Electronic supplementary material

Bis(amido) Rare-earth Complexes Coordinated by Tridentate Amidinate Ligand: Synthesis, Structure and Catalytic Activity in Polymerization of Isoprene and rac-Lactide

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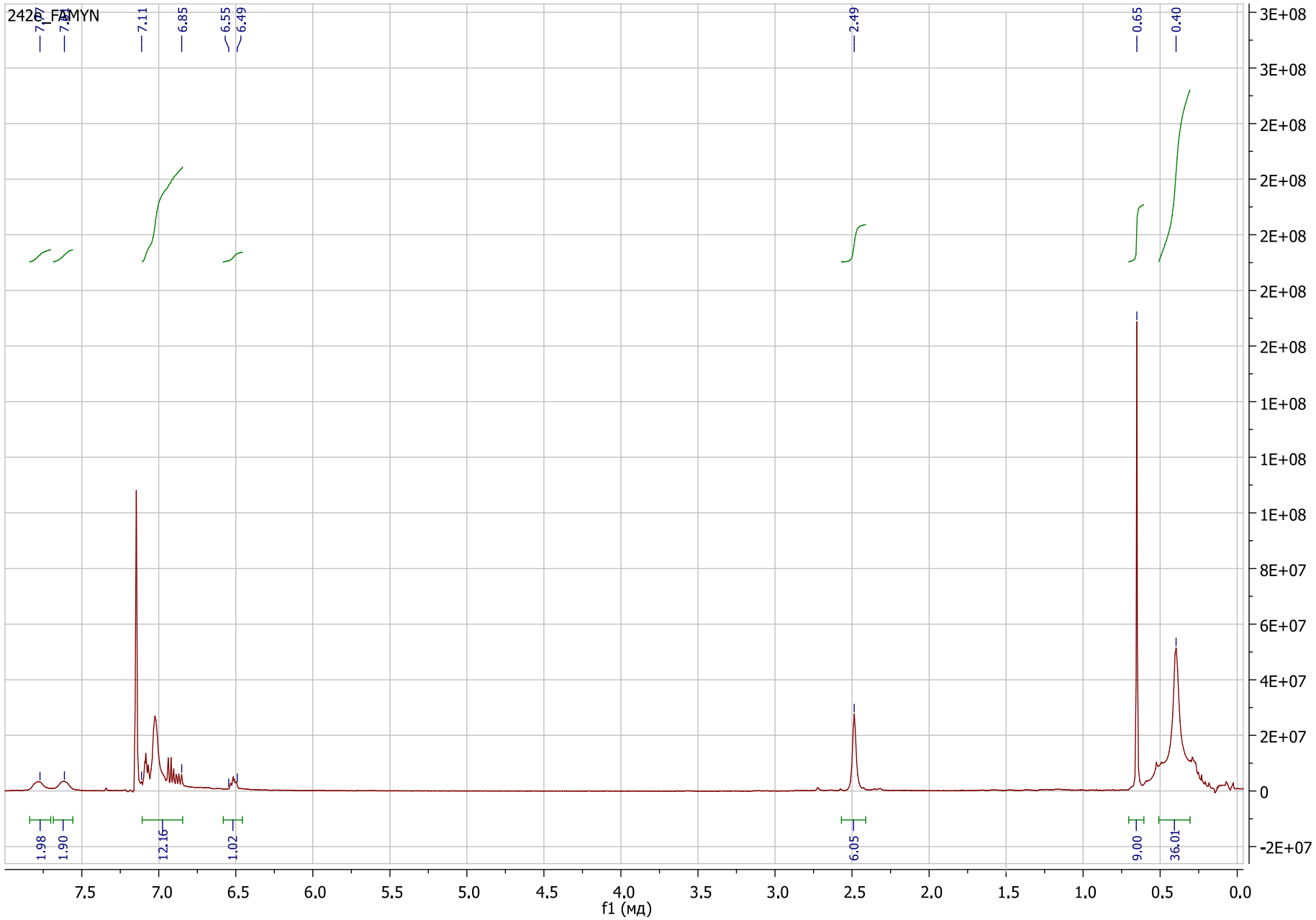
Table 1S. Crystallographic data and structure refinement details for **2**–**4**.

