Supplementary data

Allo-gibberic acid-based aminodiols, aminotetraols, and 1,2,3-triazoles: stereoselective synthesis and antiproliferative activity

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Table S2, Docking models for selected compounds S243 – S254

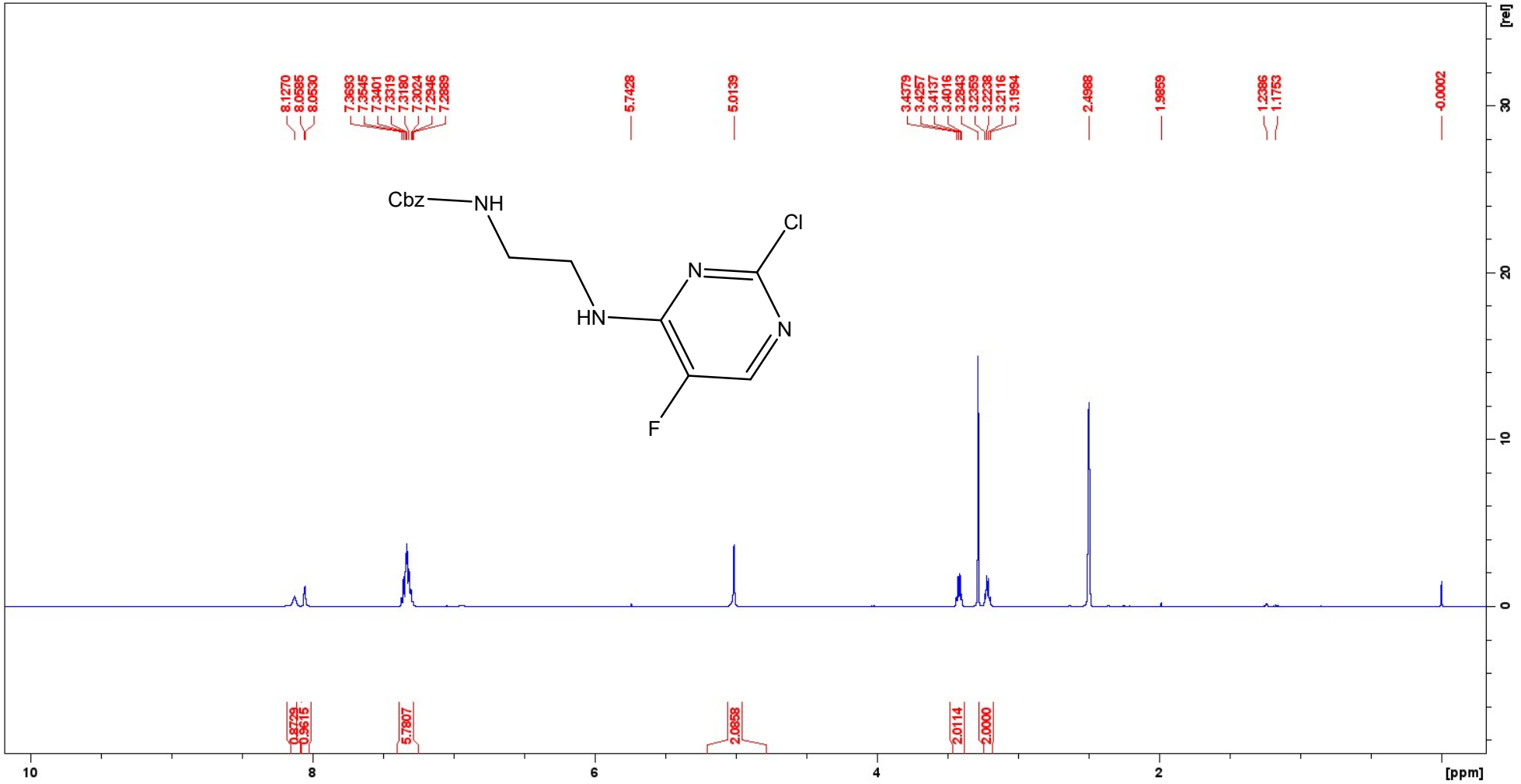
Table S1: Antiproliferative effects of the investigated compounds

	Cc	Growth inhibition (%) ± SEM					
	μM	HeLa	SiHa	MCF-7	MDA-MB-231	A2780	NIH/3T3
9	10	31.37 ± 1.46	34.99 ± 1.41	36.21 ± 2.68	< 20	23.42 ± 1.32	21.76 ± 2.03
	30	47.65 ± 2.83	39.79 ± 1.89	85.89 ± 0.93	65.20 ± 1.96	52.37 ± 2.58	37.58 ± 2.32
10	10	35.83 ± 0.72	28.22 ± 1.26	47.43 ± 1.52	27.04 ± 2.80	23.21 ± 1.49	< 20
	30	99.13 ± 0.29	95.63 ± 1.42	96.27 ± 0.21	98.07 ± 0.36	98.88 ± 0.14	93.81 ± 1.96
11	10	35.47 ± 0.94	30.18 ± 1.24	39.15 ± 1.69	< 20	23.64 ± 1.20	< 20
	30	98.05 ± 0.72	94.59 ± 2.63	96.32 ± 0.23	97.62 ± 0.41	97.45 ± 0.36	97.65 ± 0.79
12	10	35.37 ± 1.85	< 20	< 20	< 20	< 20	< 20
	30	98.91 ± 0.39	96.35 ± 0.49	97.39 ± 0.46	99.01 ± 0.42	98.22 ± 0.16	96.35 ± 0.61
13	10	53.92 ± 2.18	34.47 ± 0.89	69.71 ± 3.91	55.19 ± 2.82	51.31 ± 0.81	33.03 ± 0.91
	30	98.26 ± 0.57	94.95 ± 0.63	95.97 ± 1.05	99.13 ± 0.92	98.01 ± 0.10	98.28 ± 0.50
14	10	52.31 ± 2.49	20.34 ± 2.80	28.36 ± 3.38	< 20	38.66 ± 1.77	< 20
	30	97.35 ± 0.73	93.30 ± 1.06	94.80 ± 1.24	97.45 ± 1.01	97.12 ± 0.34	97.31 ± 0.51
15	10	61.72 ± 2.04	36.59 ± 2.46	53.47 ± 2.44	< 20	59.02 ± 1.66	27.62 ± 1.45
	30	99.93 ± 0.05	100.40 ± 0.23	99.35 ± 0.23	99.94 ± 0.13	99.84 ± 0.15	99.65 ± 0.23
16	10	43.31 ± 3.63	< 20	20.39 ± 3.51	< 20	43.37 ± 3.01	< 20
	30	97.83 ± 0.67	94.60 ± 0.70	95.18 ± 1.14	98.17 ± 0.89	97.45 ± 0.16.	97.93 ± 0.59
17	10	25.10 ± 0.88	< 20	< 20	< 20	< 20	< 20
	30	29.48 ± 1.98	< 20	31.53 ± 2.04	< 20	< 20	27.23 ± 2.37
18	10	99.27 ± 0.13	99.82 ± 0.22	99.31 ± 0.19	99.12 ± 0.35	98.78 ± 0.33	99.30 ± 0.26
	30	99.44 ± 0.13	100.30 ± 0.25	99.46 ± 0.17	99.50 ± 0.24	99.27 ± 0.23	99.44 ± 0.23
	IC_{50}	3.08 ± 0.07	3.44 ± 0.15	2.12 ± 0.85	1.98 ± 0.35	1.61 ± 0.11	4.36 ± 0.21
19	10	24.80 ± 2.19	29.60 ± 1.73	35.57 ± 2.73	< 20	< 20	< 20
	30	95.47 ± 2.45	81.10 ± 3.07	93.65 ± 0.73	98.44 ± 0.37	98.36 ± 0.28	40.00 ± 1.49
20	10	27.38 ± 1.71	34.64 ± 1.01	36.42 ± 1.20	< 20	22.12 ± 0.47	< 20
	30	99.12 ± 0.35	97.18 ± 1.29	96.51 ± 0.27	98.60 ± 0.42	98.99 ± 0.14	98.34 ± 0.47
21	10	27.37 ± 1.56	26.68 ± 1.12	38.09 ± 1.97	< 20	< 20	< 20
	30	98.93 ± 0.40	95.17 ± 1.74	96.76 ± 0.22	96.62 ± 1.66	98.89 ± 0.18	42.75 ± 3.68
22	10	46.39 ± 1.05	36.07 ± 3.79	91.70 ± 1.95	96.79 ± 1.04	53.99 ± 2.62	91.91 ± 2.72
	30	97.59 ± 0.63	92.94 ± 1.37	94.97 ± 1.41	99.29 ± 1.15	98.24 ± 0.07	97.43 ± 0.41
23	10	99.69 ± 0.06	99.79 ± 0.23	99.29 ± 0.09	99.60 ± 0.09	97.50 ± 0.16	99.25 ± 0.21
	30	100.60 ±0.56	100.30 ± 0.13	100.10 ± 0.07	100.10 ± 0.14	99.12 ± 0.28	99.82 ± 0.23
	IC_{50}	3.31 ± 0.24	3.52 ± 0.01	3.32 ± 0.95	5.05 ± 0.46	6.26 ± 0.18	4.54 ± 0.18
24	10	97.27 ± 0.68	76.61 ± 1.83	94.57 ± 1.54	98.36 ± 1.19	96.97 ± 0.29	97.23 ± 0.59
	30	96.97 ± 0.69	92.18 ± 1.46	94.67 ± 1.38	98.19 ± 1.08	97.50 ± 0.16	96.98 ± 0.54
	IC_{50}	3.95 ± 0.06	3.86 ± 0.03	3.94 ± 0.25	5.57 ± 0.72	6.48 ± 0.04	4.92 ± 0.15
25	10	99.94 ± 0.09	101.10 ± 0.38	99.50 ± 0.32	100.10 ± 0.12	100.10 ± 0.18	99.65 ± 0.18
	30	99.72 ± 0.11	100.20 ± 0.11	99.86 ± 0.13	99.72 ± 0.14	99.66 ± 0.20	99.56 ± 0.31
	IC_{50}	3.44 ± 0.34	2.99 ± 0.15	3.46 ± 0.59	4.45 ± 0.19	5.11 ± 0.98	4.31 ± 0.18
26	10	85.34 ± 2.45	91.94 ± 1.01	98.84 ± 0.35	99.26 ± 0.21	87.97 ± 2.79	92.79 ± 1.19
	30	99.52 ± 0.16	100.20 ± 0.16	99.91 ± 0.22	99.71 ± 0.30	99.42 ± 0.14	99.54 ± 0.19
	IC_{50}	3.82 ± 0.30	4.64 ± 0.17	3.92 ± 0.22	5.04 ± 0.03	5.99 ± 0.76	5.14 ± 0.21
27	10	< 20	< 20	< 20	< 20	< 20	< 20
	30	28.15 ± 2.89	< 20	< 20	< 20	< 20	< 20
28	10	99.42 ± 0.15	100.10 ± 0.21	98.91 ± 0.24	99.11 ± 0.33	99.71 ± 0.23	99.16 ± 0.41
	30	99.01 ± 0.14	99.71 ± 0.24	99.48 ± 0.26	99.04 ± 0.28	98.98 ± 0.29	99.03 ± 0.44
	IC_{50}	2.68 ± 0.76	3.09 ± 0.19	1.49 ± 0.02	3.48 ± 0.47	3.31 ± 0.40	4.16 ± 0.07
30	10	< 20	< 20	< 20	< 20	< 20	< 20

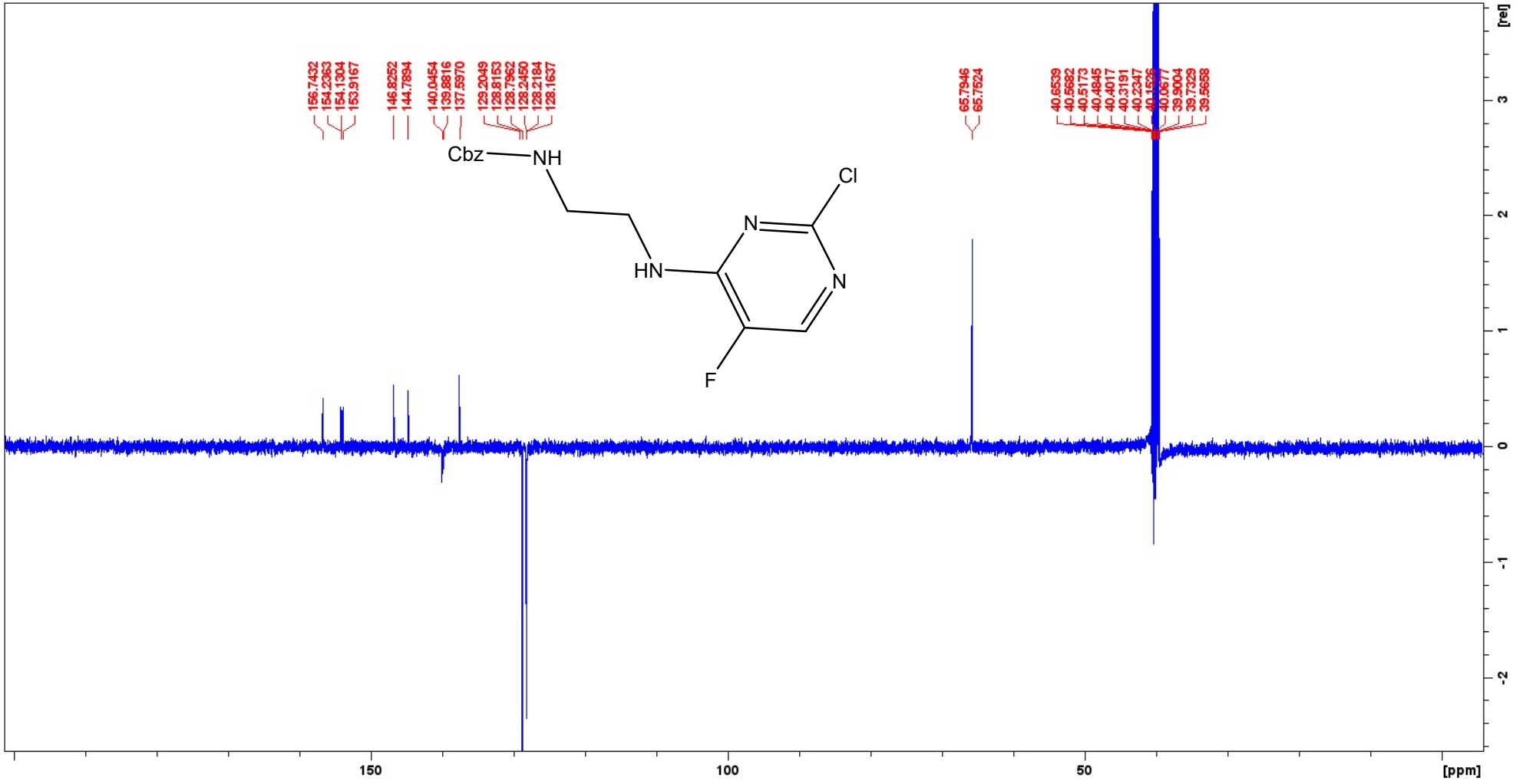
	30	< 20	26.19 ± 2.93	< 20	< 20	< 20	< 20
31	10	< 20	< 20	< 20	< 20	< 20	< 20
	30	< 20	< 20	24.61 ± 1.84	< 20	< 20	< 20
32	10	95.32 ± 0.92	97.59 ± 0.36	93.53 ± 0.38	98.09 ± 0.19	99.03 ± 0.21	97.11 ± 0.23
	30	98.55 ± 0.46	96.45 ± 0.22	96.87 ± 0.44	98.12 ± 0.59	99.65 ± 0.32	97.44 ± 0.28
	IC_{50}	4.10 ± 0.02	5.68 ± 0.68	3.70 ± 0.05	5.51 ± 0.25	5.42 ± 0.98	4.48 ± 0.28
33	10	97.94 ± 0.24	84.55 ± 3.58	93.21 ± 0.76	93.46 ± 0.64	96.75 ± 0.64	83.73 ± 0.82
	30	98.96 ± 0.29	96.58 ± 0.59	94.45 ± 0.88	98.34 ± 0.66	99.77 ± 0.25	96.62 ± 0.33
	IC_{50}	4.37 ± 0.05	6.04 ± 0.68	3.53 ± 0.19	6.26 ± 0.36	4.90 ± 0.54	5.53 ± 0.19
34	10	< 20	< 20	< 20	< 20	< 20	< 20
	30	< 20	23.30 ± 2.43	< 20	< 20	< 20	< 20
35	10	< 20	< 20	< 20	< 20	< 20	< 20
	30	< 20	< 20	< 20	< 20	< 20	< 20
36	10	< 20	< 20	< 20	< 20	< 20	< 20
	30	< 20	29.31 ± 0.95	24.11 ± 1.66	< 20	< 20	< 20
37	10	< 20	< 20	< 20	< 20	< 20	< 20
	30	< 20	21.60 ± 0.72	< 20	< 20	< 20	< 20
38	10	95.20 ± 0.29	90.65 ± 0.88	86.22 ± 1.71	88.39 ± 2.26	93.82 ± 1.01	67.36 ± 1.57
	30	97.57 ± 0.81	95.80 ± 0.53	98.29 ± 0.27	97.53 ± 0.66	99.51 ± 0.30	96.90 ± 0.46
	IC_{50}	4.48 ± 0.19	6.13 ± 1.26	4.65 ± 0.16	7.74 ± 0.13	5.65 ± 0.89	7.00 ± 0.23
39	10	96.43 ± 0.25	81.07 ± 0.48	82.70 ± 2.27	82.08 ± 0.32	81.15 ± 2.07	78.12 ± 0.39
	30	98.45 ± 0.22	93.82 ± 0.58	91.61 ± 0.46	93.47 ± 1.01	98.63 ± 0.29	72.77 ± 0.62
	IC_{50}	5.31 ± 0.21	8.23 ± 0.14	5.80 ± 1.26	8.05 ± 0.29	5.99 ± 0.24	8.31 ± 0.76
40	10	< 20	< 20	< 20	< 20	< 20	< 20
	30	21.43 ± 1.69	28.27 ± 0.65	28.07 ± 2.38	< 20	< 20	< 20
41	10	< 20	< 20	< 20	< 20	< 20	< 20
	30	< 20	< 20	26.20 ± 2.18	< 20	< 20	< 20
Cisplatin*	10	42.61 ± 2.33	60.98 ± 0.92	53.03 ± 2.29	67.51 ± 1.01	83.57 ± 1.21	73.88 ± 1.63
	30	99.93 ± 0.26	88.95 ± 0.53	86.90 ± 1.22	87.75 ± 1.10	95.02 ± 0.28	97.10 ± 0.15

*: data from reference 10.3390/ijms24021121 (Bai D, Int J Mol Sci 2023

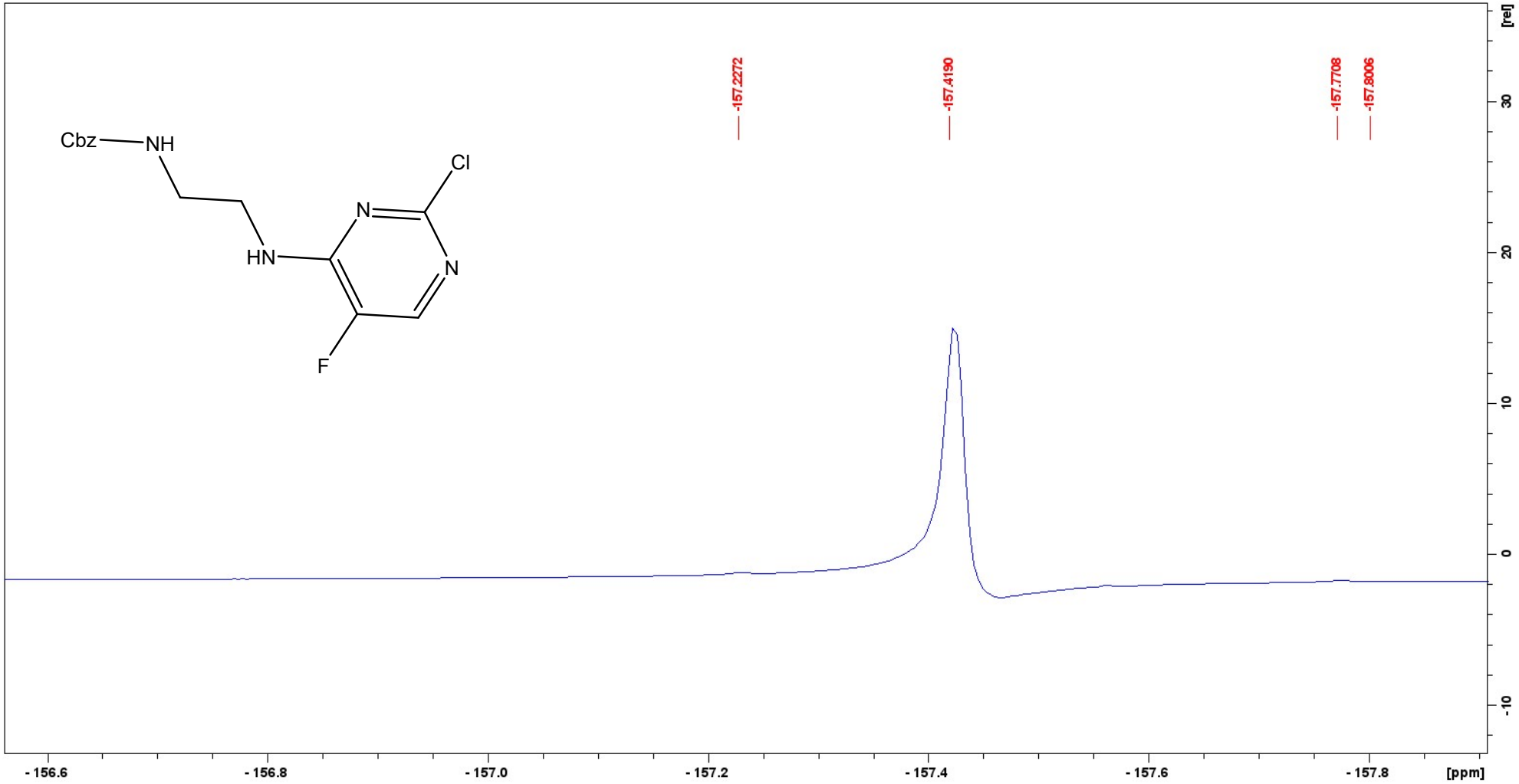
^{1}H-NMR (500 MHz) of Benzyl (2-((2-chloro-5-fluoropyrimidin-4-yl)amino)ethyl)carbamate **R1**



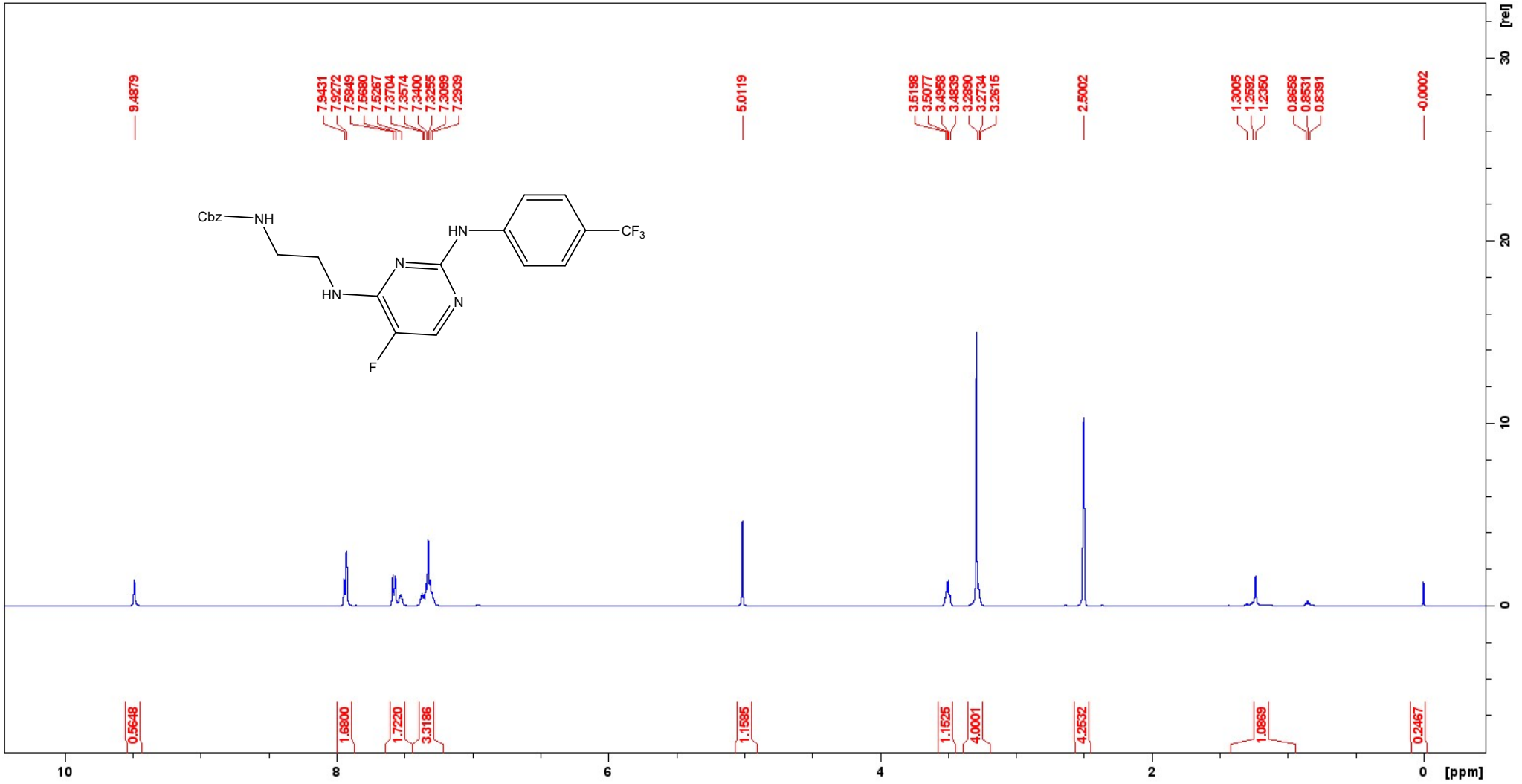
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of Benzyl (2-((2-chloro-5-fluoropyrimidin-4-yl)amino)ethyl)carbamate **R1**



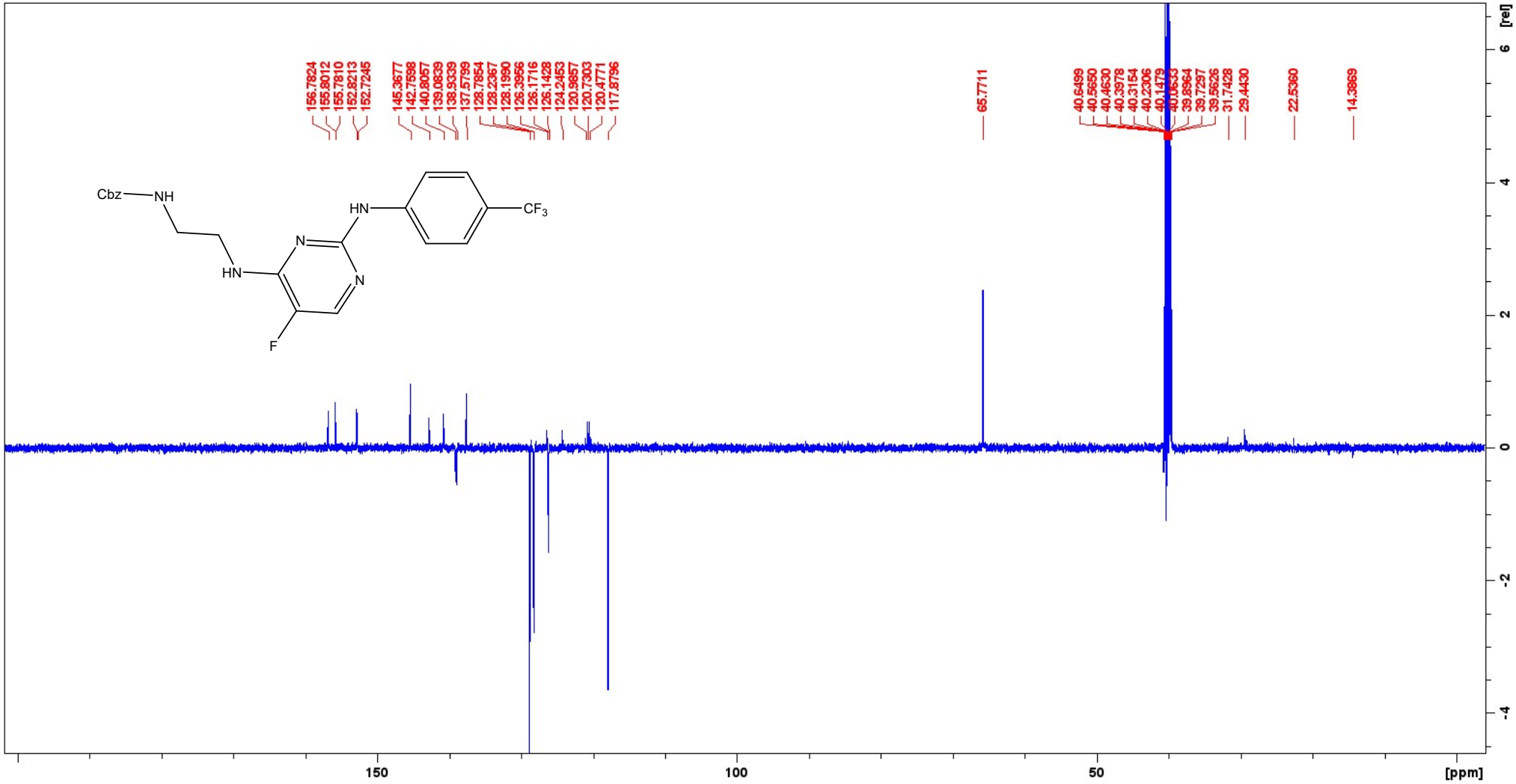
^{19}F *J*-MOD NMR (470 MHz) of Benzyl (2-((2-chloro-5-fluoropyrimidin-4-yl)amino)ethyl)carbamate **R1**



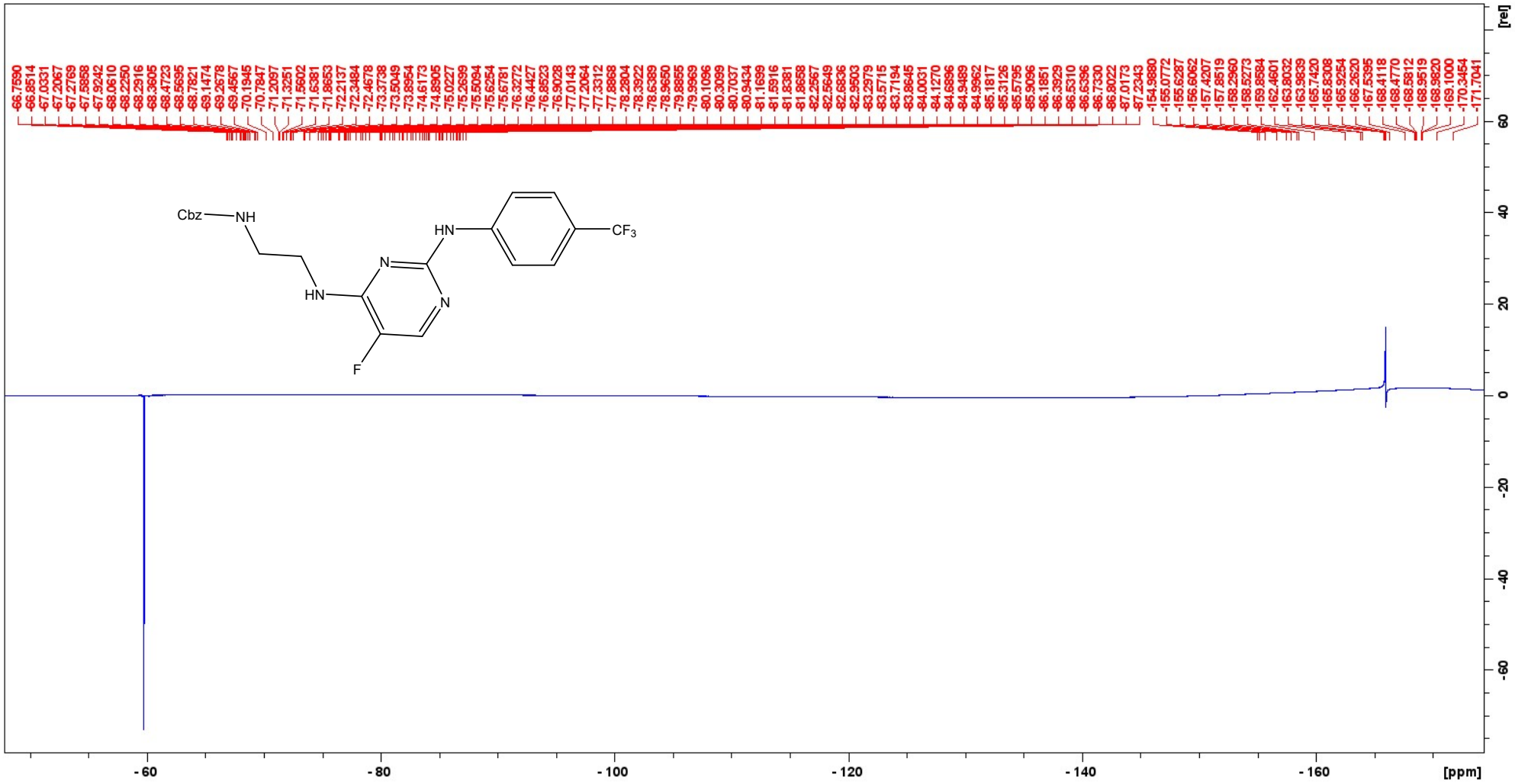
^{1}H-NMR (500 MHz) of Benzyl (2-((5-fluoro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)ethyl)carbamate **R2**



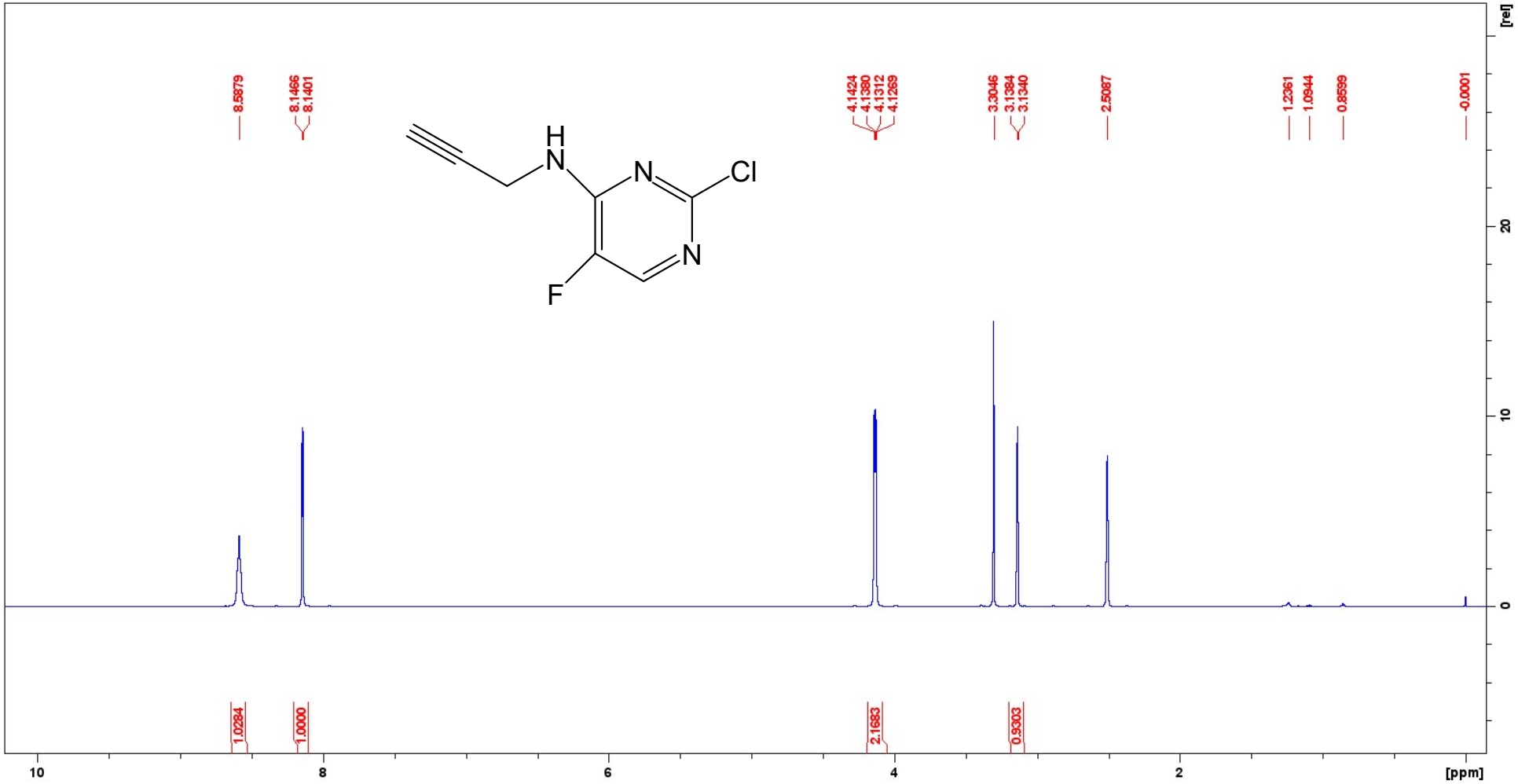
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of Benzyl (2-((5-fluoro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)ethyl)carbamate **R2**



