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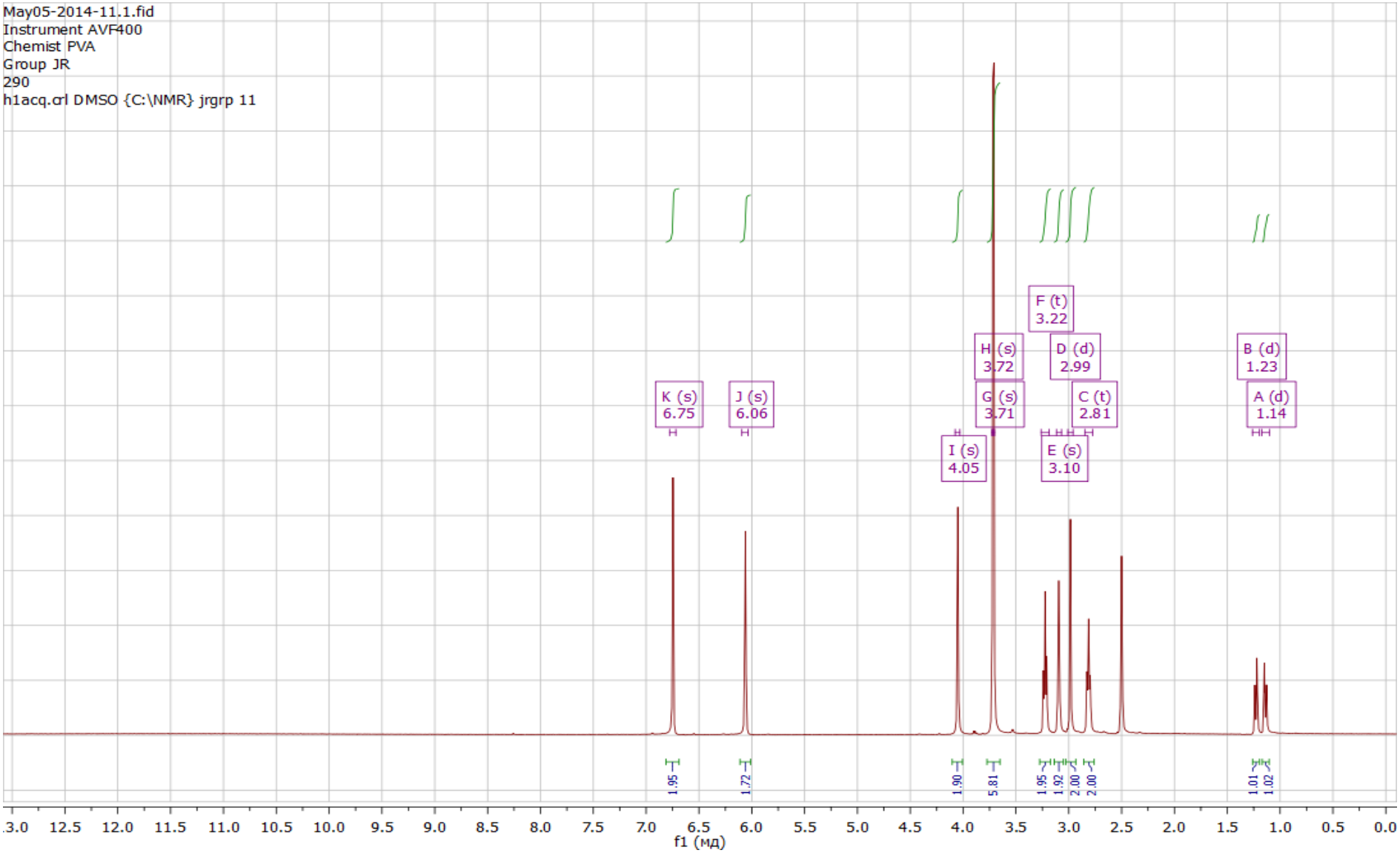
Supporting information for article:

The formation of the salt and neutral molecule co-crystal from equimolar solution of 6,7-dimethoxy-1,2,3,4-tetrahydroisoquinoline (heliamine) and bicyclo[2.2.1]hept-5-ene-*endo*-2,3-dicarboxylic acid