Compound	**2**	**3**	**4**
Empiricalformula	$C_{43}H_{68}N_4OPSi_4Y$	$C_{43}H_{68}N_4OPSi_4Nd$	$C_{43}H_{68}N_4OPSi_4La$
Formulaweight	889.25	944.58	939.25
T [K]	100(2)		
Wavelength [Å]	0.71073		
Crystalsystem	Monoclinic		
Spacegroup	C2/c		
a [Å]	21.2784(9)	21.4494(2)	21.5190(6)
b [Å]	12.6709(5)	12.75910(10)	12.7854(3)
c [Å]	36.8622(15)	37.4670(4)	36.8722(10)
α [°]	90	90	90
β [°]	105.1430(10)	108.1100(10)	105.513(3)
γ [°]	90	90	90
Volume [$Å^3$]	9593.6(7)	9745.82(17)	9775.1(5)
Z	8	8	8
$\rho_{calcd.}$ [g cm^{-3}]	1.231	1.288	1.276
Absorptioncoefficient [mm^{-1}]	1.384	1.231	1.039
F(000)	3776	3944	3920
Crystalsize [mm]	0.42×0.25×0.18	0.45×0.30×0.15	0.42×0.25×0.18
θ range for data collection [°]	1.90 to 29.00	3.16 to 29.00	3.16 to 29.00
Indexranges	-28≤h≤28, -17≤k≤16, -49≤l≤49	-29≤h≤29, -17≤k≤17, -51≤l≤51	-29≤h≤28, -17≤k≤17, -50≤l≤46
Reflectionscollected	50161	93016	28859
Independentreflections	12692	12919	12946
Rint	0.0415	0.0420	0.0577
