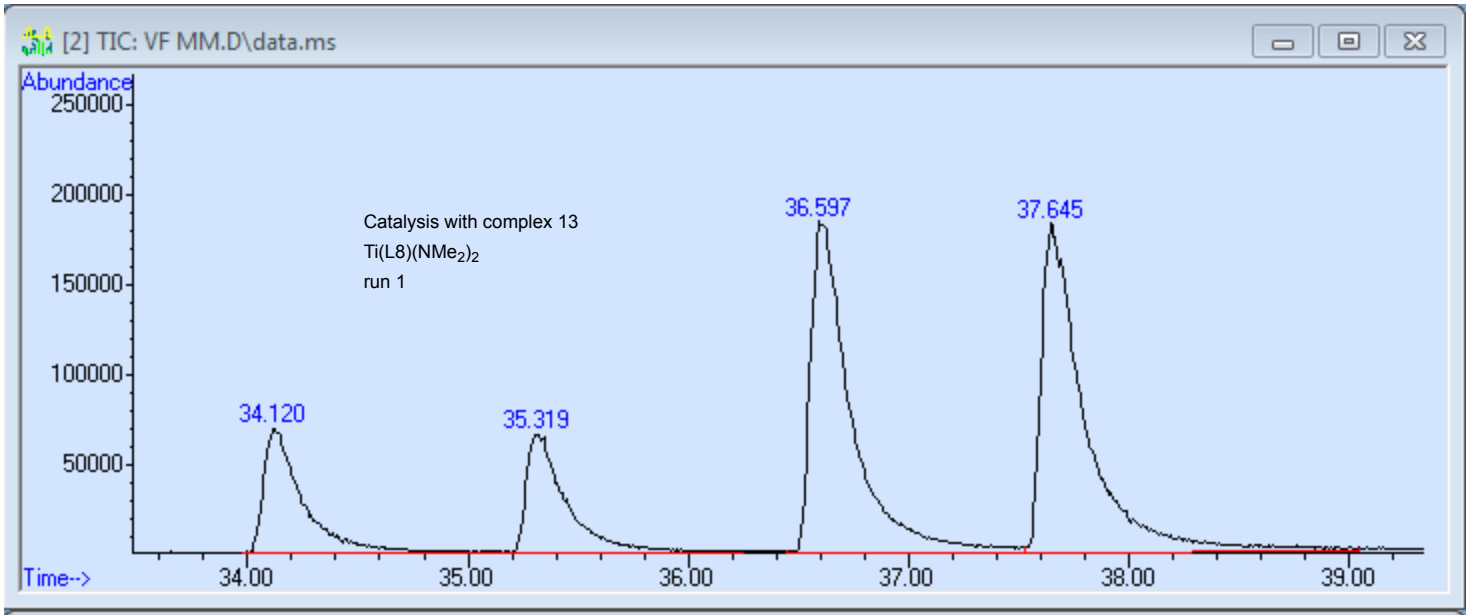
Data Path : D:\MassHunter\GCMS\1\data\Johnson Lab\
Data File : PF MM 2.D
Acq On : 23 Jul 2018 15:45
Operator : arj
Sample :
Misc :
ALS Vial : 3 Sample Multiplier: 1

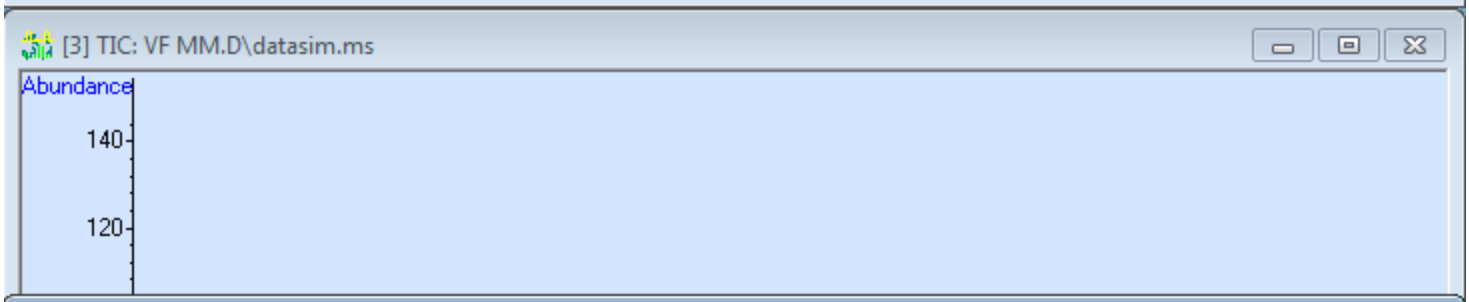
Integration Parameters: autoint1.e
Integrator: ChemStation

Method : D:\MassHunter\GCMS\1\data\Johnson Lab\ph3 Ti.D\chiraldexbDM_400split.M
Title :

Signal : TIC: PF MM 2.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	34.115	3855	3880	4024	M2	67571	8306957	44.37%	15.683%
2	35.318	4024	4040	4153	M2	62204	7325312	39.13%	13.830%
3	36.593	4189	4211	4334	M2	159147	18721637	100.00%	35.345%
4	37.657	4334	4353	4480	M	146834	18614155	99.43%	35.142%





D:\MassHunter\GCMS\1\data\Johnson Lab\VF MM.D\rteres.txt

Area Percent Report

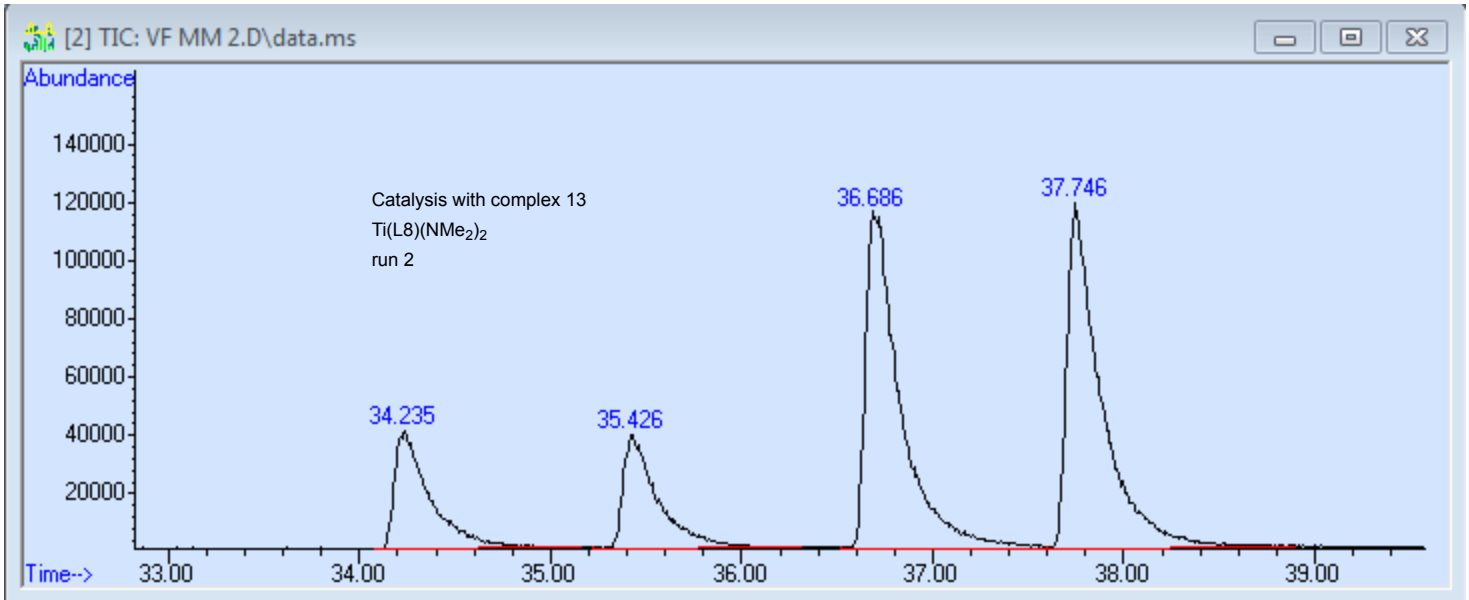
Data Path : D:\MassHunter\GCMS\1\data\Johnson Lab\
Data File : VF MM.D
Acq On : 10 Jul 2018 11:18
Operator : arj
Sample :
Misc :
ALS Vial : 2 Sample Multiplier: 1