Svitlana V. Shishkina, Ivan A. Isaiev, Viktoriya V. Urzhuntseva and Vitalii A. Palchykov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Group JR
290
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H (s)
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G (s)
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F (t)
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1.72
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5.81
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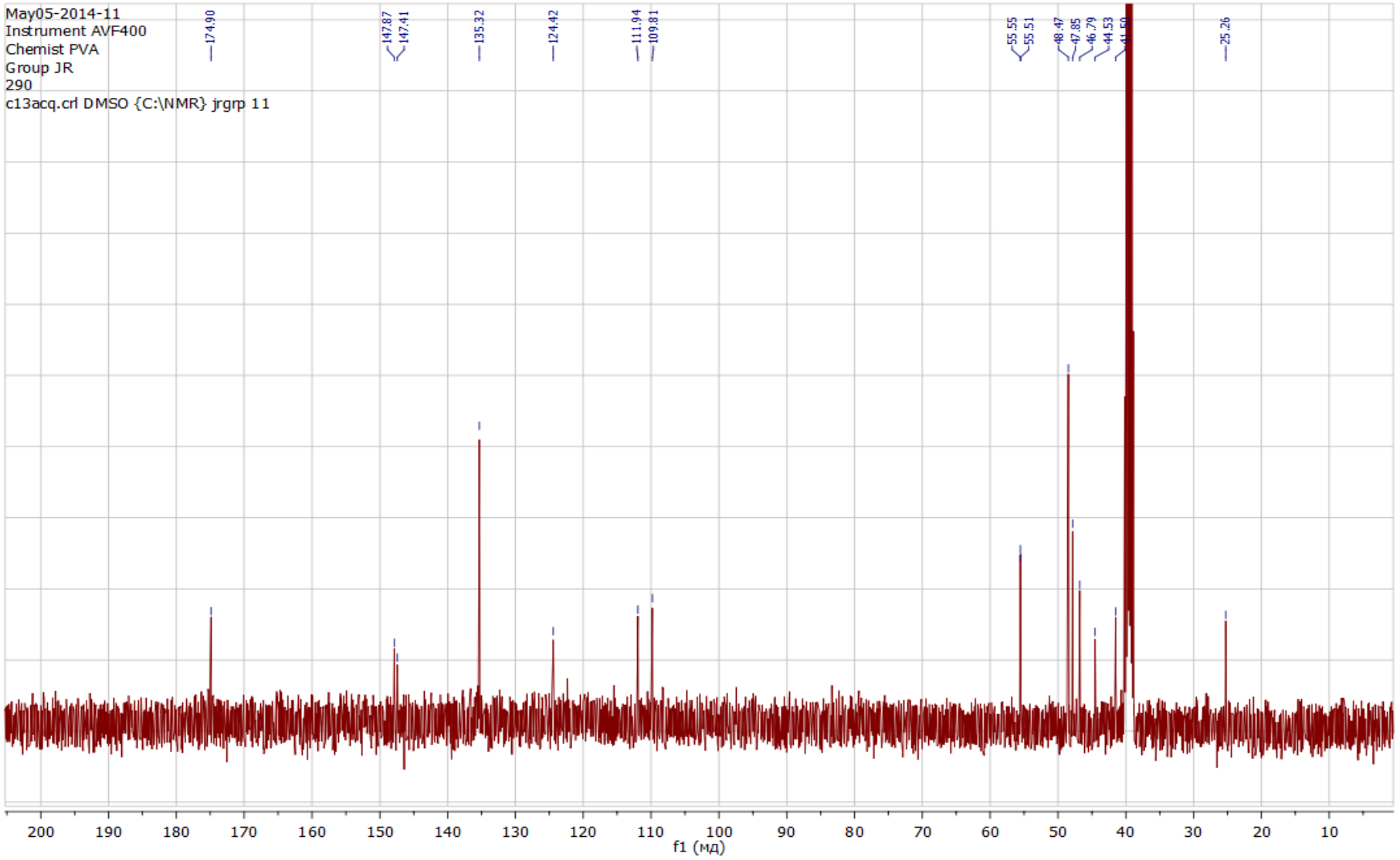
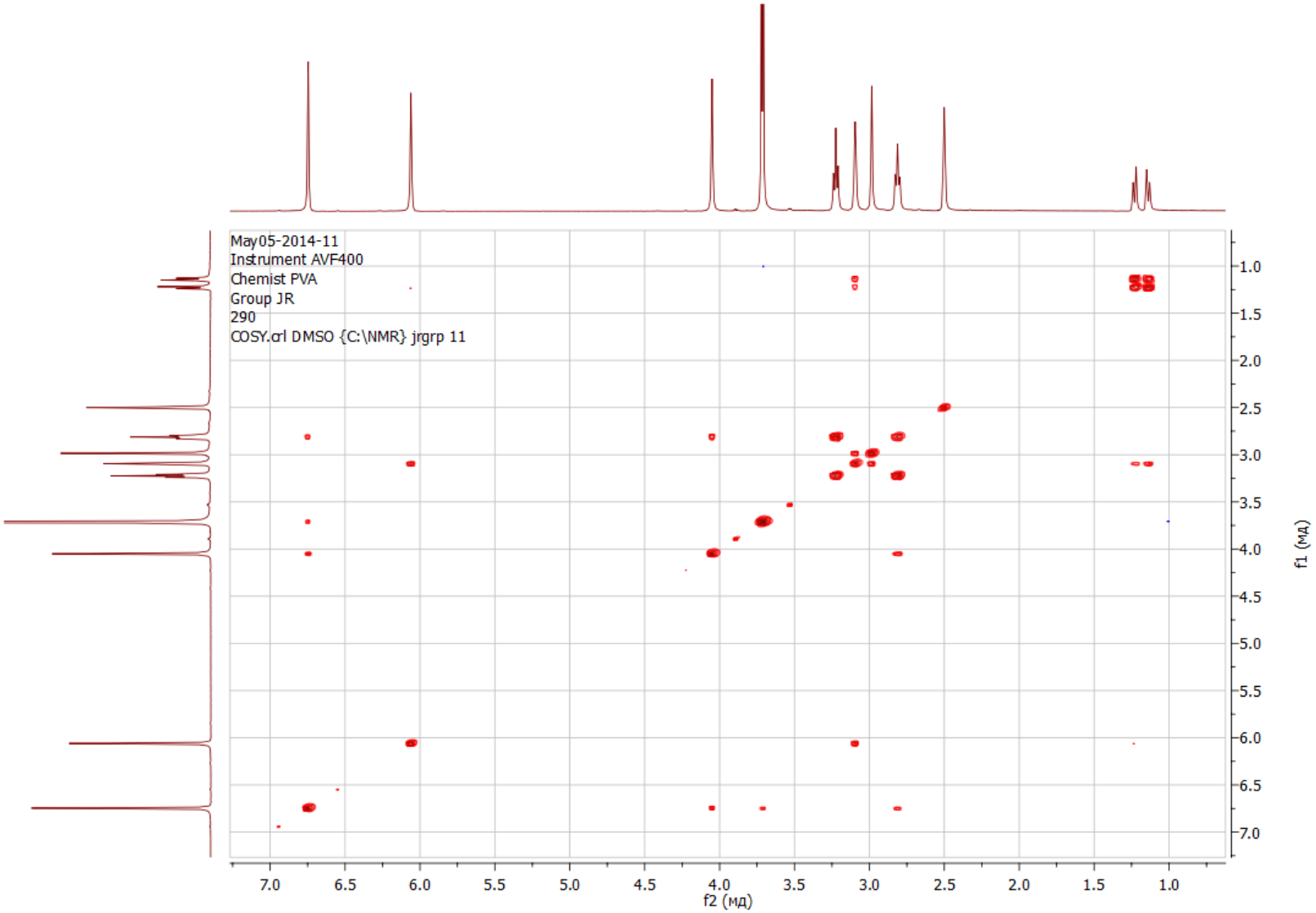
2.00
2.00
1.01
1.02
f1 (мд)