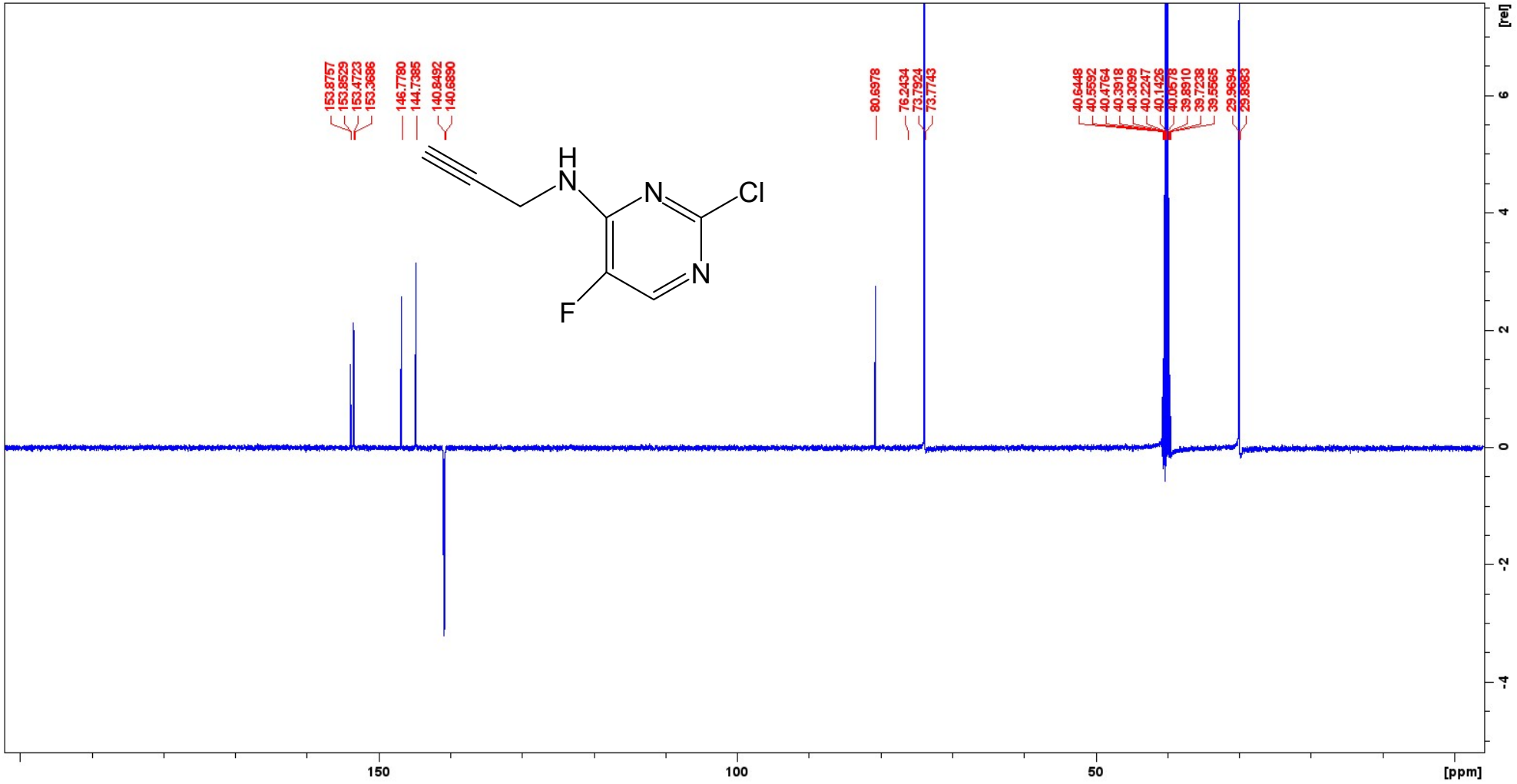
^{19}F *J*-MOD NMR (470 MHz) of Benzyl (2-((5-fluoro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)ethyl)carbamate **R2**



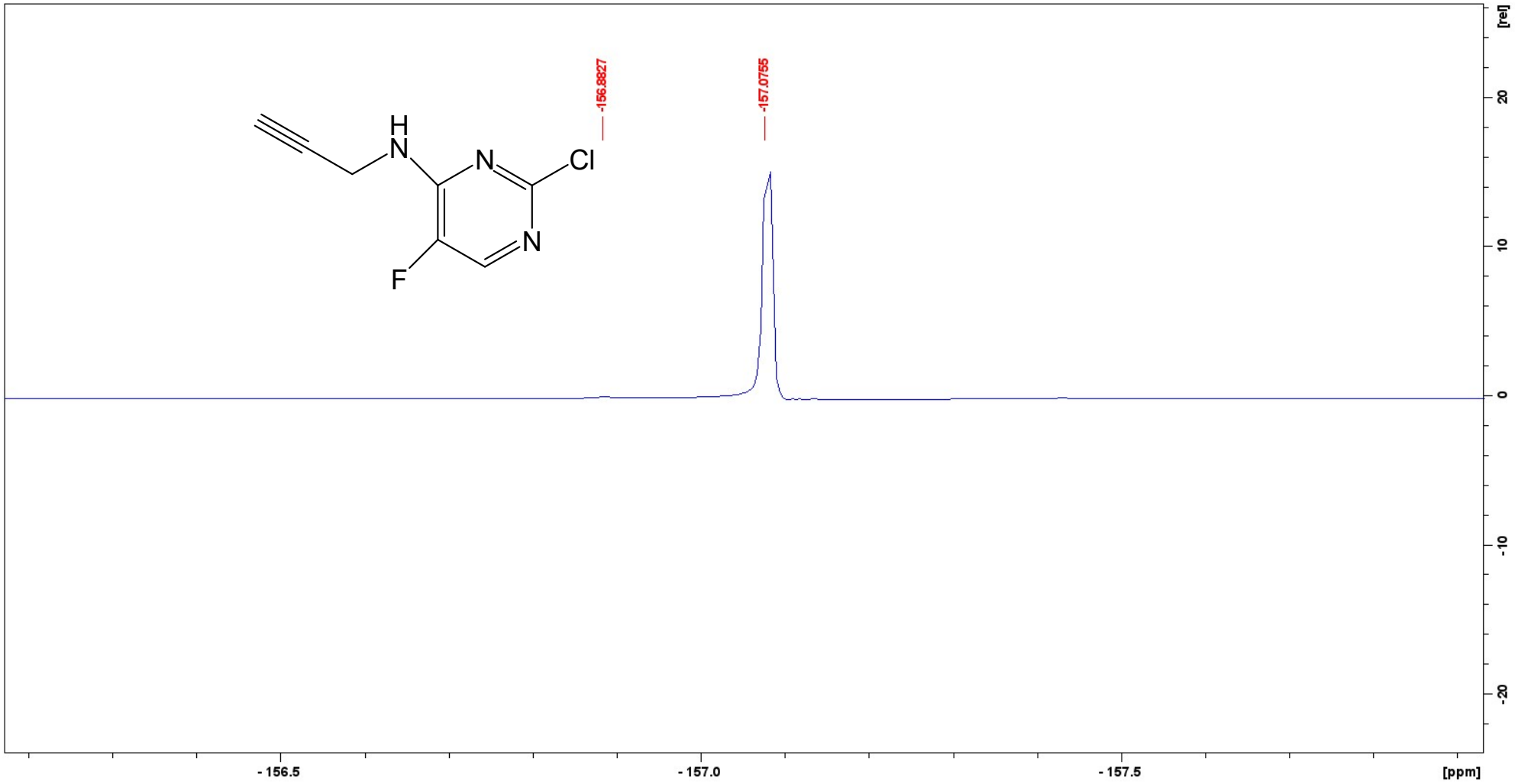
^{1}H-NMR (500 MHz) of 2-Chloro-5-fluoro-N-(prop-2-yn-1-yl)pyrimidin-4-amine **R3**



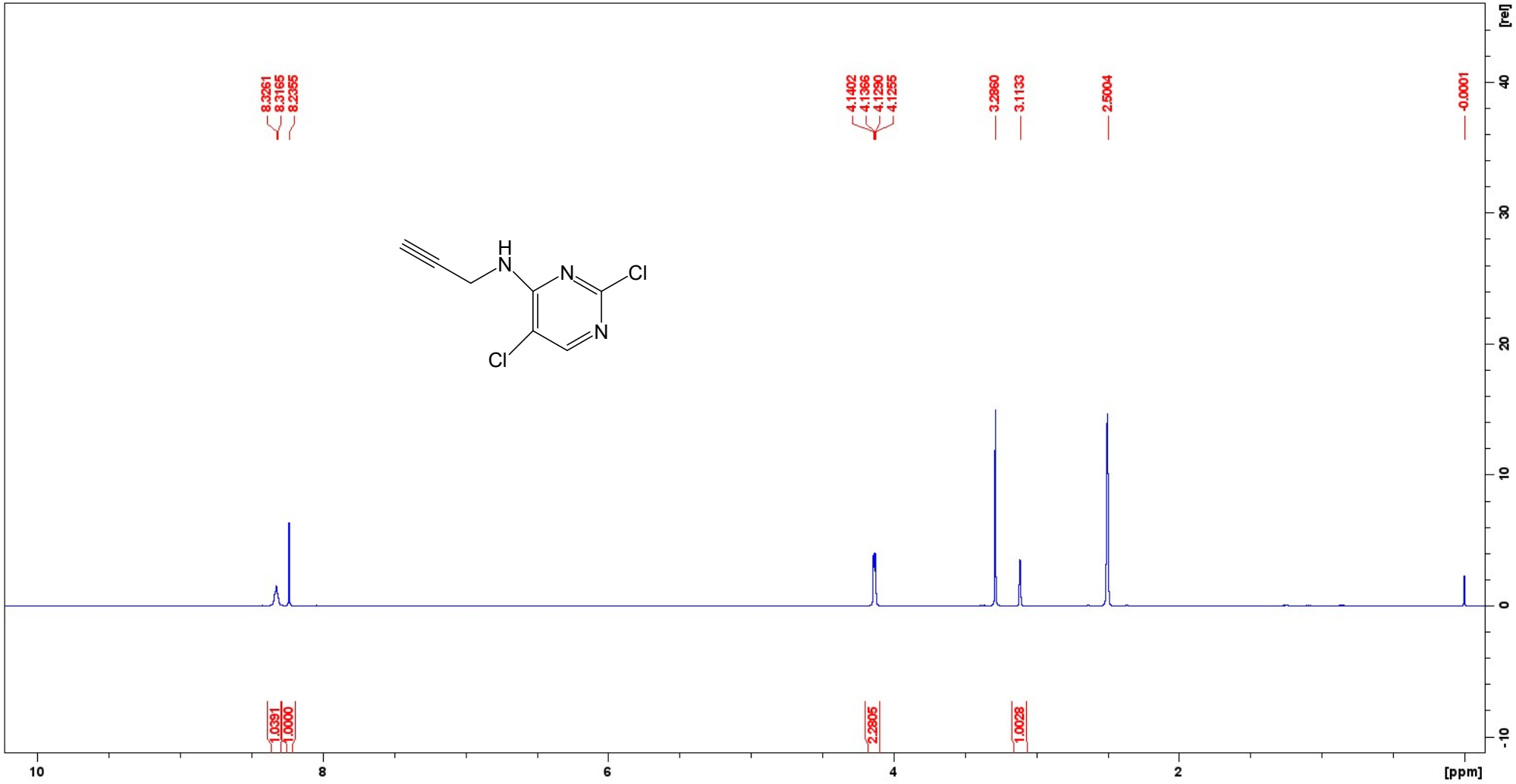
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of 2-Chloro-5-fluoro-N-(prop-2-yn-1-yl)pyrimidin-4-amine **R3**



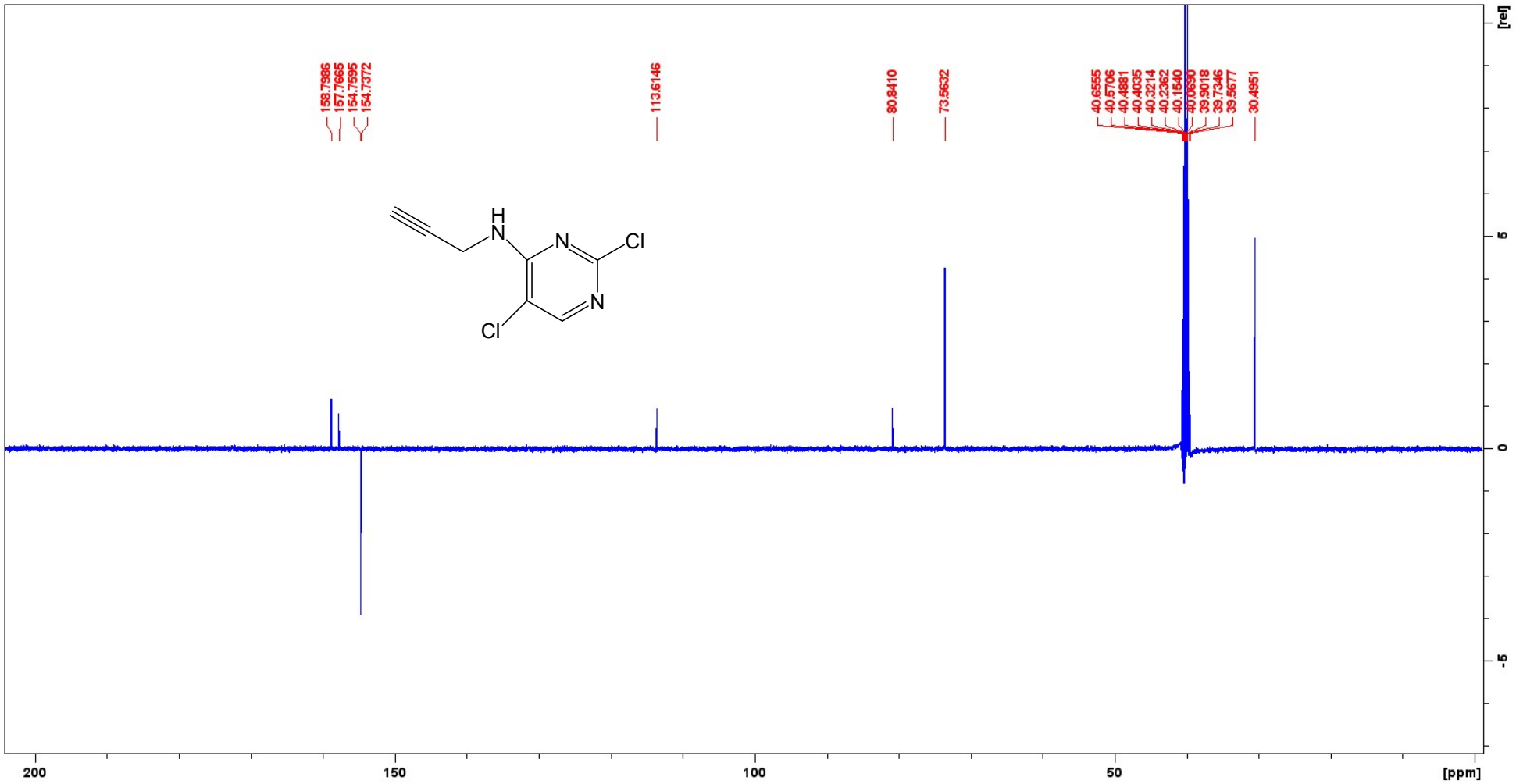
^{19}F *J*-MOD NMR (470 MHz) of 2-Chloro-5-fluoro-N-(prop-2-yn-1-yl)pyrimidin-4-amine **R3**



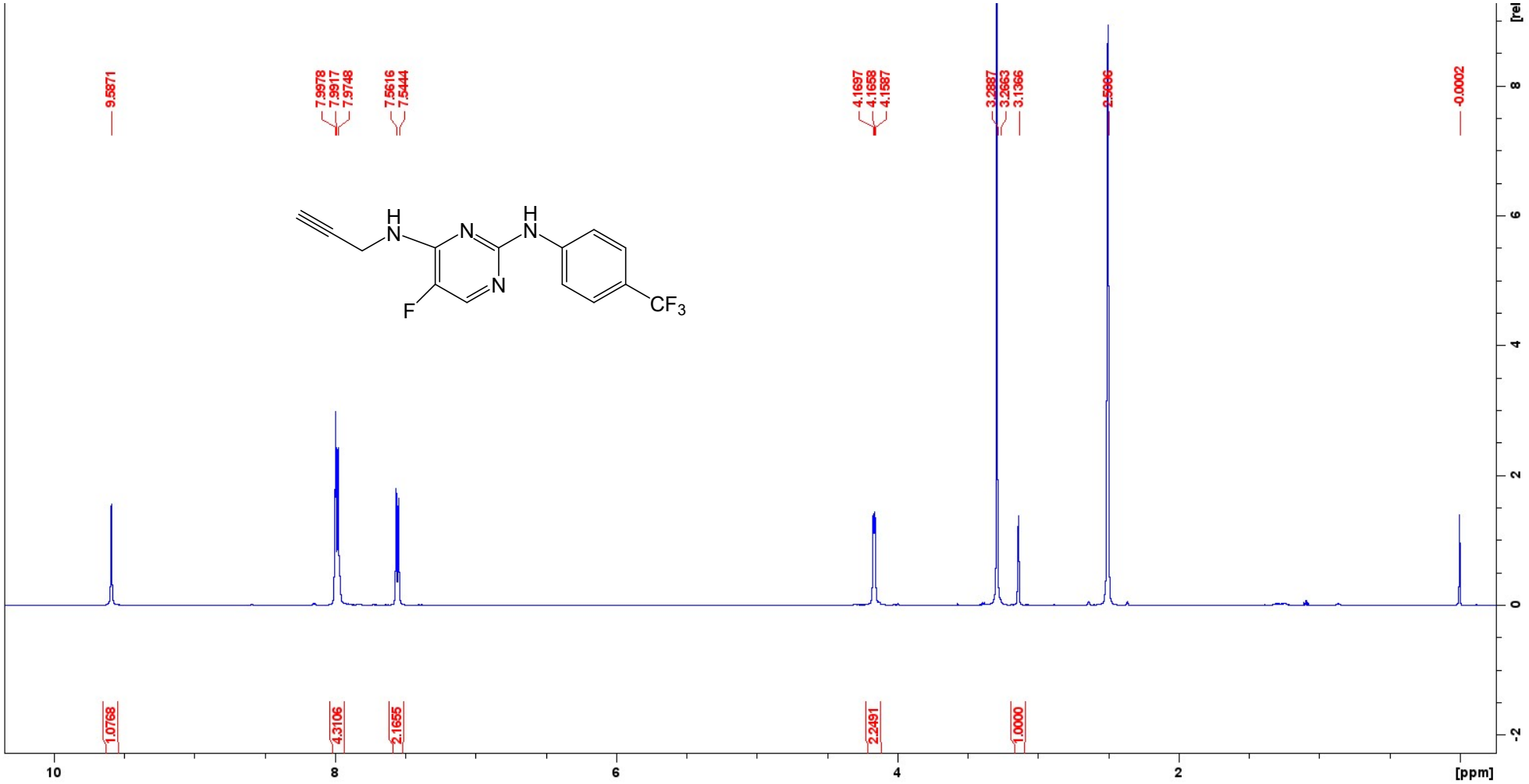
^{1}H-NMR (500 MHz) of 2,5-Dichloro-N-(prop-2-yn-1-yl)pyrimidin-4-amine **R4**



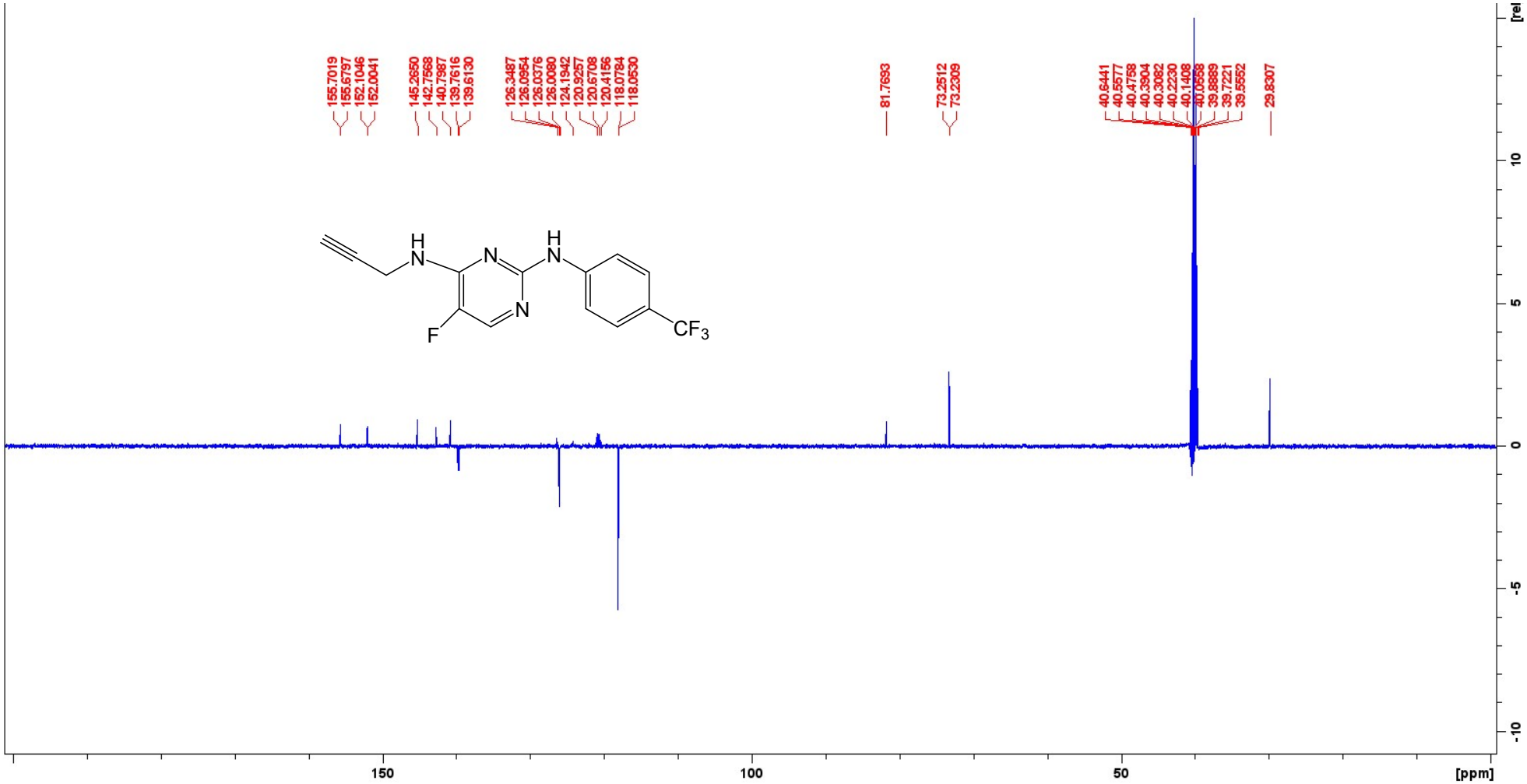
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of 2,5-Dichloro-N-(prop-2-yn-1-yl)pyrimidin-4-amine **R4**



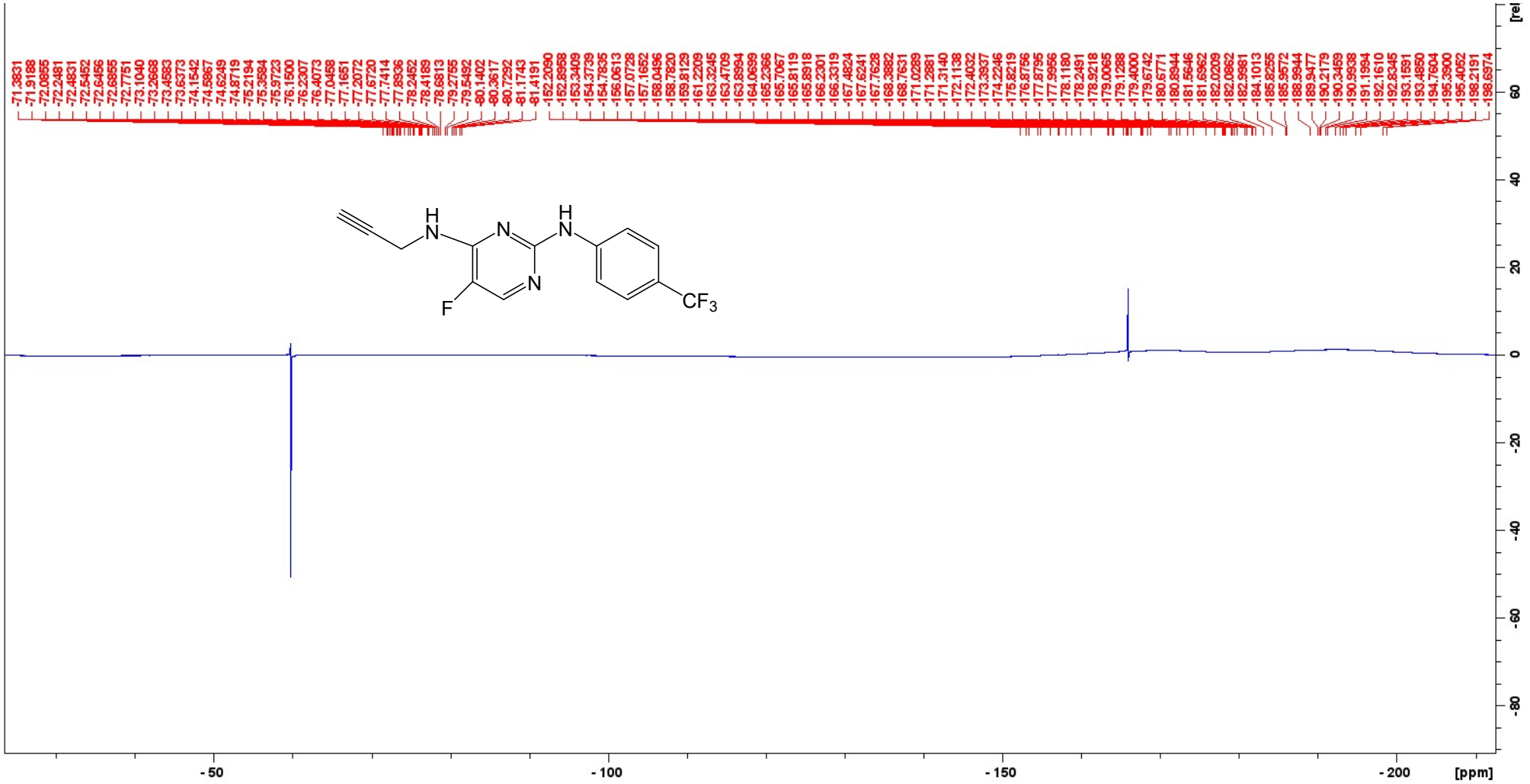
^{1}H-NMR (500 MHz) of 5-Fluoro-*N*^{4}-(prop-2-yn-1-yl)-*N*^{2}-(4-(trifluoromethyl)phenyl)pyrimidine-2,4-diamine **R5**



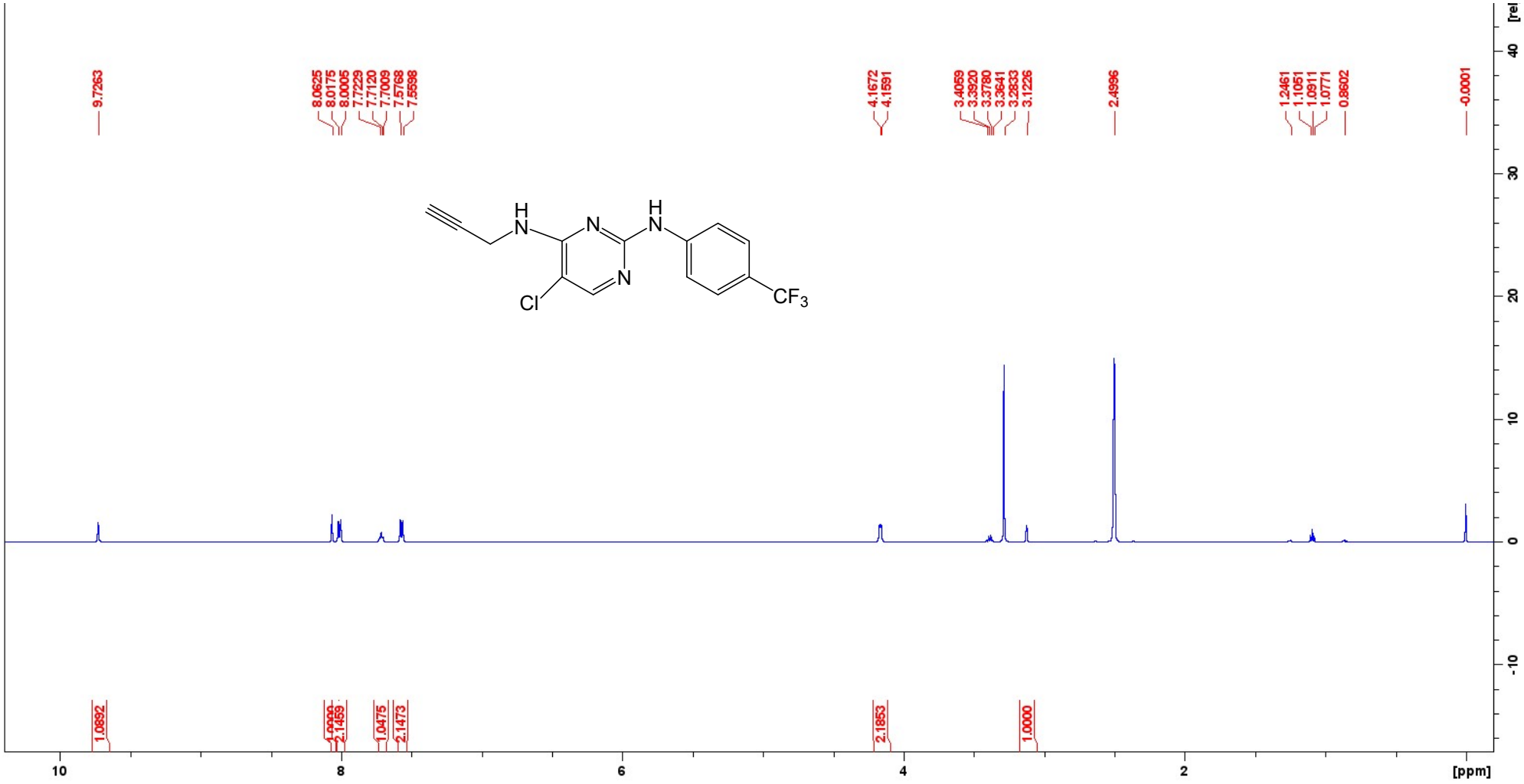
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of 5-Fluoro-N^4-(prop-2-yn-1-yl)-N^2-(4-(trifluoromethyl)phenyl)pyrimidine-2,4-diamine **R5**



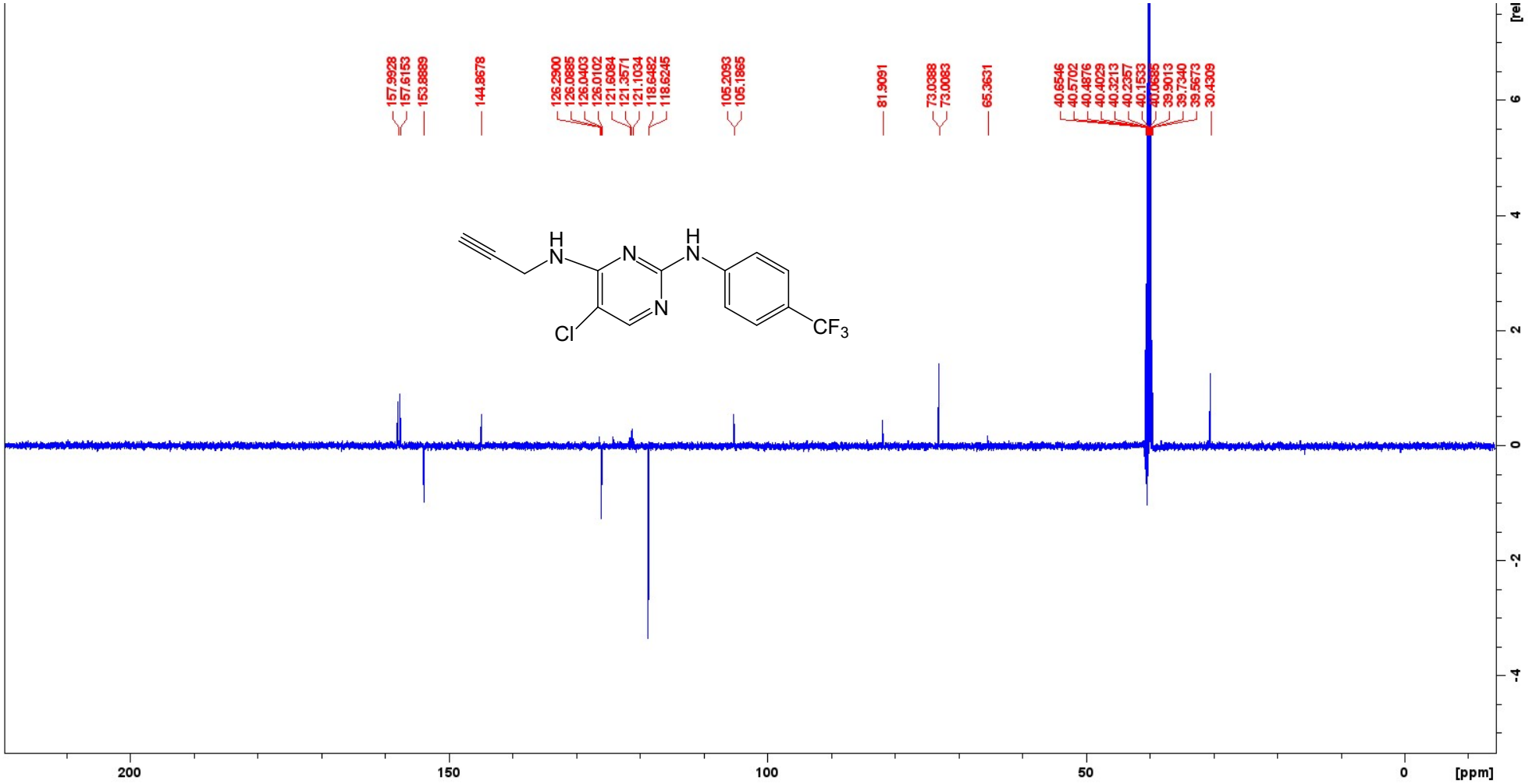
^{19}F *J*-MOD NMR (470 MHz) of 5-Fluoro-N^4-(prop-2-yn-1-yl)-N^2-(4-(trifluoromethyl)phenyl)pyrimidine-2,4-diamine **R5**