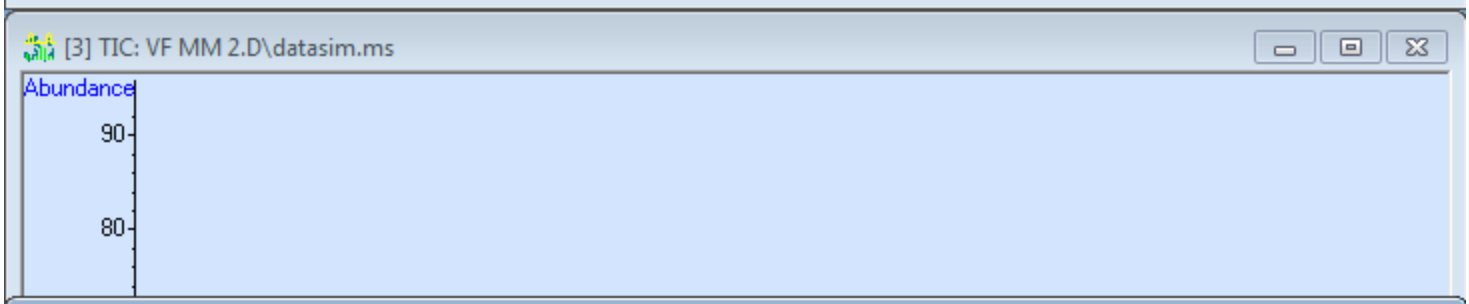
Integration Parameters: autoint1.e
Integrator: ChemStation

Method : D:\MassHunter\GCMS\1\data\Johnson Lab\ph3 Ti.D\chiraldexbDM_400split.M
Title :

Signal : TIC: VF MM.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	34.120	3861	3880	4024	M3	69269	8711001	34.05%	13.103%
2	35.319	4024	4040	4165	M3	66002	8429822	32.95%	12.680%
3	36.597	4191	4211	4336	M2	185304	23761103	92.89%	35.740%
4	37.645	4336	4351	4538	M3	184008	25581199	100.00%	38.478%





D:\MassHunter\GCMS\1\data\Johnson Lab\VF MM 2.D\rteres.txt

Area Percent Report

Data Path : D:\MassHunter\GCMS\1\data\Johnson Lab\
Data File : VF MM 2.D
Acq On : 23 Jul 2018 14:34
Operator : arj
Sample :
Misc :
ALS Vial : 2 Sample Multiplier: 1

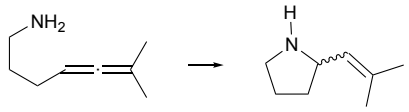
Integration Parameters: autoint1.e
Integrator: ChemStation

Method : D:\MassHunter\GCMS\1\data\Johnson Lab\ph3 Ti.D\chiraldexbDM_400split.M
Title :

Signal : TIC: VF MM 2.D\data.ms

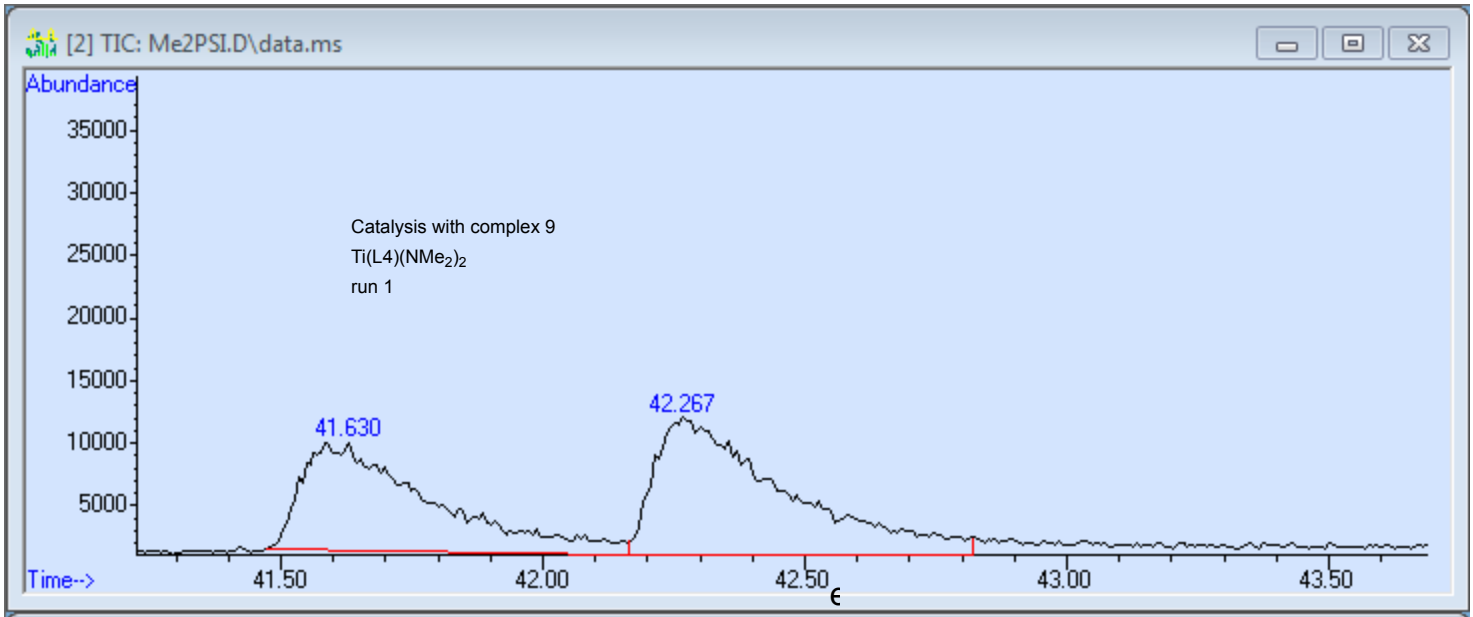
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	34.235	3875	3896	4020	M3	40681	5136736	34.59%	12.919%
2	35.426	4027	4055	4174	M2	39397	4943891	33.29%	12.434%
3	36.686	4201	4223	4345	M3	116121	14830082	99.87%	37.299%
4	37.746	4345	4365	4519	M2	118797	14848944	100.00%	37.347%

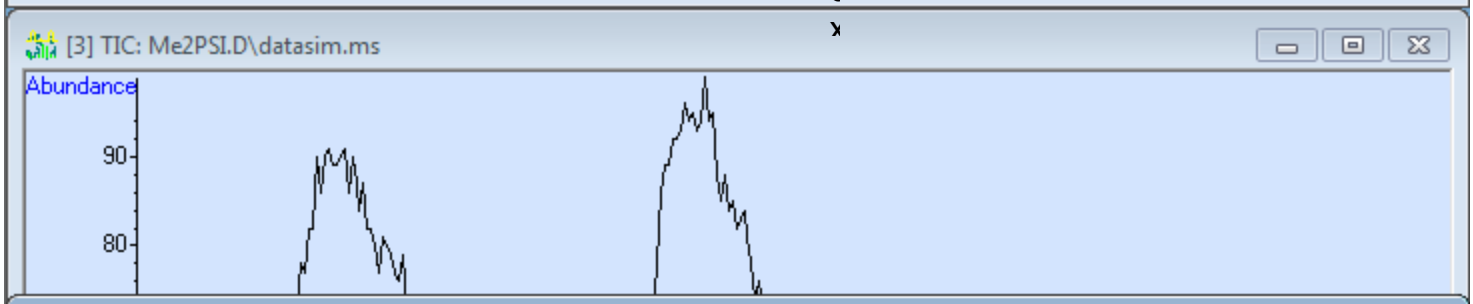
Hydroamination of 6-methyl-hepta-4,5-dienylamine 1c at 135 °C with *in situ* catalysts (5 mol% catalyst).



1b **3b**

41.3, 42.1 min





D:\MassHunter\GCMS\1\data\Johnson Lab\Me2PSI.D\rteres.txt

Area Percent Report

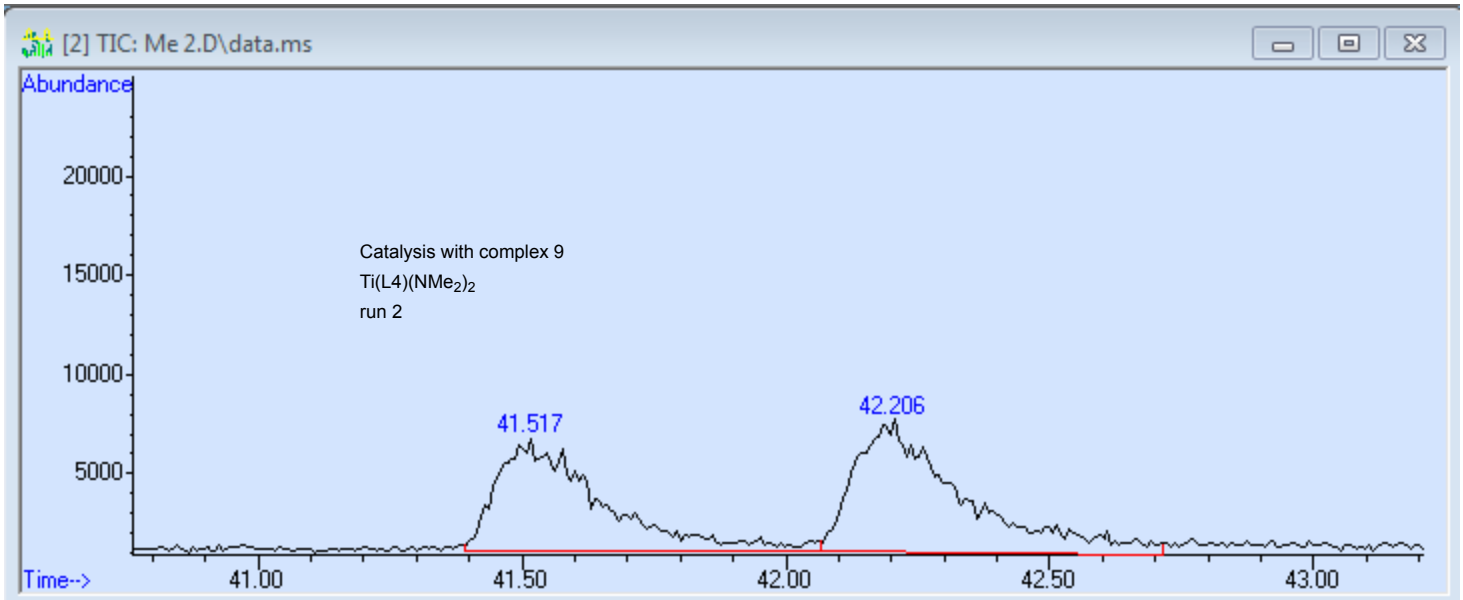
Data Path : D:\MassHunter\GCMS\1\data\Johnson Lab\
Data File : Me2PSI.D
Acq On : 06 Jul 2018 14:25
Operator : arj
Sample :
Misc :
ALS Vial : 2 Sample Multiplier: 1