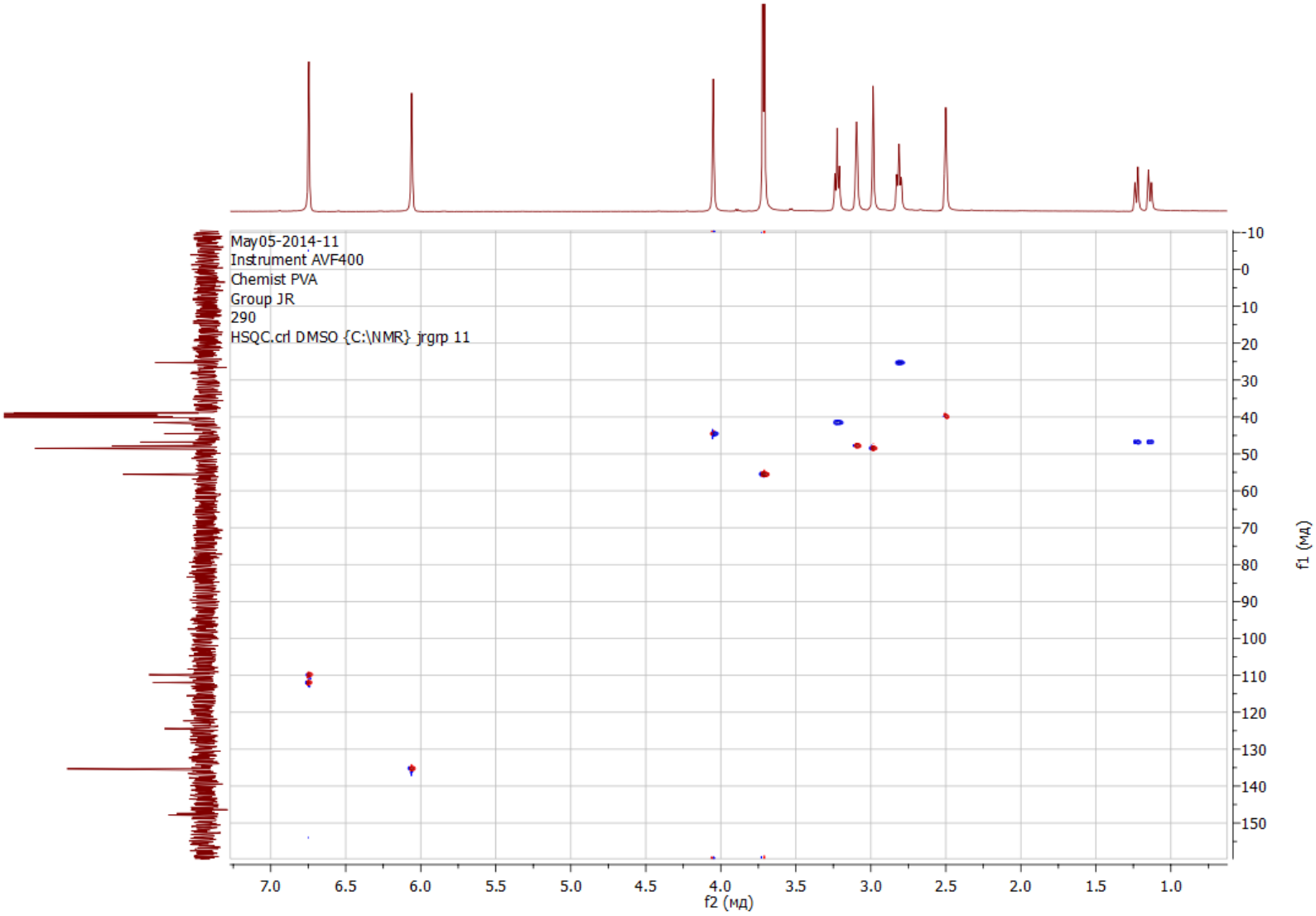
^{1}H NMR spectrum of obtained compound (DMSO-d_6, 400 MHz)