Completenessto θ [%]	99.8	99.8	99.7
Data/restraints/parameters	12692 / 0 / 504	12919 / 0 / 504	12946 / 0 / 504
Goodness-of-fit on F^2	1.043	1.123	1.024
Final R indices [I>2σ(I)]	R_1 = 0.0394, wR_2 = 0.0857	R_1 = 0.0287, wR_2 = 0.0592	R_1 = 0.0531, wR_2 = 0.0746
R indices (alldata)	R_1 = 0.0604, wR_2 = 0.0911	R_1 = 0.0335, wR_2 = 0.0606	R_1 = 0.0849, wR_2 = 0.0811
Largest diff. peak and hole [e$Å^{-3}$]	0.555 / -0.393	0.686 / -1.111	0.780 / -1.127



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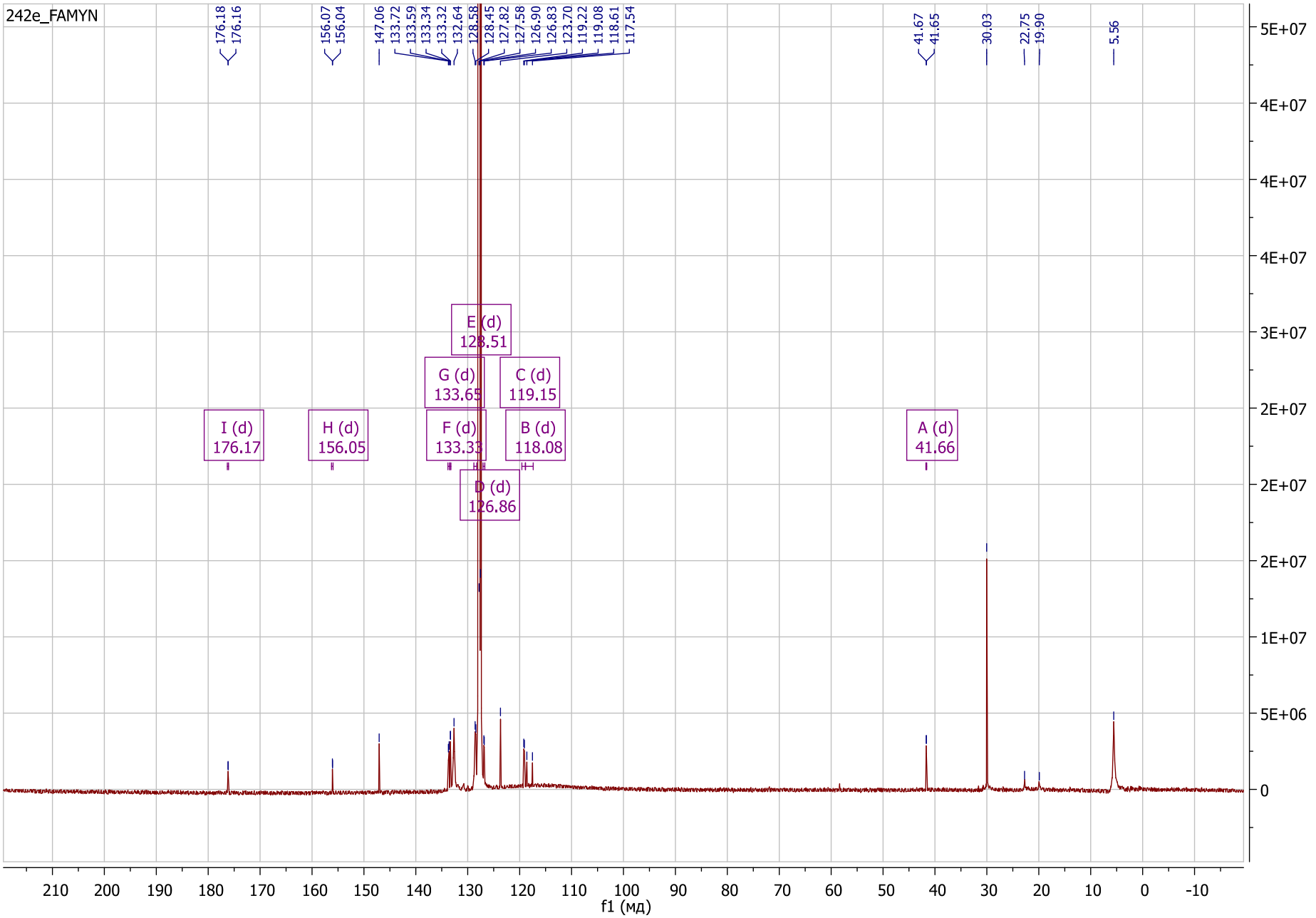

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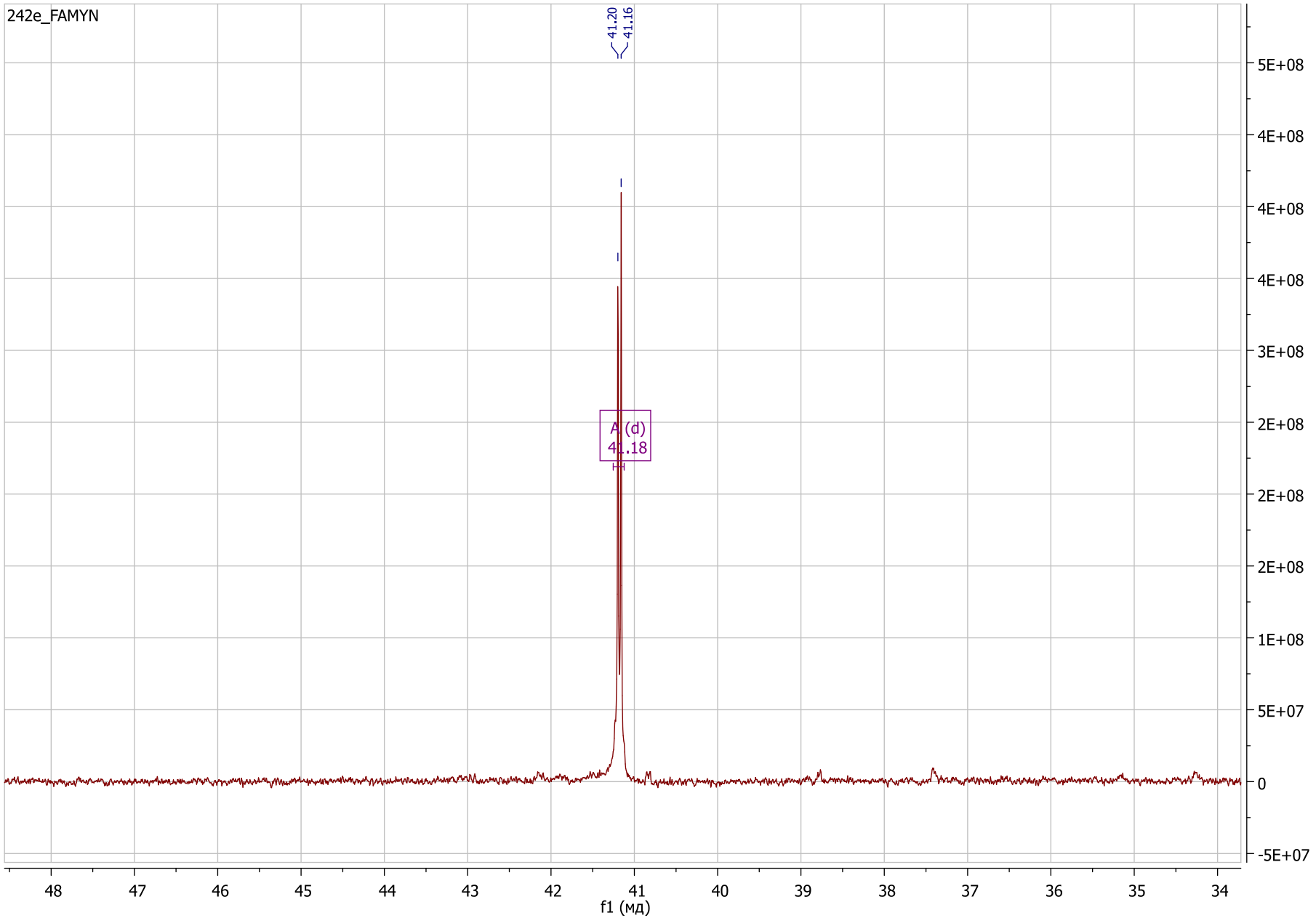