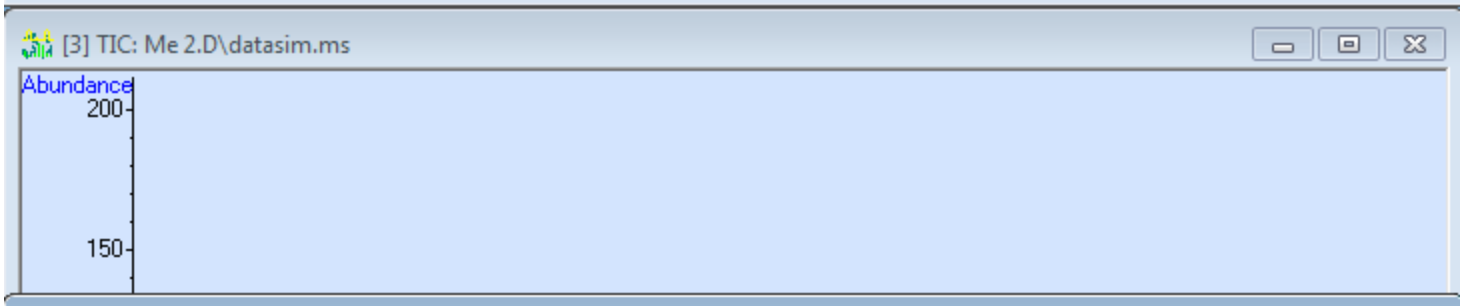
Integration Parameters: autoint1.e
Integrator: ChemStation

Method : D:\MassHunter\GCMS\1\data\Johnson Lab\ph3 Ti.D\chiraldexbDM_400split.M
Title :

Signal : TIC: Me2PSI.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	41.630	4863	4884	4955	M10	8609	1498226	78.63%	44.017%
2	42.267	4955	4969	5043	M8	10978	1905528	100.00%	55.983%





D:\MassHunter\GCMS\1\data\Johnson Lab\Me 2.D\rteres.txt

Area Percent Report

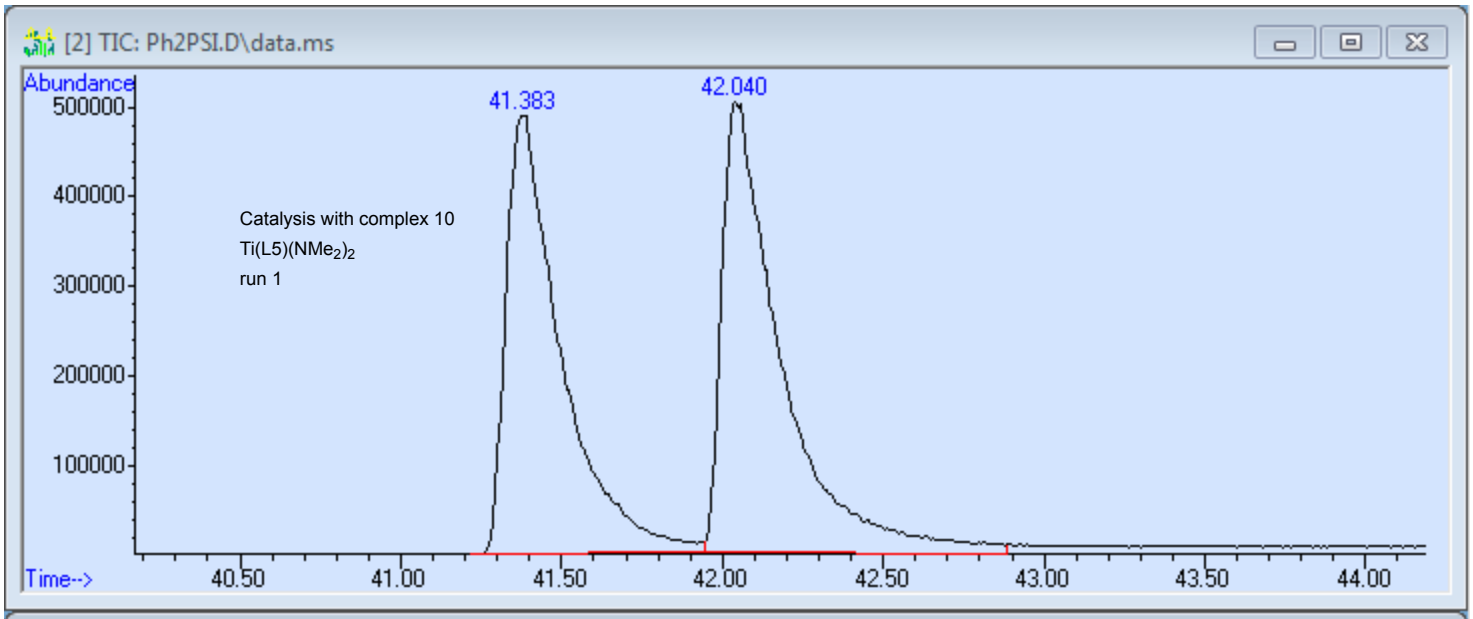
Data Path : D:\MassHunter\GCMS\1\data\Johnson Lab\
Data File : Me 2.D
Acq On : 25 Jul 2018 14:21
Operator : arj
Sample :
Misc :
ALS Vial : 2 Sample Multiplier: 1

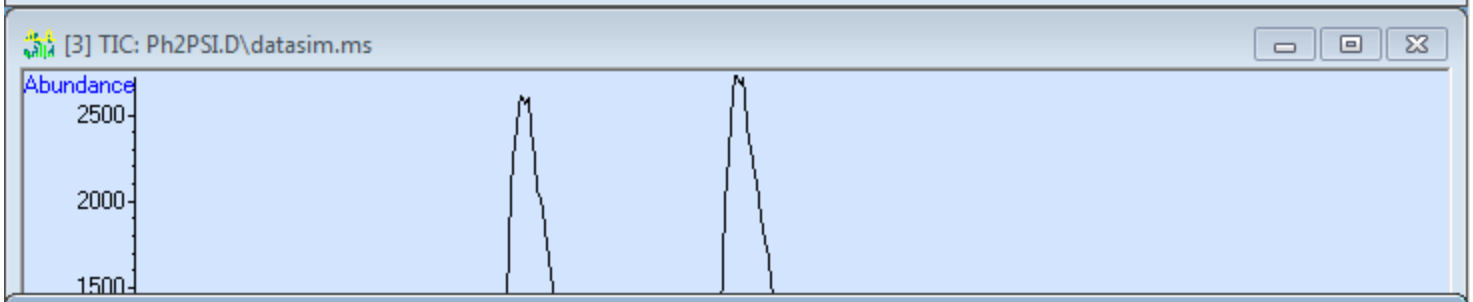
Integration Parameters: autoint1.e
Integrator: ChemStation

Method : D:\MassHunter\GCMS\1\data\Johnson Lab\ph3 Ti.D\chiraldexbDM_400split.M
Title :

Signal : TIC: Me 2.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	41.517	4852	4869	4942	M	5693	768465	82.75%	45.282%
2	42.206	4942	4961	5029	M7	6657	928609	100.00%	54.718%