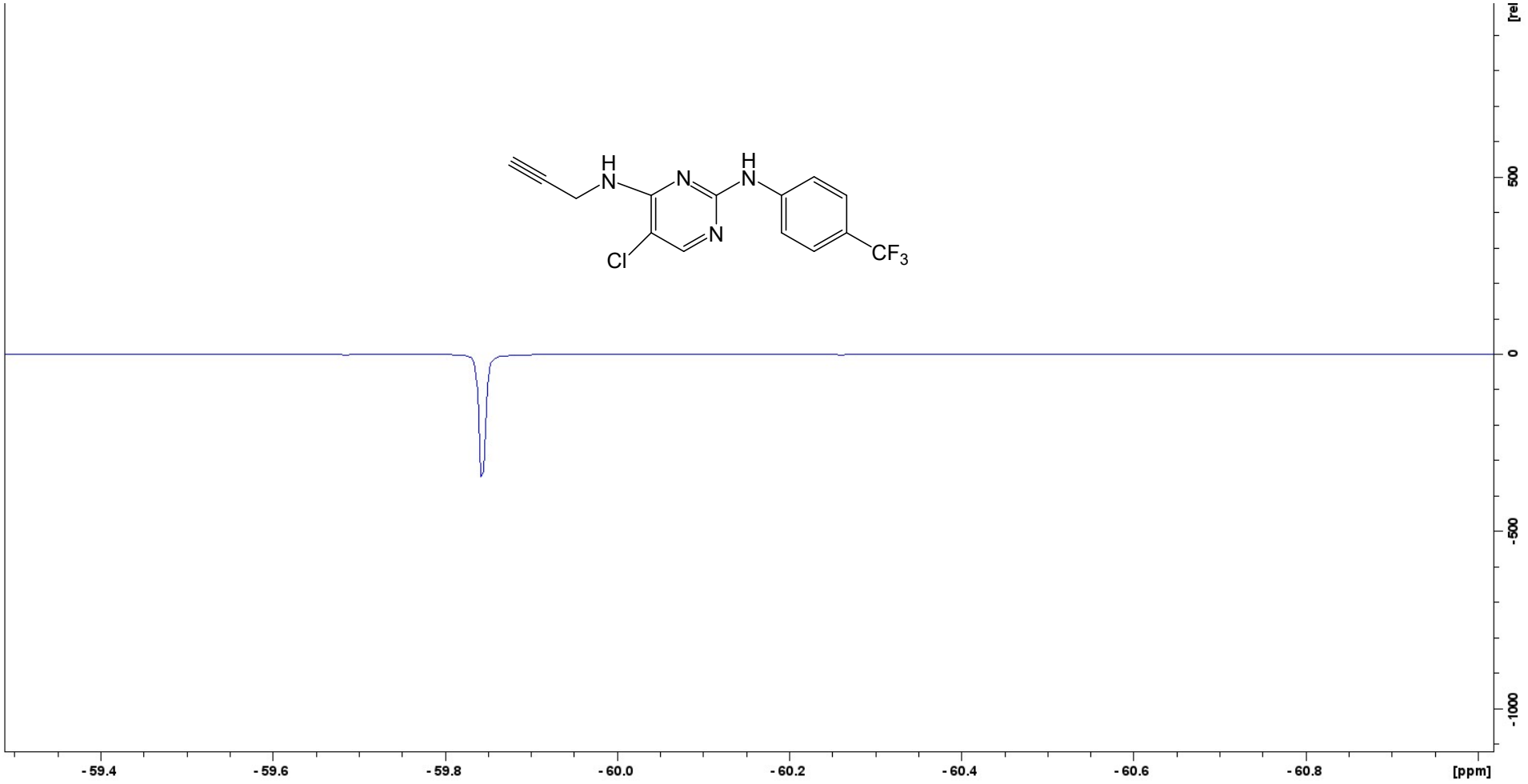
^{1}H-NMR (500 MHz) of 5-Chloro-*N*^{4}-(prop-2-yn-1-yl)-*N*^{2}-(4-(trifluoromethyl)phenyl)pyrimidine-2,4-diamine **R6**



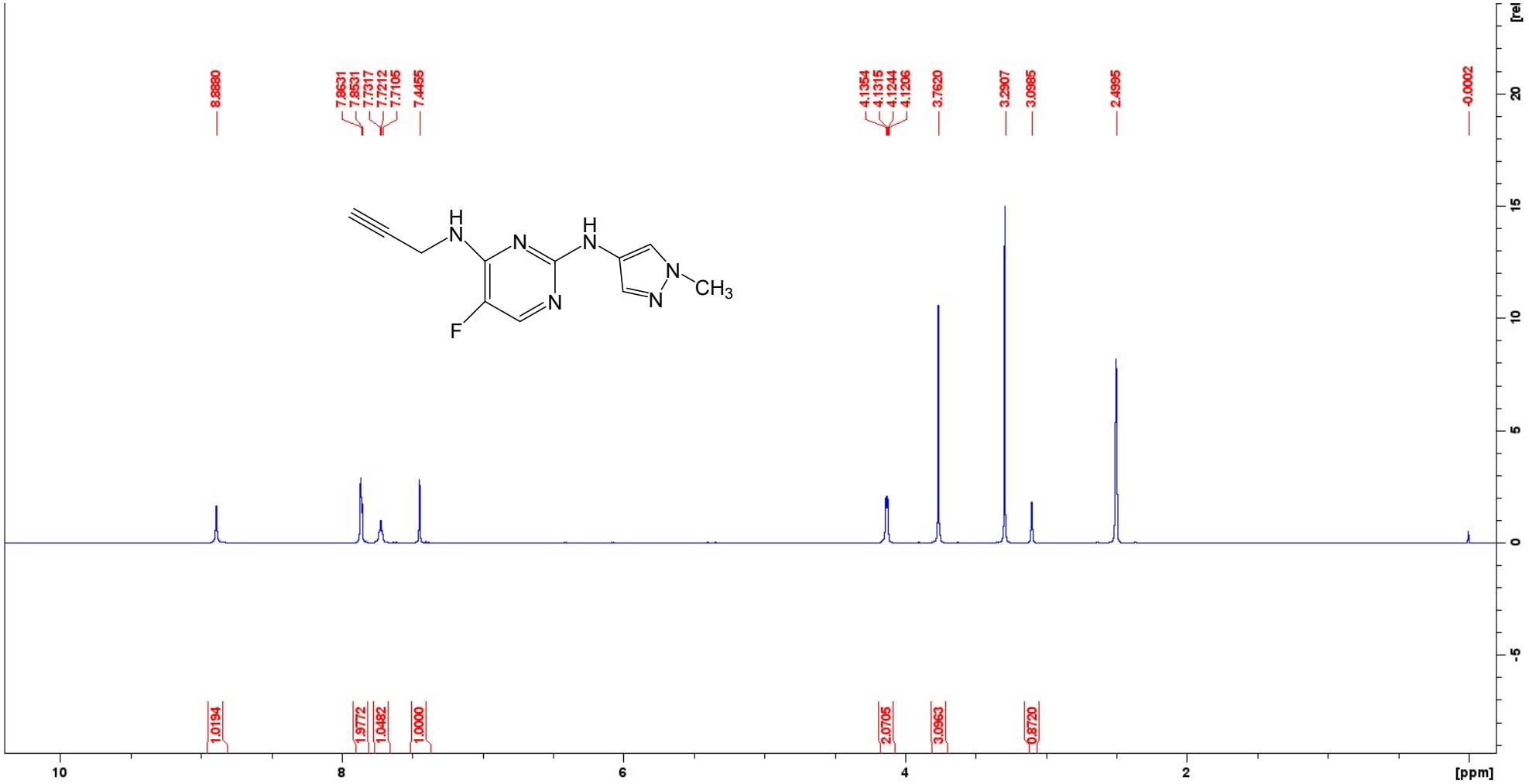
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of 5-Chloro-N^4-(prop-2-yn-1-yl)-N^2-(4-(trifluoromethyl)phenyl)pyrimidine-2,4-diamine **R6**



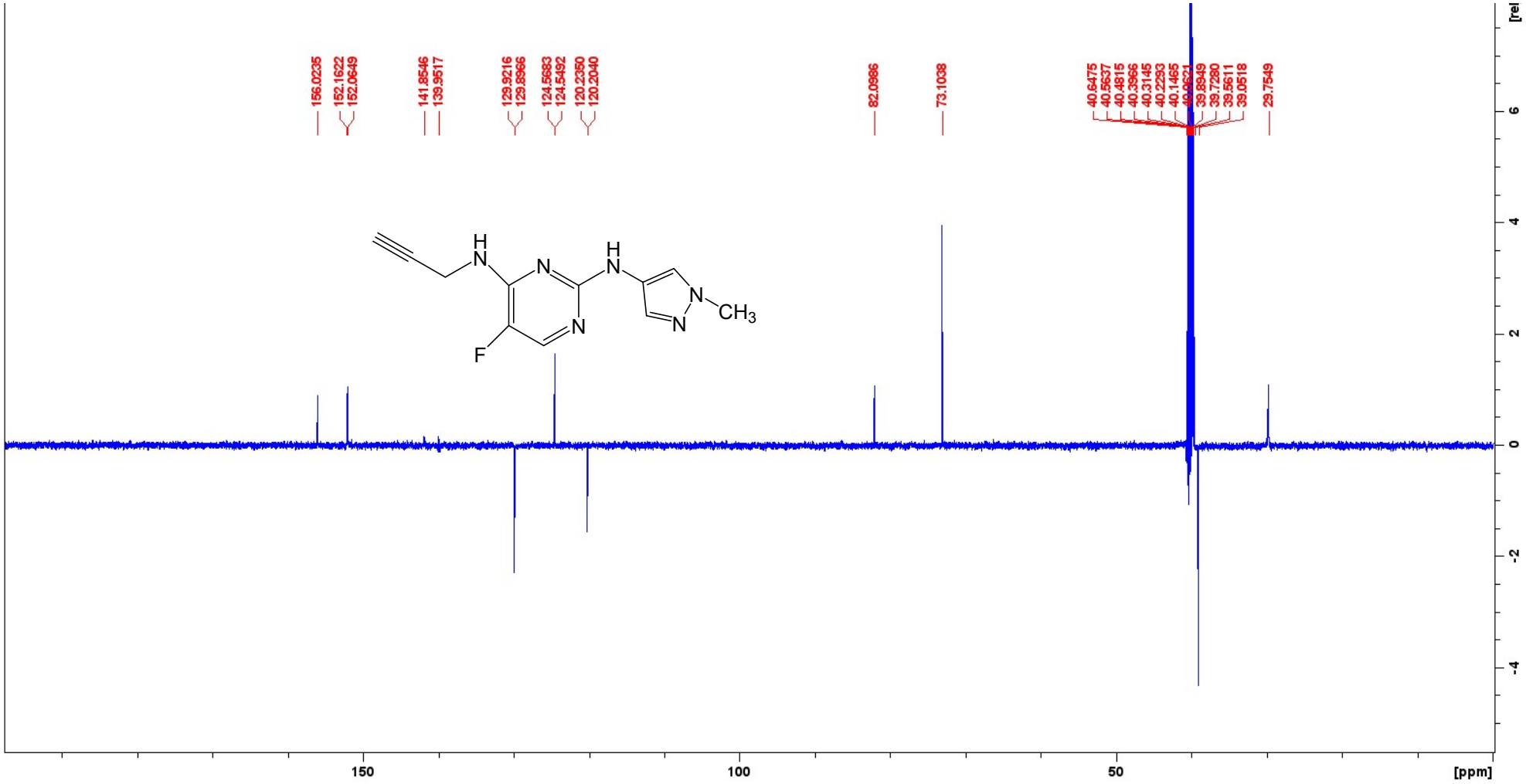
^{19}F *J*-MOD NMR (470 MHz) of 5-Chloro-N^4-(prop-2-yn-1-yl)-N^2-(4-(trifluoromethyl)phenyl)pyrimidine-2,4-diamine **R6**



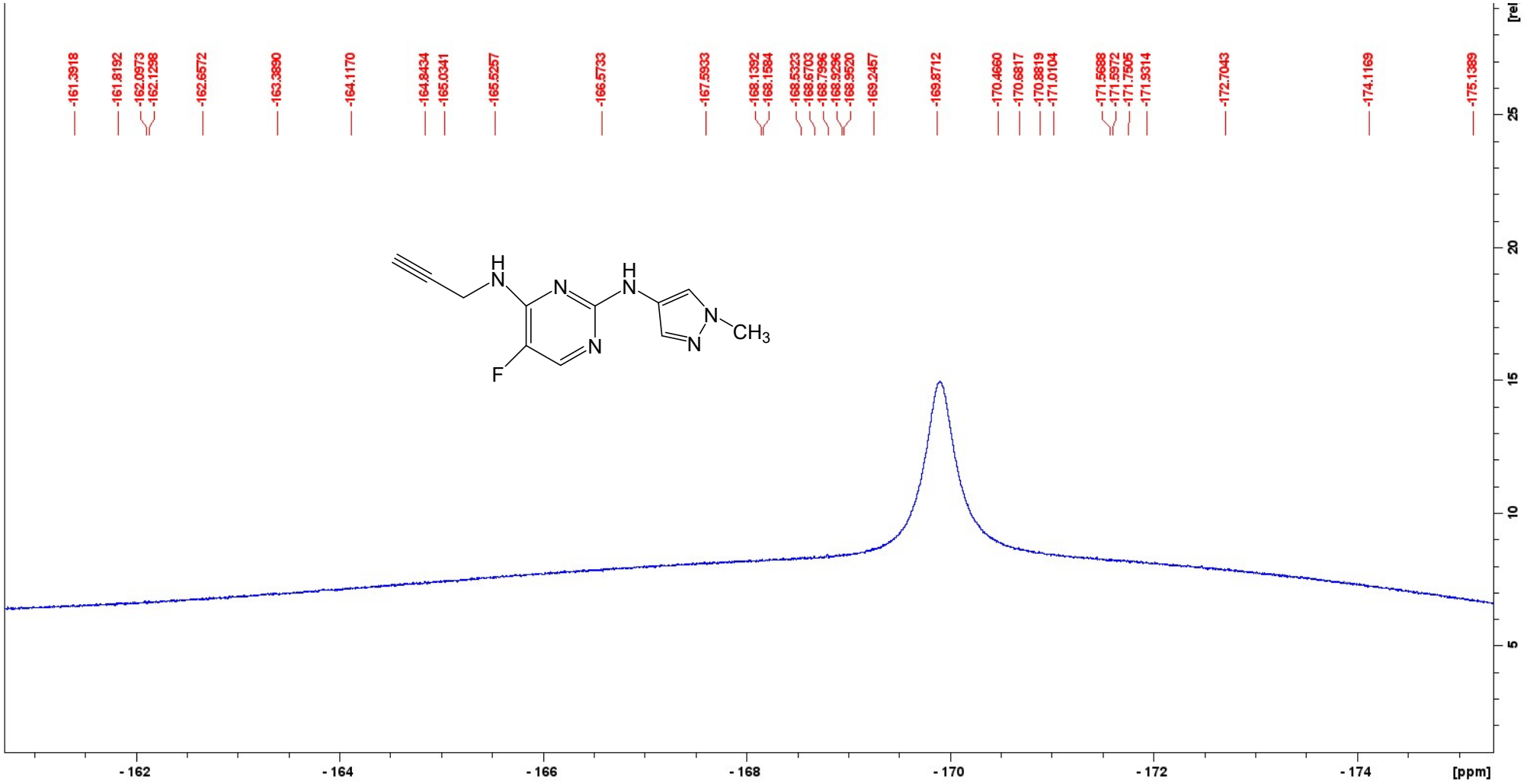
^{1}H-NMR (500 MHz) of 5-Fluoro-*N*^{2}-(1-methyl-1H-pyrazol-4-yl)-*N*^{4}-(prop-2-yn-1-yl)pyrimidine-2,4-diamine **R7**



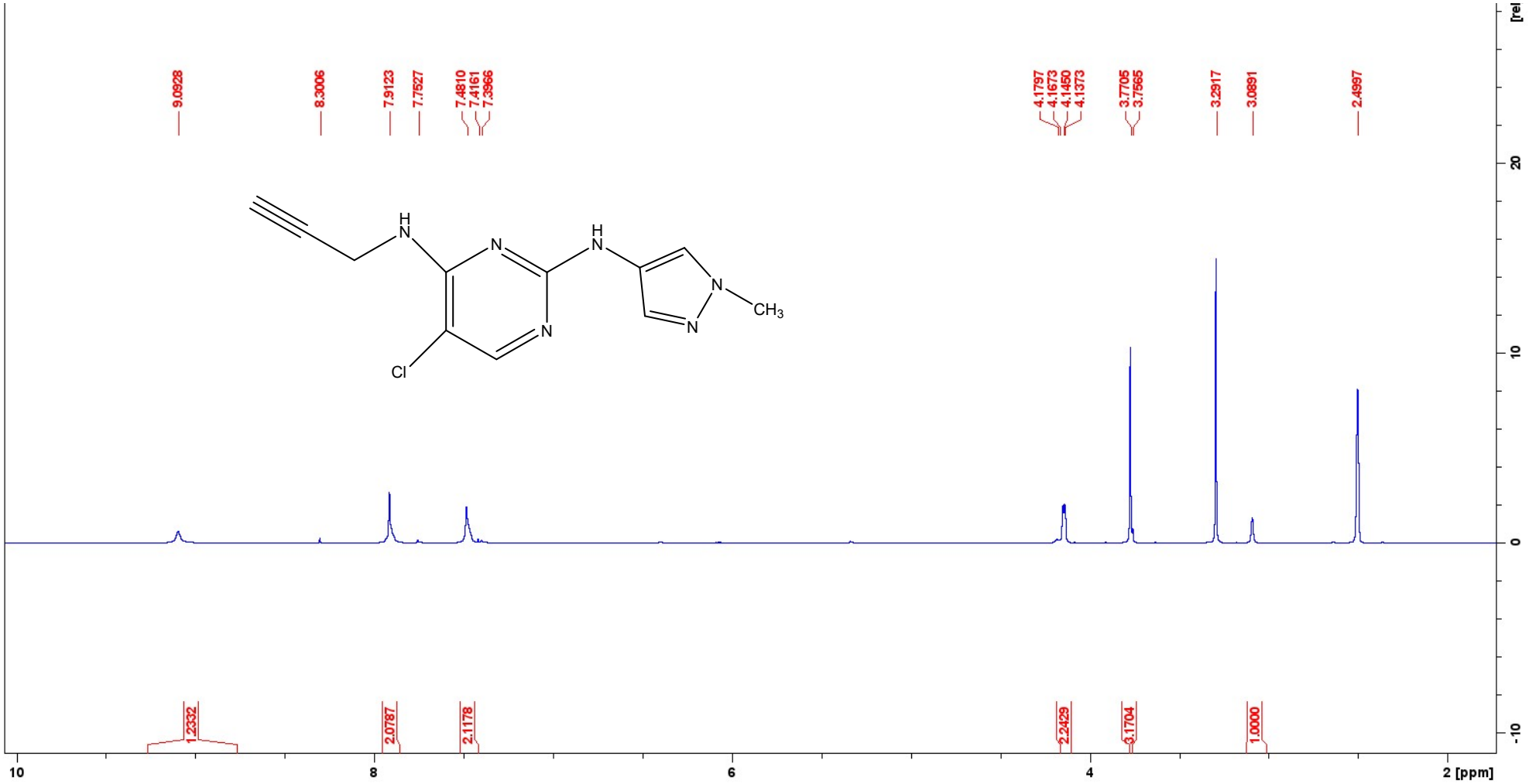
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of 5-Fluoro-N^2-(1-methyl-1H-pyrazol-4-yl)-N^4-(prop-2-yn-1-yl)pyrimidine-2,4-diamine **R7**



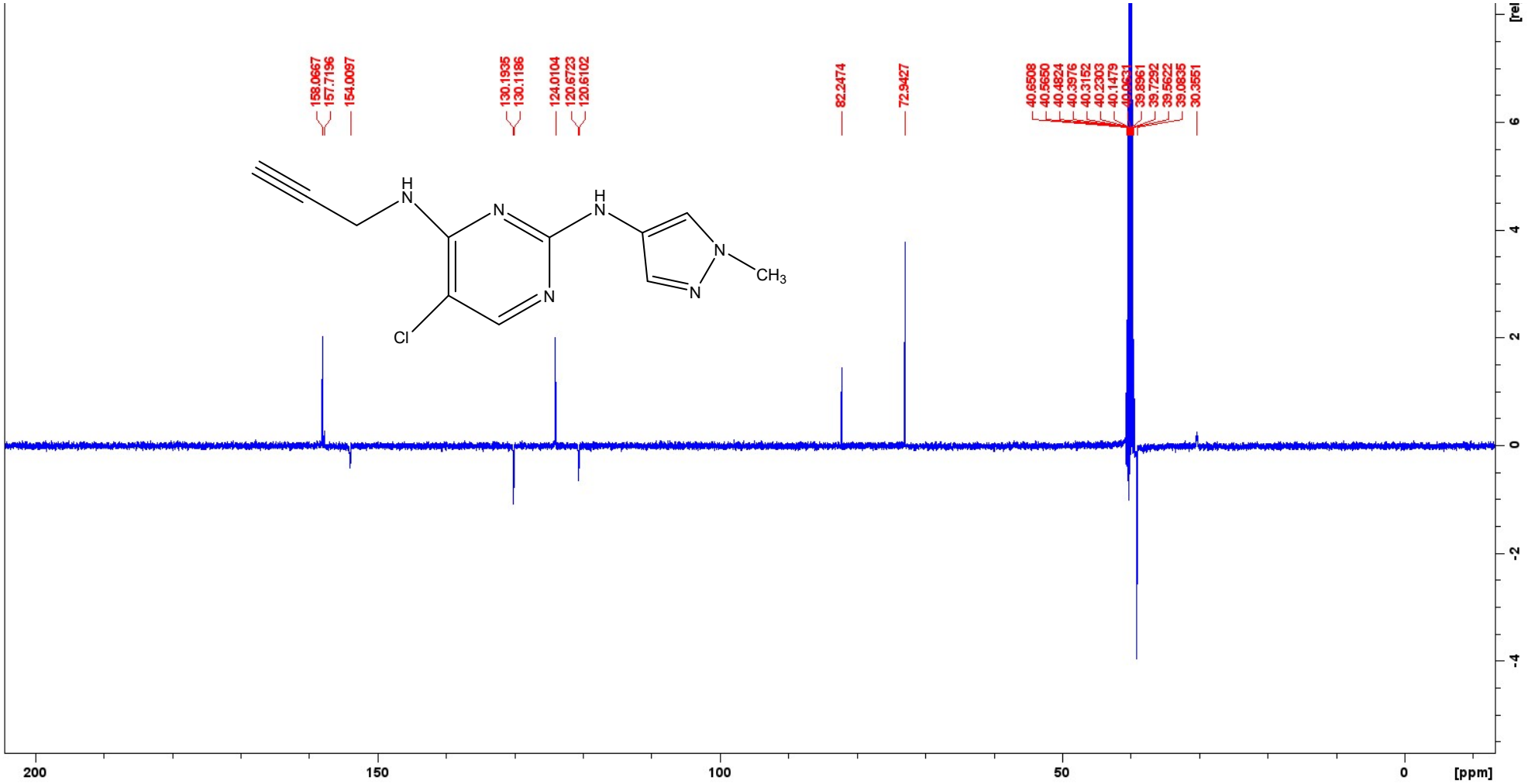
^{19}F *J*-MOD NMR (470 MHz) of 5-Fluoro-N^2-(1-methyl-1H-pyrazol-4-yl)-N^4-(prop-2-yn-1-yl)pyrimidine-2,4-diamine **R7**



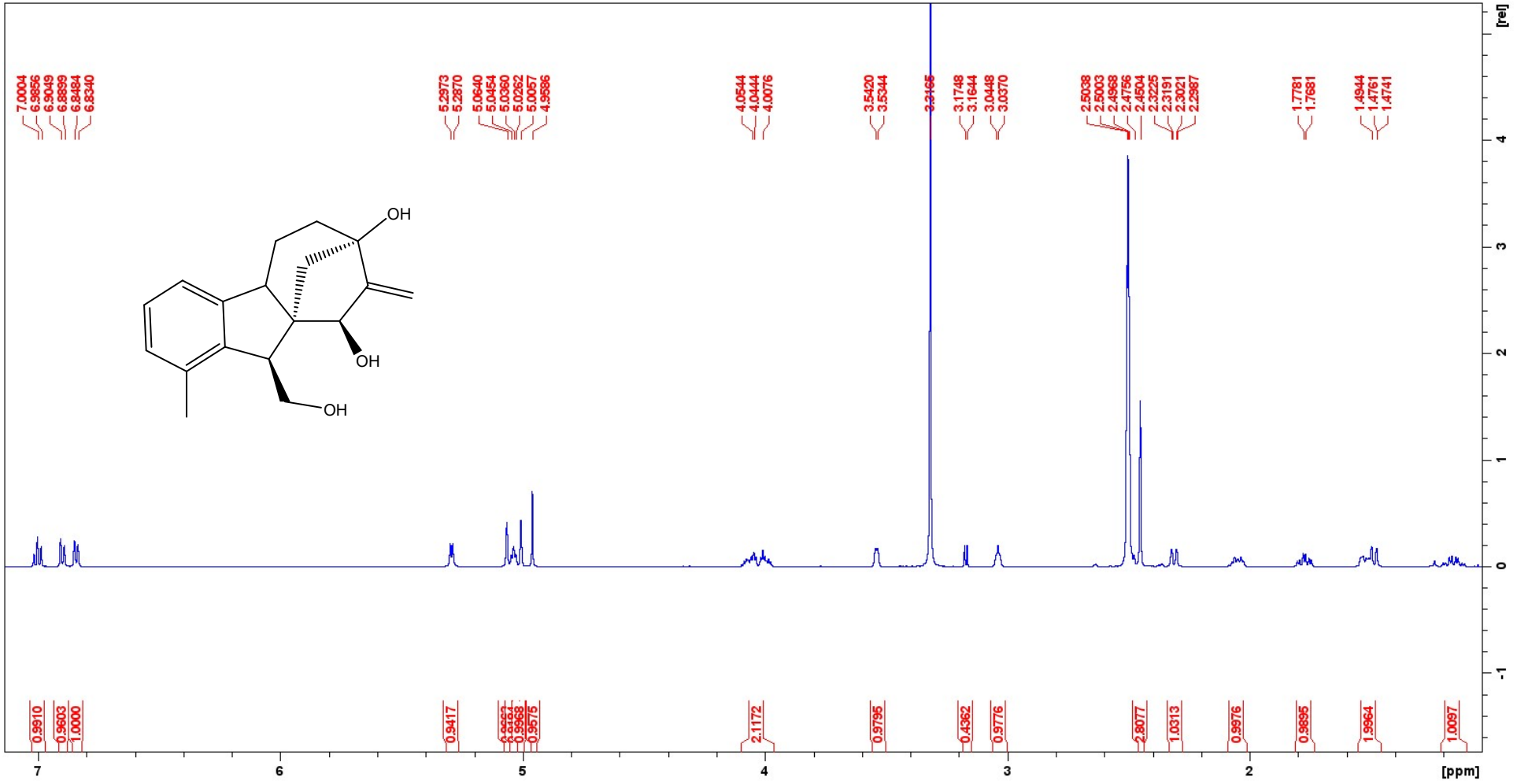
^{1}H-NMR (500 MHz) of 5-Chloro-*N*^{2}-(1-methyl-1*H*-pyrazol-4-yl)-*N*^{4}-(prop-2-yn-1-yl)pyrimidine-2,4-diamine **R8**



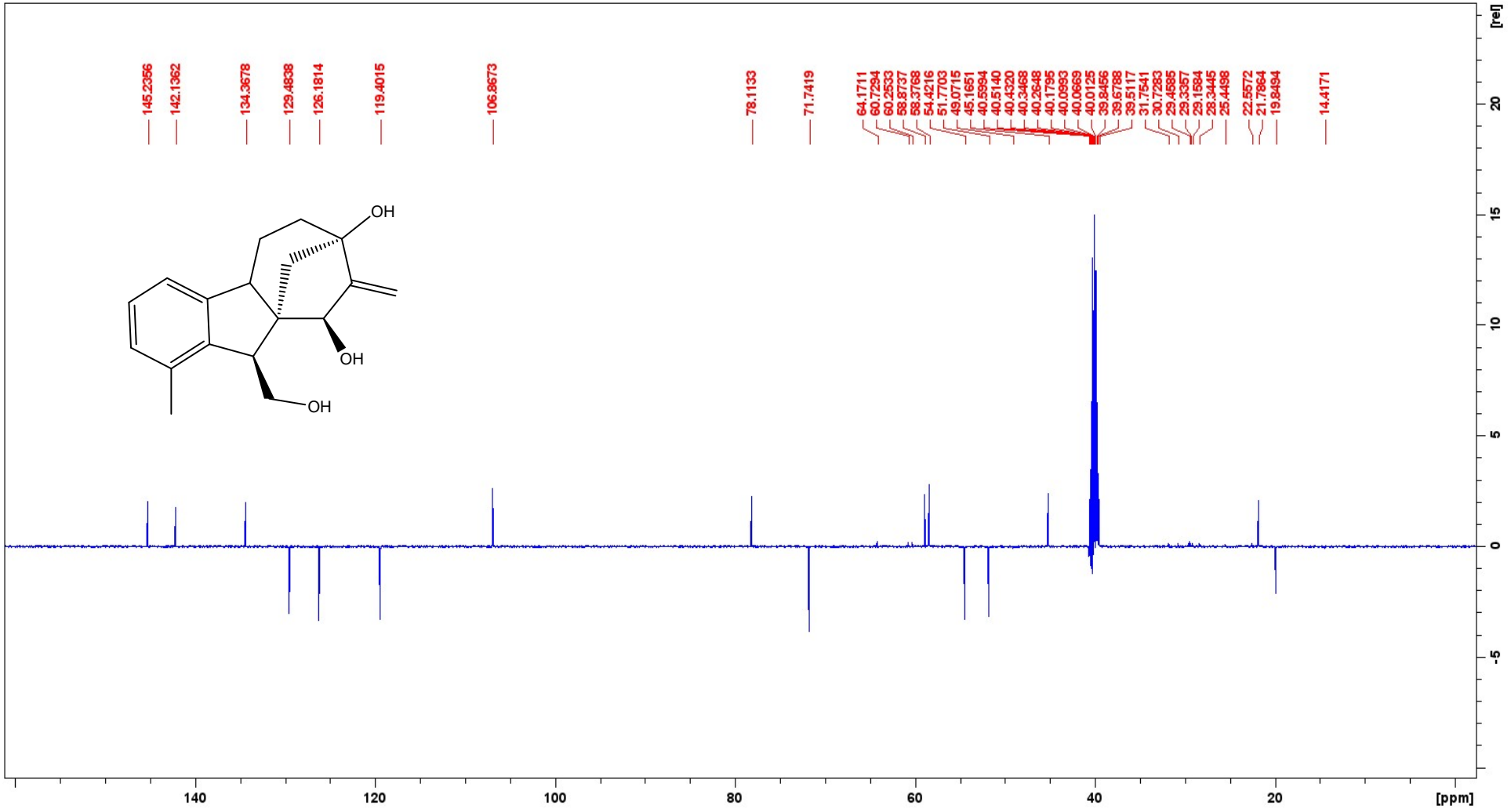
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of 5-Chloro-N^2-(1-methyl-1*H*-pyrazol-4-yl)-N^4-(prop-2-yn-1-yl)pyrimidine-2,4-diamine **R8**



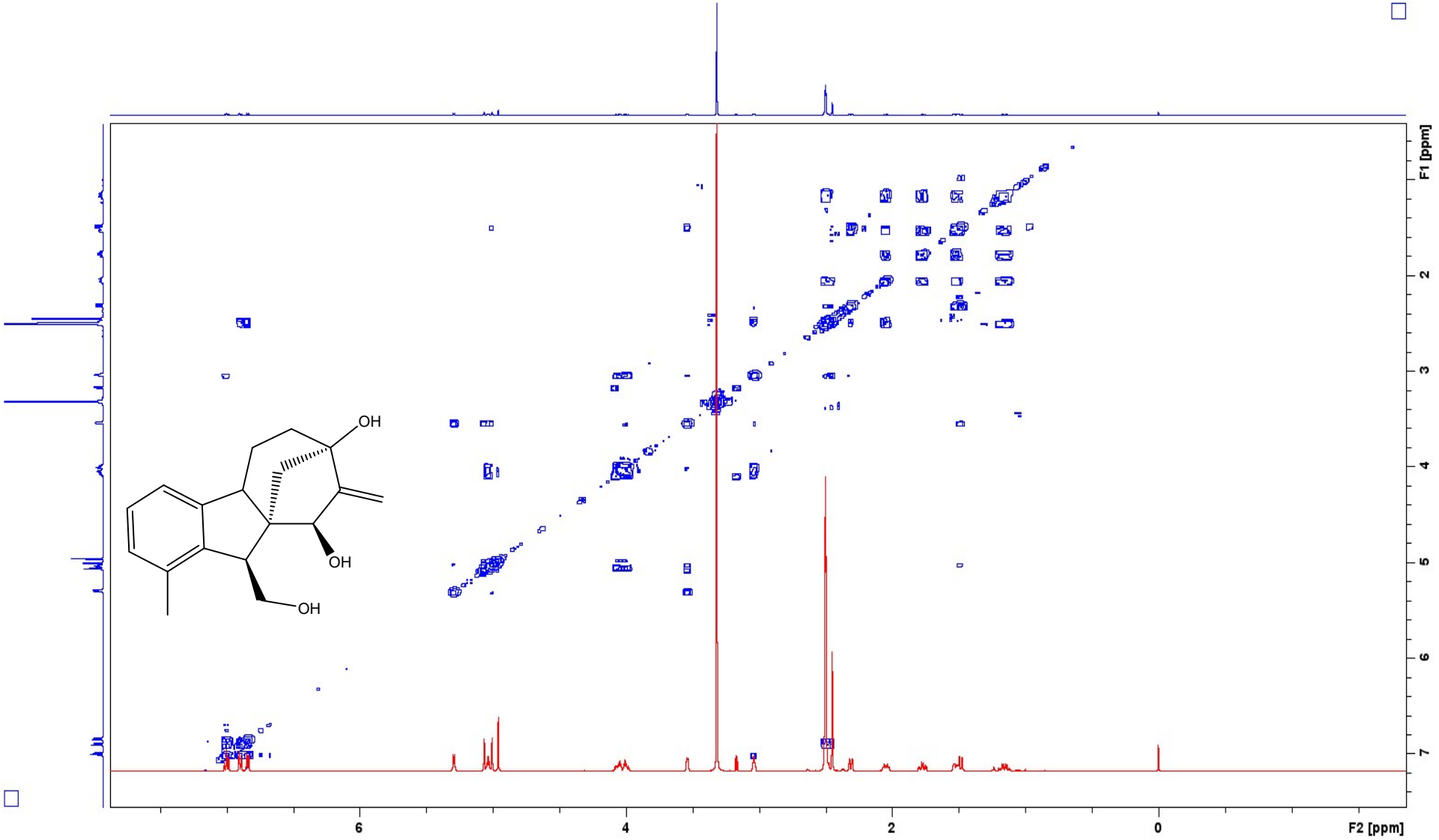
^{1}H-NMR (500 MHz) of (4b*R*,7*S*,9*S*,9a*R*,10*S*)-10-(Hydroxymethyl)-1-methyl-8-methylene-4b,5,6,8,9,10-hexahydro-7*H*-7,9a-methanobenzo[a]azulene-7,9-diol **6**