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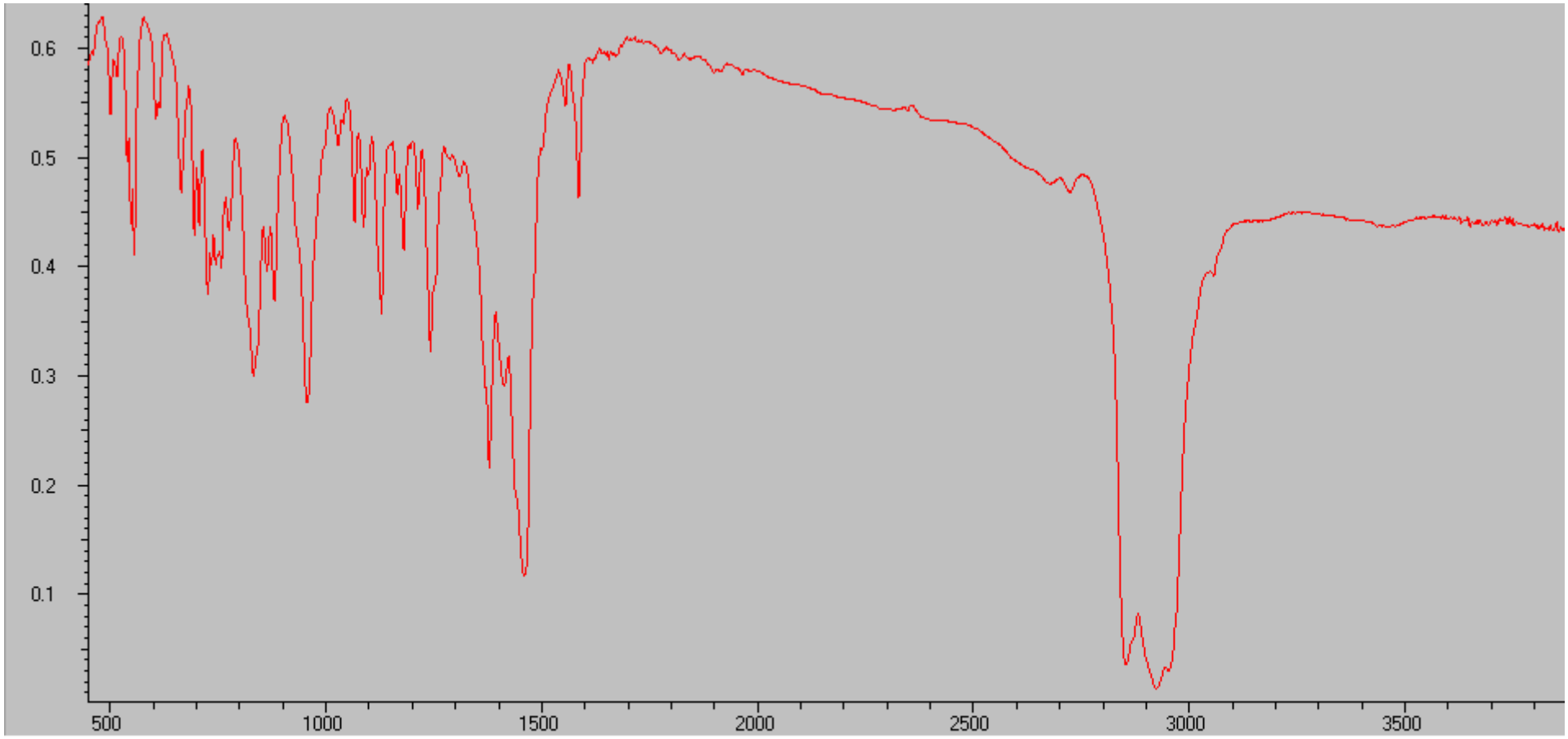

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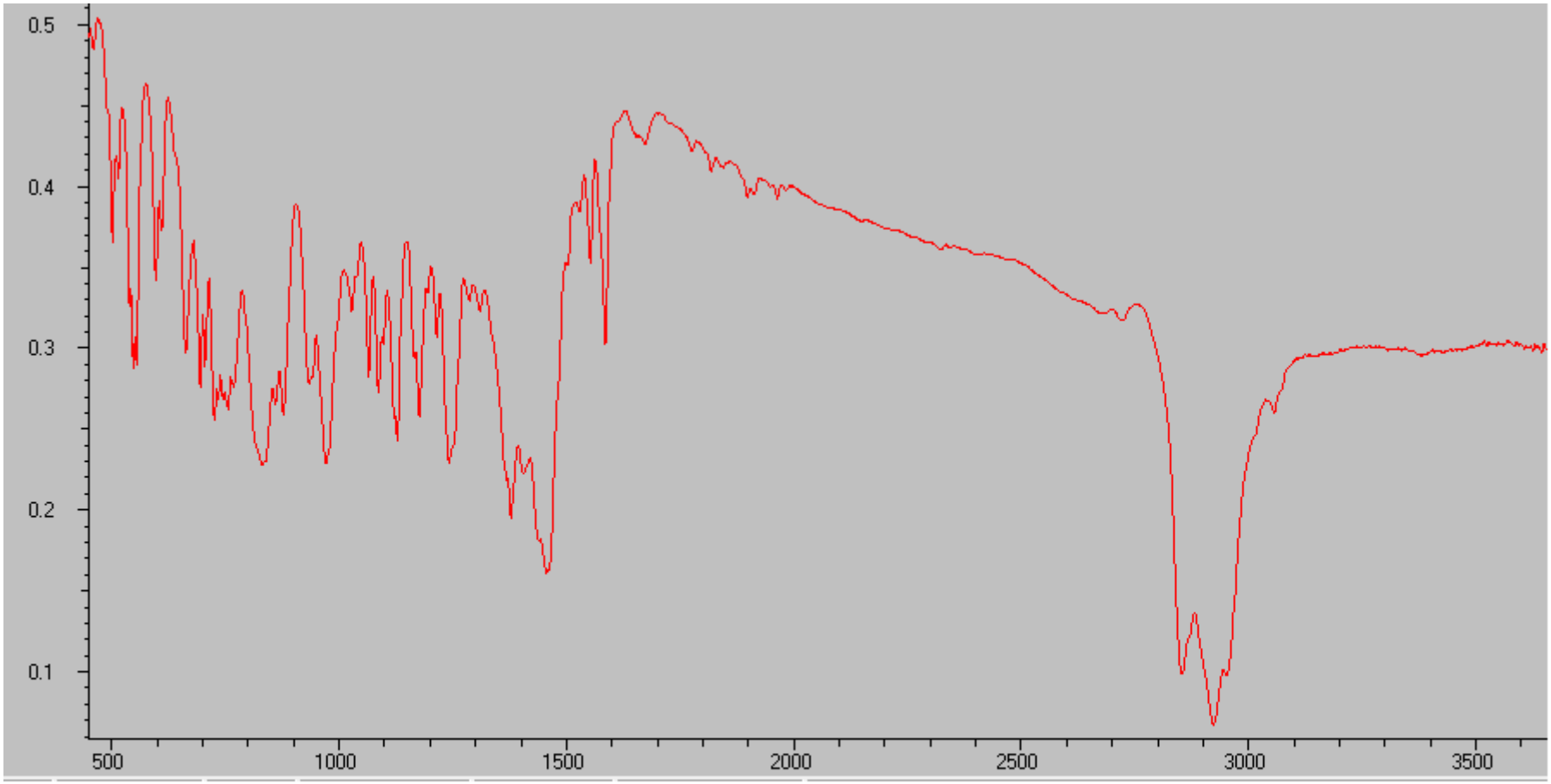

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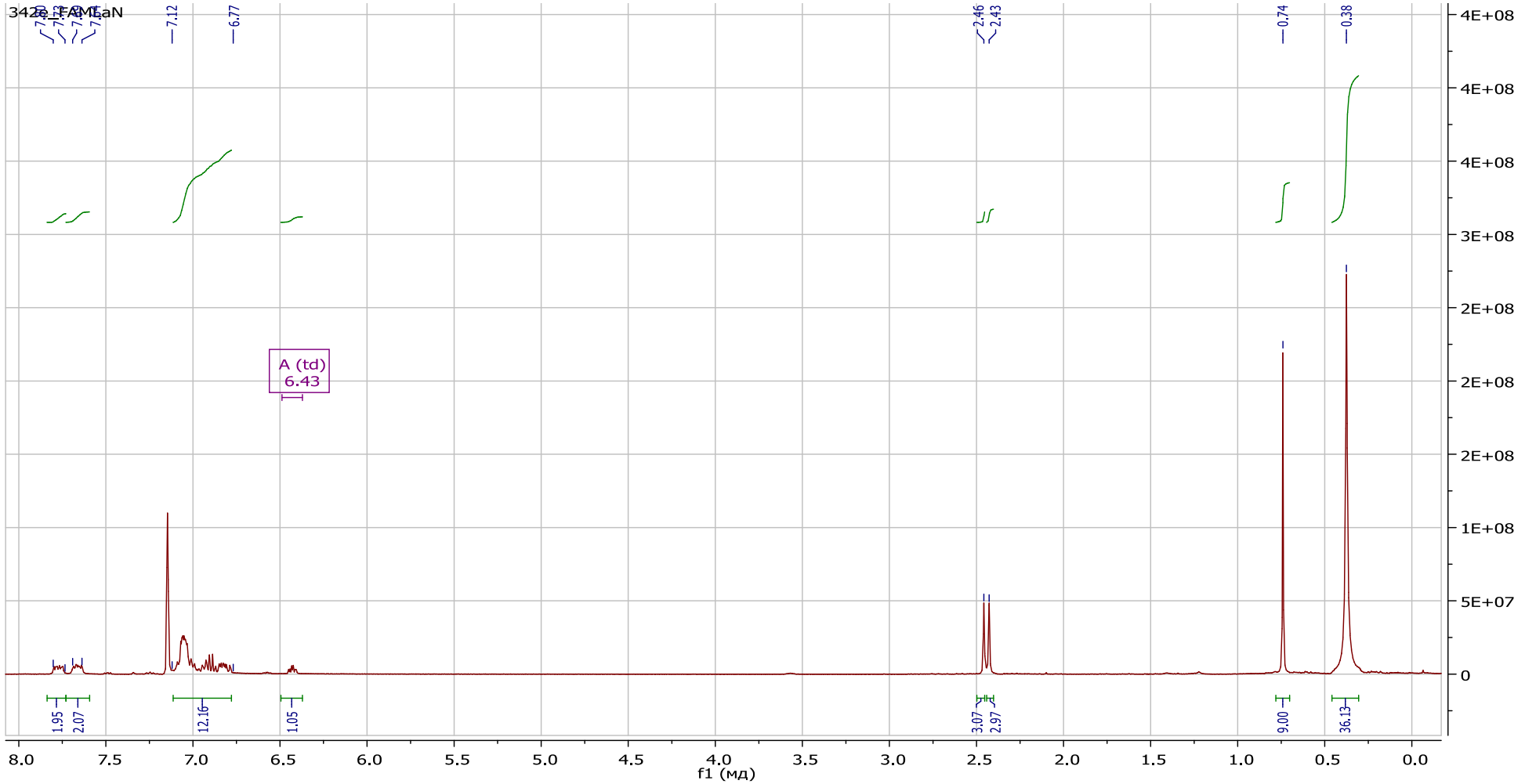