D:\MassHunter\GCMS\1\data\Johnson Lab\Ph2PSI.D\rteres.txt

Area Percent Report

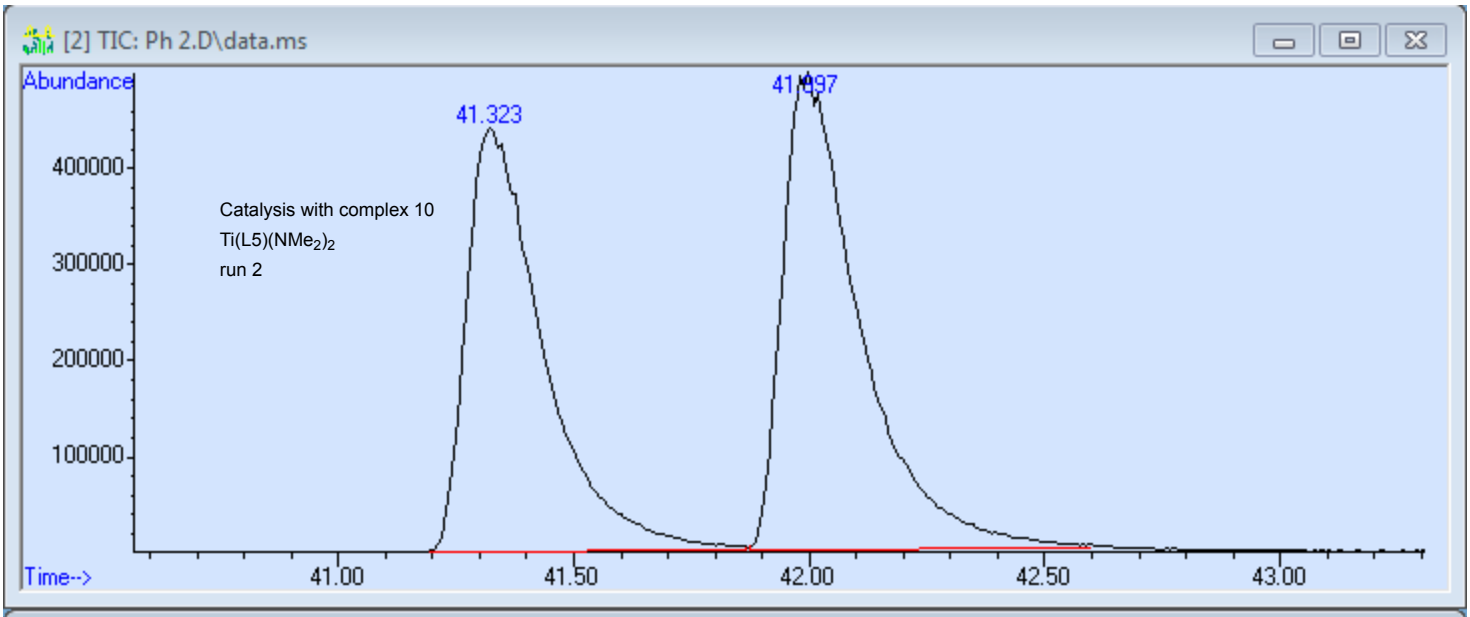
Data Path : D:\MassHunter\GCMS\1\data\Johnson Lab\
Data File : Ph2PSI.D
Acq On : 06 Jul 2018 13:15
Operator : arj
Sample :
Misc :
ALS Vial : 1 Sample Multiplier: 1

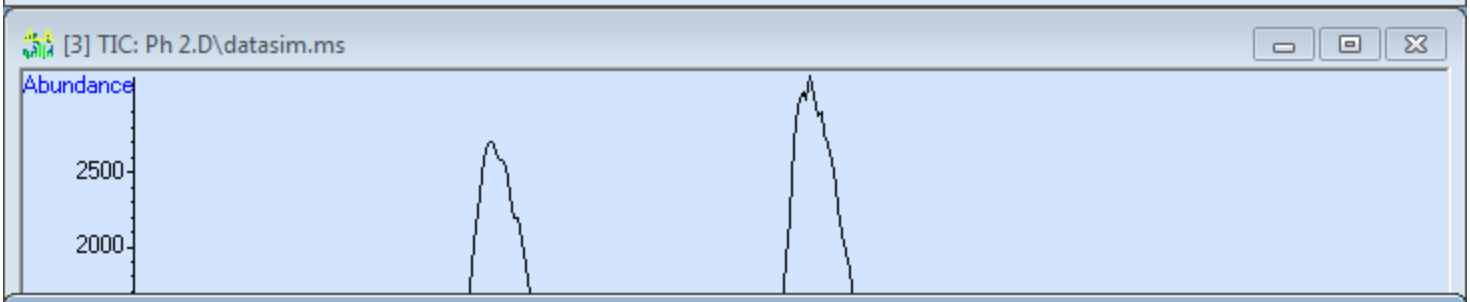
Integration Parameters: autoint1.e
Integrator: ChemStation

Method : D:\MassHunter\GCMS\1\data\Johnson Lab\ph3 Ti.D\chiraldexbDM_400split.M
Title :

Signal : TIC: Ph2PSI.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	41.383	4829	4851	4926	M	489322	58460450	90.37%	47.471%
2	42.040	4926	4939	5052	M2	503899	64688423	100.00%	52.529%





D:\MassHunter\GCMS\1\data\Johnson Lab\Ph 2.D\rteres.txt

Area Percent Report

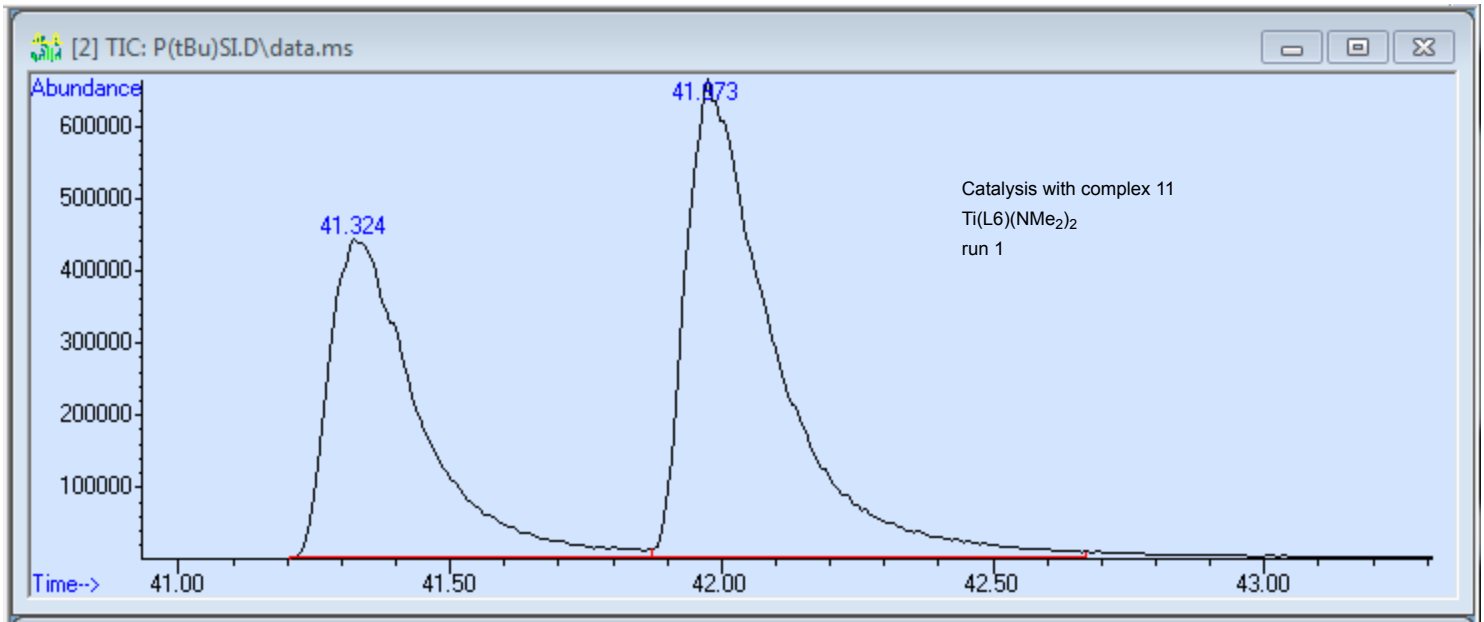
Data Path : D:\MassHunter\GCMS\1\data\Johnson Lab\
Data File : Ph 2.D
Acq On : 25 Jul 2018 13:10
Operator : arj
Sample :
Misc :
ALS Vial : 1 Sample Multiplier: 1

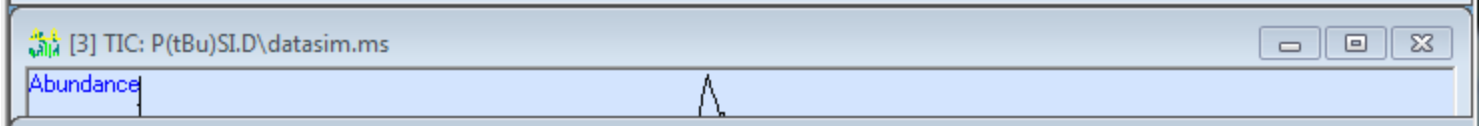
Integration Parameters: autoint1.e
Integrator: ChemStation