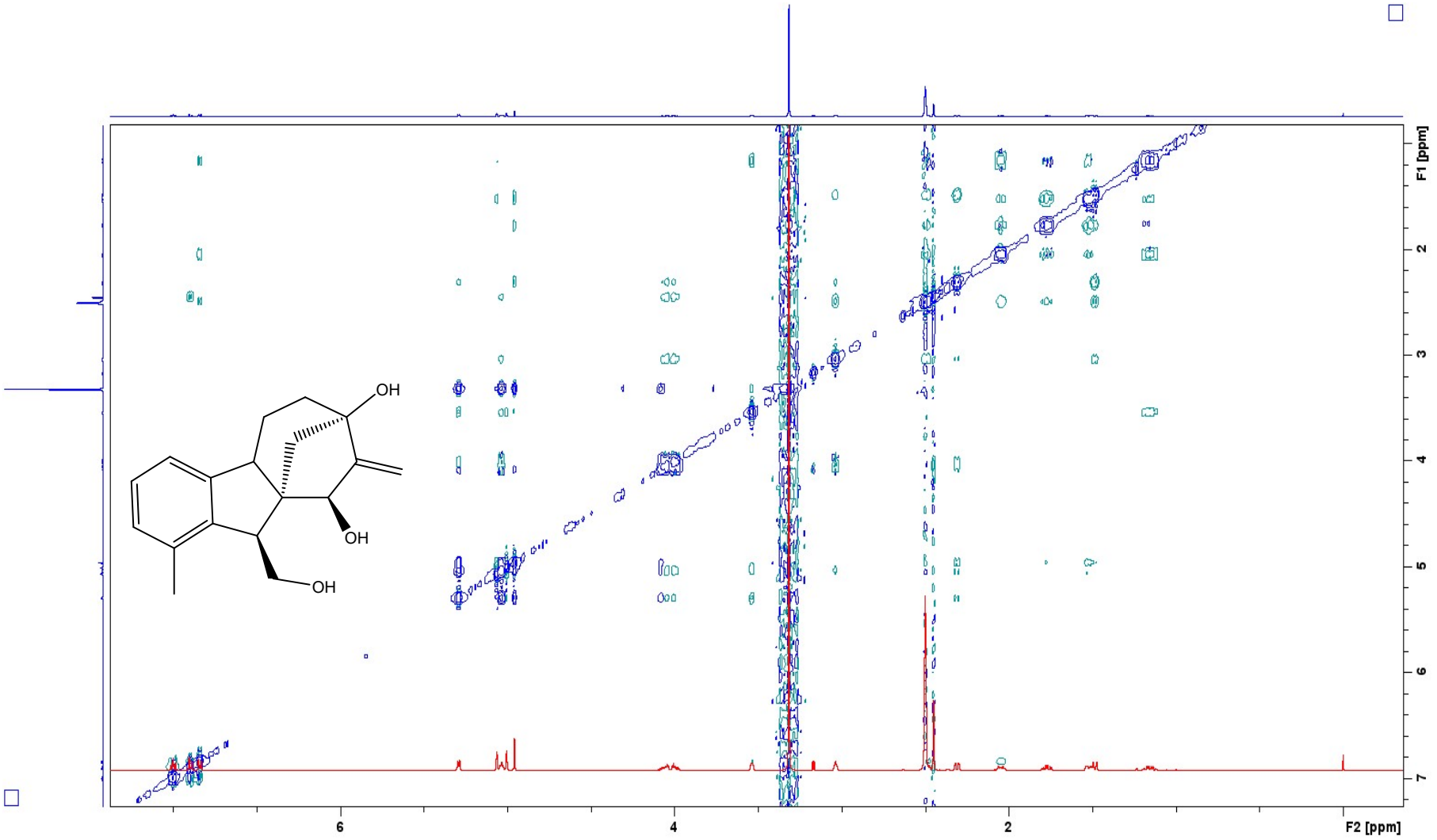
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of (4b*R*,7*S*,9*S*,9a*R*,10*S*)-10-(Hydroxymethyl)-1-methyl-8-methylene-4b,5,6,8,9,10-hexahydro-7*H*-7,9a-methanobenzo[a]azulene-7,9-diol **6**



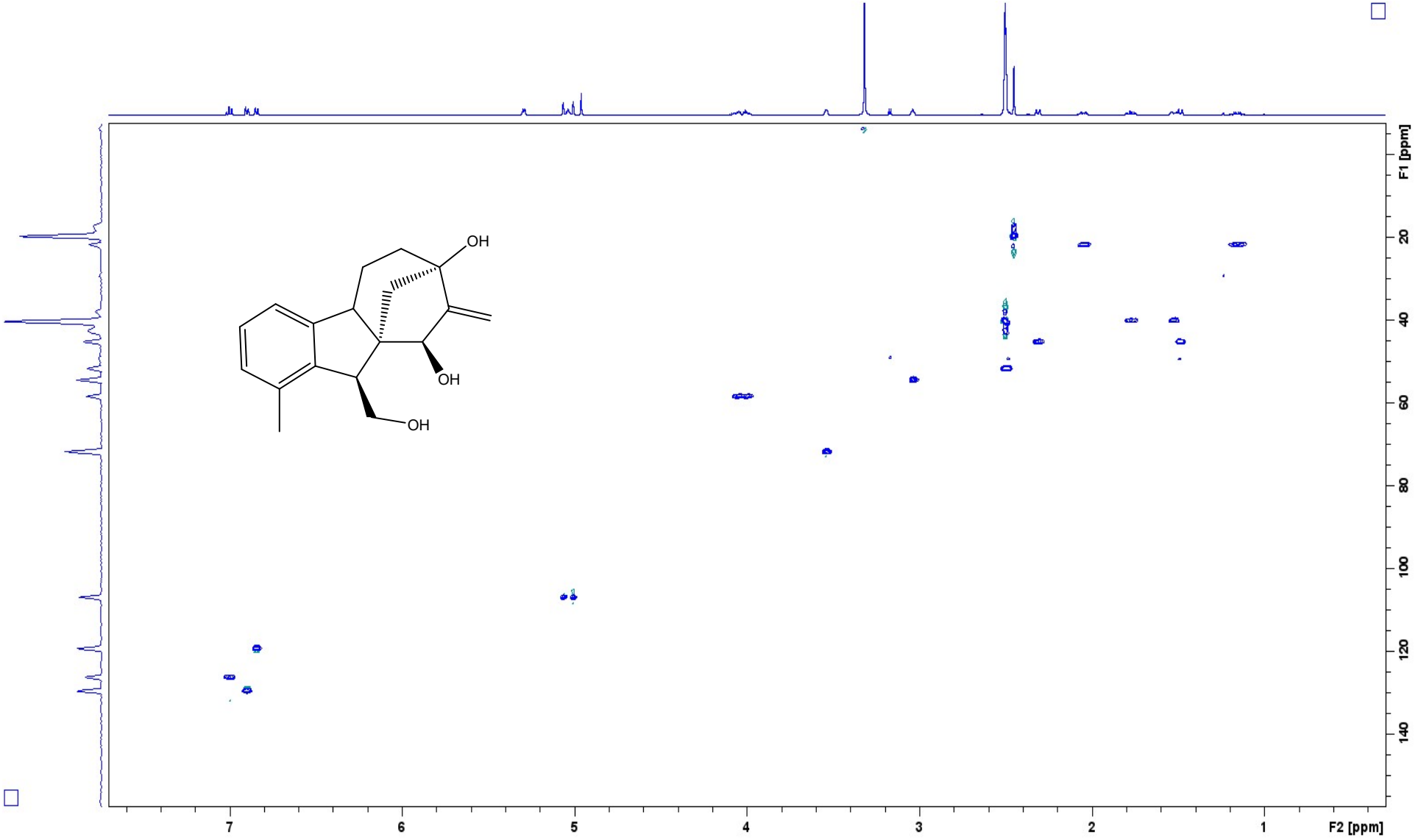
COSY of (4b*R*,7*S*,9*S*,9a*R*,10*S*)-10-(Hydroxymethyl)-1-methyl-8-methylene-4b,5,6,8,9,10-hexahydro-7*H*-7,9a-methanobenzo[a]azulene-7,9-diol **6**



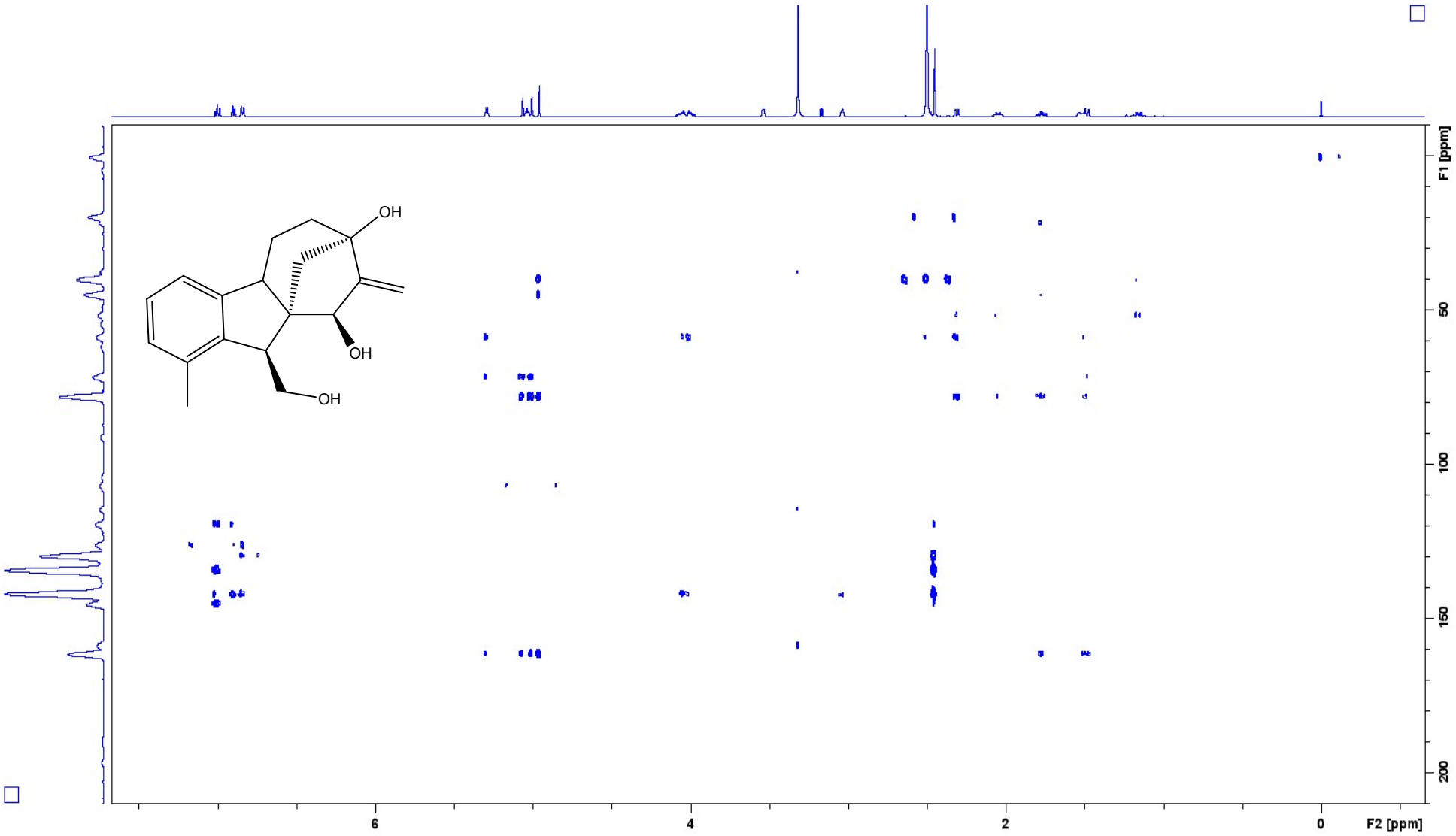
NOESY of (4b*R*,7*S*,9*S*,9a*R*,10*S*)-10-(Hydroxymethyl)-1-methyl-8-methylene-4b,5,6,8,9,10-hexahydro-7*H*-7,9a-methanobenzo[a]azulene-7,9-diol **6**



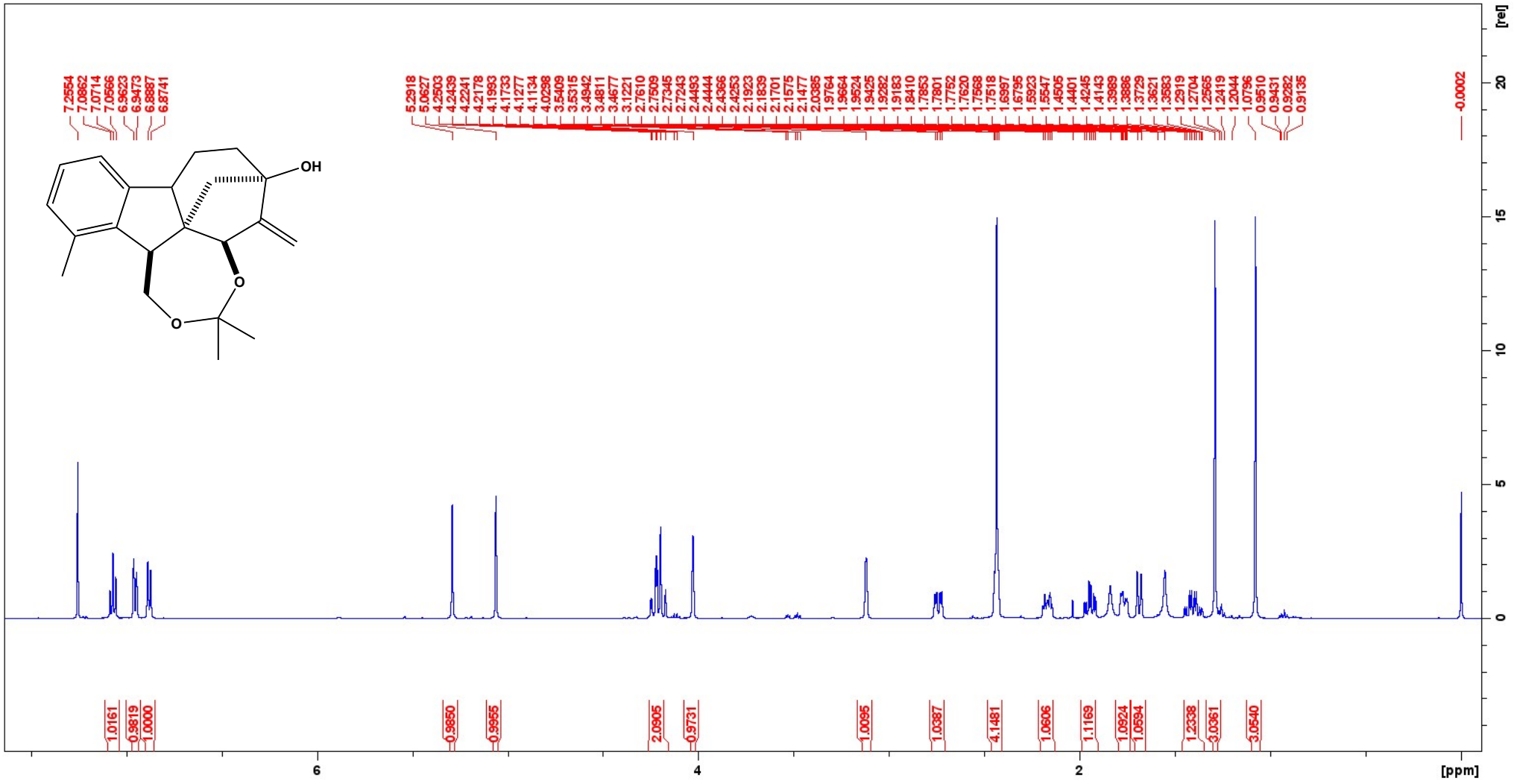
HSQC of (4b*R*,7*S*,9*S*,9a*R*,10*S*)-10-(Hydroxymethyl)-1-methyl-8-methylene-4b,5,6,8,9,10-hexahydro-7*H*-7,9a-methanobenzo[a]azulene-7,9-diol **6**



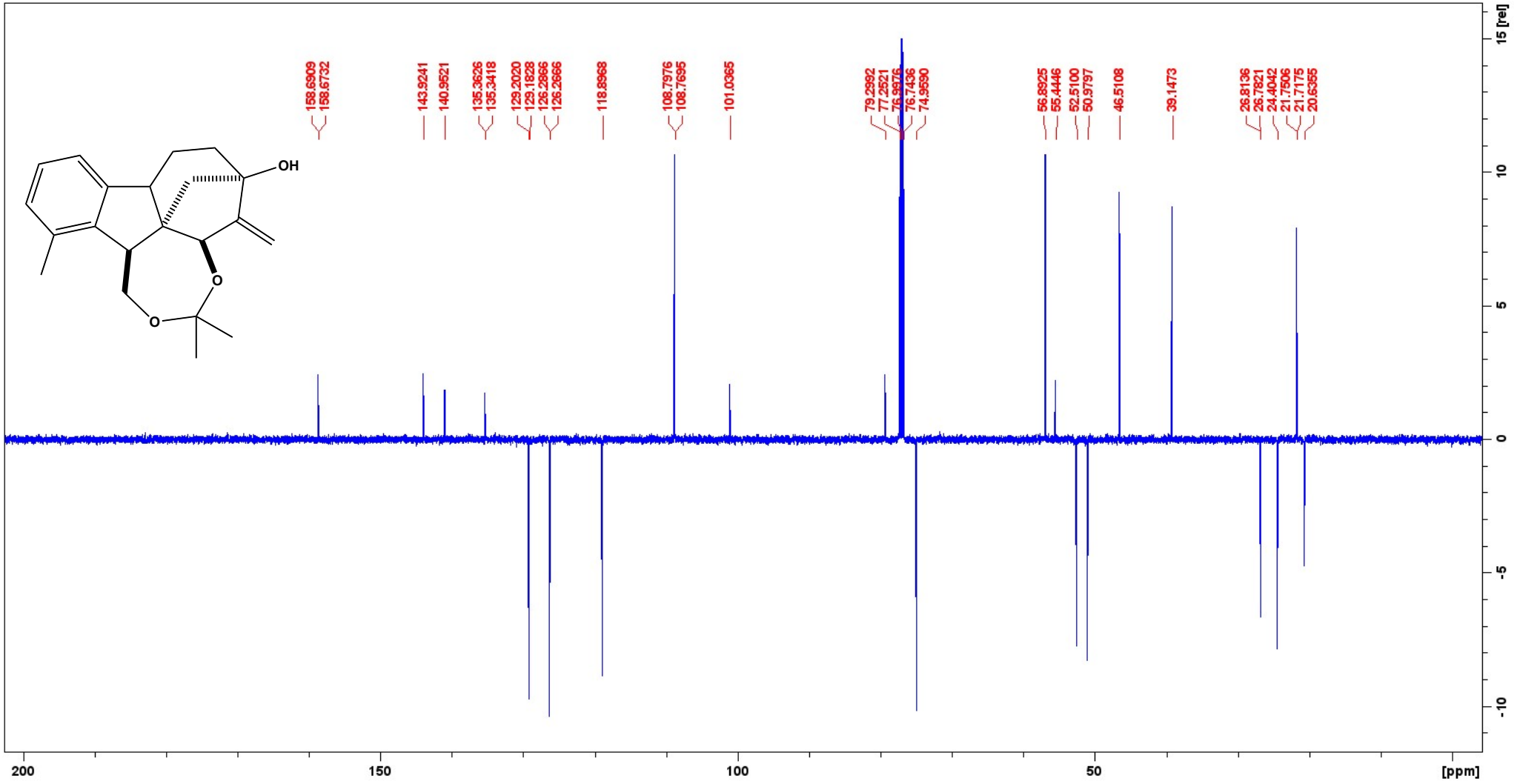
HMBC of (4b*R*,7*S*,9*S*,9a*R*,10*S*)-10-(Hydroxymethyl)-1-methyl-8-methylene-4b,5,6,8,9,10-hexahydro-7*H*-7,9a-methanobenzo[a]azulene-7,9-diol **6**



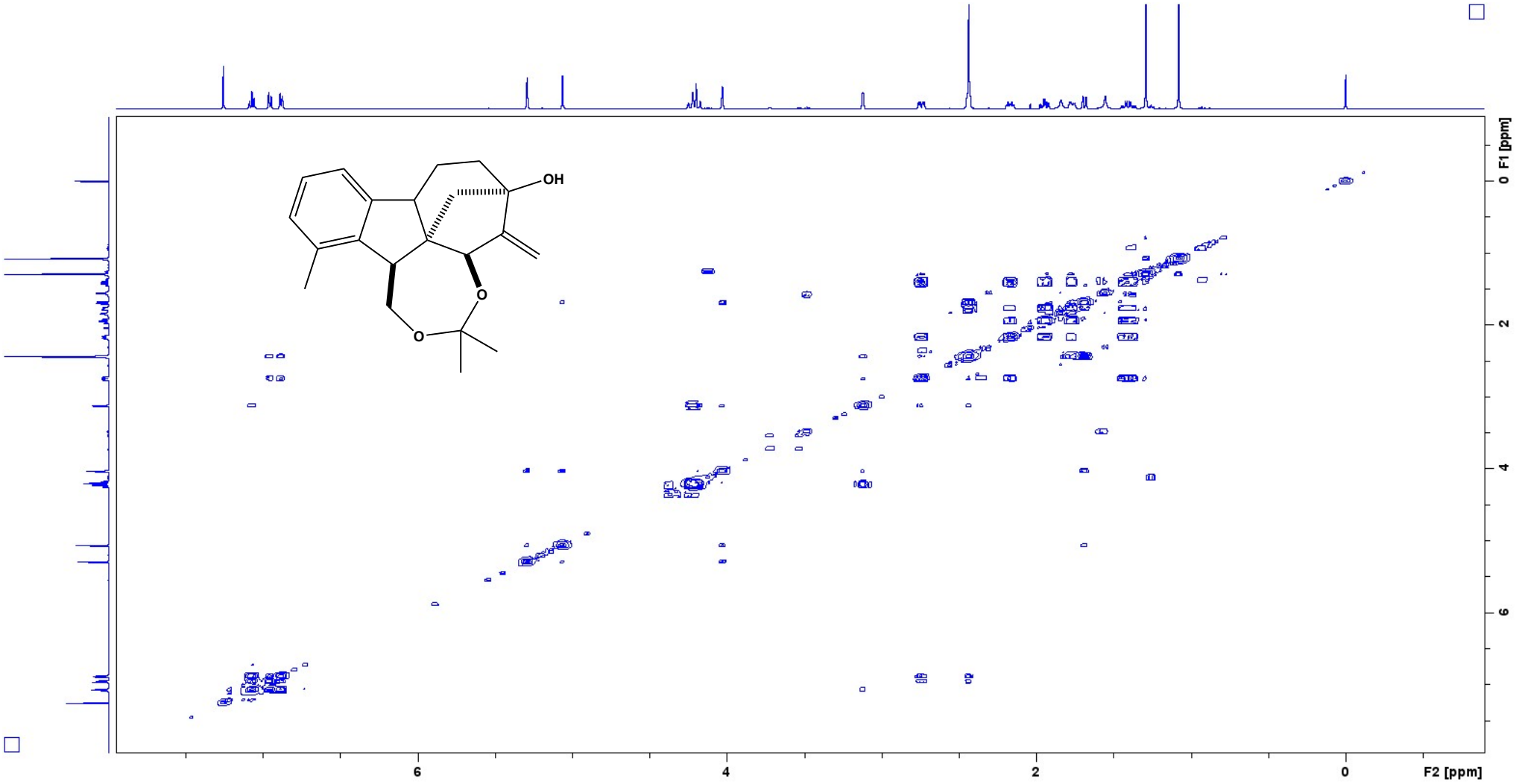
^{1}H-NMR (500 MHz) of (4a*R*,4a1*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-methylene-4a,5,7,8,8a,12b-hexahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepin-6(1*H*)-ol **7**



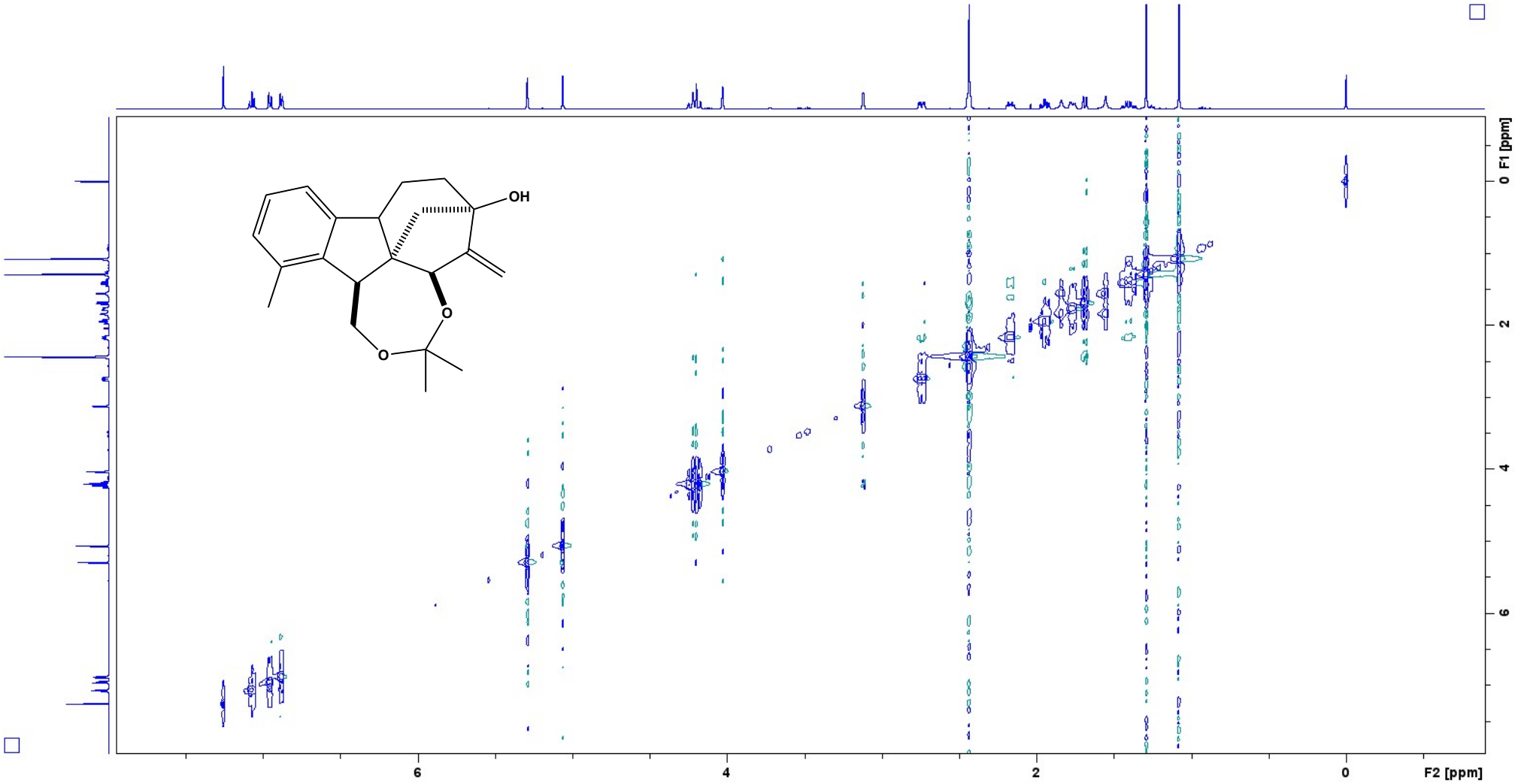
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of (4a*R*,4a1*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-methylene-4a,5,7,8,8a,12b-hexahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepin-6(1*H*)-ol **7**



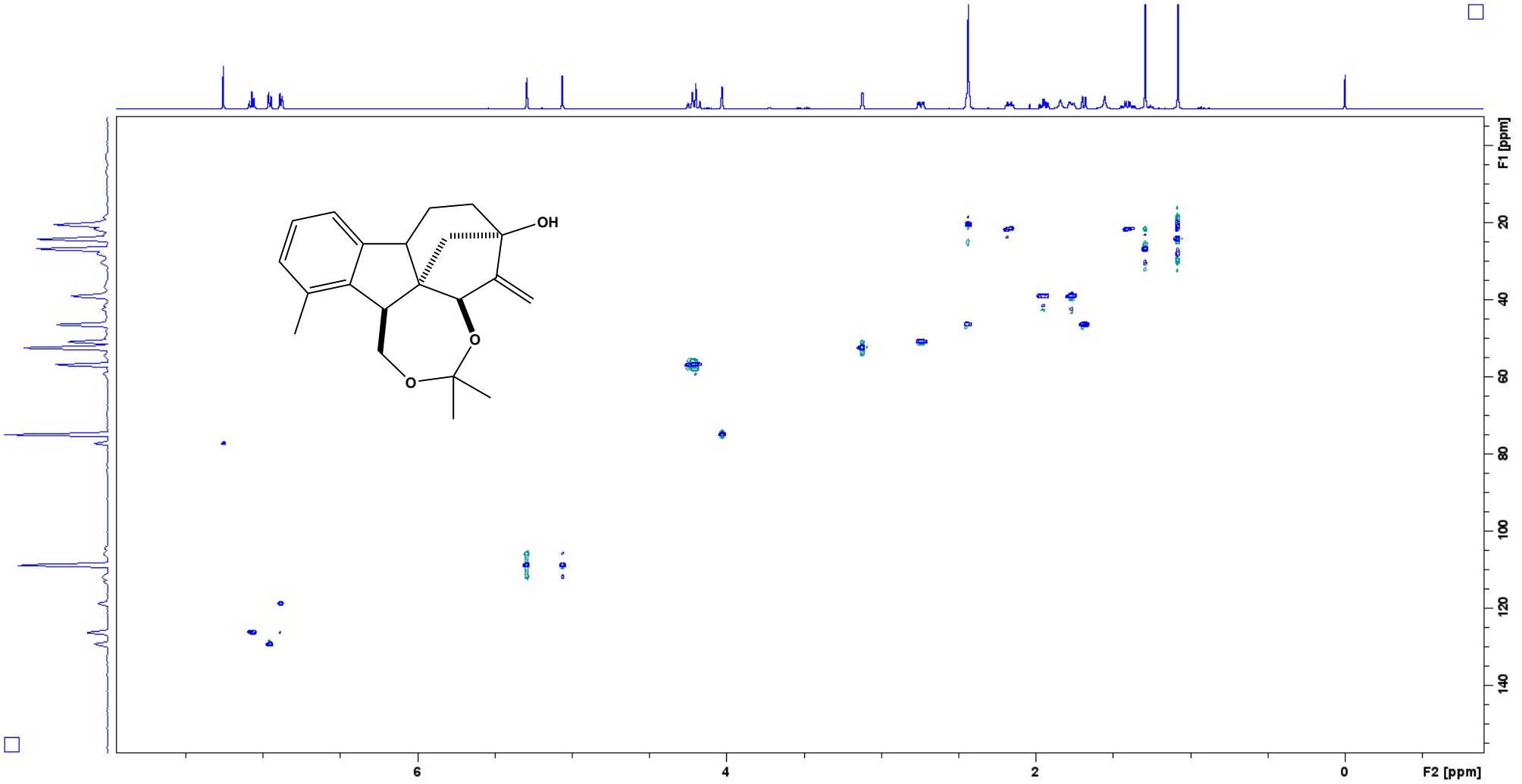
COSY of (4a*R*,4a1*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-methylene-4a,5,7,8,8a,12b-hexahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepin-6(1*H*)-ol **7**



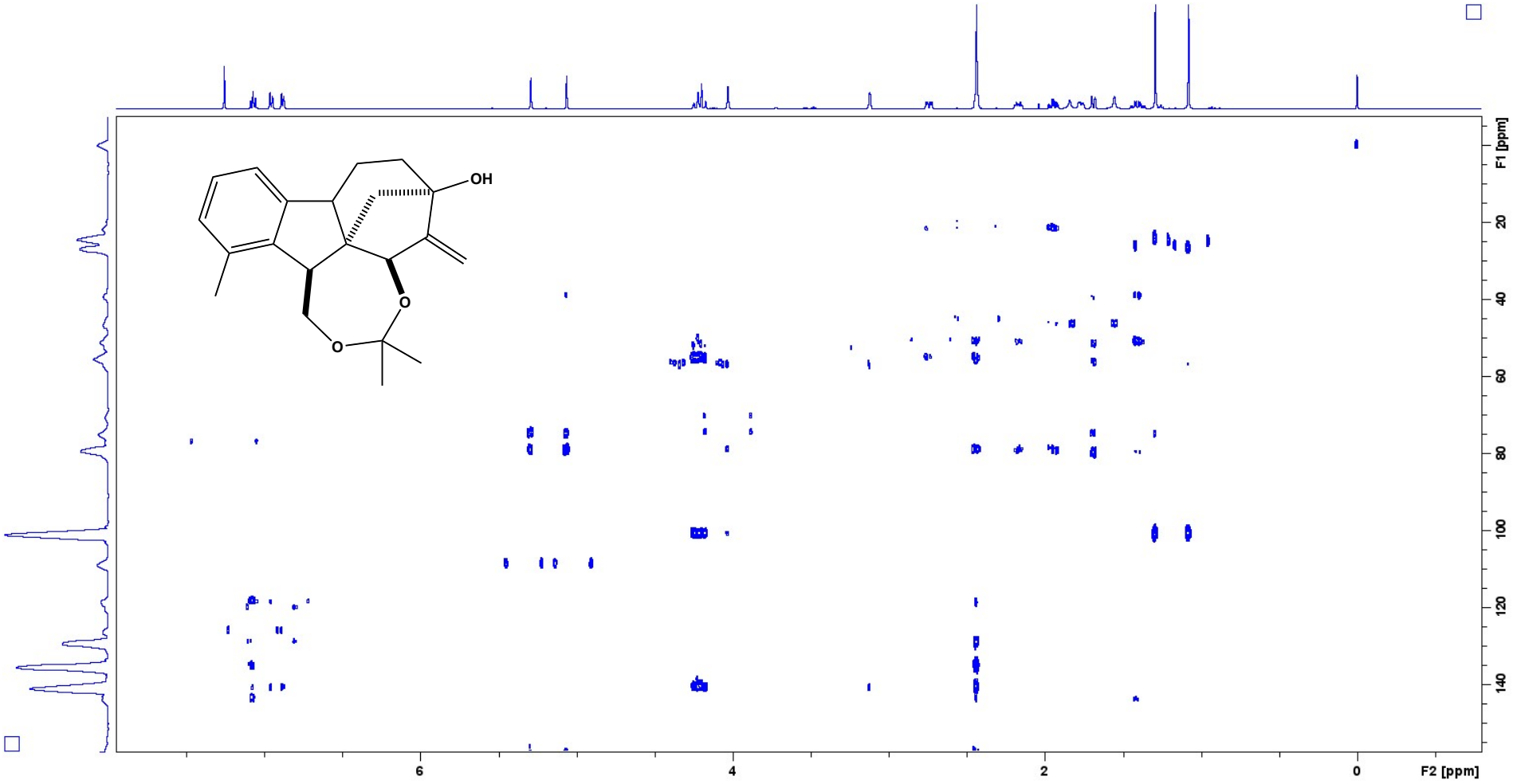
NOESY of (4a*R*,4a1*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-methylene-4a,5,7,8,8a,12b-hexahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepin-6(1*H*)-ol **7**



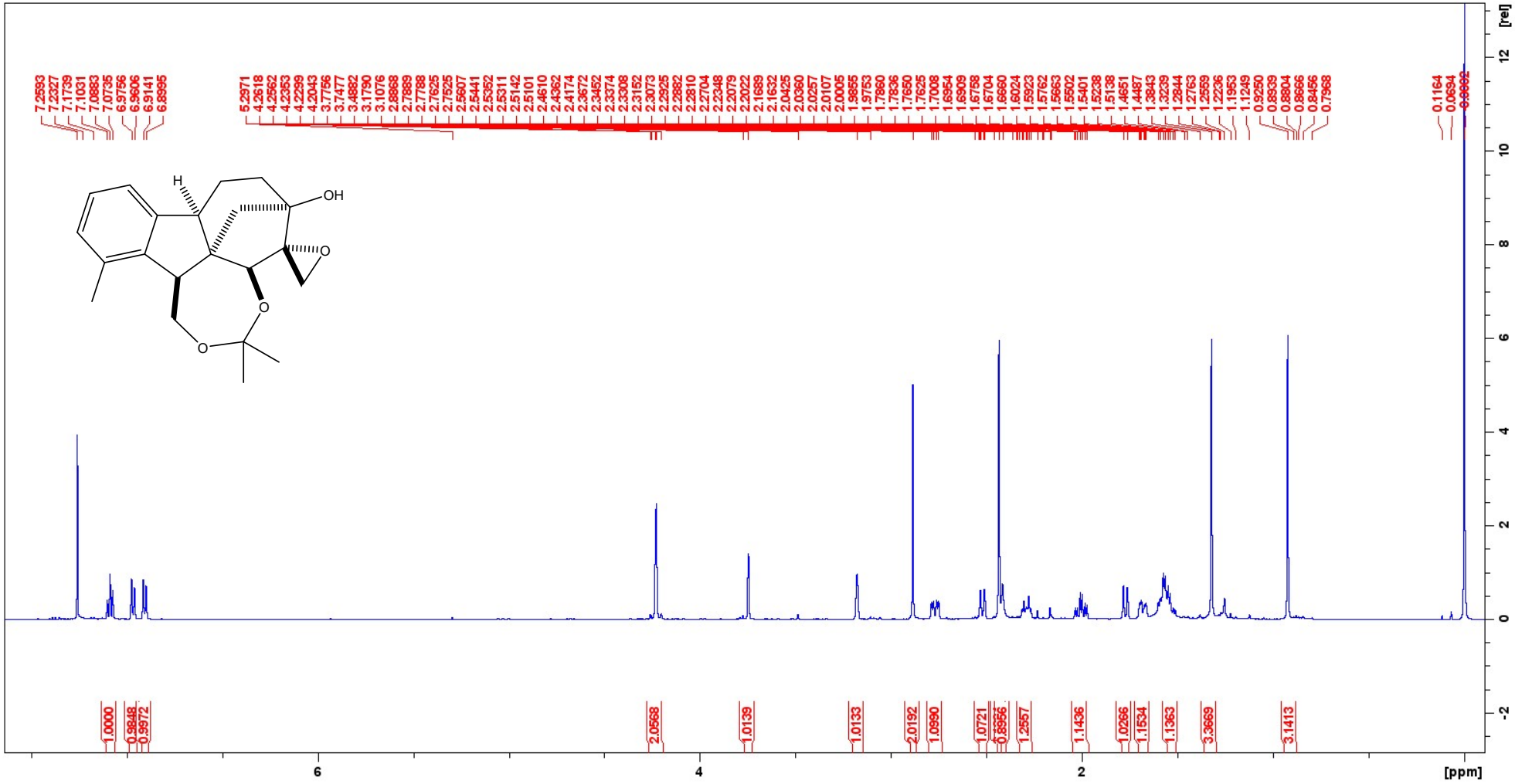
HSQC of (4a*R*,4a1*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-methylene-4a,5,7,8,8a,12b-hexahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepin-6(1*H*)-ol **7**