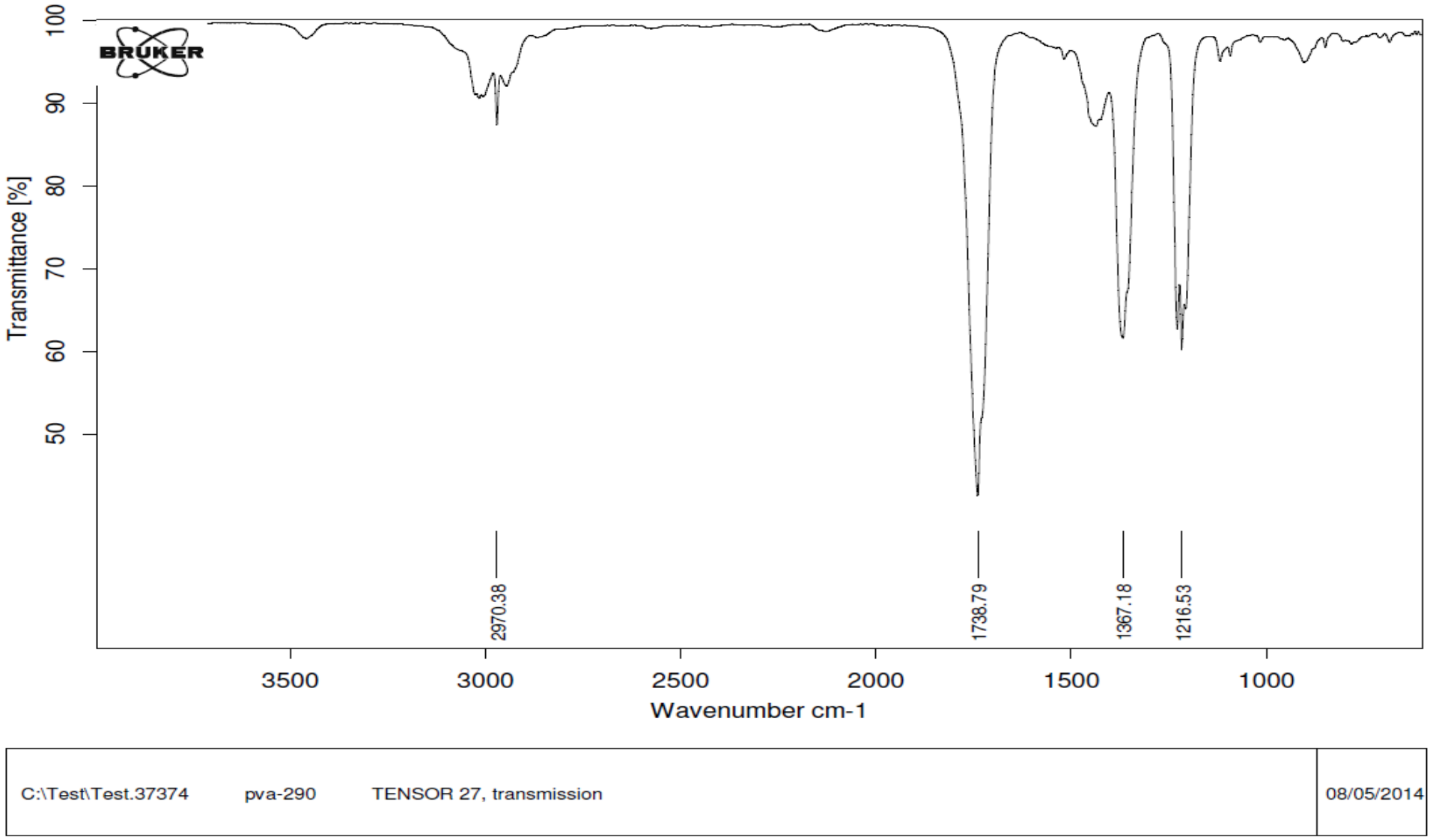
^{13}C NMR spectrum of obtained compound (DMSO-d_6, 100 MHz)