Method : D:\MassHunter\GCMS\1\data\Johnson Lab\ph3 Ti.D\chiraldexbDM_400split.M
Title :

Signal : TIC: Ph 2.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	41.323	4826	4843	4915	M2	441099	50410366	88.02%	46.814%
2	41.997	4917	4933	5013	M2	497445	57271297	100.00%	53.186%





D:\MassHunter\GCMS\1\data\Johnson Lab\P(tBu)SI.D\rteres.txt

Area Percent Report

Data Path : D:\MassHunter\GCMS\1\data\Johnson Lab\
Data File : P(tBu)SI.D
Acq On : 06 Jul 2018 06:33
Operator : arj
Sample :
Misc :
ALS Vial : 1 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : D:\MassHunter\GCMS\1\data\Johnson Lab\ph3 Ti.D\chiraldexbDM_400split.M
Title :

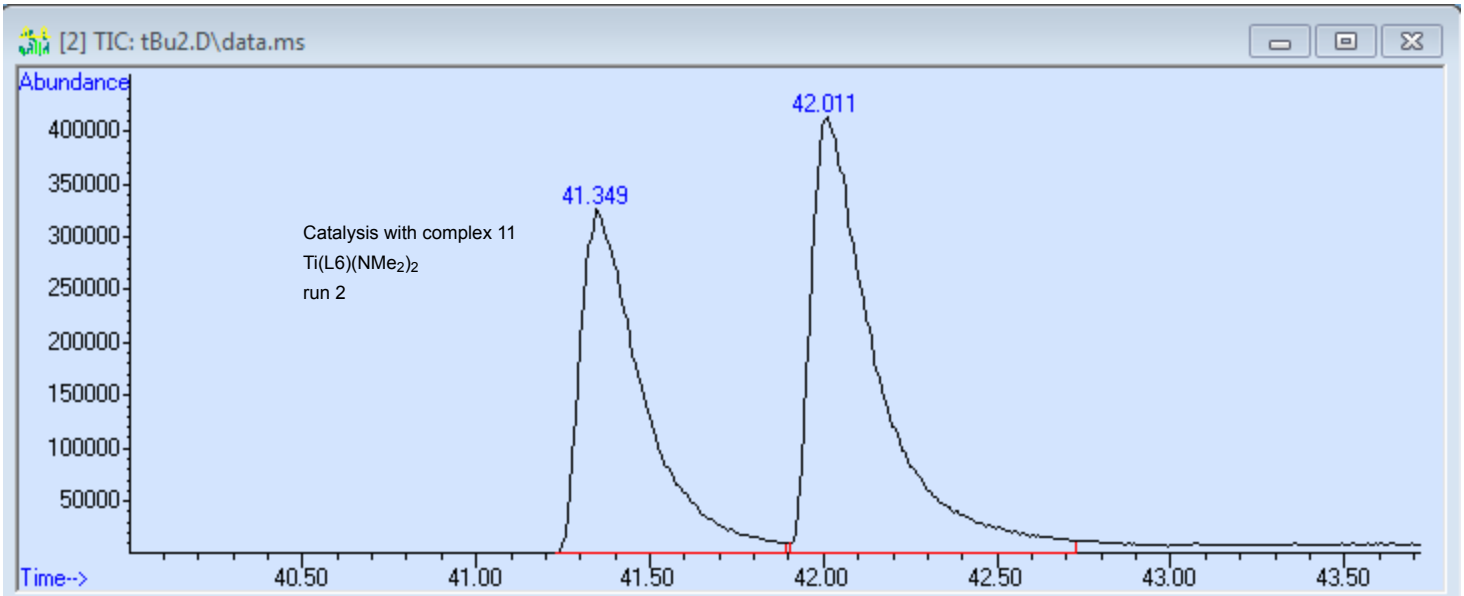
Signal : TIC: P(tBu)SI.D\data.ms

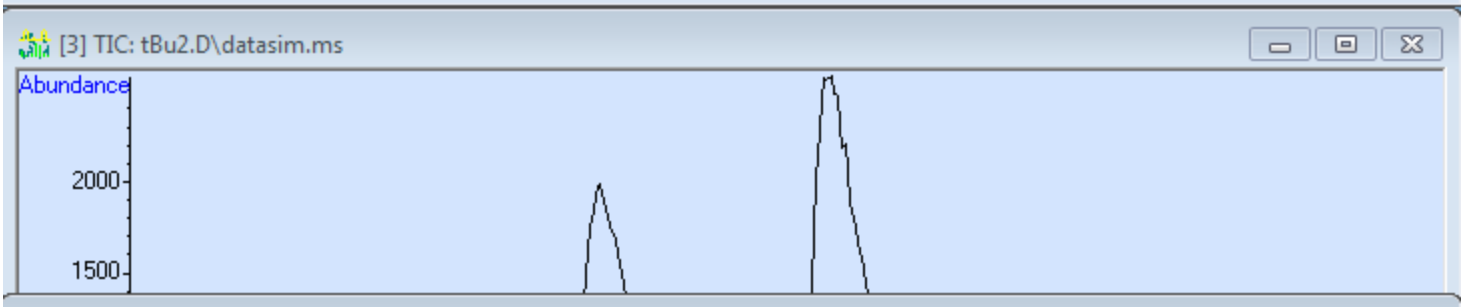
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	41.324	4827	4843	4916	M2	439419	50993378	67.66%	40.357%
2	41.973	4916	4930	5023	M	661625	75363679	100.00%	59.643%

Sum of corrected areas: 126357057

Signal : TIC: P(tBu)SI.D\datasim.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total





D:\MassHunter\GCMS\1\data\Johnson Lab\tBu2.D\rteres.txt

Area Percent Report

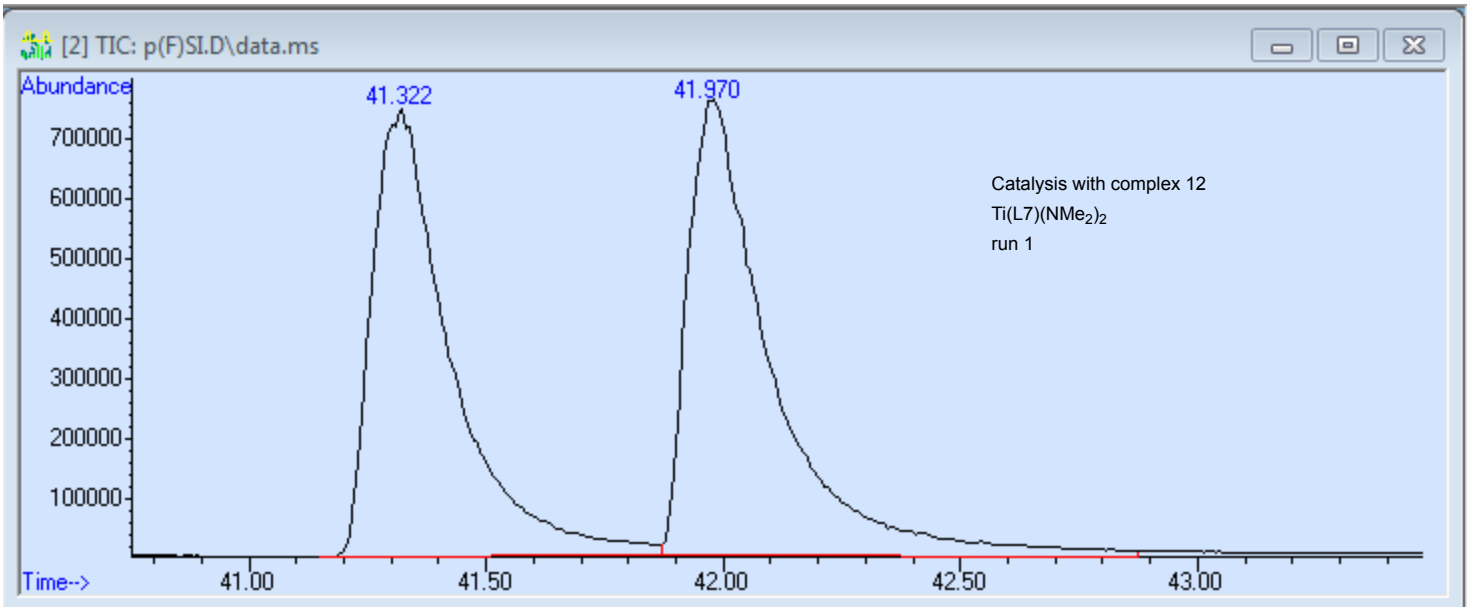
Data Path : D:\MassHunter\GCMS\1\data\Johnson Lab\
Data File : tBu2.D
Acq On : 06 Jul 2018 15:27
Operator : arj
Sample :
Misc :
ALS Vial : 3 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : D:\MassHunter\GCMS\1\data\Johnson Lab\ph3 Ti.D\chiraldexbDM_400split.M
Title :