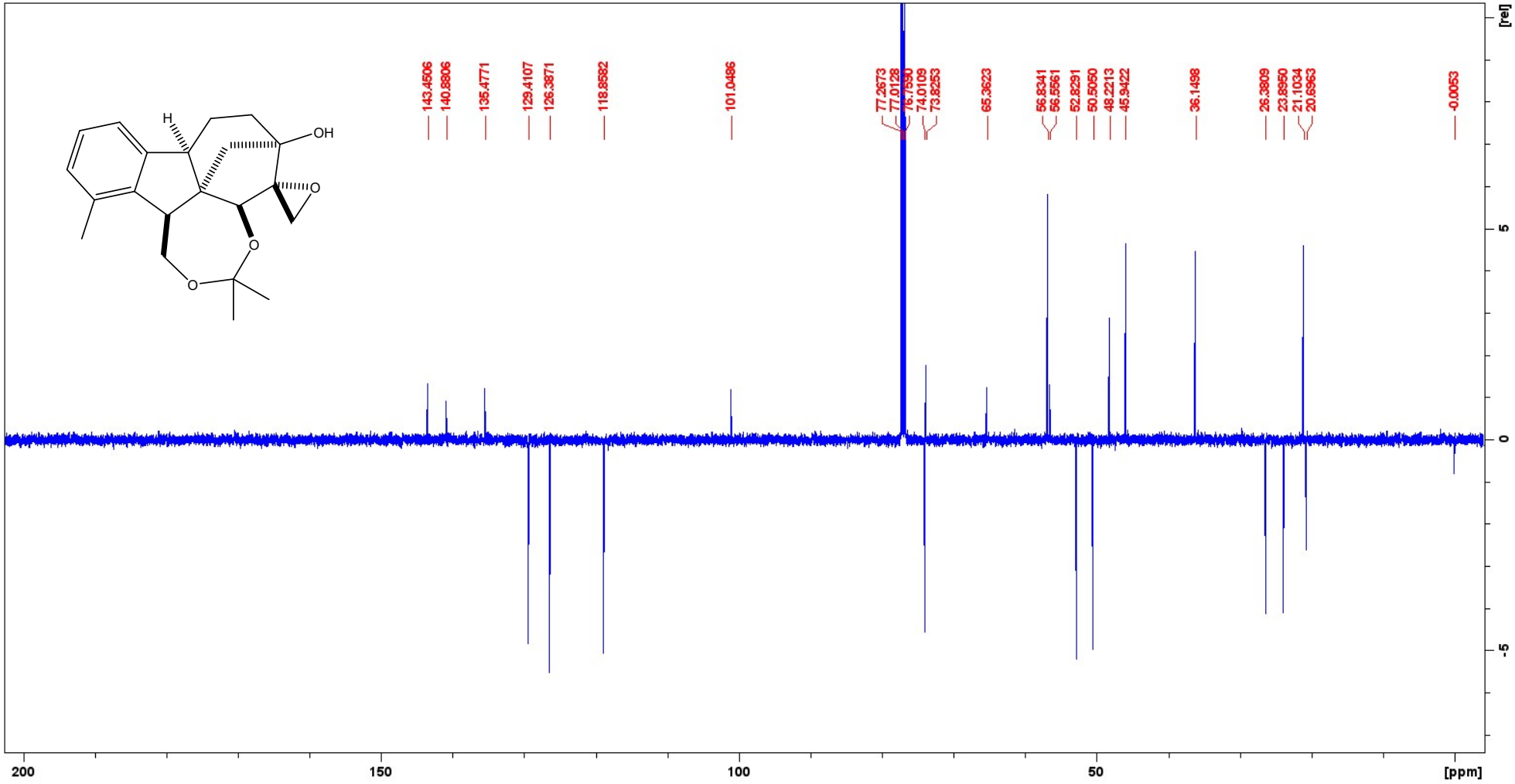
HMBC of (4a*R*,4a1*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-methylene-4a,5,7,8,8a,12b-hexahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepin-6(1*H*)-ol **7**



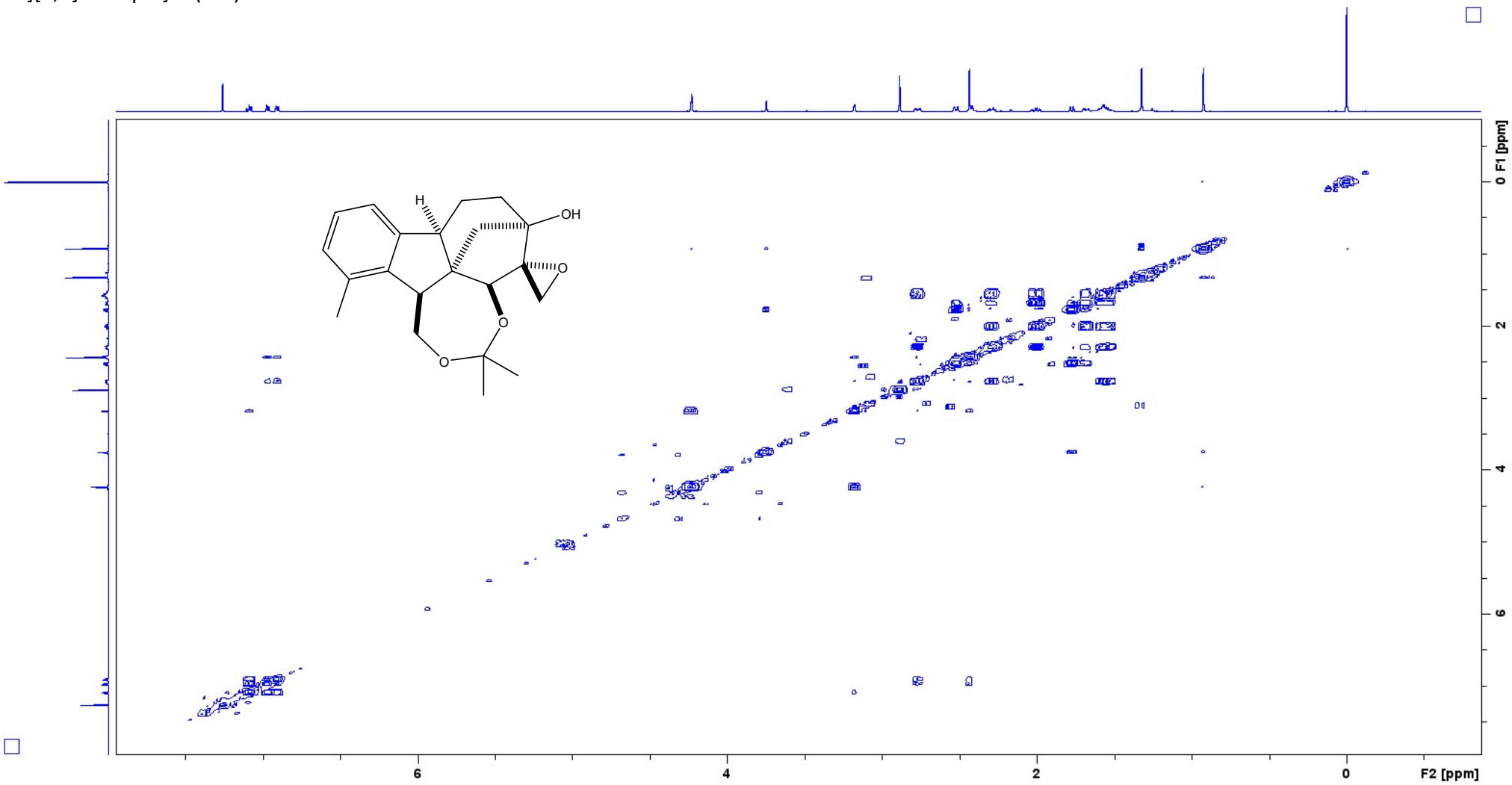
^{1}H-NMR (500 MHz) of (2*R*,4a'*S*,4a^{1}'*R*,6'S,12b'S)-3',3',12'-Trimethyl-7',8',8a',12b'-tetrahydro-4a'H-spiro[oxirane-2,5'-[4a^{1},6]methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepin]-6'(1'*H*)-ol **8**



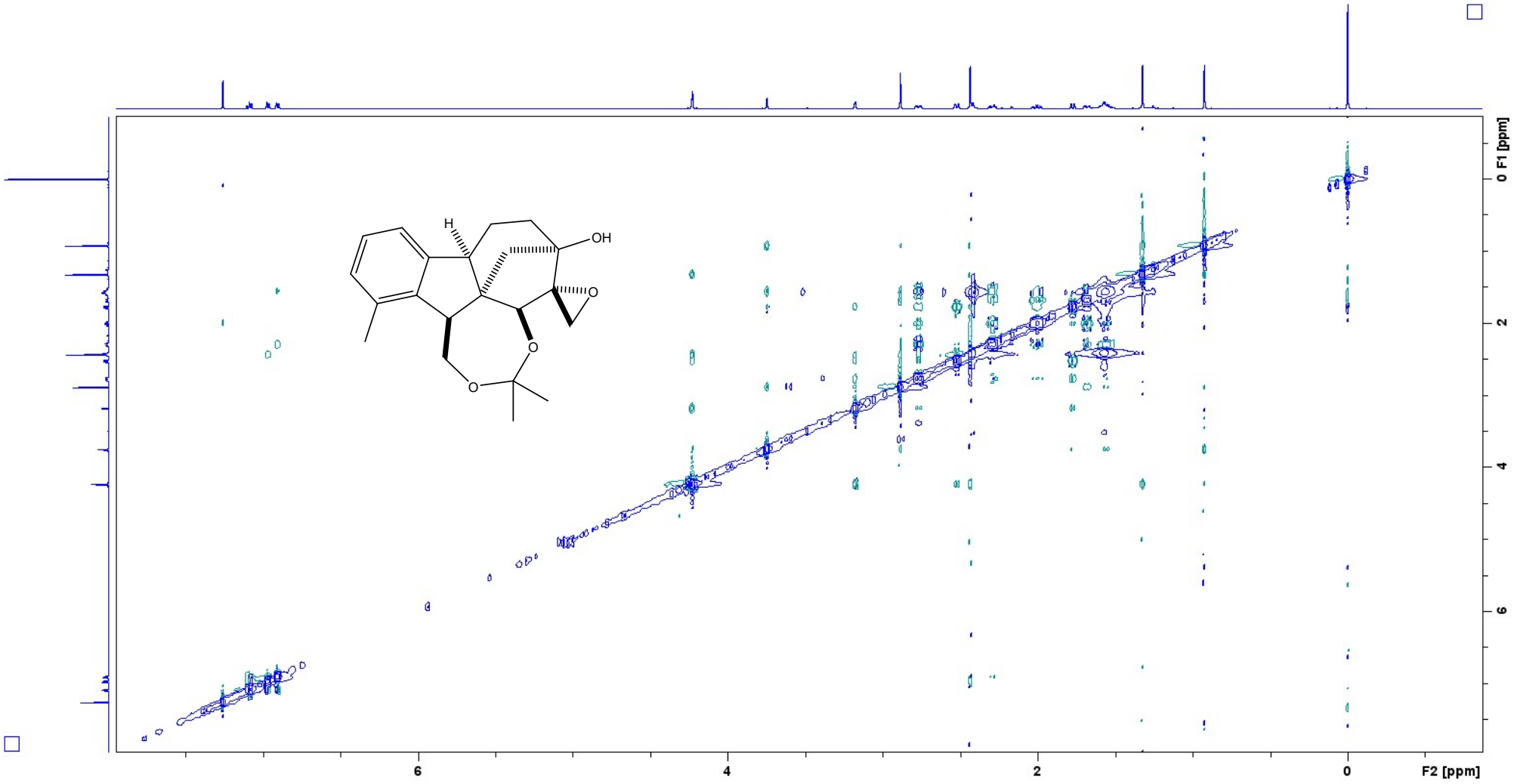
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of (2*R*,4a'*S*,4a^{1}'*R*,6'S,12b'S)-3',3',12'-Trimethyl-7',8',8a',12b'-tetrahydro-4a'H-spiro[oxirane-2,5'-[4a^{1},6]methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepin]-6'(1'*H*)-ol **8**



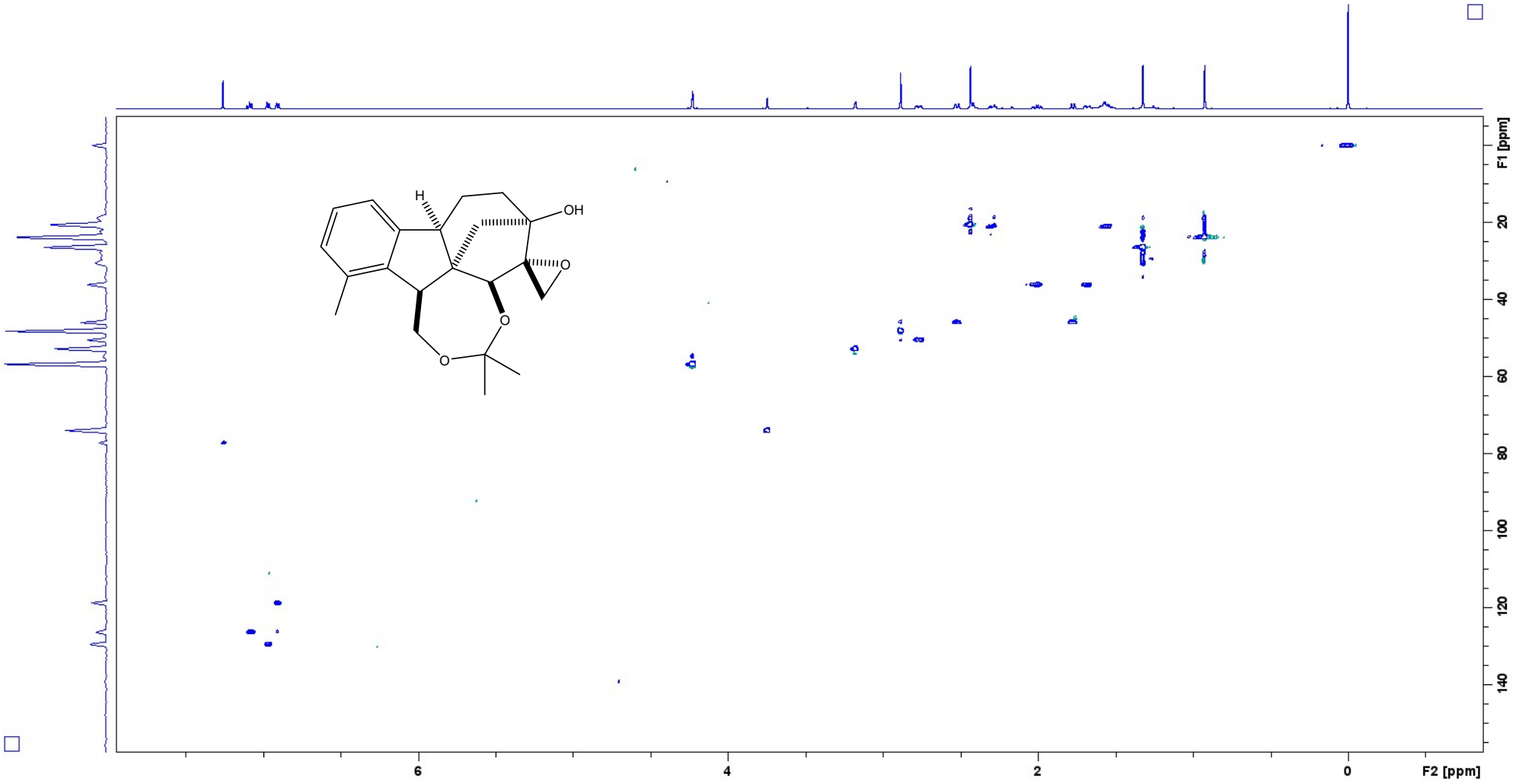
COSY of (2*R*,4a'*S*,4a[1]'*R*,6'S,12b'S)-3',3',12'-Trimethyl-7',8',8a',12b'-tetrahydro-4a'H-spiro[oxirane-2,5'-[4a[1],6]methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepin]-6'(1'*H*)-ol **8**



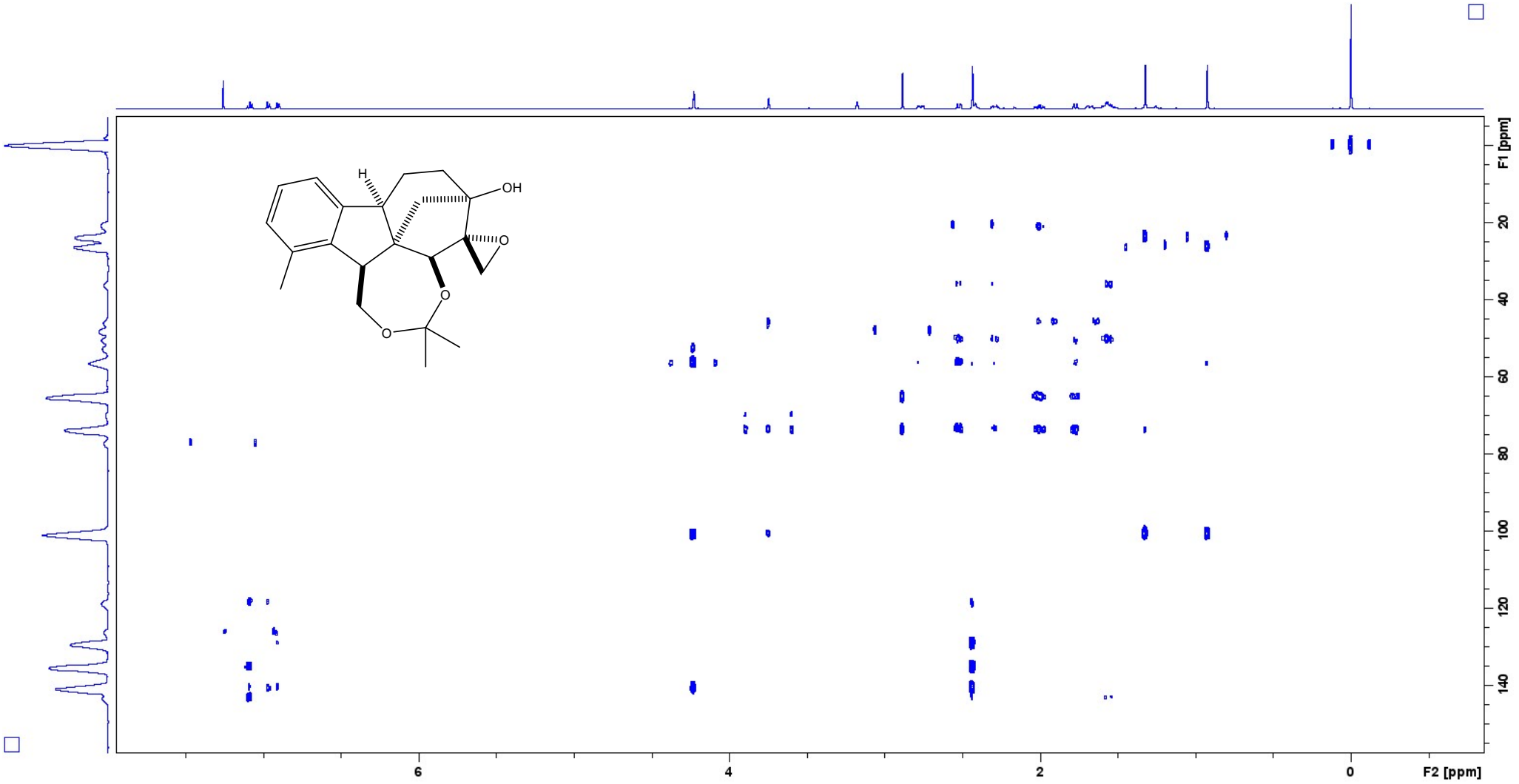
NOESY of (2*R*,4a'*S*,4a[1]'*R*,6'S,12b'S)-3',3',12'-Trimethyl-7',8',8a',12b'-tetrahydro-4a'H-spiro[oxirane-2,5'-[4a[1],6]methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepin]-6'(1'*H*)-ol **8**



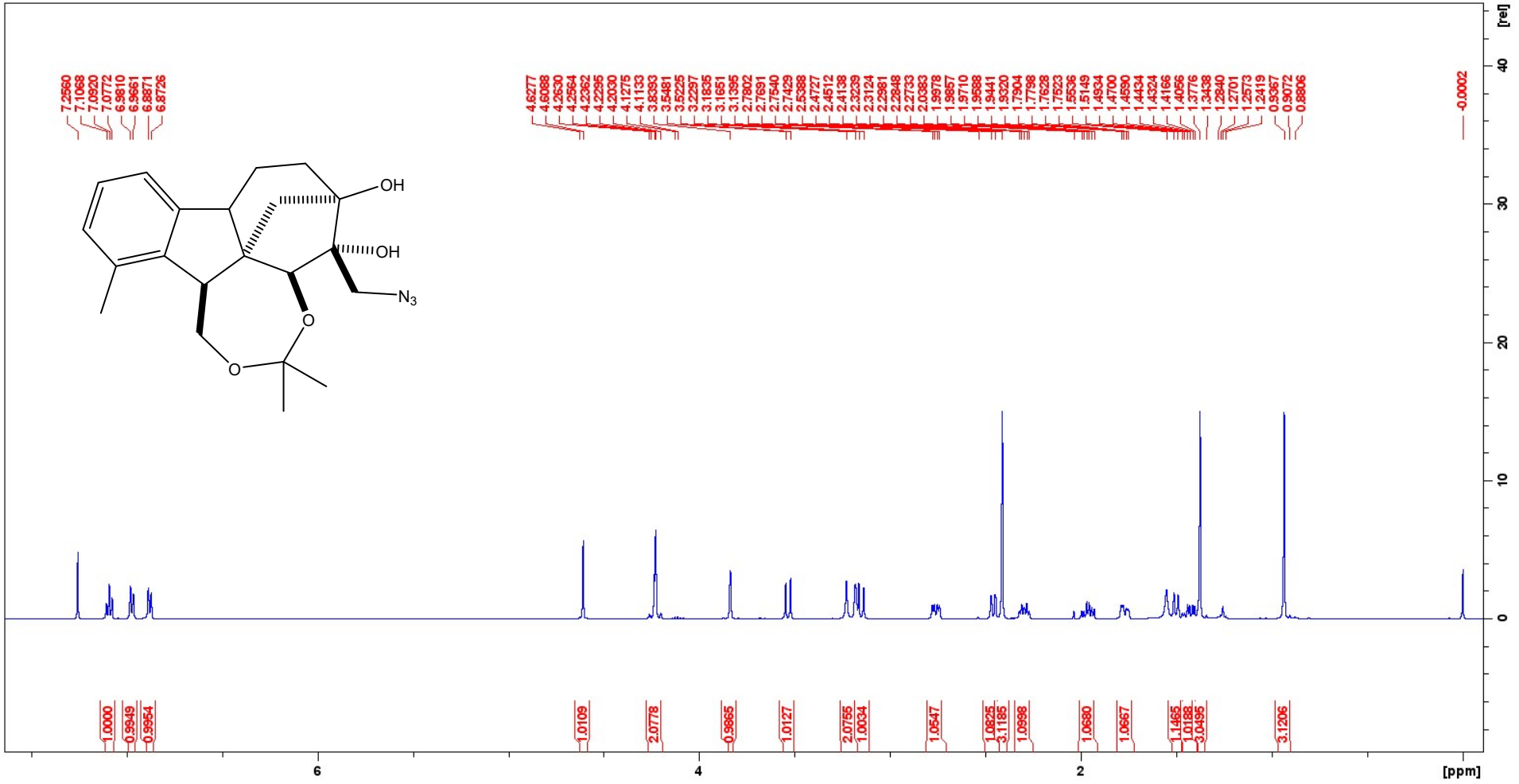
HSQC of (2*R*,4a'*S*,4a[1]'*R*,6'S,12b'S)-3',3',12'-Trimethyl-7',8',8a',12b'-tetrahydro-4a'H-spiro[oxirane-2,5'-[4a[1],6]methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepin]-6'(1'*H*)-ol **8**



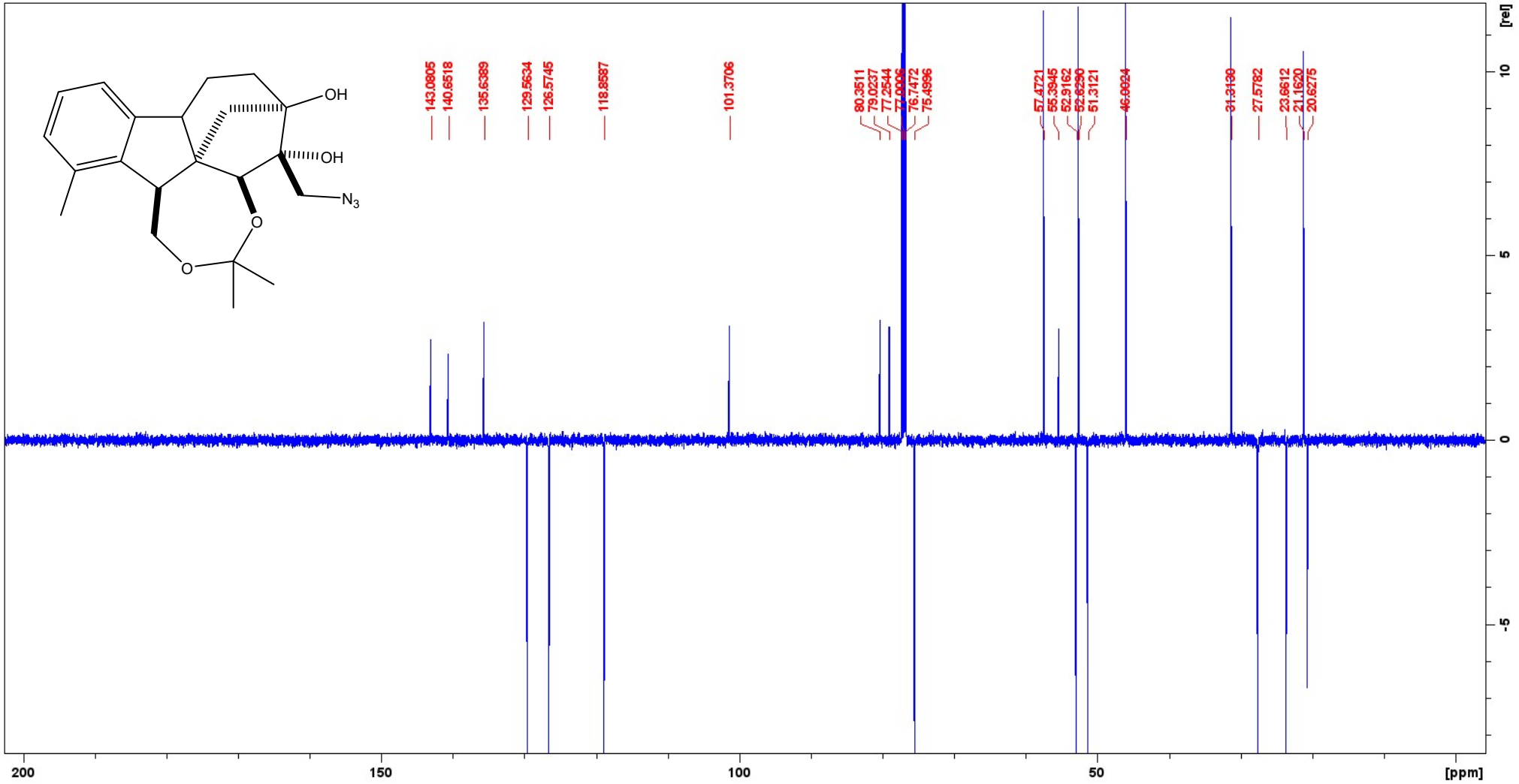
HMBC of (2*R*,4a'*S*,4a^{1}'*R*,6'S,12b'S)-3',3',12'-Trimethyl-7',8',8a',12b'-tetrahydro-4a'H-spiro[oxirane-2,5'-[4a^{1},6]methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepin]-6'(1'*H*)-ol **8**



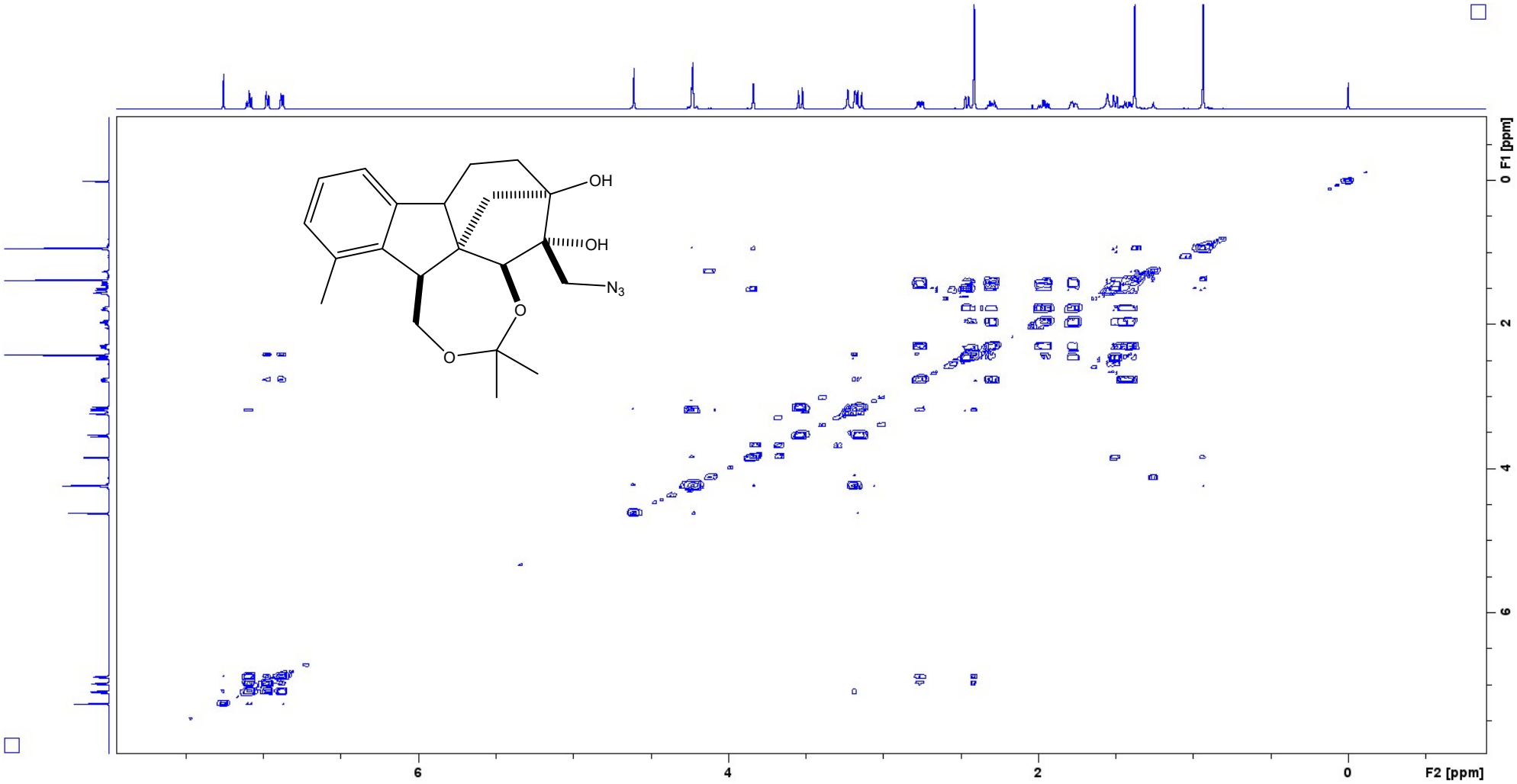
^{1}H-NMR (500 MHz) of (4a*R*,4a^{1}*R*,5*R*,6*S*,12b*S*)-5-(Azidomethyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^{1},6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1H)-diol **29**



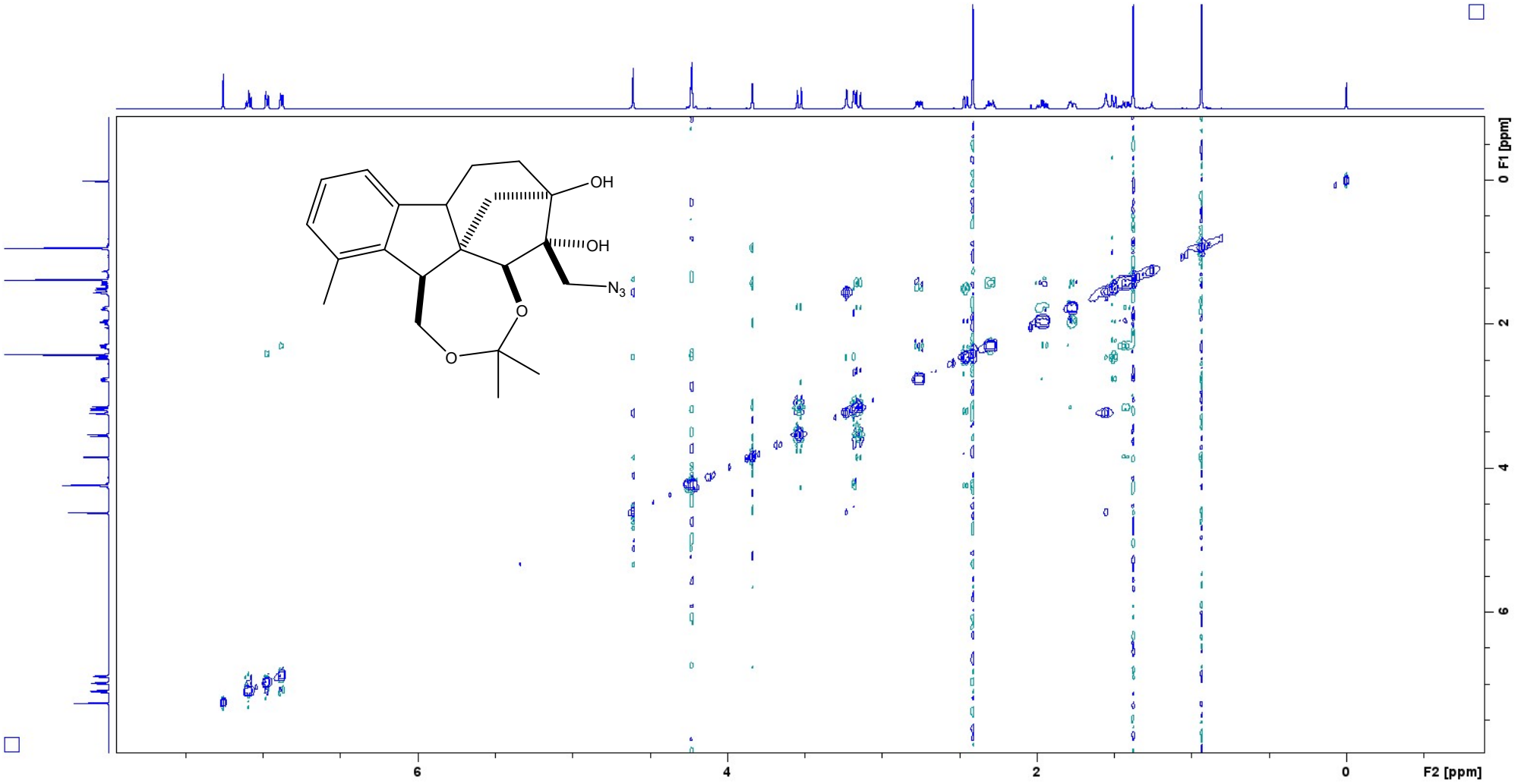
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of (4a*R*,4a^{1}*R*,5*R*,6*S*,12b*S*)-5-(Azidomethyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^{1},6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1H)-diol **29**