^{1}H-^{1}H COSY spectrum of obtained compound (DMSO-d_6, 400 MHz)



^{1}H-^{13}C HMQC spectrum of obtained compound (DMSO-d_6, 400/100 MHz)



IR spectrum of obtained compound

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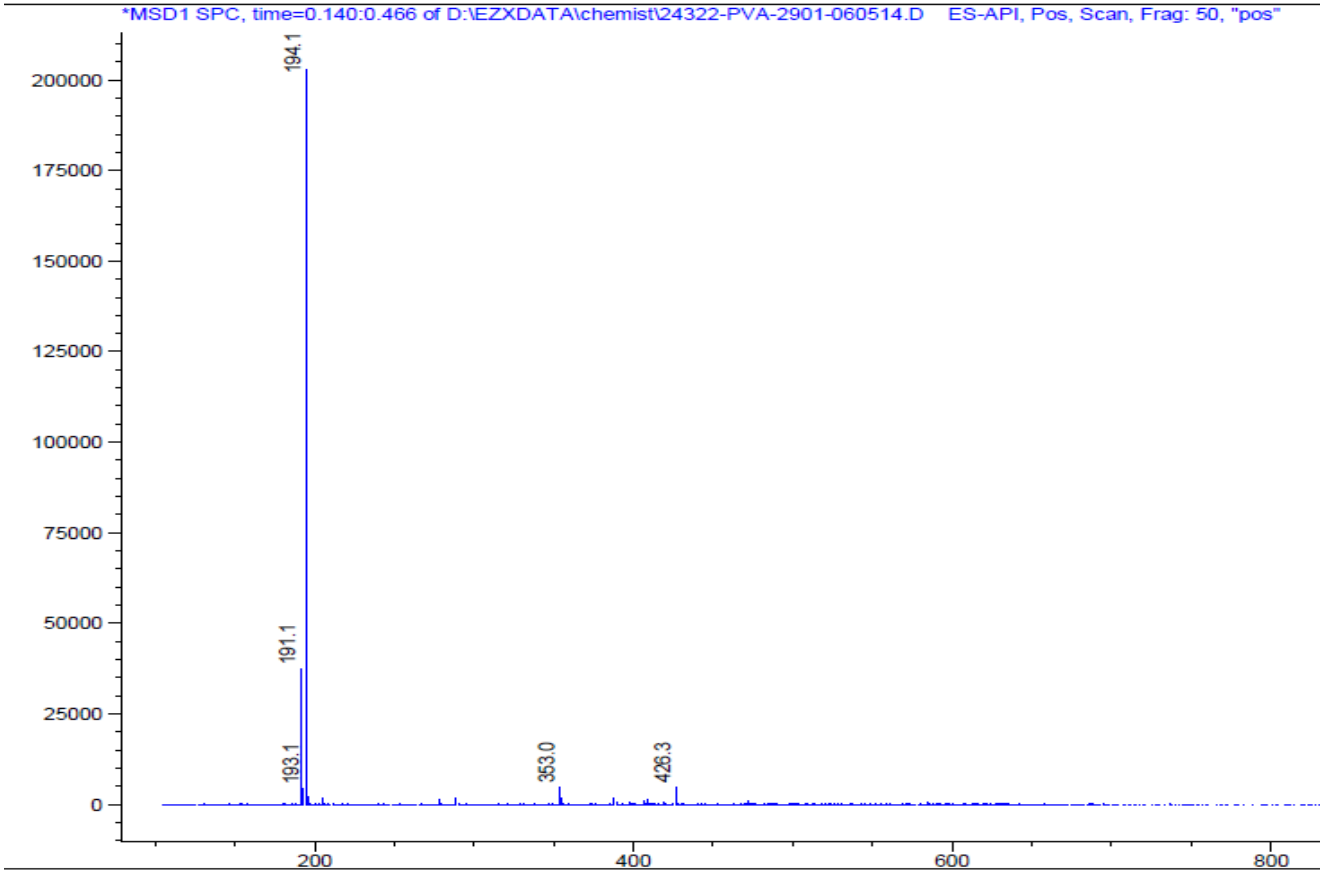
User Name: Yuliia Velichenko
Sample Name: PVA-290
Location: P1-A-03
Sample Info: Easy-Access Method: '1_POS1000' ->
Method Info: Positive open access method
105-1000



MS (ES-API) spectrum of obtained compound (positive mode)

Table S1. Full pairwise interaction energies (kcal/mol) of each of the molecules with neighboring ones in the salt-co-crystal**.**