Signal : TIC: tBu2.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	41.349	4830	4846	4919	M	326482	41025720	74.67%	42.750%
2	42.011	4921	4935	5031	M2	412331	54940503	100.00%	57.250%



D:\MassHunter\GCMS\1\data\Johnson Lab\p(F)SI.D\rteres.txt

Area Percent Report

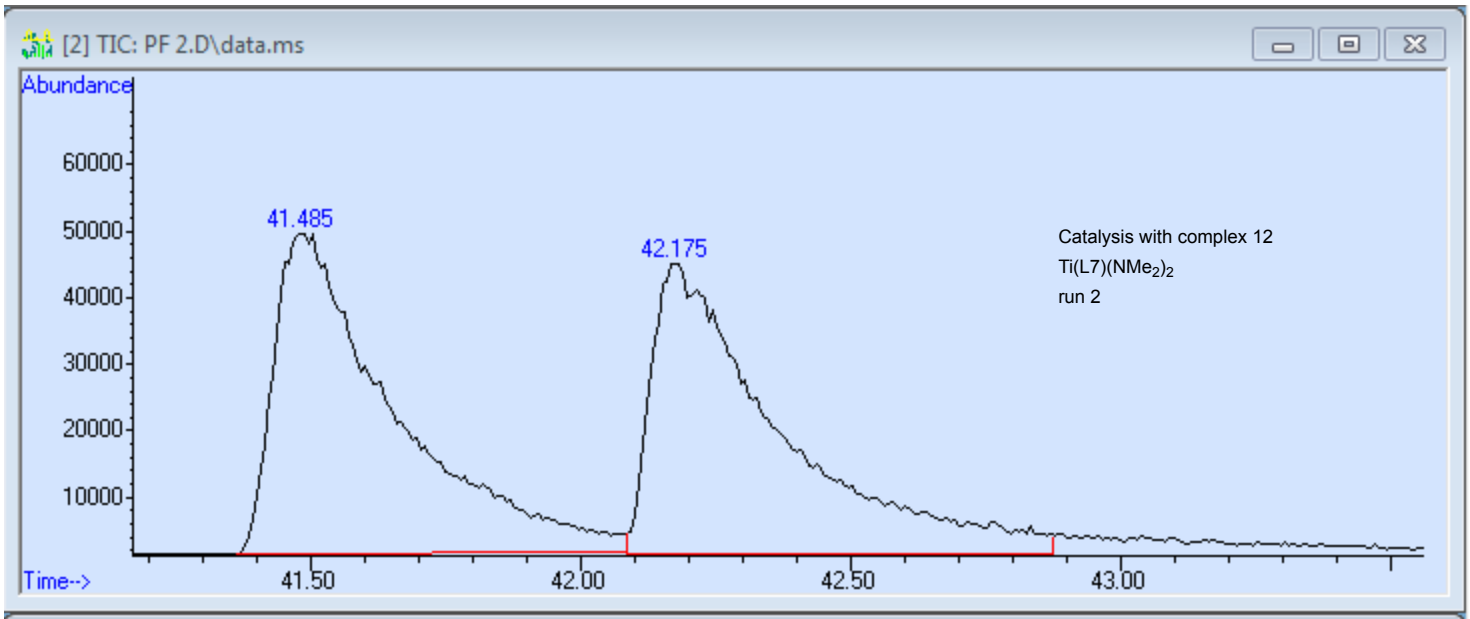
Data Path : D:\MassHunter\GCMS\1\data\Johnson Lab\
Data File : p(F)SI.D
Acq On : 06 Jul 2018 03:48
Operator : arj
Sample :
Misc :
ALS Vial : 3 Sample Multiplier: 1

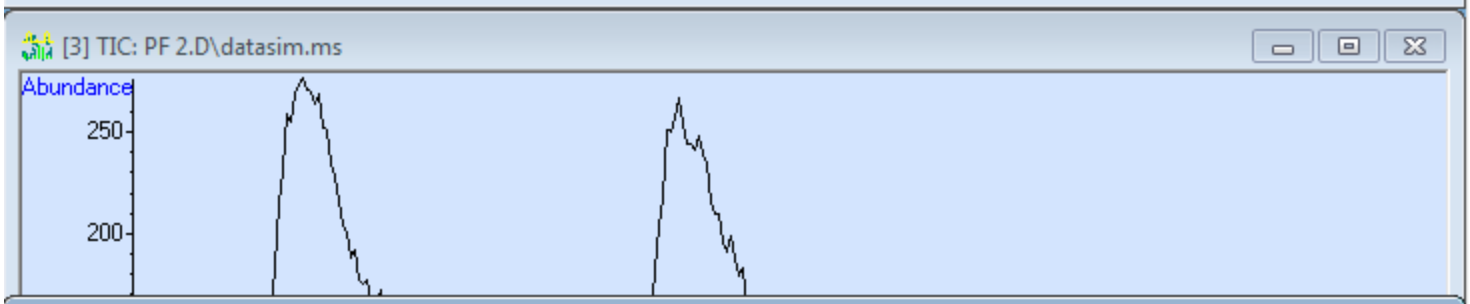
Integration Parameters: autoint1.e
Integrator: ChemStation

Method : D:\MassHunter\GCMS\1\data\Johnson Lab\ph3 Ti.D\chiraldexbDM_400split.M
Title :

Signal : TIC: p(F)SI.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	41.322	4820	4843	4916	M	748271	86585245	92.63%	48.088%
2	41.970	4916	4929	5050	M2	766543	93470246	100.00%	51.912%





D:\MassHunter\GCMS\1\data\Johnson Lab\PF 2.D\rteres.txt

Area Percent Report

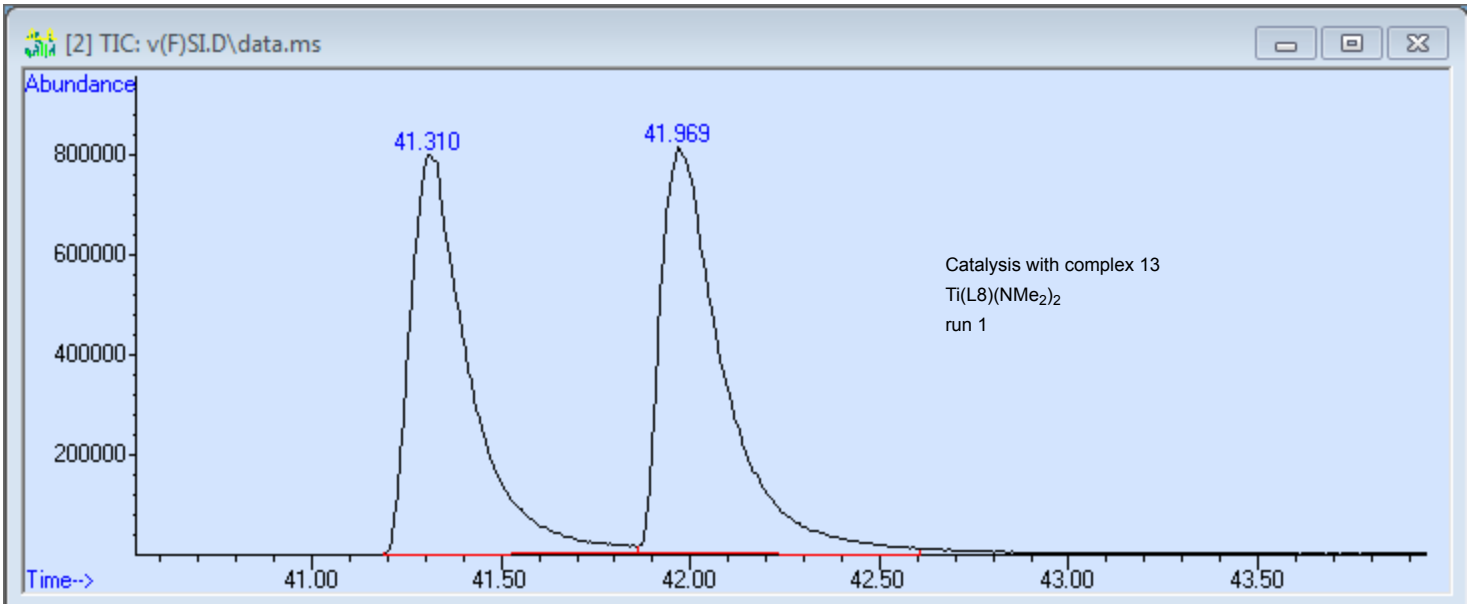
Data Path : D:\MassHunter\GCMS\1\data\Johnson Lab\
Data File : PF 2.D
Acq On : 10 Jul 2018 13:39
Operator : arj
Sample :
Misc :
ALS Vial : 4 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : D:\MassHunter\GCMS\1\data\Johnson Lab\ph3 Ti.D\chiraldexbDM_400split.M
Title :

Signal : TIC: PF 2.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	41.485	4848	4865	4945	M	48392	7456299	100.00%	50.926%
2	42.175	4945	4957	5050	M2	43765	7185092	96.36%	49.074%