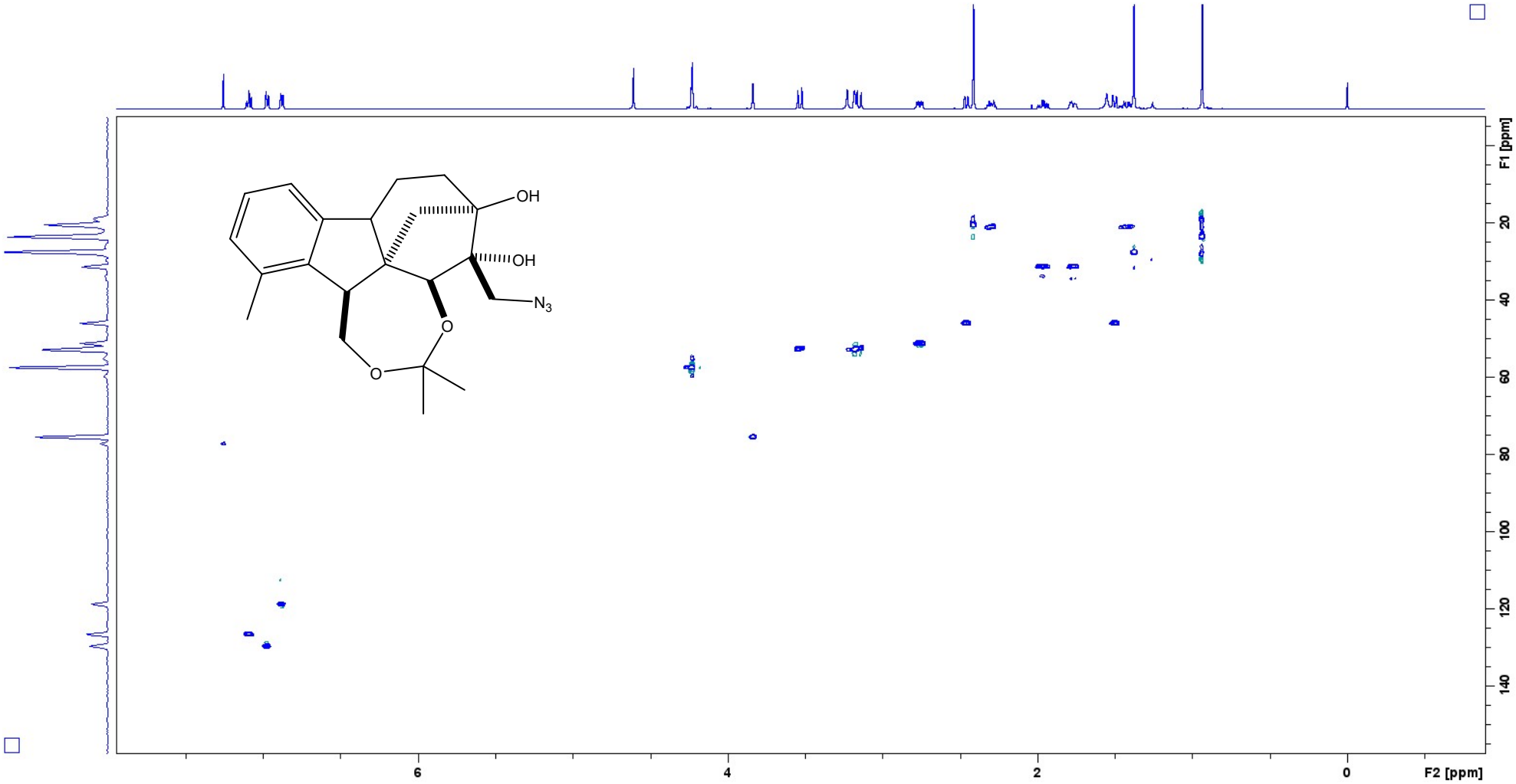
COSY of (4a*R*,4a^1*R*,5*R*,6*S*,12b*S*)-5-(Azidomethyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1H)-diol **29**



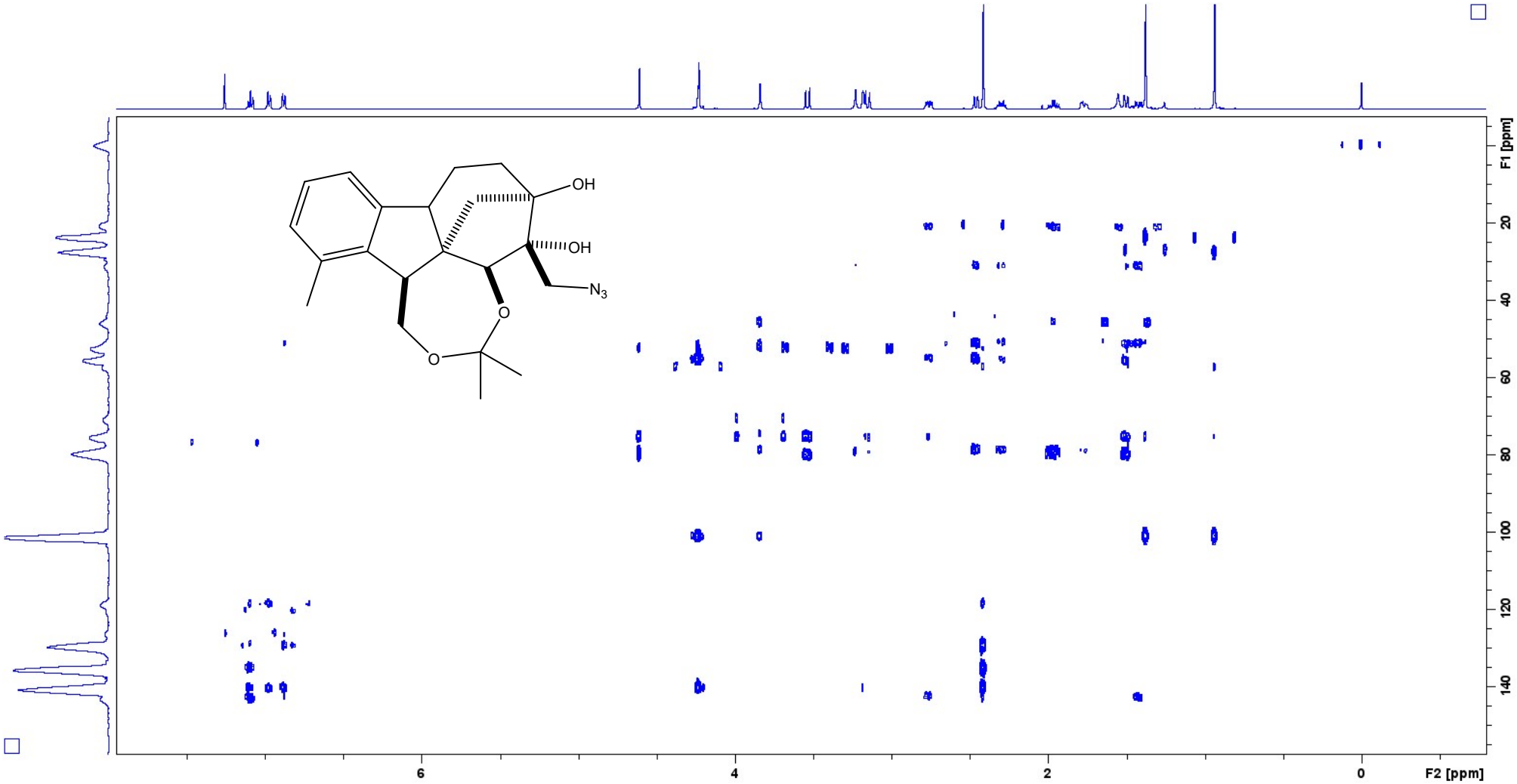
NOESY of (4a*R*,4a^1*R*,5*R*,6*S*,12b*S*)-5-(Azidomethyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1H)-diol **29**



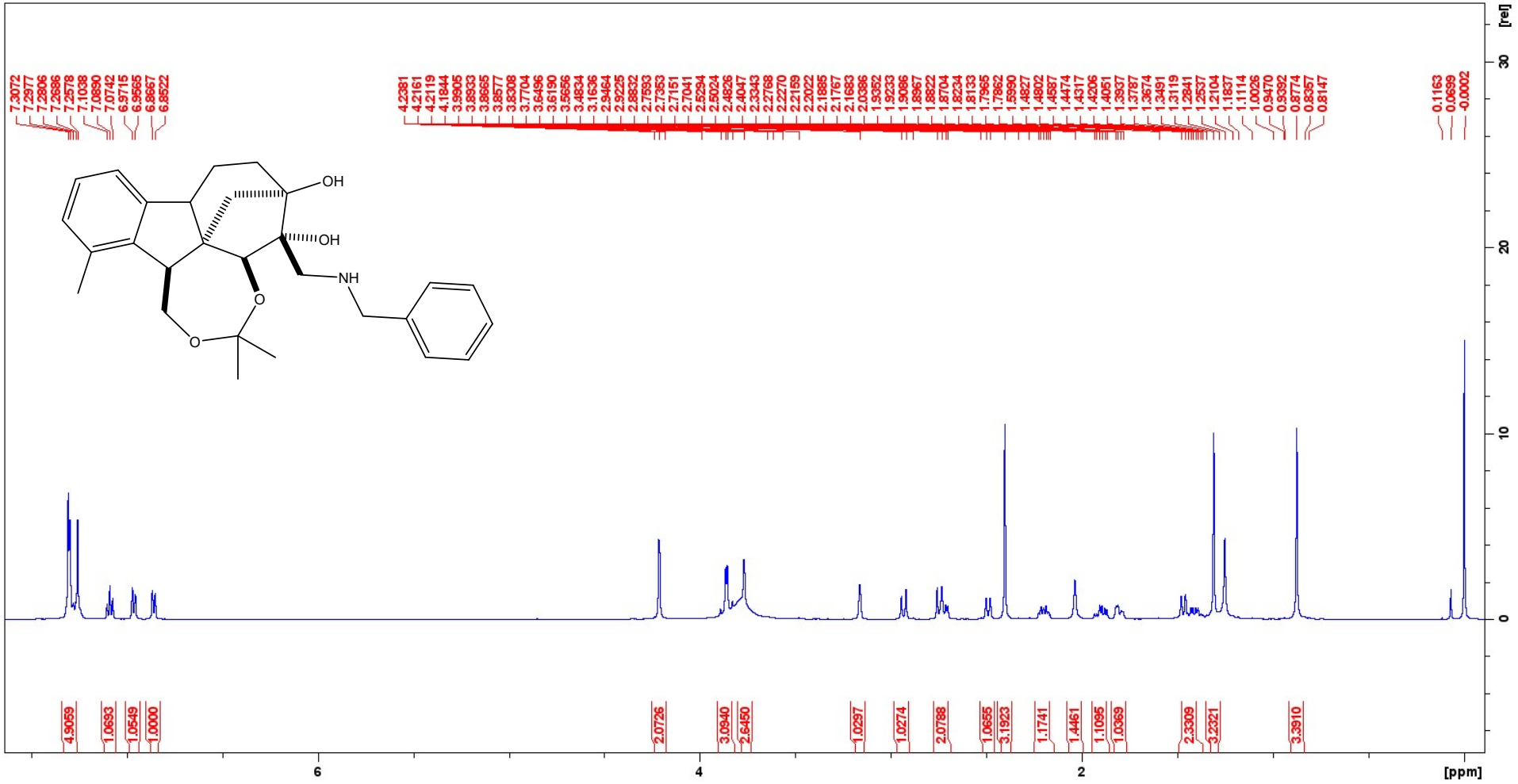
HSQC of (4a*R*,4a^1*R*,5*R*,6*S*,12b*S*)-5-(Azidomethyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1H)-diol **29**



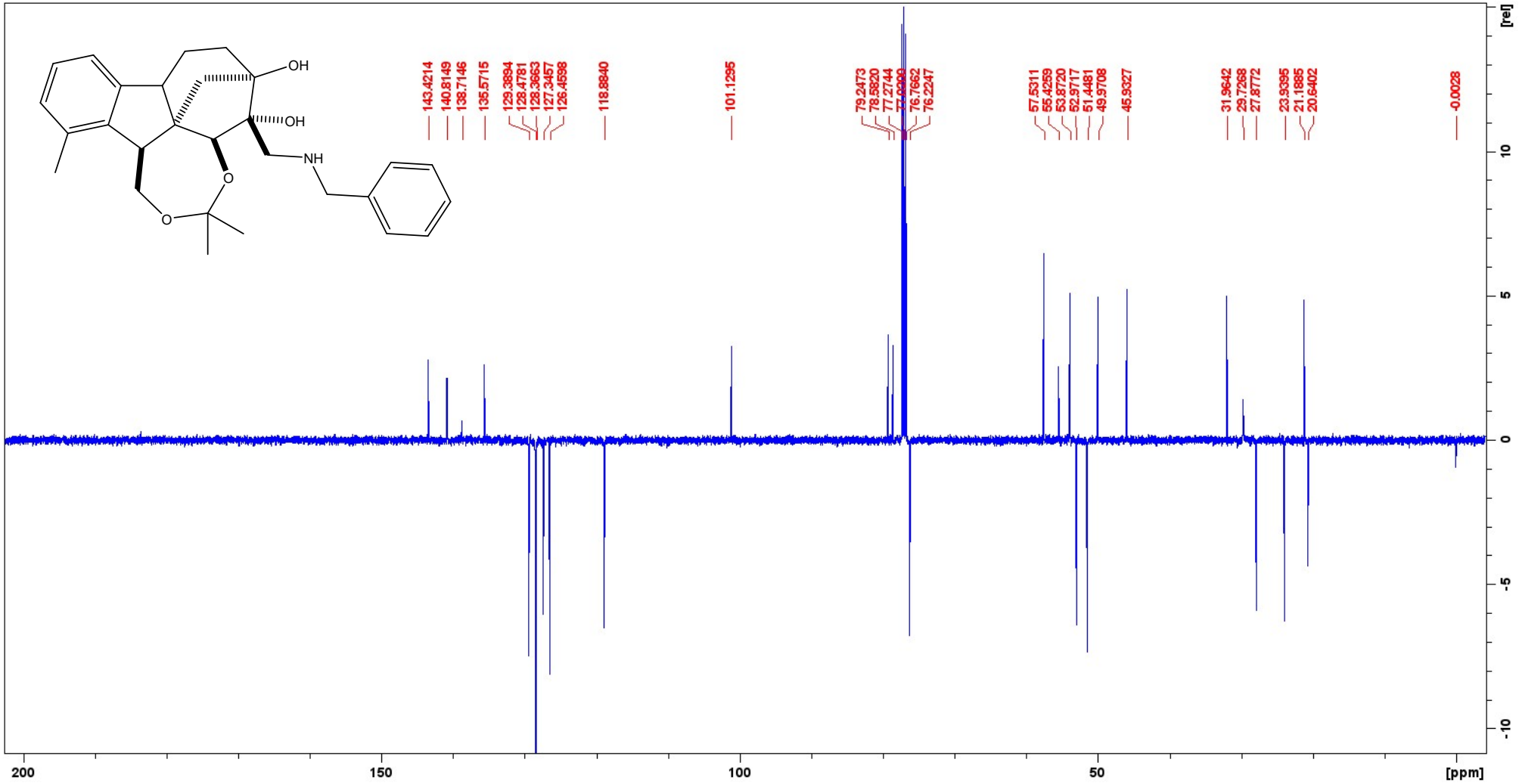
HMBC of (4a*R*,4a^1*R*,5*R*,6*S*,12b*S*)-5-(Azidomethyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1H)-diol **29**



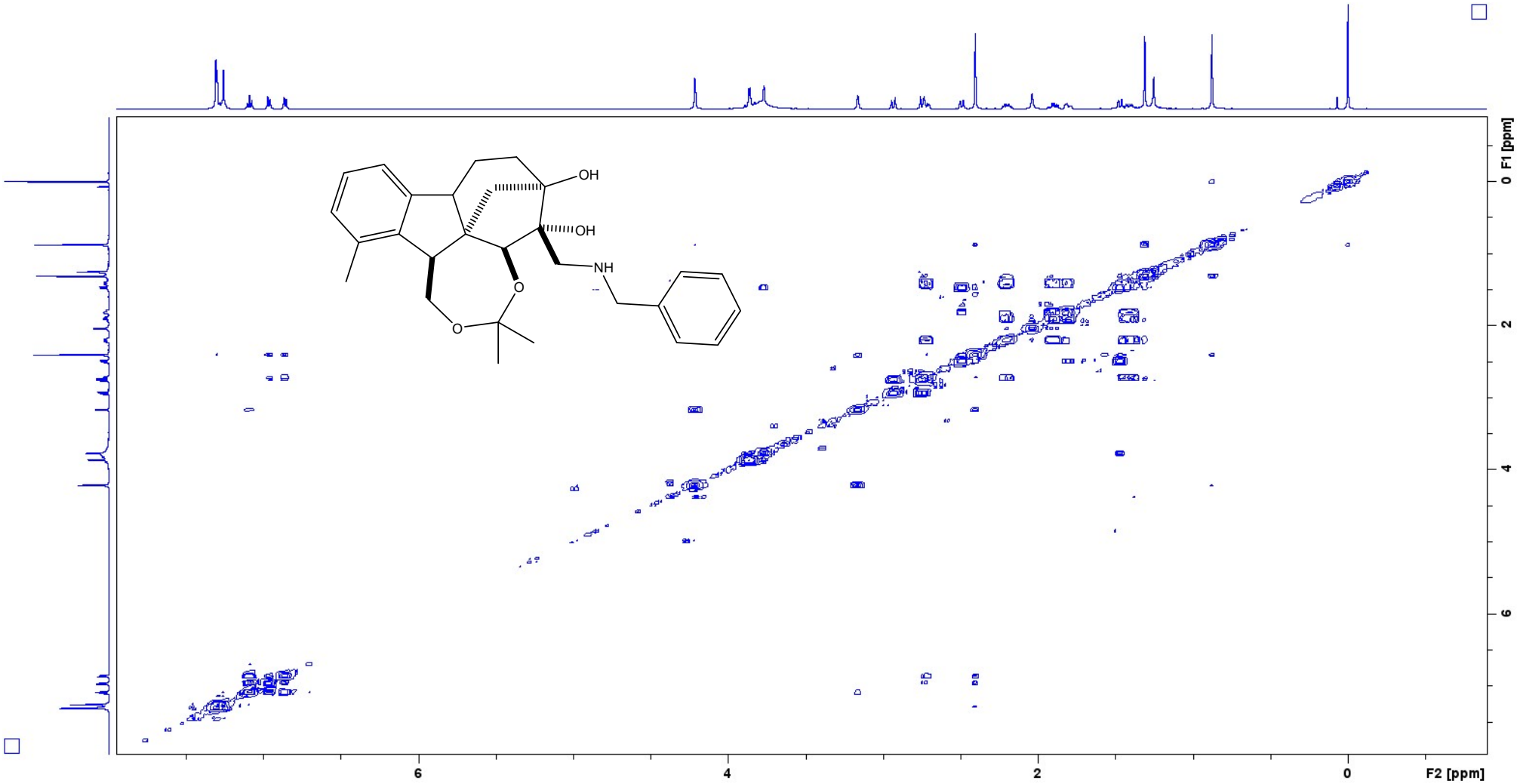
^{1}H-NMR (500 MHz) of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-5-((Benzylamino)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^{1},6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **9**



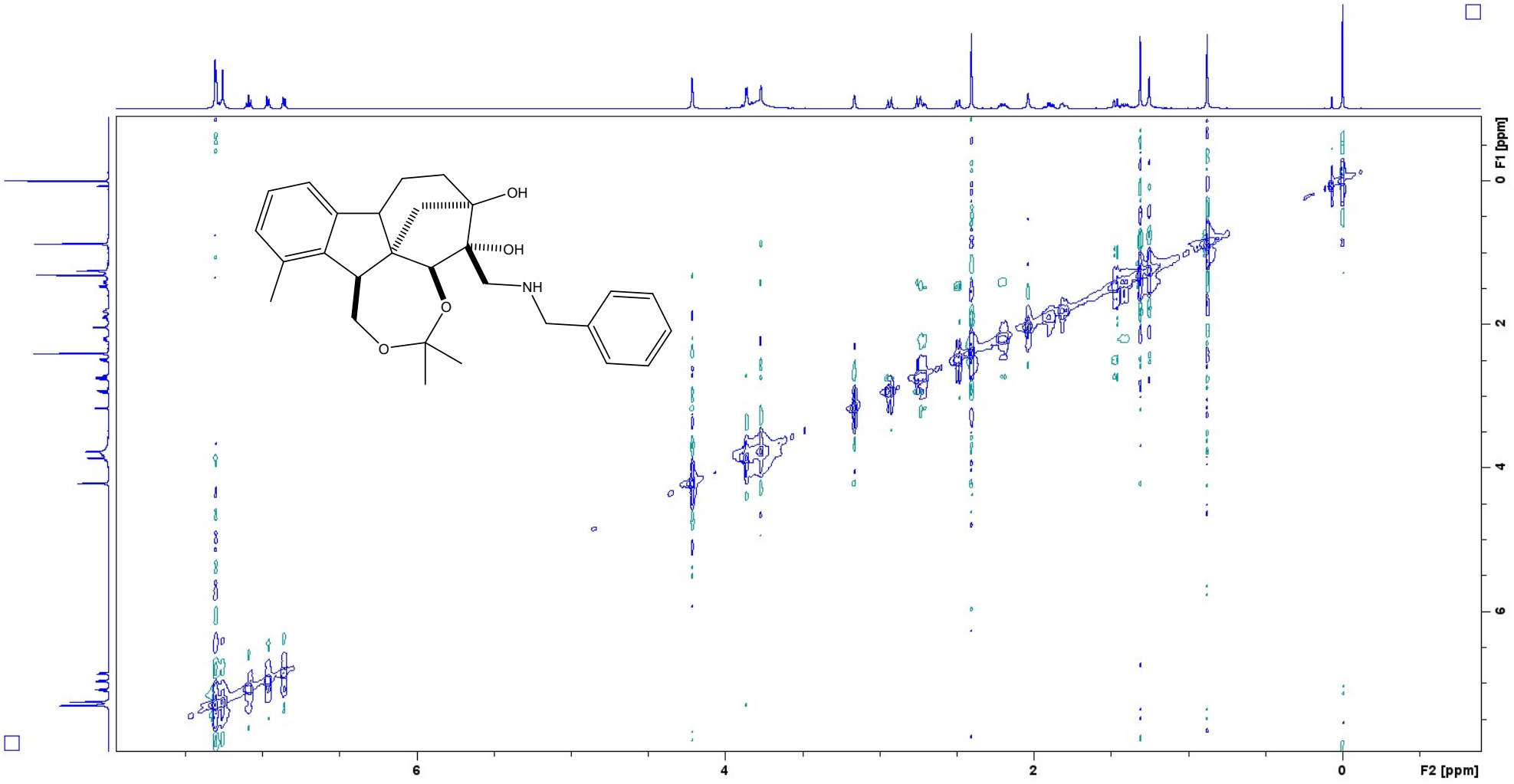
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-5-((Benzylamino)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^{1},6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **9**



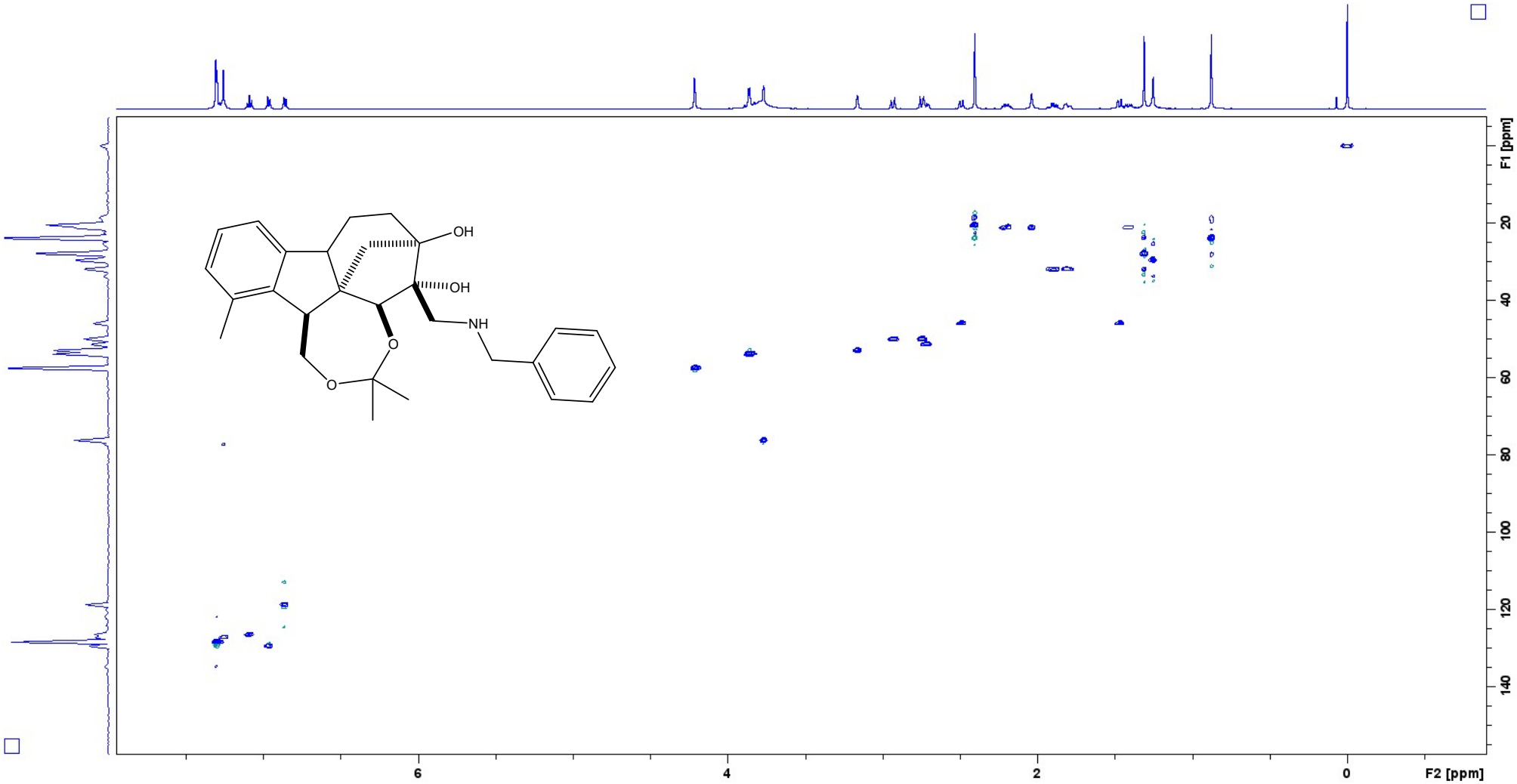
COSY of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-5-((Benzylamino)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **9**



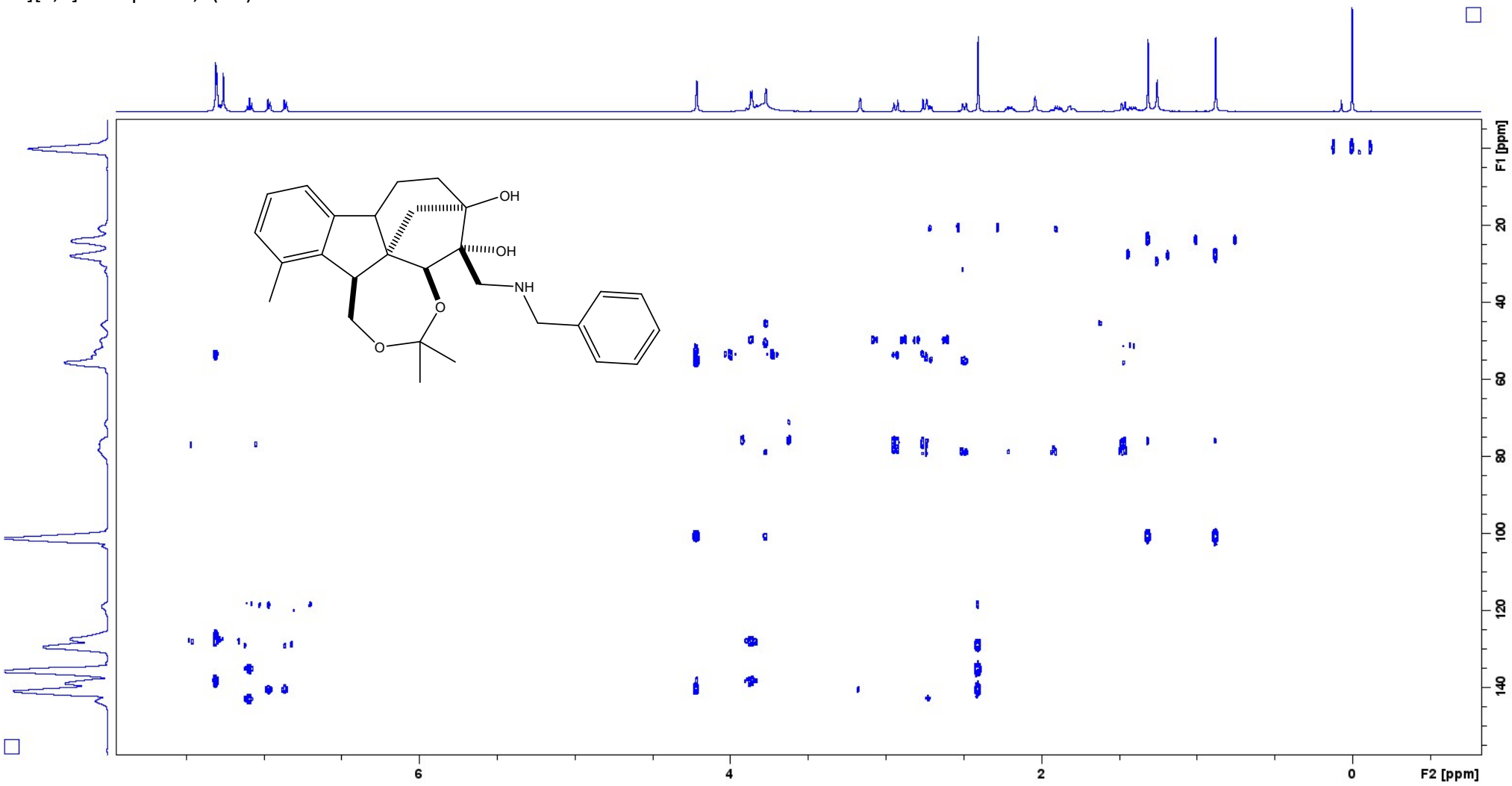
NOESY of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-5-((Benzylamino)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **9**



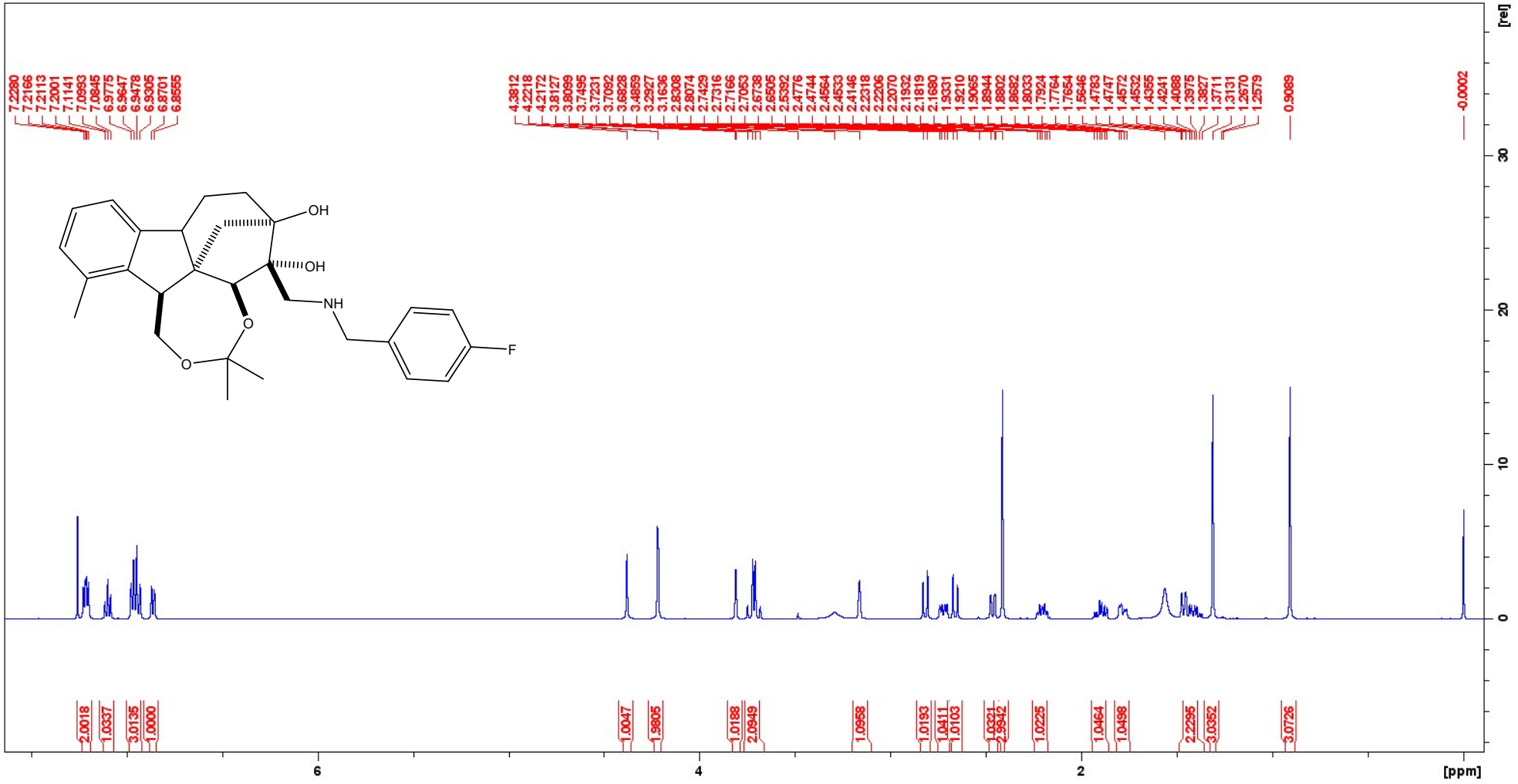
HSQC of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-5-((Benzylamino)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **9**



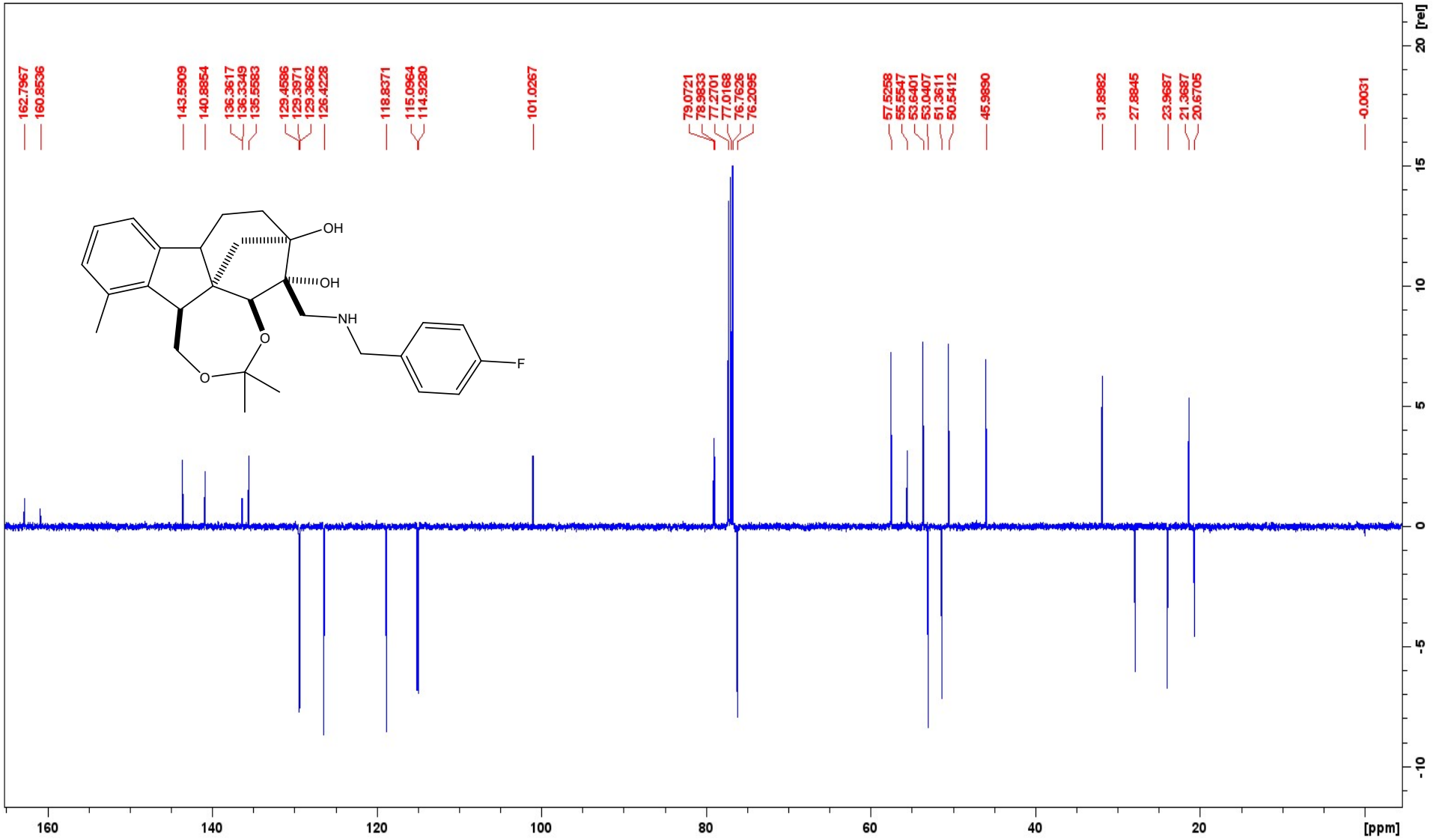
HMBC of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-5-((Benzylamino)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **9**