Dimer	Molecules	Symmetry operation	E_{int}, kJ/mol	Contribution to the total interaction energy, %
dim 1	**A-D**	x,y,z	-16.7	4.8
dim 2	**A-B**	x,y,z	-25.1	7.1
dim 3	**A-B**	x,y,-1+z	-92.0	26.2
dim 4	**A-D**	1+x,y,z	-12.6	3.6
dim 5	**A-C**	1+x,y,z	-25.1	7.1
dim 6	**A-C**	1+x,y,-1+z	-12.6	3.6
dim 7	**A-C**	1-x,1-y,1-z	-20.9	5.9
dim 8	**A-A**	2-x,1-y,-z	-4.2	1.2
dim 9	**A-A**	2-x,1-y,1-z	0	0
dim 10	**A-B**	2-x,1-y,1-z	-108.8	31.0
dim 11	**A-A**	x,3/2-y,1/2+z	-8.4	2.4
dim 12	**A-D**	x,3/2-y,1/2+z	0	0
dim 13	**A-A**	x,3/2-y,-1/2+z	-8.4	2.4
dim 14	**A-B**	x,3/2-y,-1/2+z	-8.4	2.4
dim 15	**A-C**	1+x,3/2-y,-1/2+z	-4.2	1.2
dim 16	**A-D**	1+x,3/2-y,-1/2+z	0	0
Total interaction energy of molecule **A** -351.5 kJ/mol				
dim 17	**B-A**	x,y,z	-20.9	3.2

dim 18	**B-D**	x,y,z	-100.4	15.2
dim 19	**B-C**	x,y,z	-12.6	1.9
dim 20	**B-A**	x,y,1+z	-92.0	13.9
dim 21	**B-D**	x,y,1+z	-29.3	4.4
dim 22	**B-C**	1+x,y,z	-4.2	0.6
dim 23	**B-C**	1-x,1-y,1-z	-75.3	11.4
dim 24	**B-D**	1-x,1-y,1-z	-96.2	14.6
dim 25	**B-C**	1-x,1-y,2-z	-75.3	11.4
dim 26	**B-A**	2-x,1-y,1-z	-108.8	16.5
dim 27	**B-A**	x,3/2-y,1/2+z	-8.4	1.3
dim 28	**B-D**	x,3/2-y,1/2+z	-8.4	1.3
		Total interaction energy of molecule **B** -661.1 kJ/mol		
dim 29	**C-B**	x,y,z	-12.6	4.1
dim 30	**C-D**	x,y,z	-8.4	2.7
dim 31	**C-D**	x,y,1+z	-25.1	8.1
dim 32	**C-B**	-1+x,y,z	-4.2	1.4
dim 33	**C-A**	-1+x,y,z	-25.1	8.1
dim 34	**C-A**	-1+x,y,1+z	-12.6	4.1
dim 35	**C-A**	1-x,1-y,1-z	-20.9	6.8
dim 36	**C-D**	1-x,1-y,1-z	-12.6	4.1
dim 37	**C-B**	1-x,1-y,1-z	-75.3	24.3
dim 38	**C-B**	1-x,1-y,2-z	-75.3	24.3

dim 39	**C-D**	x,3/2-y,1/2+z	-4.2	1.4
dim 40	**C-A**	-1+x,3/2-y,1/2+z	-4.2	1.4
		Total interaction energy of molecule **C** -309.6 kJ/mol		
dim 41	**D-B**	x,y,z	-100.4	27.9
dim 42	**D-C**	x,y,z	-8.4	2.3
dim 43	**D-A**	x,y,z	-16.7	4.6
dim 44	**D-C**	x,y,-1+z	-25.1	7.0
dim 45	**D-B**	x,y,-1+z	-29.3	8.1
dim 46	**D-A**	-1+x,y,z	-12.6	3.5
dim 47	**D-D**	1-x,1-y,-z	0	0
dim 48	**D-B**	1-x,1-y,1-z	-96.2	26.7
dim 49	**D-C**	1-x,1-y,1-z	-12.6	3.5
dim 50	**D-D**	x,3/2-y,1/2+z	-8.4	2.3
dim 51	**D-C**	x,3/2-y,-1/2+z	-4.2	1.2
dim 52	**D-D**	x,3/2-y,-1/2+z	-8.4	2.3
dim 53	**D-A**	x,3/2-y,-1/2+z	0	0
dim 54	**D-B**	x,3/2-y,-1/2+z	-8.4	2.3
dim 55	**D-A**	-1+x,3/2-y,1/2+z	0	0
		Total interaction energy of molecule **D** -359.8 kJ/mol		