D:\MassHunter\GCMS\1\data\Johnson Lab\v(F)SI.D\rteres.txt

Area Percent Report

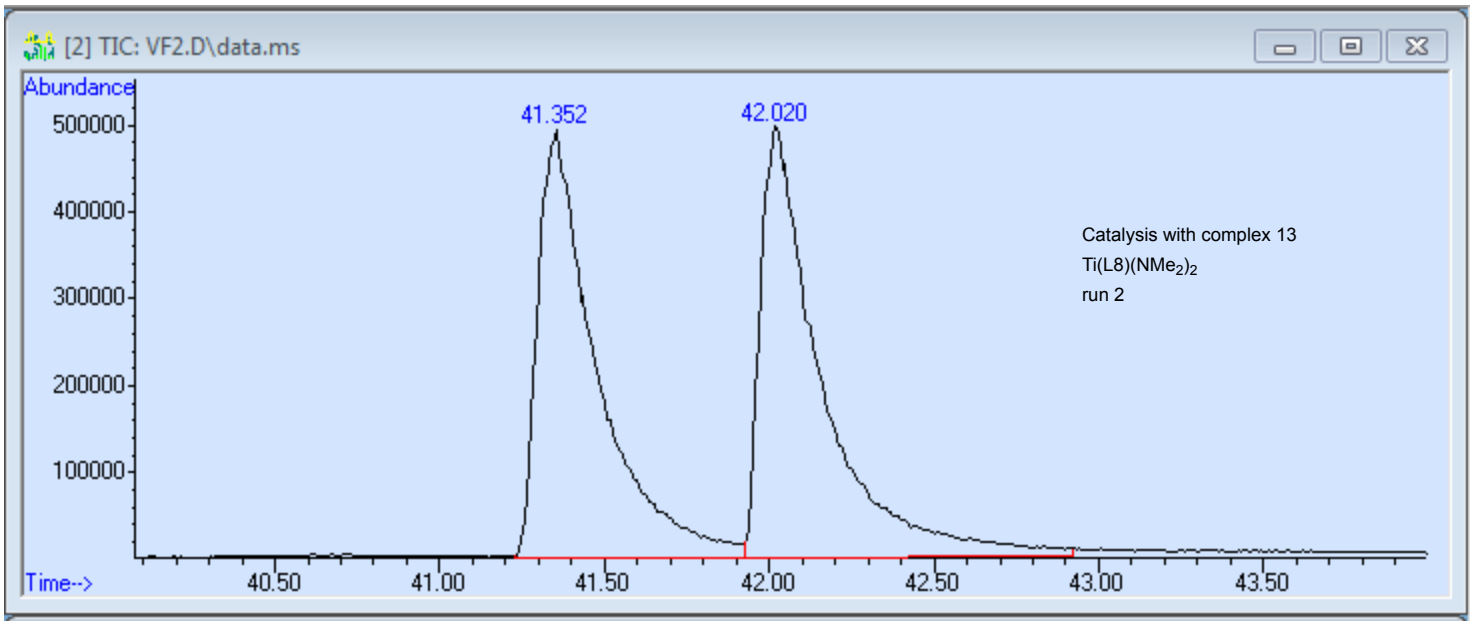
Data Path : D:\MassHunter\GCMS\1\data\Johnson Lab\
Data File : v(F)SI.D
Acq On : 06 Jul 2018 01:02
Operator : arj
Sample :
Misc :
ALS Vial : 2 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : D:\MassHunter\GCMS\1\data\Johnson Lab\ph3 Ti.D\chiraldexbDM_400split.M
Title :

Signal : TIC: v(F)SI.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	41.310	4825	4841	4915	M2	797074	87055659	91.62%	47.814%
2	41.969	4915	4929	5015	M	811306	95014841	100.00%	52.186%



D:\MassHunter\GCMS\1\data\Johnson Lab\VF2.D\rteres.txt

Area Percent Report

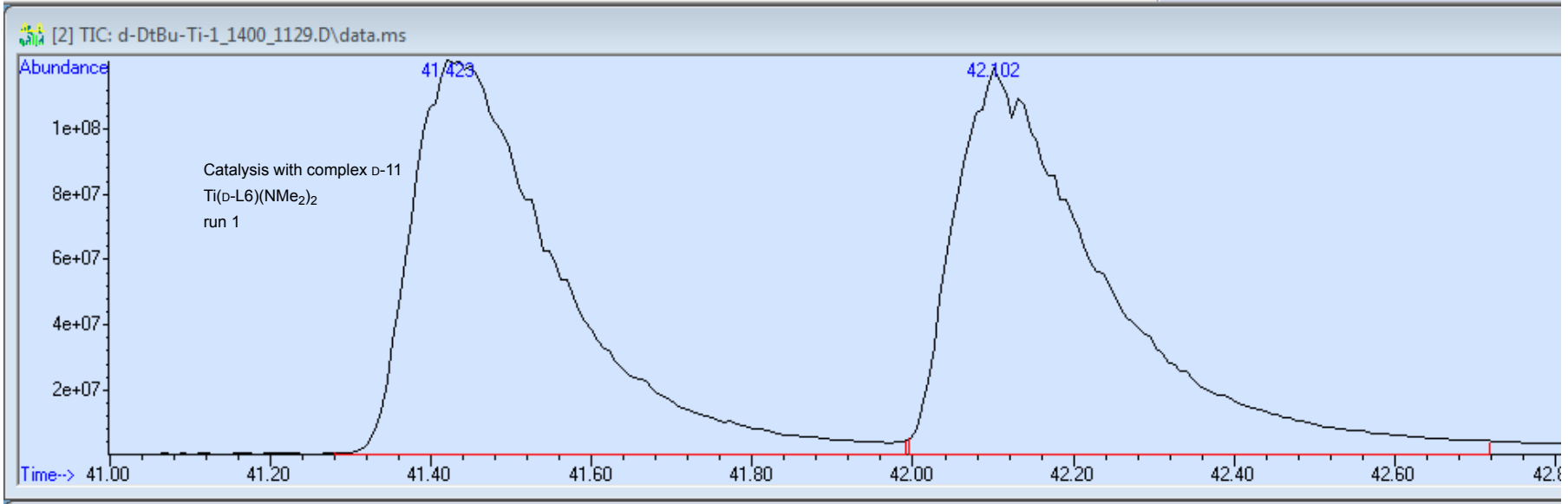
Data Path : D:\MassHunter\GCMS\1\data\Johnson Lab\
Data File : VF2.D
Acq On : 06 Jul 2018 16:38
Operator : arj
Sample :
Misc :
ALS Vial : 4 Sample Multiplier: 1

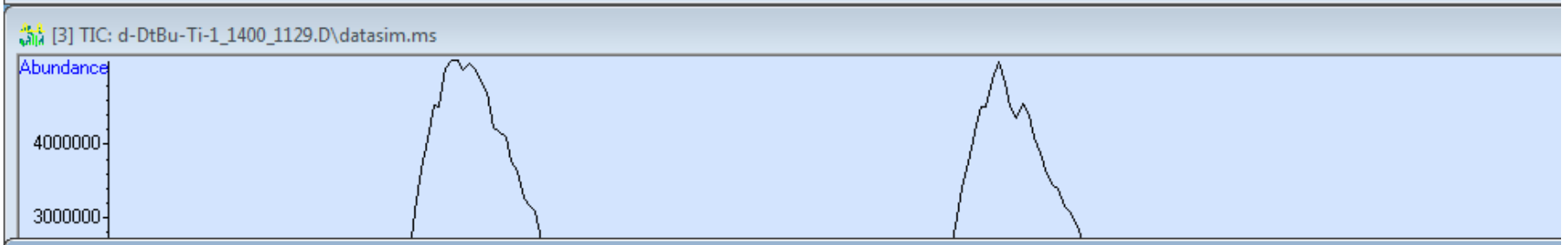
Integration Parameters: autoint1.e
Integrator: ChemStation

Method : D:\MassHunter\GCMS\1\data\Johnson Lab\ph3 Ti.D\chiraldexbDM_400split.M
Title :

Signal : TIC: VF2.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	41.352	4830	4847	4924	M2	494115	61560017	95.89%	48.951%
2	42.020	4924	4936	5057	M2	497545	64199617	100.00%	51.049%





D:\MassHunter\GCMS\1\data\Johnson Lab\d-DtBu-Ti-1_1400_1129.D\rteres.txt

Area Percent Report

Data Path : D:\MassHunter\GCMS\1\data\Johnson Lab\
Data File : d-DtBu-Ti-1_1400_1129.D
Acq On : 29 Nov 2018 09:56
Operator : fs
Sample : di-tBu-Ti
Misc :
ALS Vial : 2 Sample Multiplier: 1