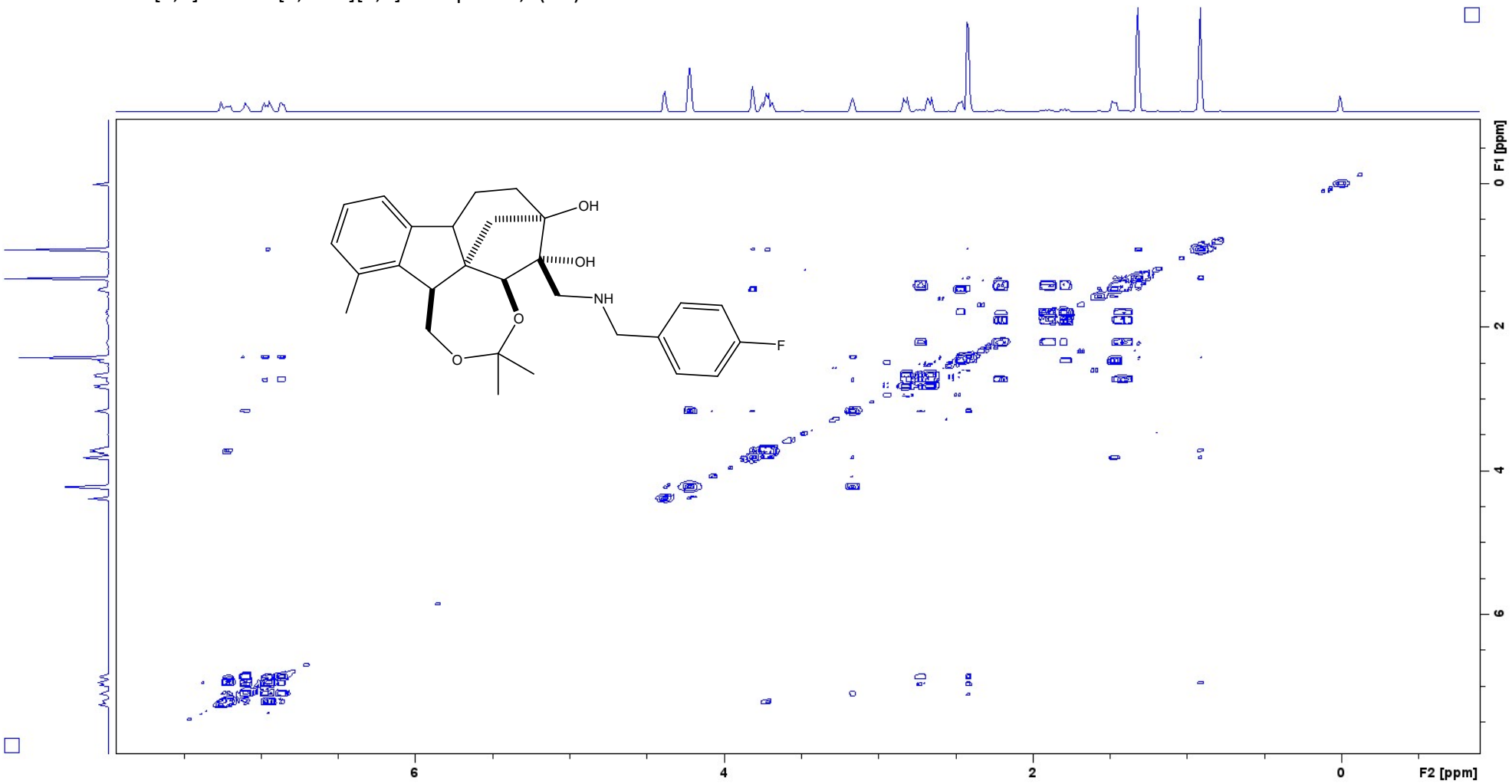
^{1}H-NMR (500 MHz) of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-5-(((4-Fluorobenzyl)amino)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^{1},6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **10**



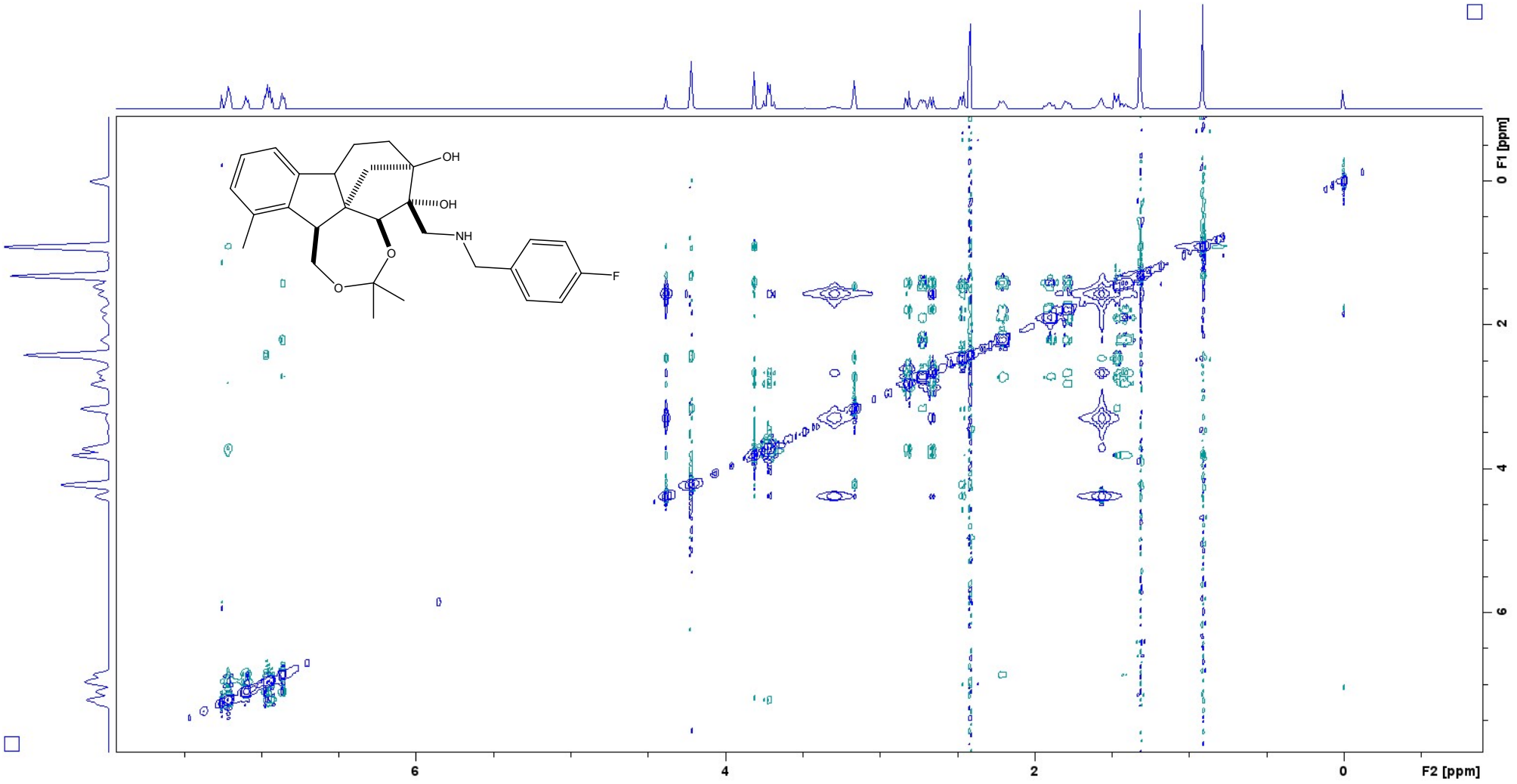
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-5-(((4-Fluorobenzyl)amino)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^{1},6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **10**



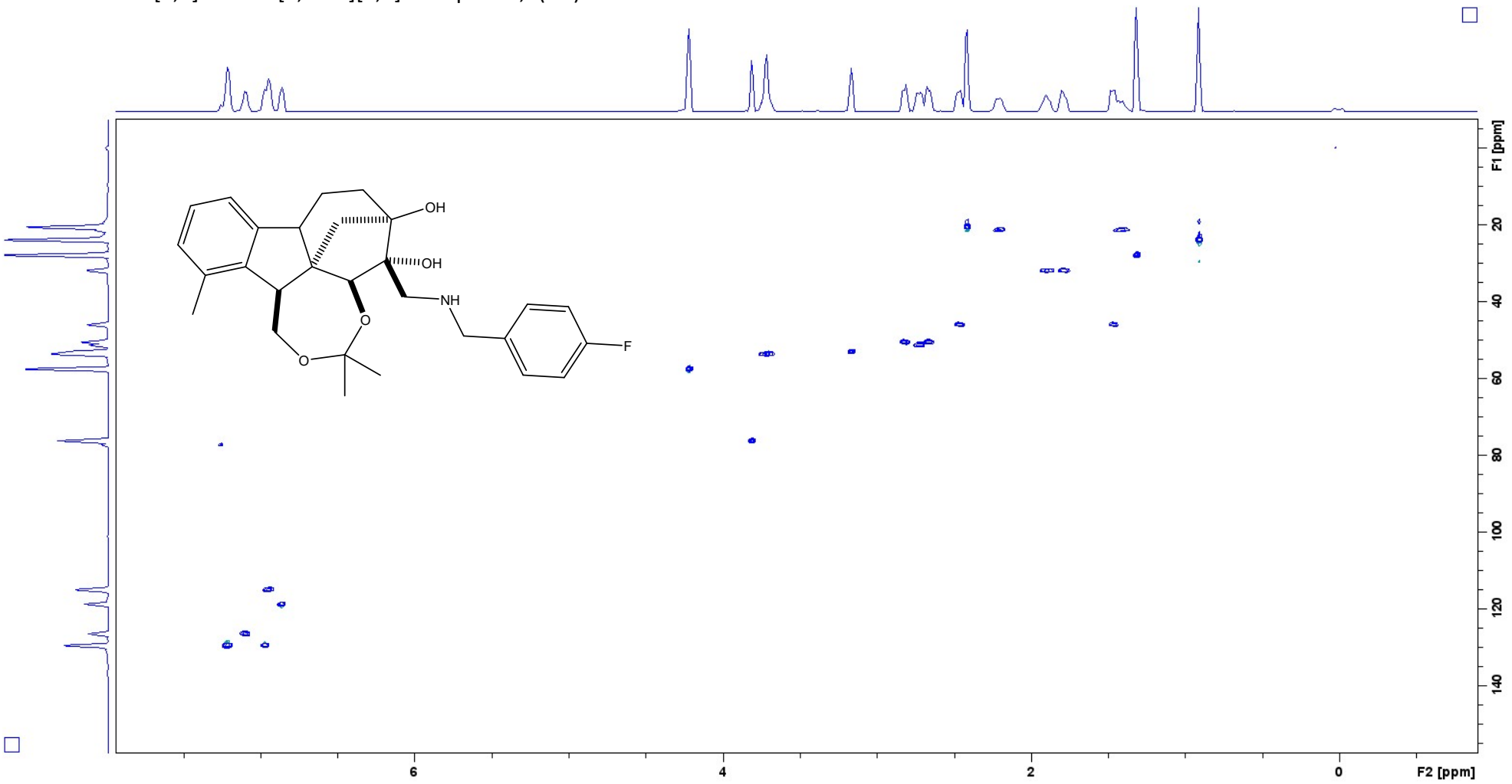
COSY of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-5-(((4-Fluorobenzyl)amino)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **10**



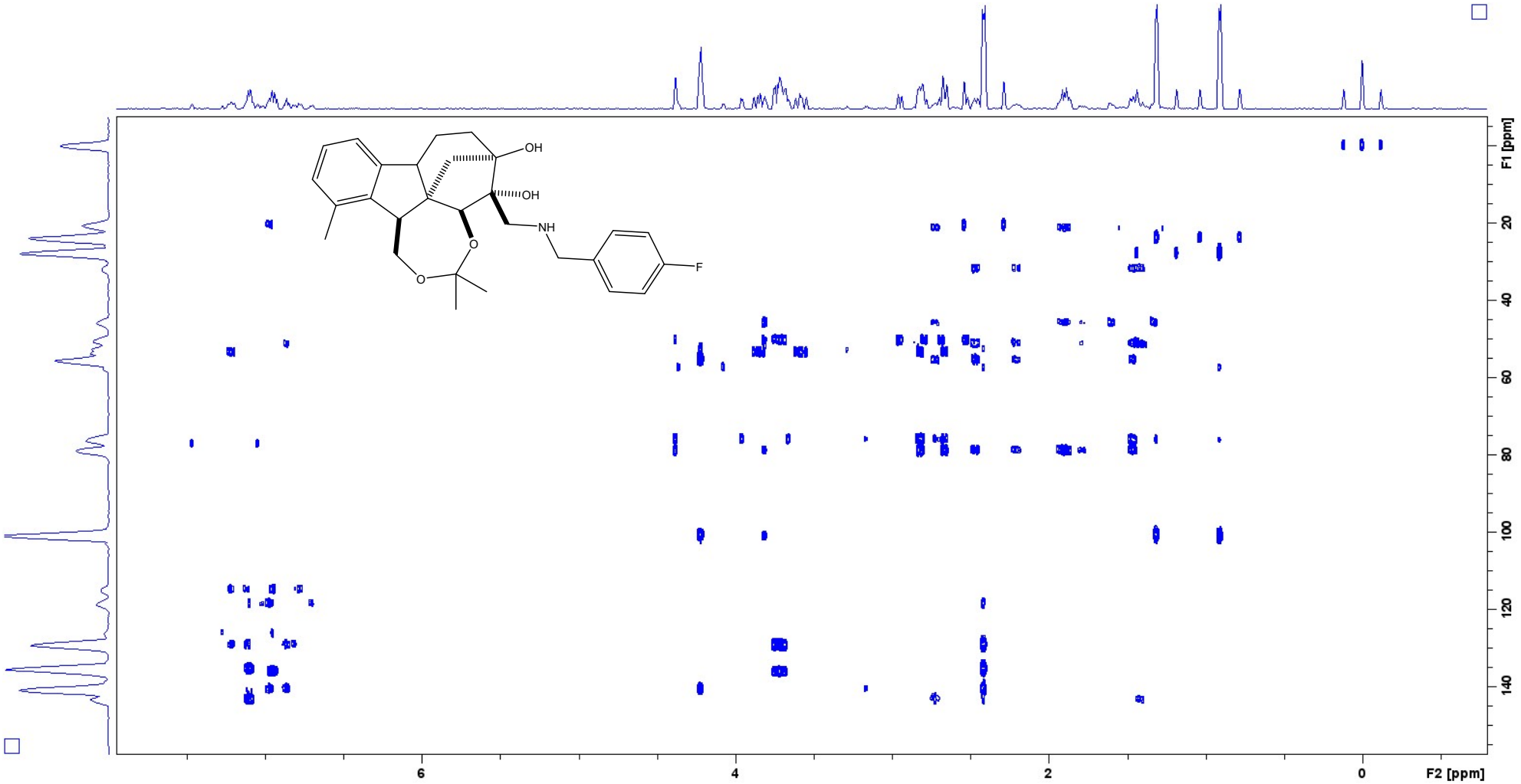
NOESY of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-5-(((4-Fluorobenzyl)amino)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **10**



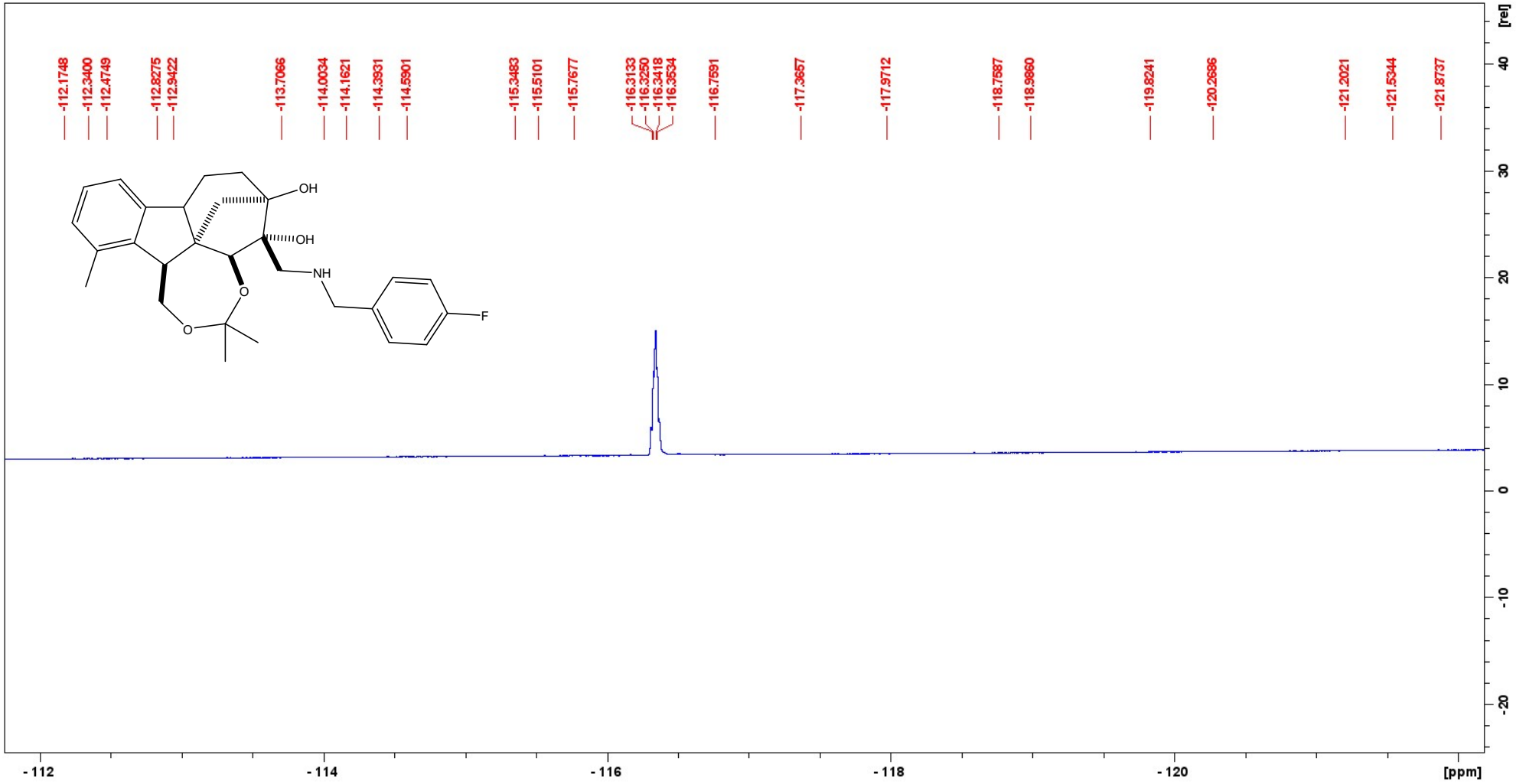
HSQC of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-5-(((4-Fluorobenzyl)amino)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **10**



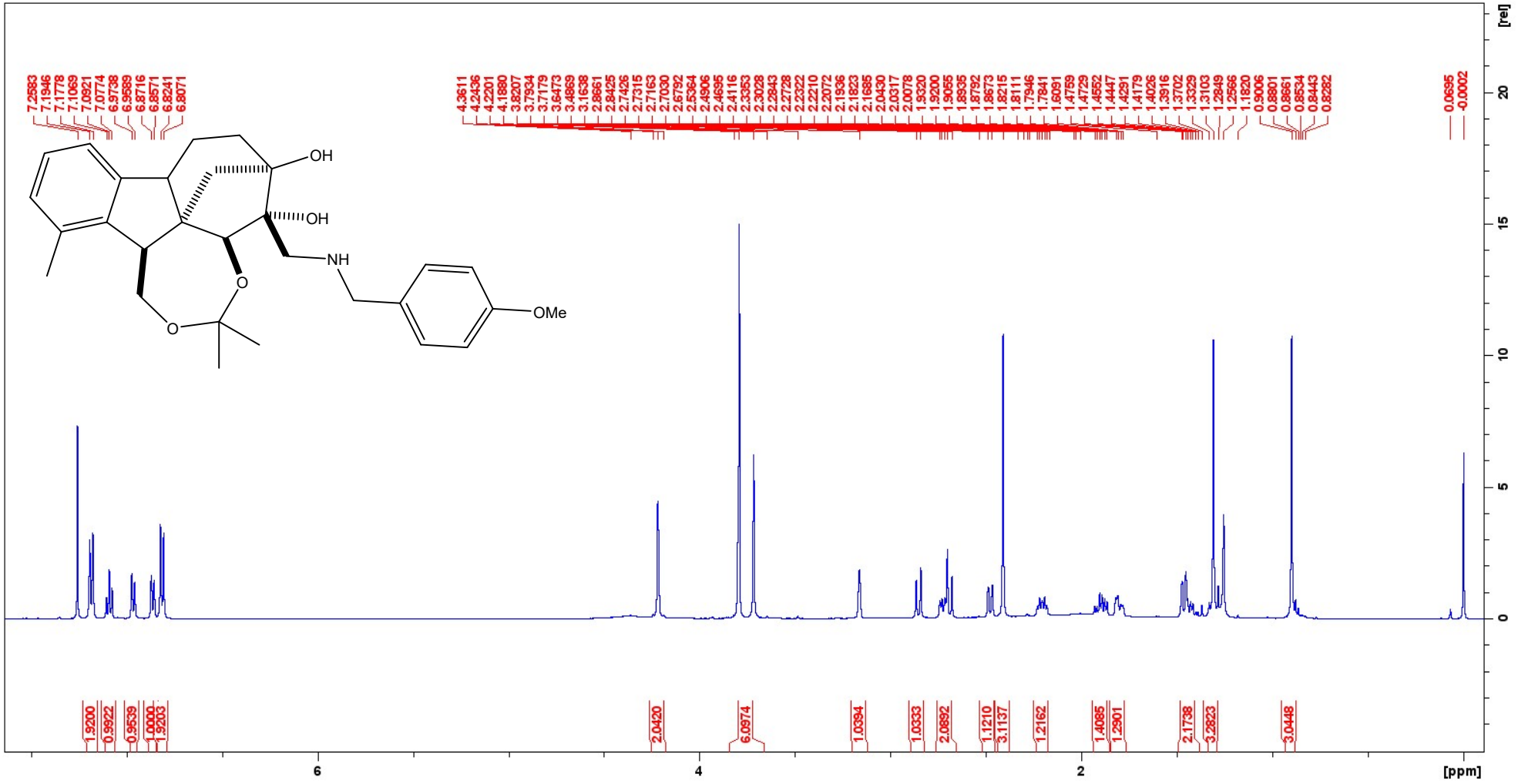
HMBC of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-5-(((4-Fluorobenzyl)amino)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **10**



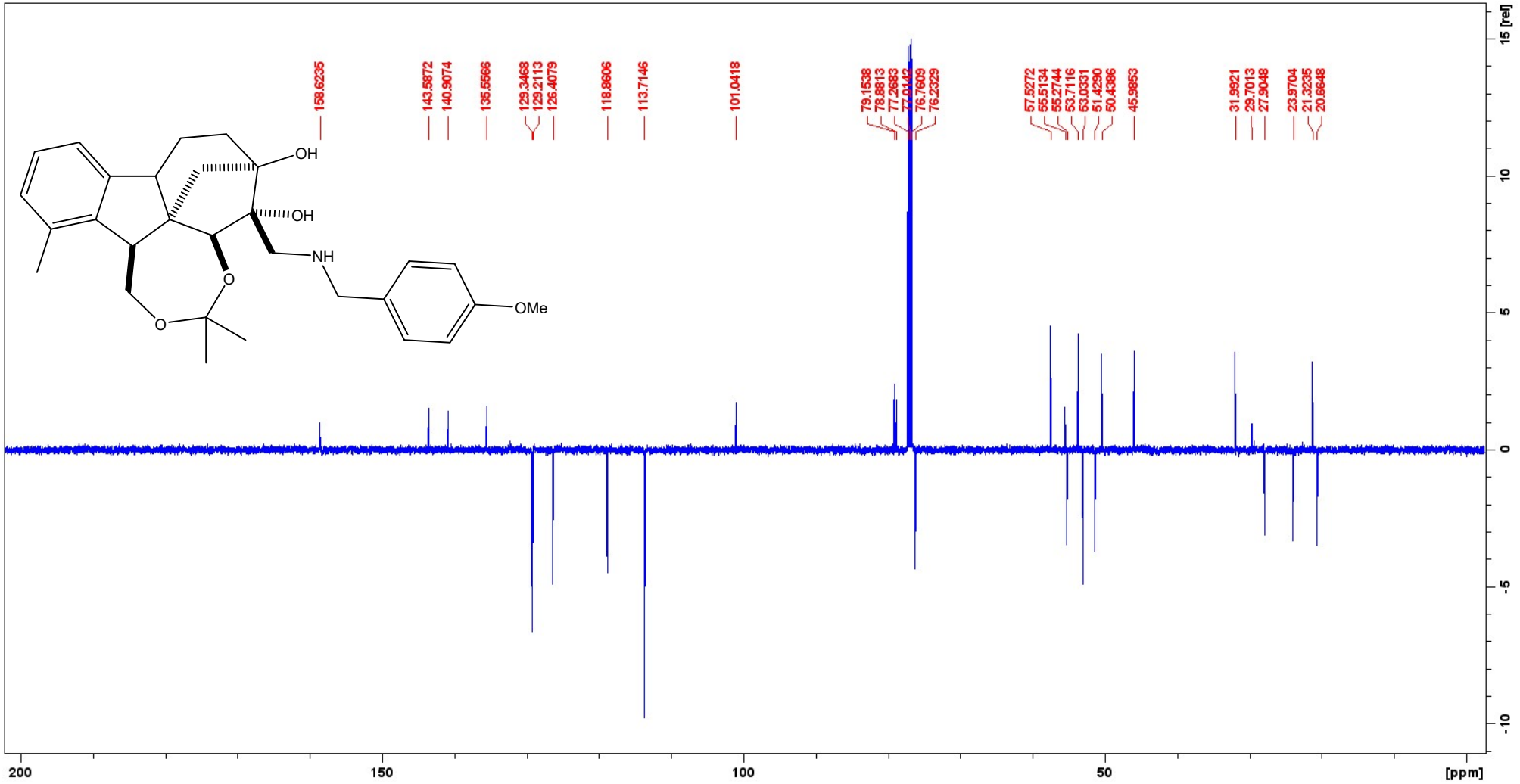
^{19}F *J*-MOD NMR (470 MHz) of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-5-(((4-Fluorobenzyl)amino)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^{1},6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **10**



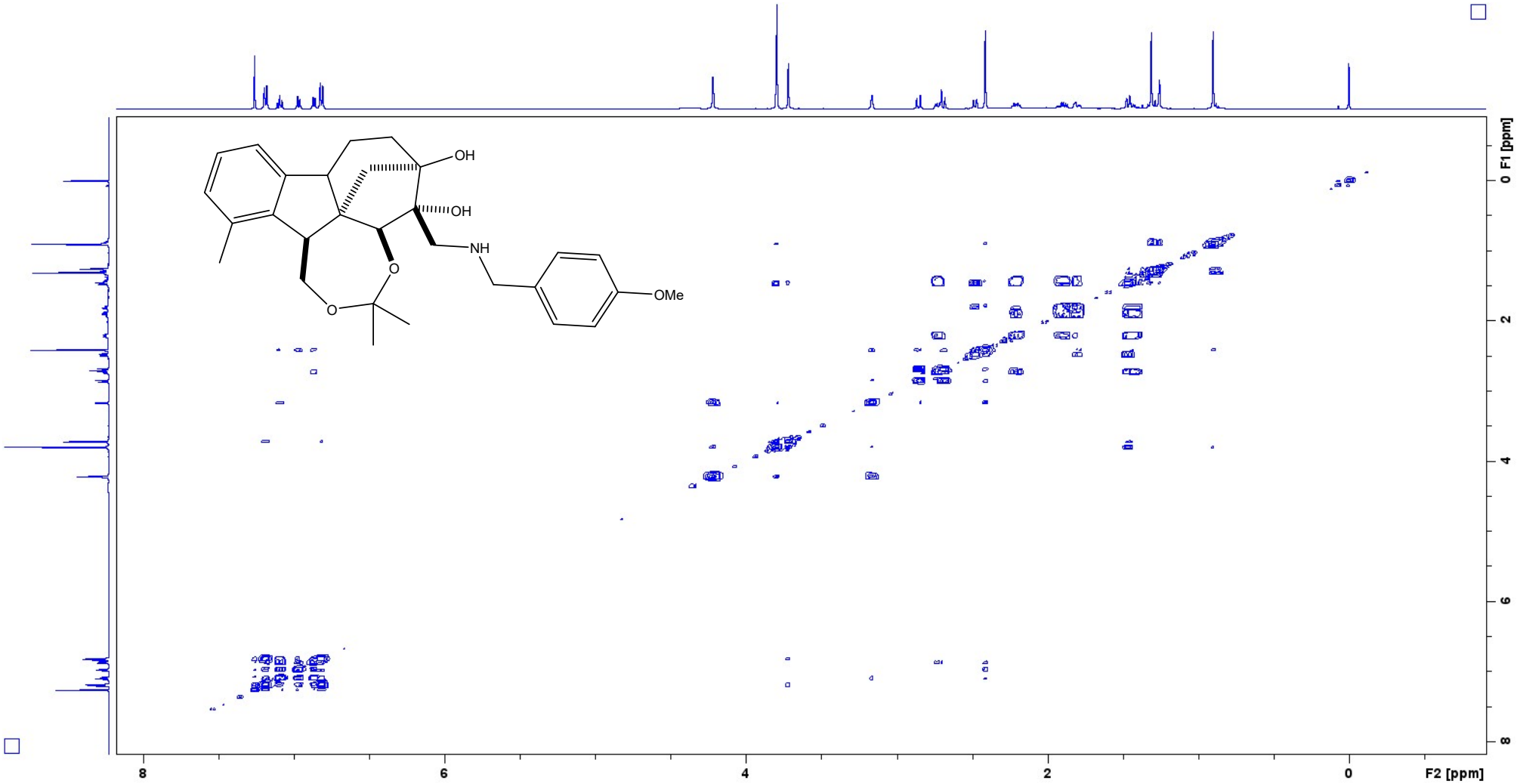
^{1}H-NMR (500 MHz) of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-5-(((4-Methoxybenzyl)amino)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^{1},6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **11**



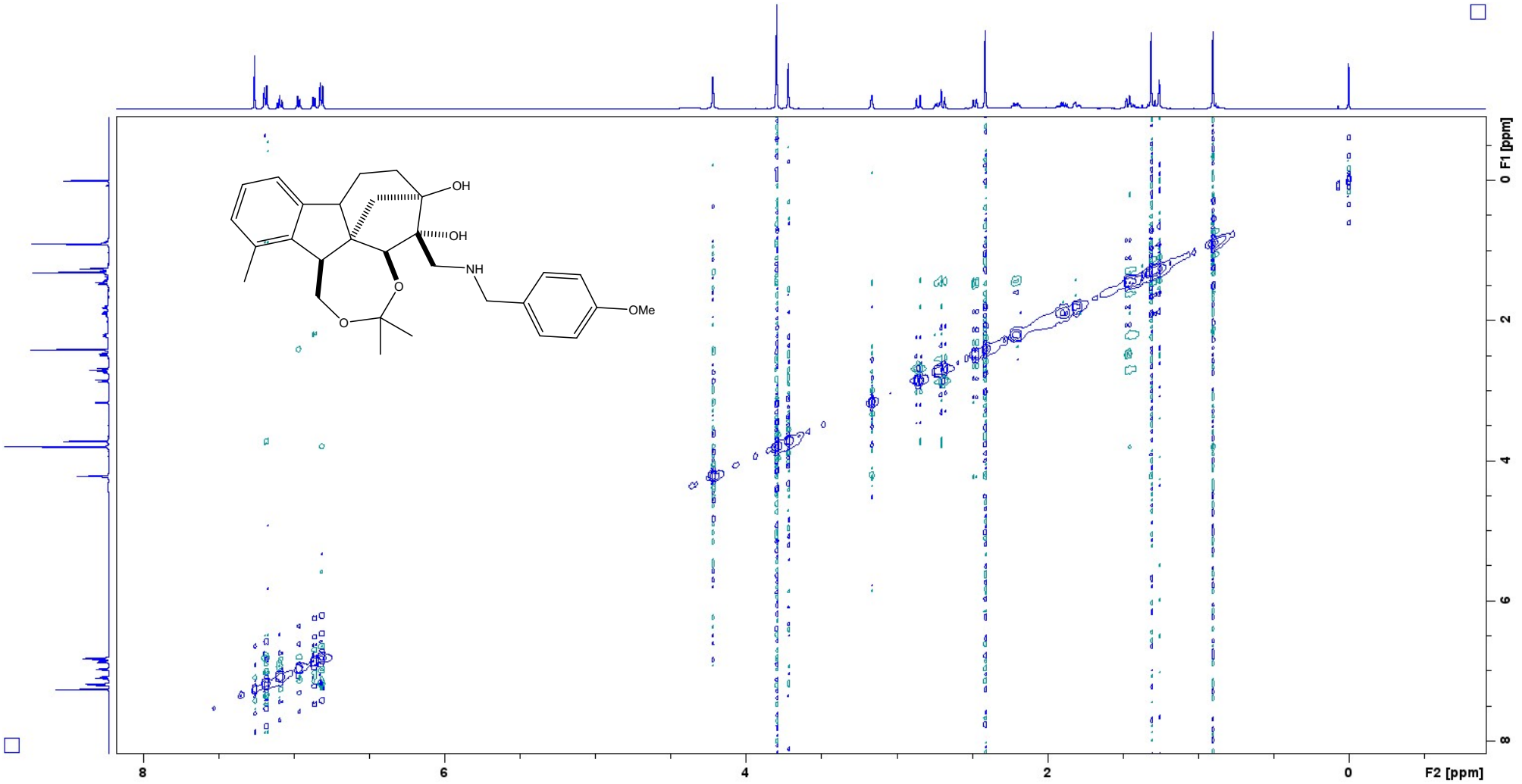
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-5-(((4-Methoxybenzyl)amino)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^{1},6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **11**