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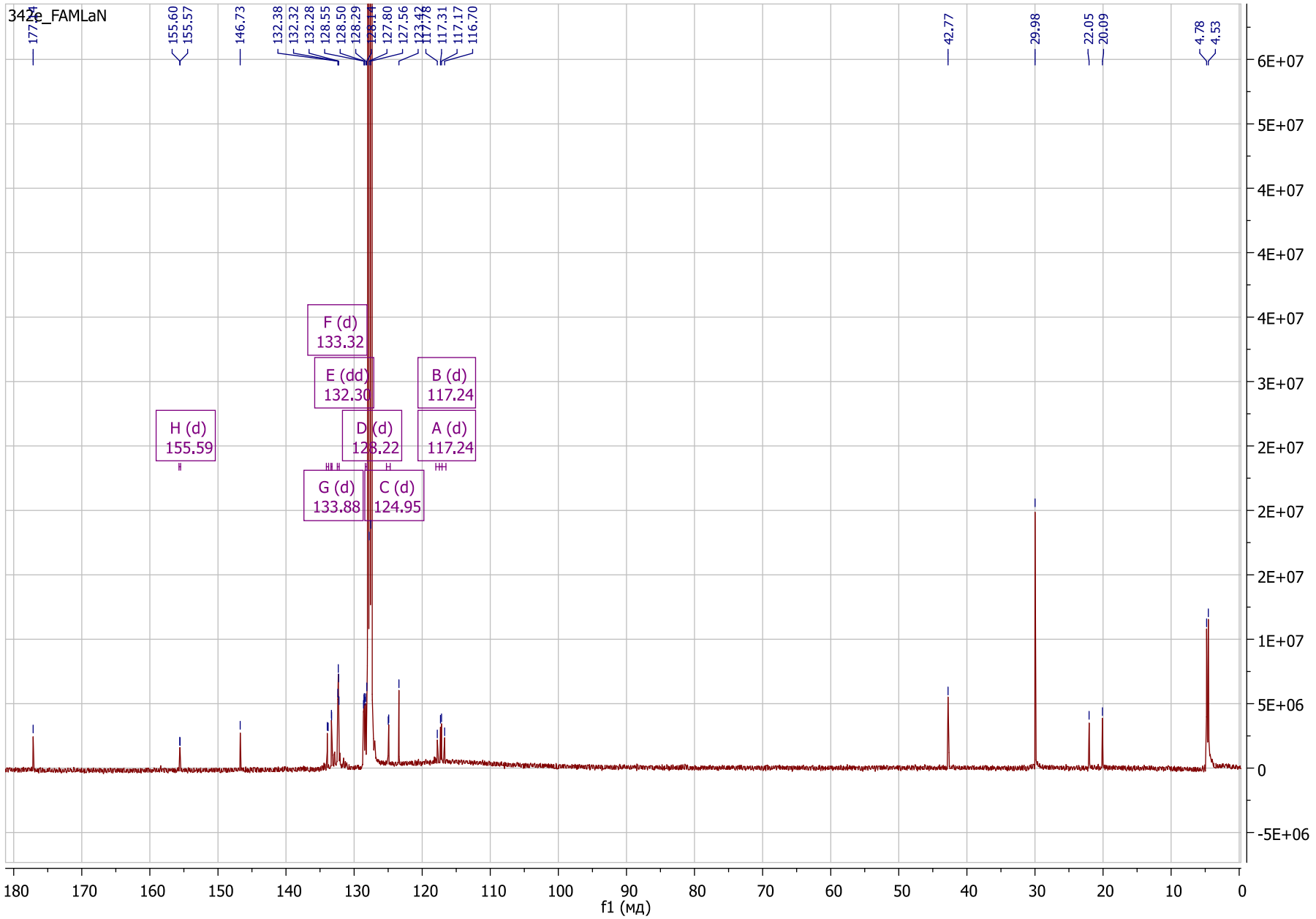

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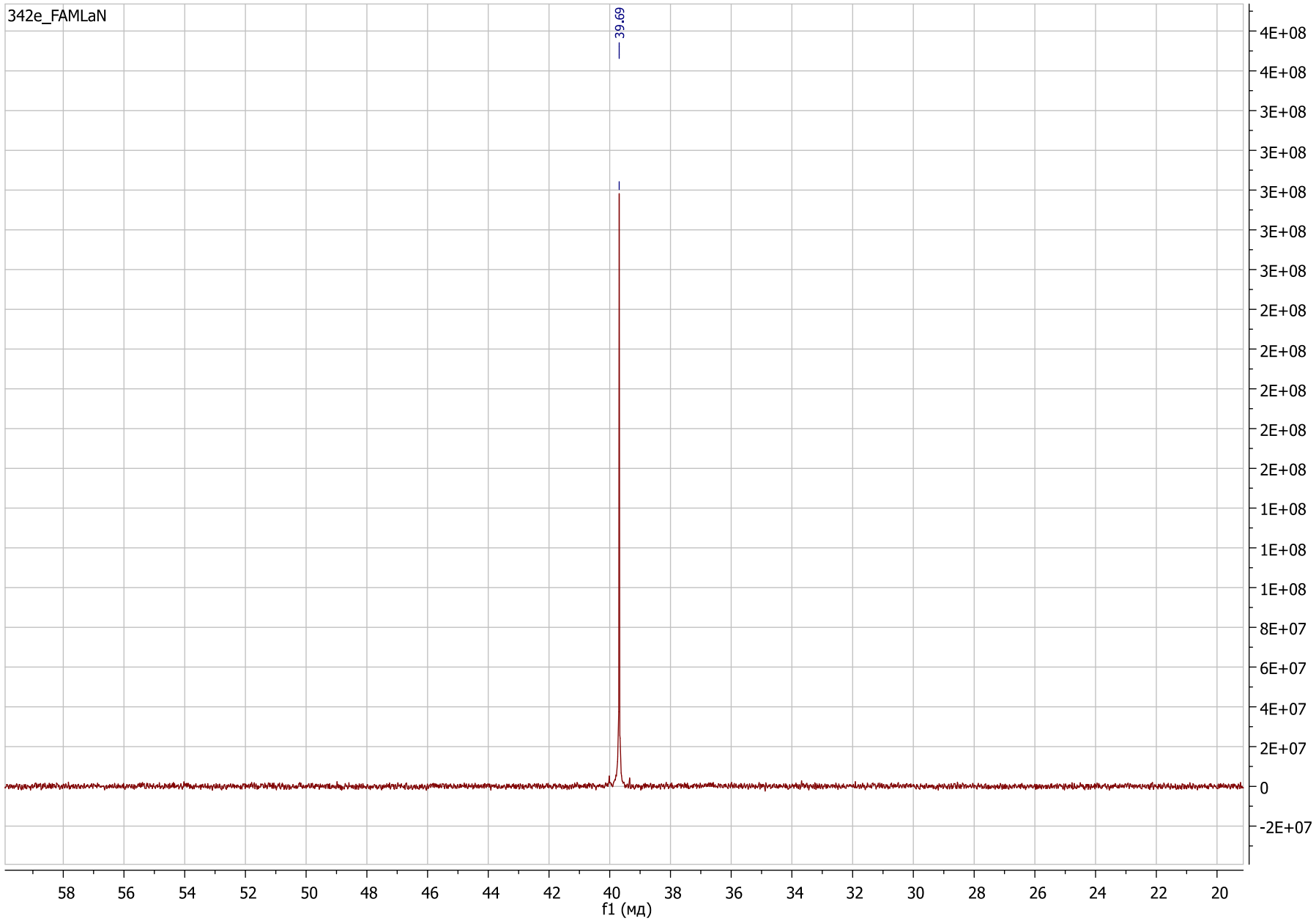

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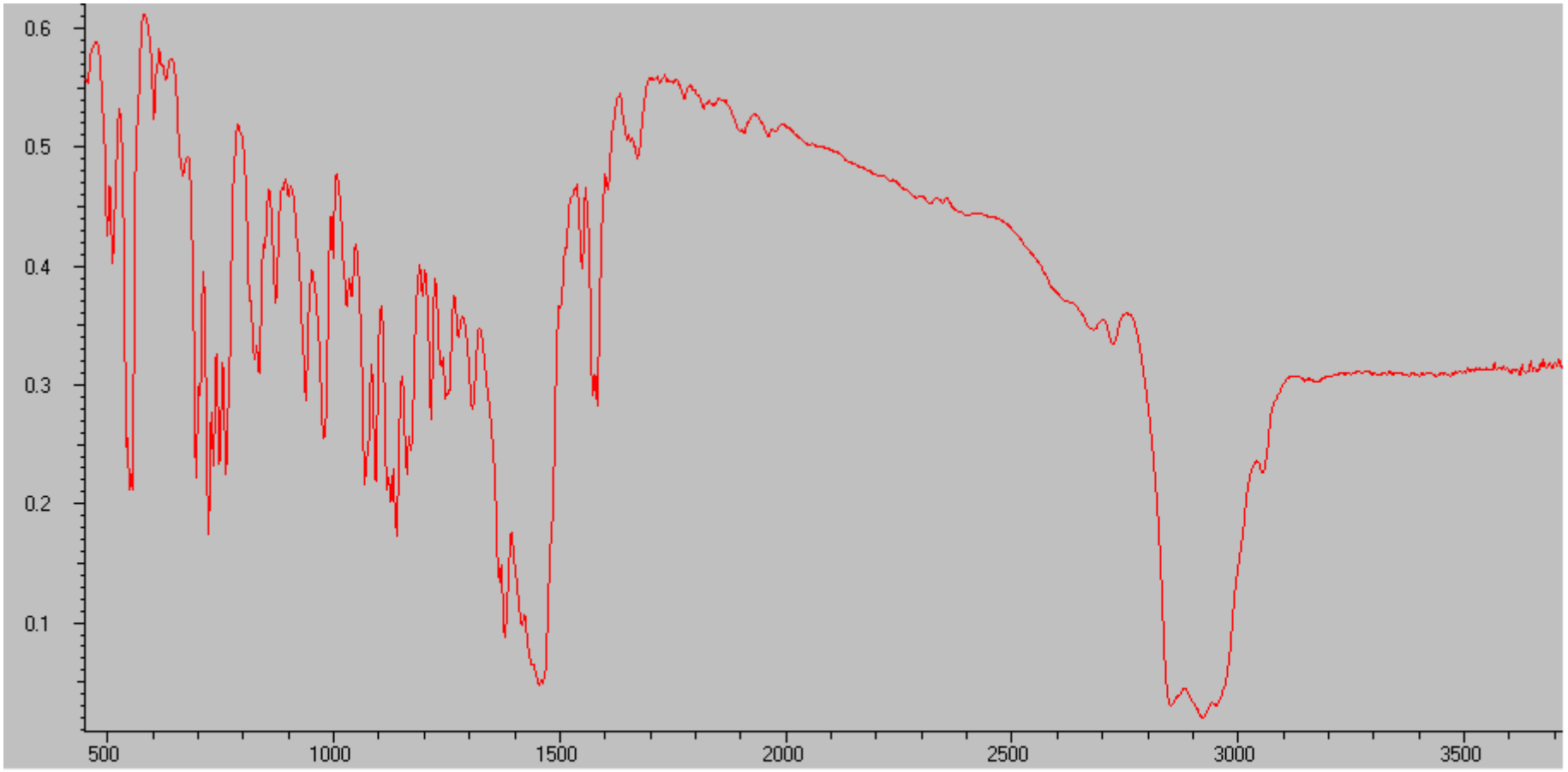

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