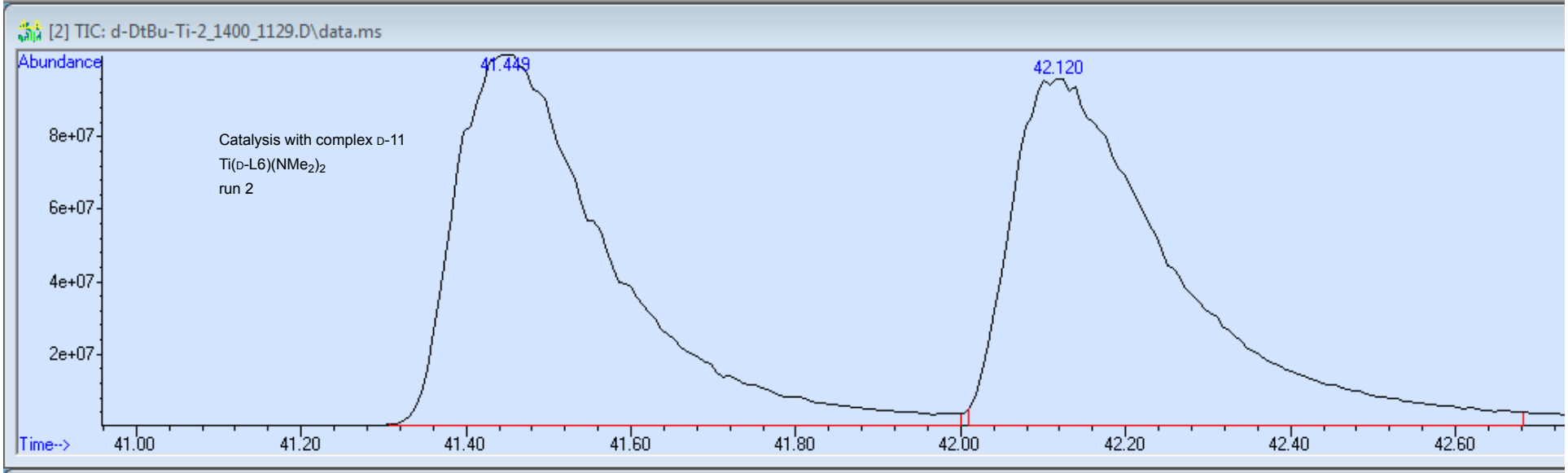
Integration Parameters: events.e
Integrator: ChemStation

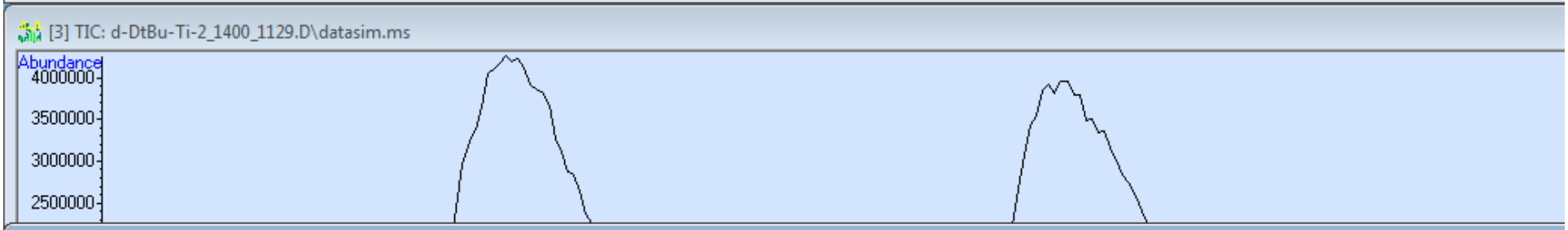
Method : D:\MassHunter\GCMS\1\data\Johnson Lab\d-DtBu-Ti-1_1test50.D\chiraldexbDM_50split.M
Title :

Signal : TIC: d-DtBu-Ti-1_1400_1129.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	41.423	4837	4856	4932	M6	121264066	15564667052	99.10%	49.774%
2	42.102	4933	4947	5029	M4	118382562	15705950014	100.00%	50.226%

Sum of corrected areas: 31270617066





D:\MassHunter\GCMS\1\data\Johnson Lab\d-DtBu-Ti-2_1400_1129.D\rteres.txt

Area Percent Report

Data Path : D:\MassHunter\GCMS\1\data\Johnson Lab\
Data File : d-DtBu-Ti-2_1400_1129.D
Acq On : 29 Nov 2018 11:07
Operator : fs
Sample : di-tBu-Ti
Misc :
ALS Vial : 3 Sample Multiplier: 1

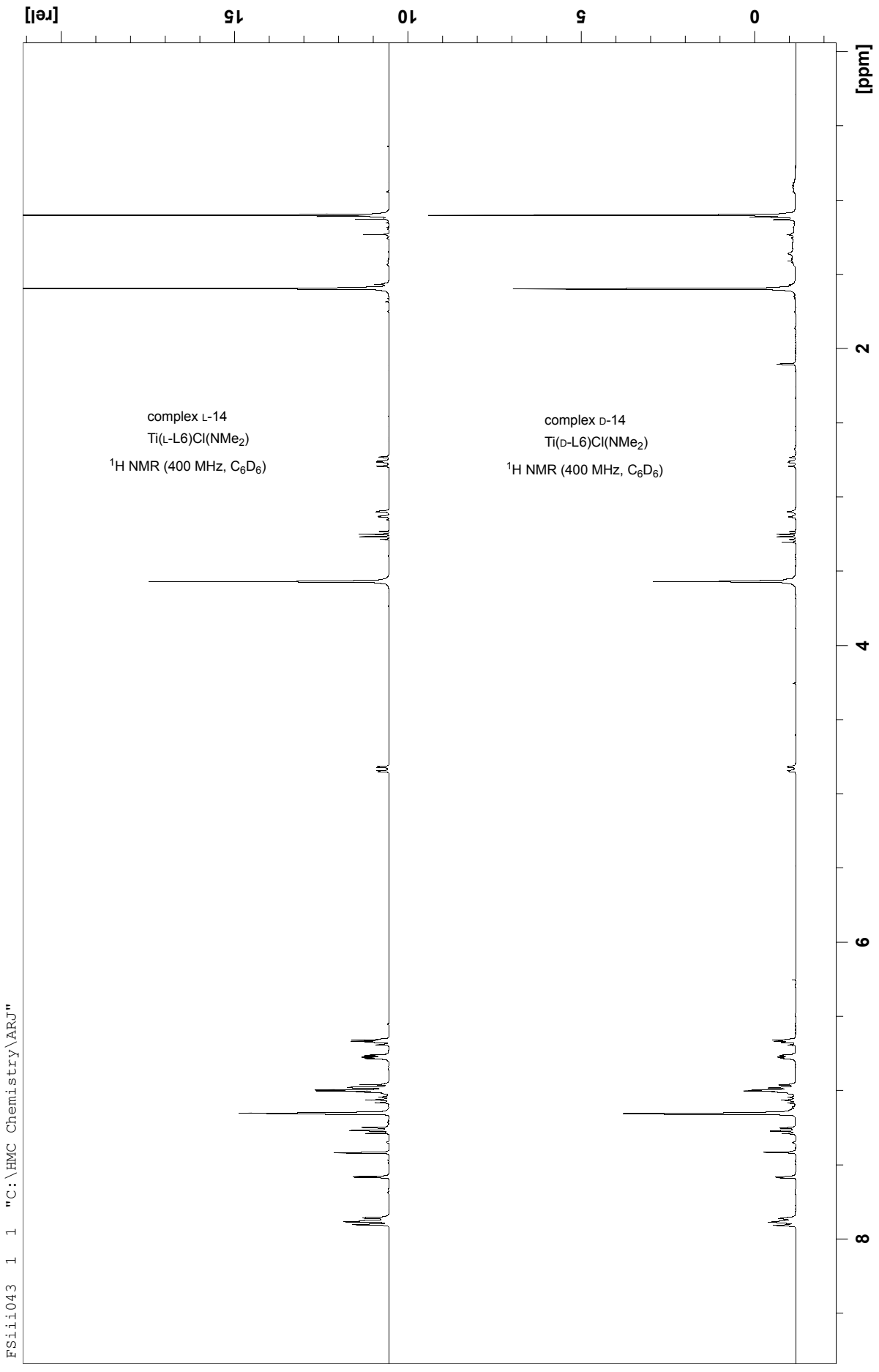
Integration Parameters: events.e
Integrator: ChemStation

Method : D:\MassHunter\GCMS\1\data\Johnson Lab\d-DtBu-Ti-1_1test50.D\chiraldexbDM_50split.M
Title :

Signal : TIC: d-DtBu-Ti-2_1400_1129.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	41.449	4841	4860	4934	M5	102202315	13458319589	100.00%	50.289%
2	42.120	4935	4949	5025	M5	96010286	13303385253	98.85%	49.711%

Sum of corrected areas: 26761704842


complex L-14
Ti(L-L6)Cl(NMe2)
1H NMR (400 MHz, C6D6)
complex D-14
Ti(D-L6)Cl(NMe2)
1H NMR (400 MHz, C6D6)
[rel]
15
10
5
0
[ppm]
2
4
6
8
FSiii043 1 1 "C:\HMC Chemistry\ARJ"