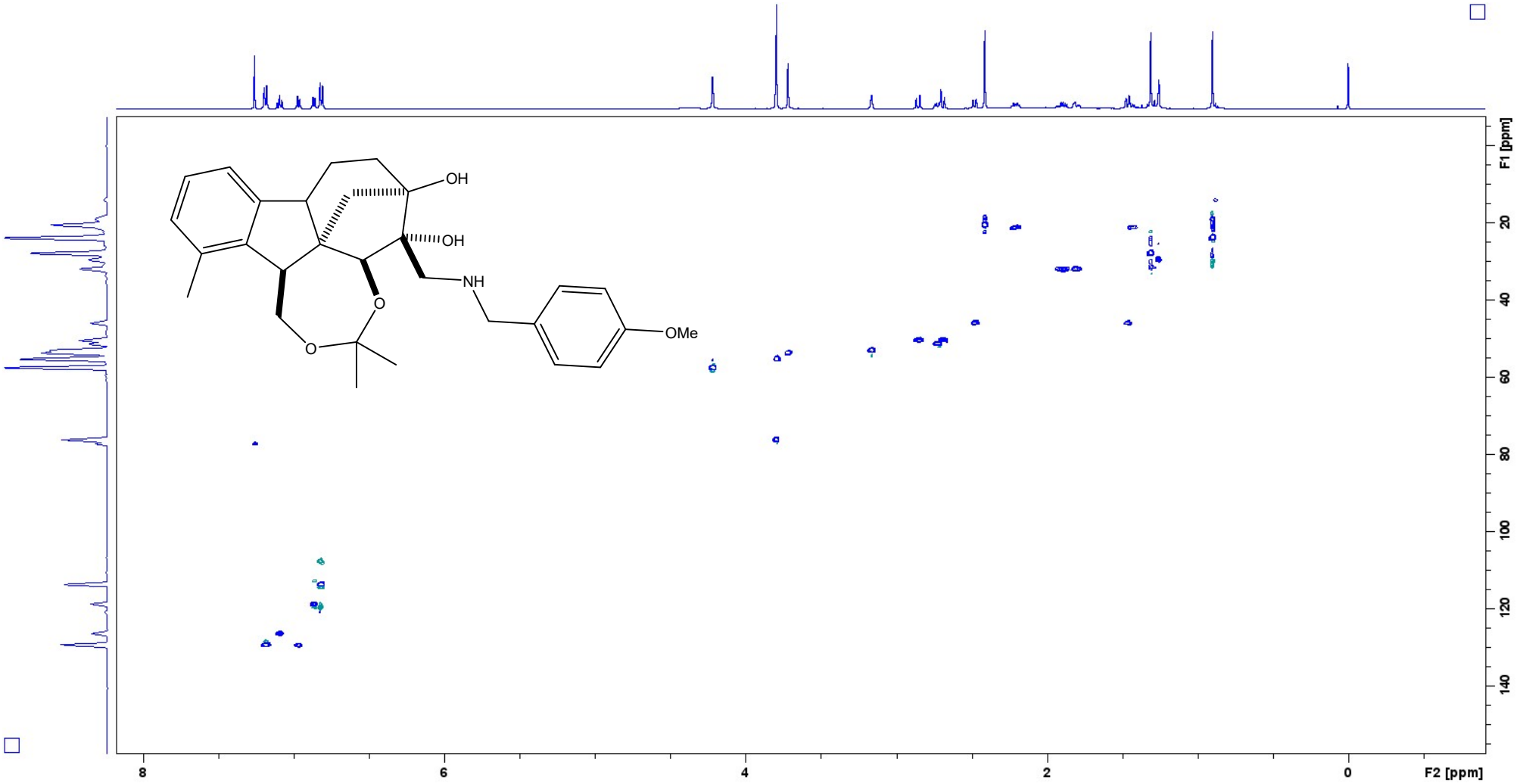
COSY of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-5-(((4-Methoxybenzyl)amino)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **11**



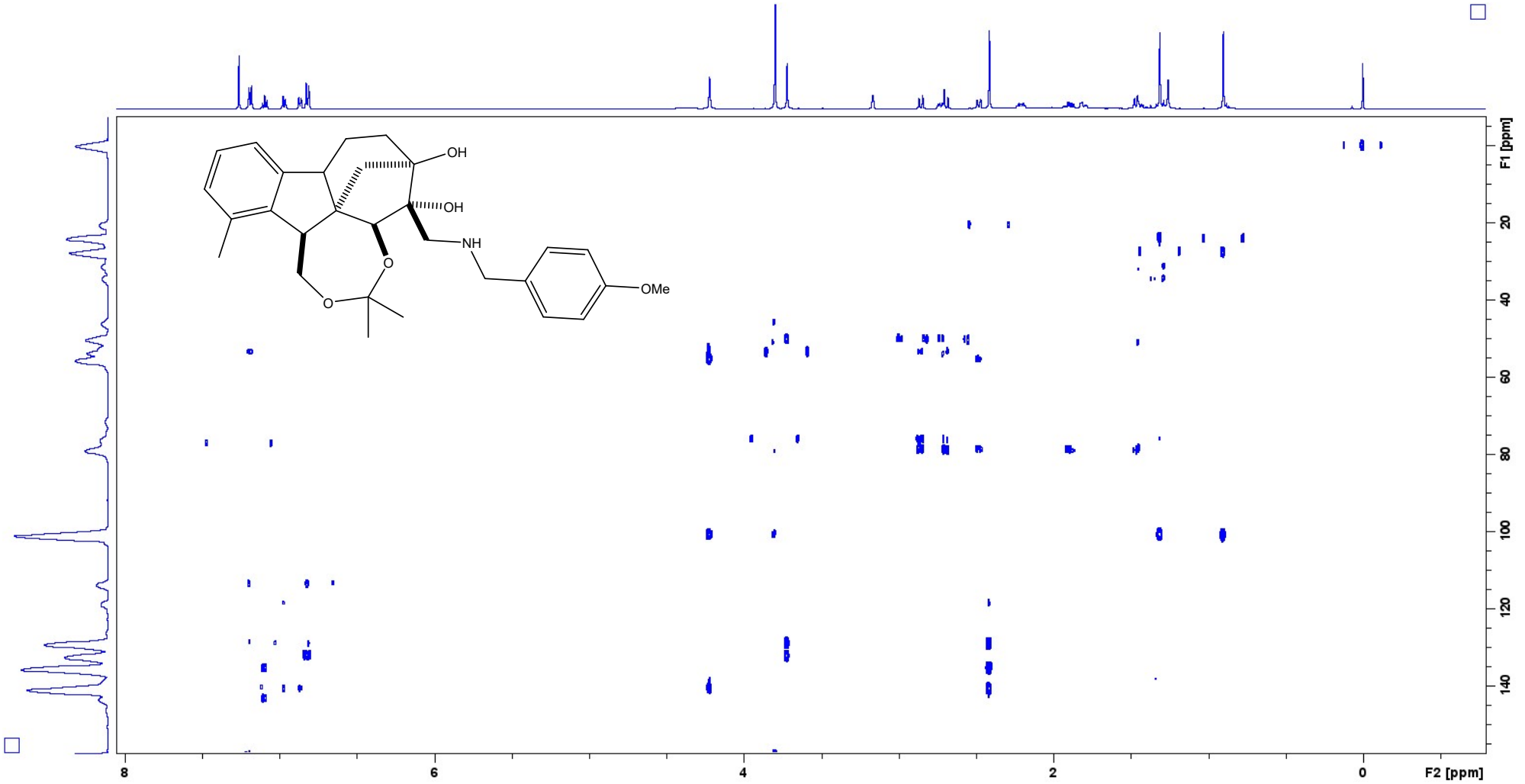
NOESY of (4a*S*,4a[1]*R*,5*R*,6*S*,12b*S*)-5-(((4-Methoxybenzyl)amino)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a[1],6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **11**



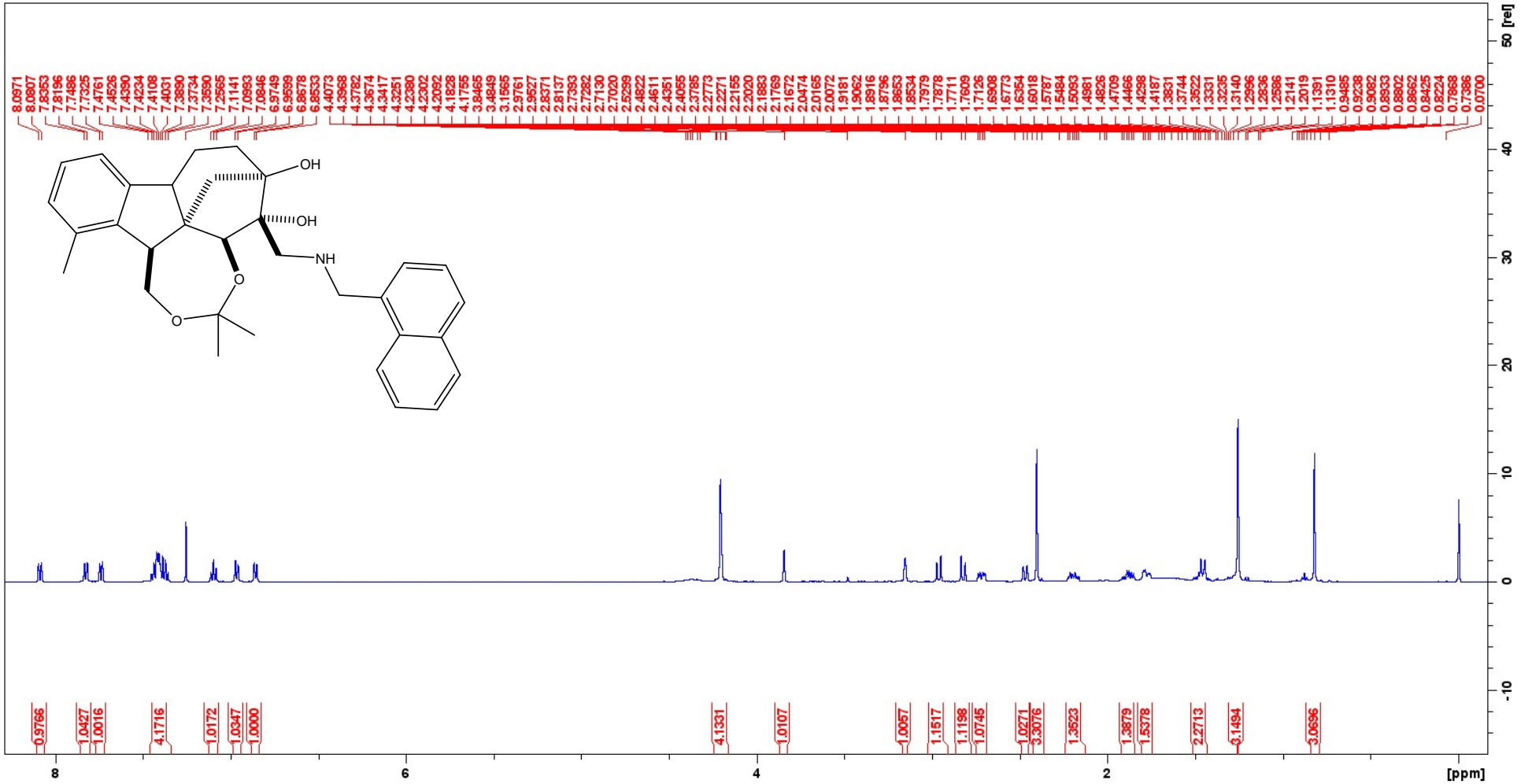
HSQC of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-5-(((4-Methoxybenzyl)amino)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **11**



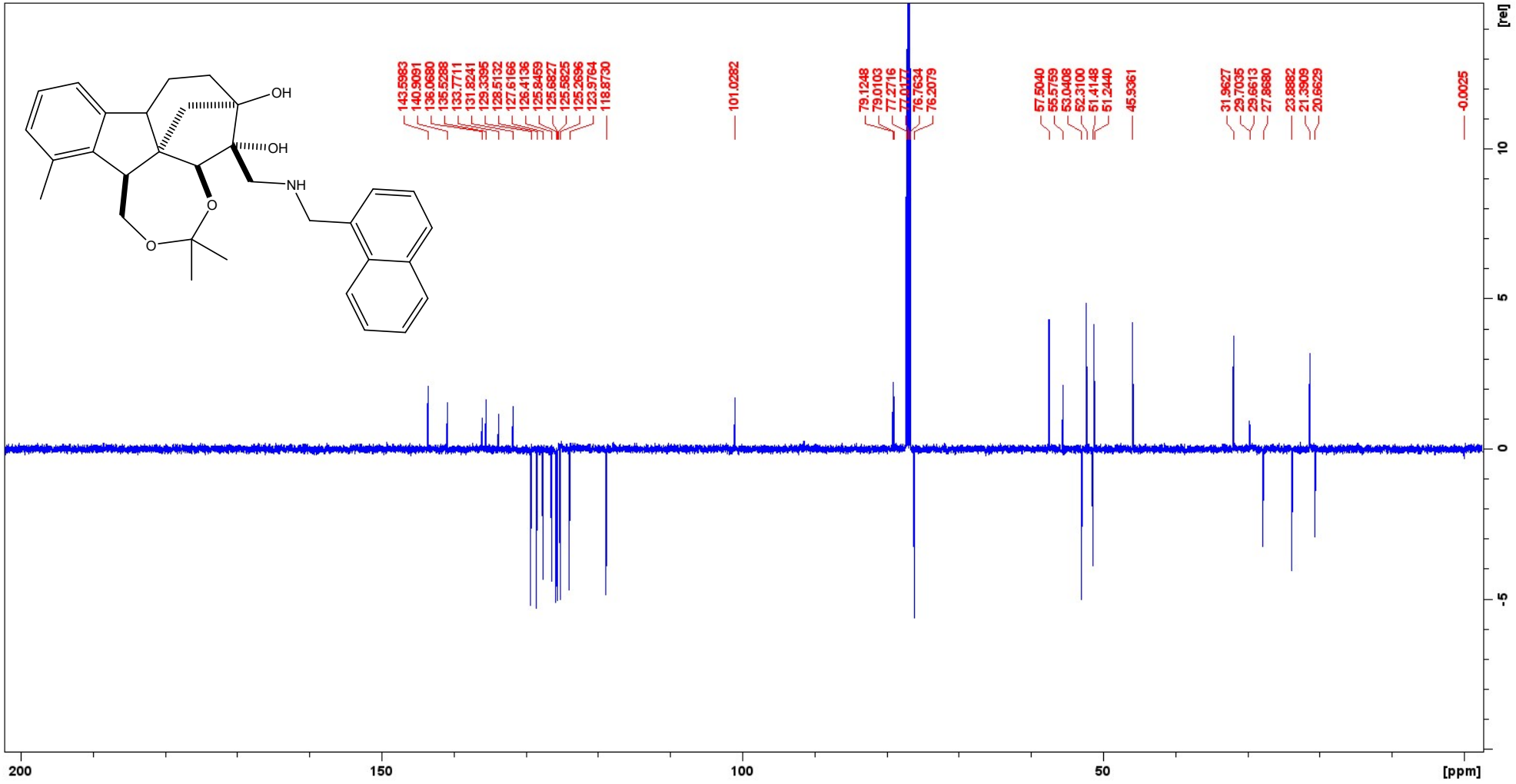
HMBC of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-5-(((4-Methoxybenzyl)amino)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **11**



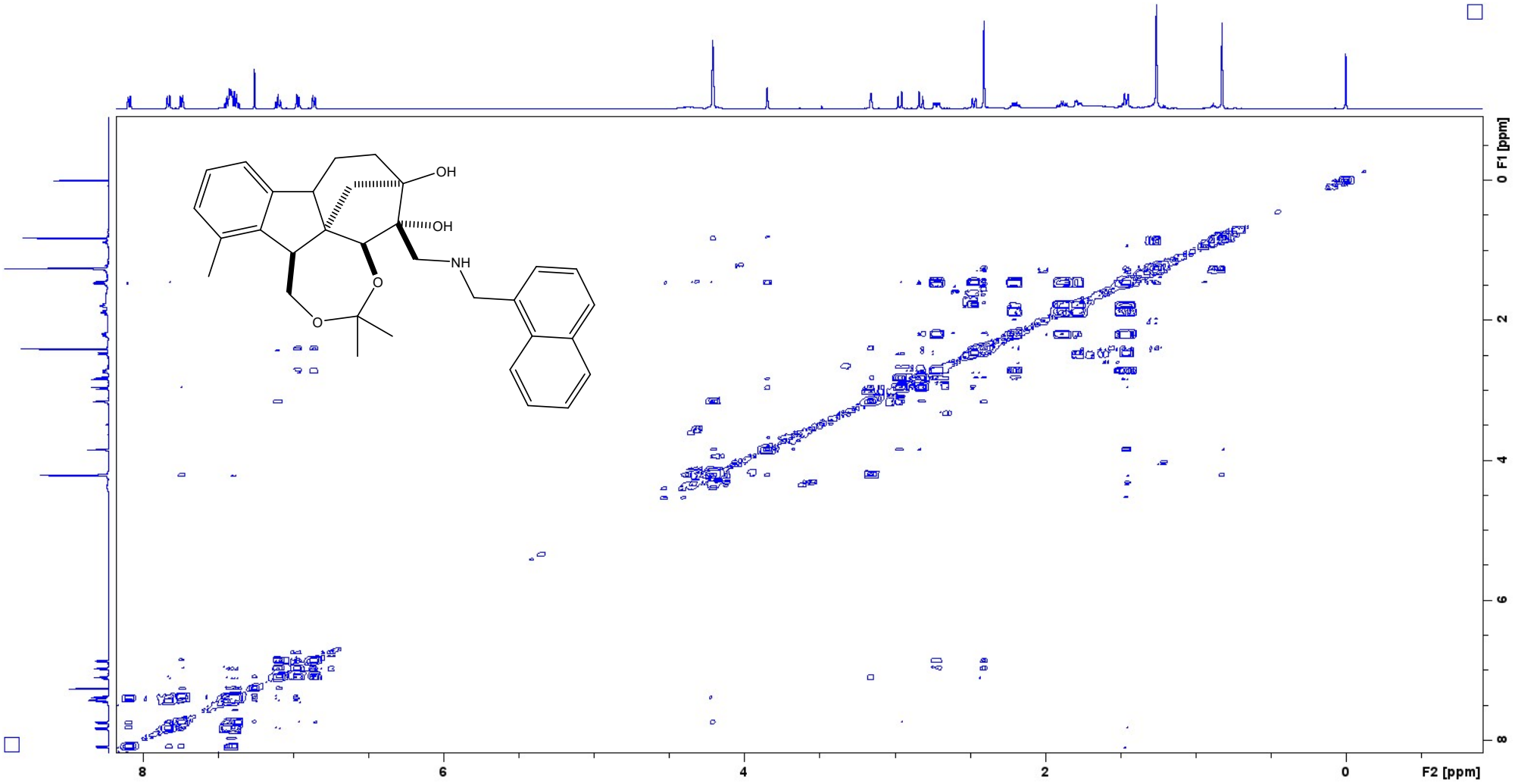
^{1}H-NMR (500 MHz) of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-(((naphthalen-1-ylmethyl)amino)methyl)-4a,5,7,8,8a,12b-hexahydro-4a^{1},6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **12**



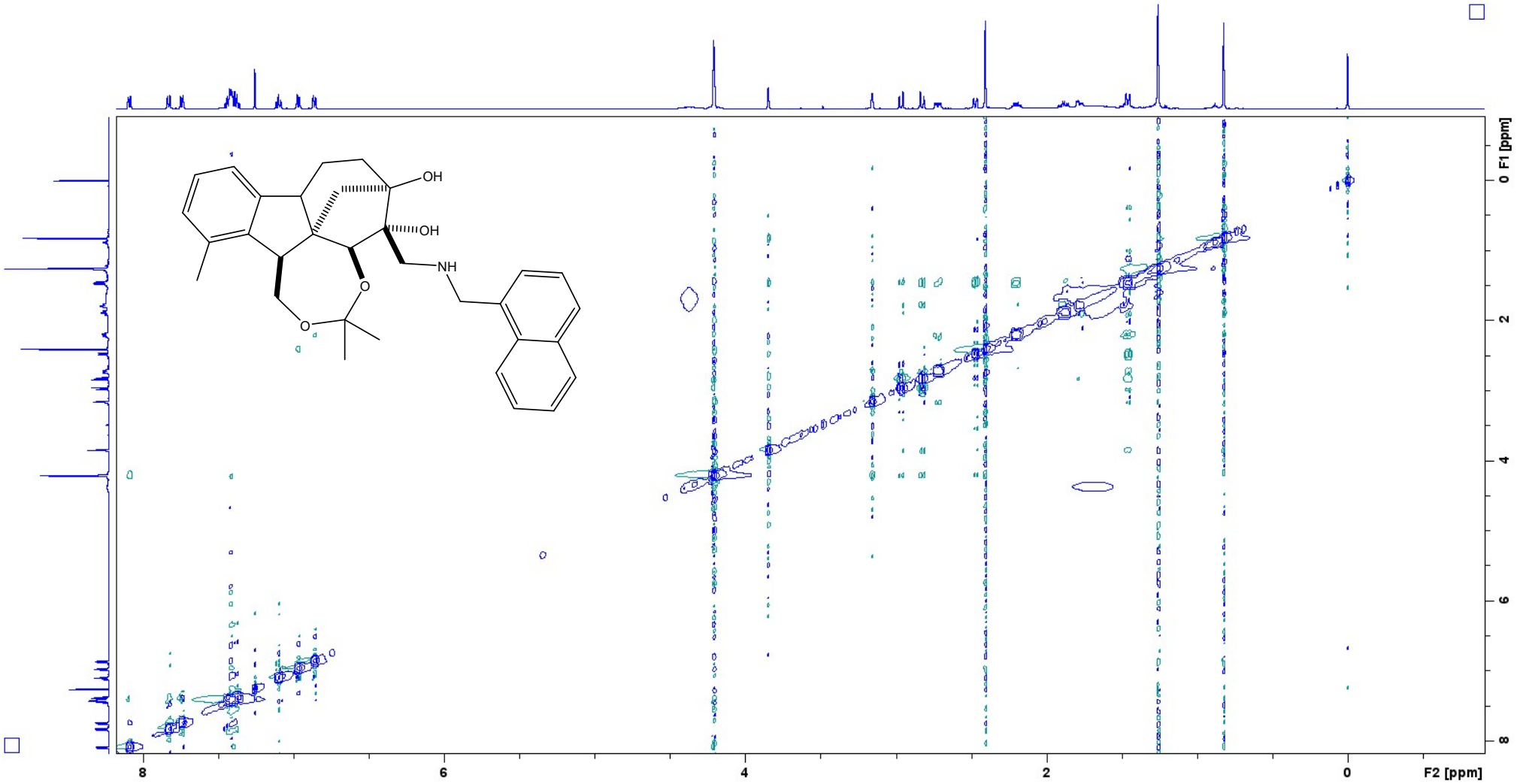
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-(((naphthalen-1-ylmethyl)amino)methyl)-4a,5,7,8,8a,12b-hexahydro-4a^{1},6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **12**



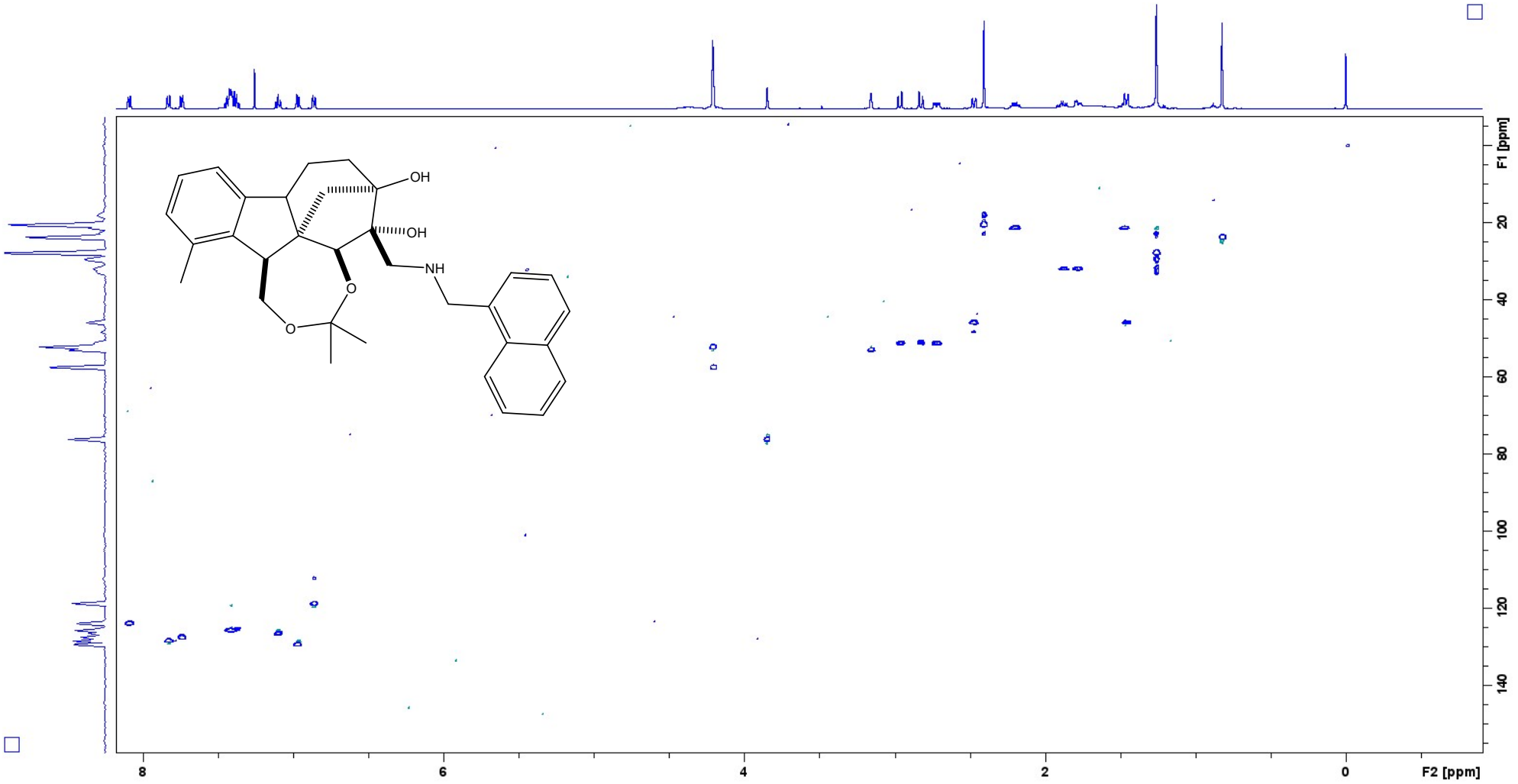
COSY of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-(((naphthalen-1-ylmethyl)amino)methyl)-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **12**



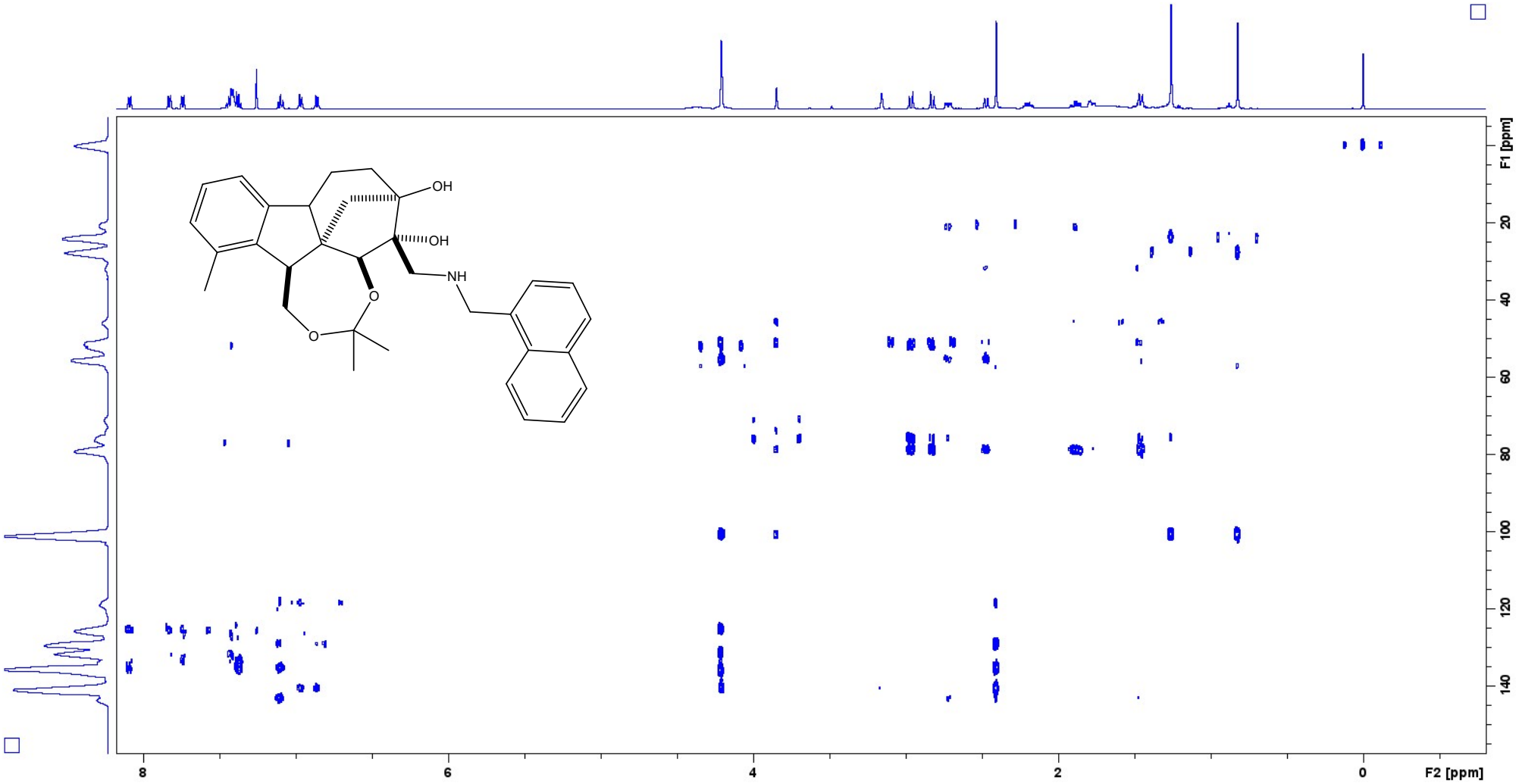
NOESY of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-(((naphthalen-1-ylmethyl)amino)methyl)-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **12**



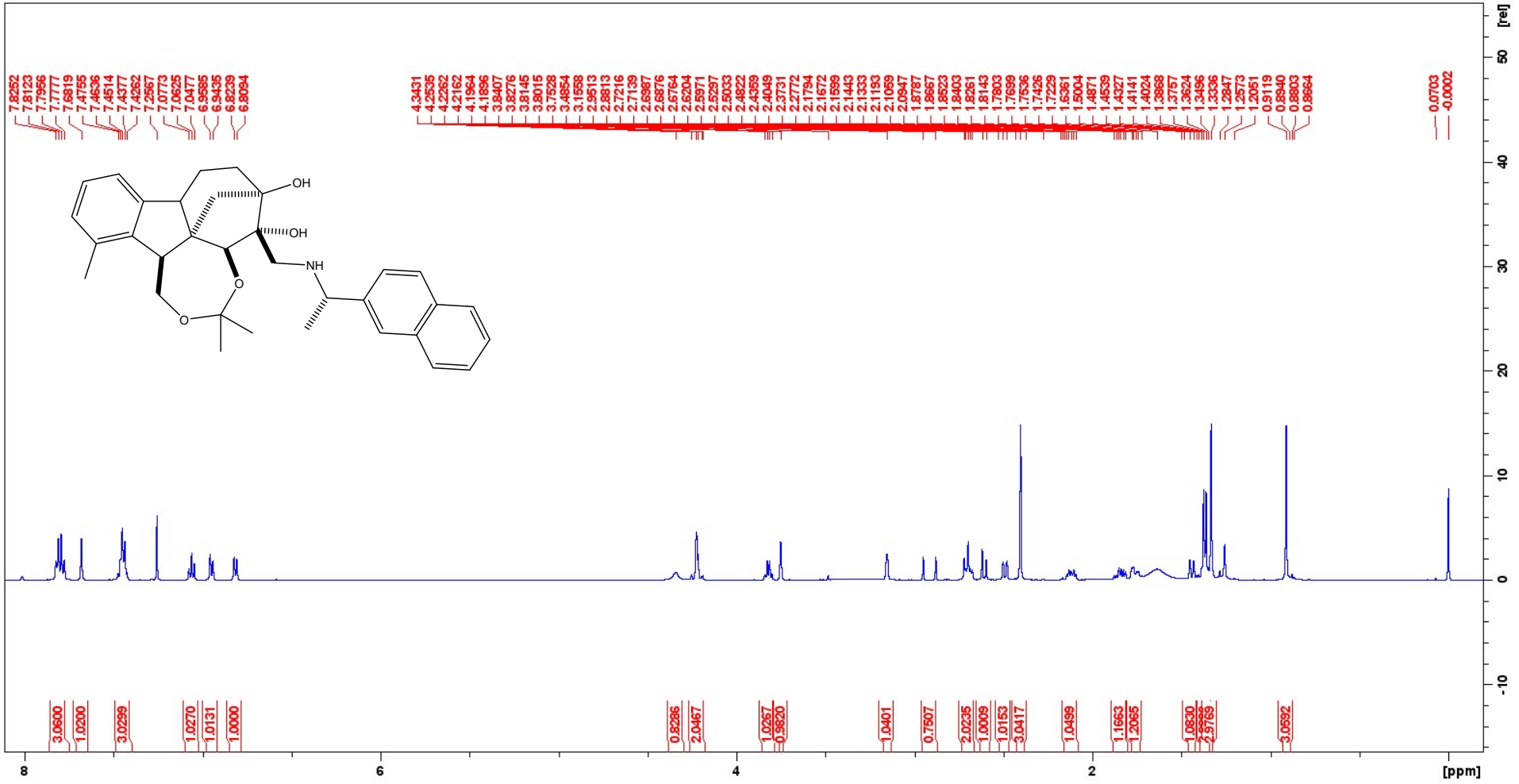
HSQC of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-(((naphthalen-1-ylmethyl)amino)methyl)-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **12**



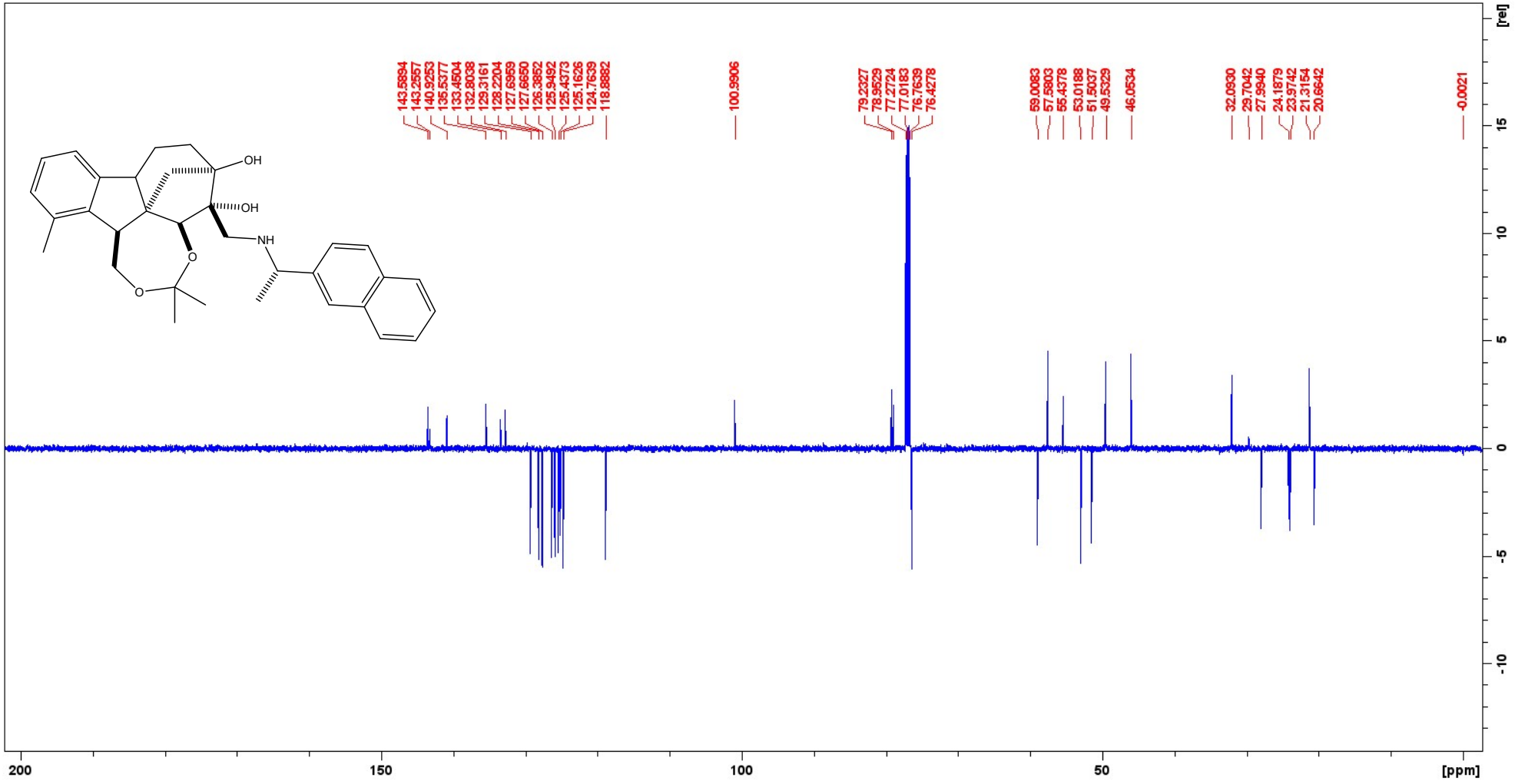
HMBC of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-(((naphthalen-1-ylmethyl)amino)methyl)-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **12**



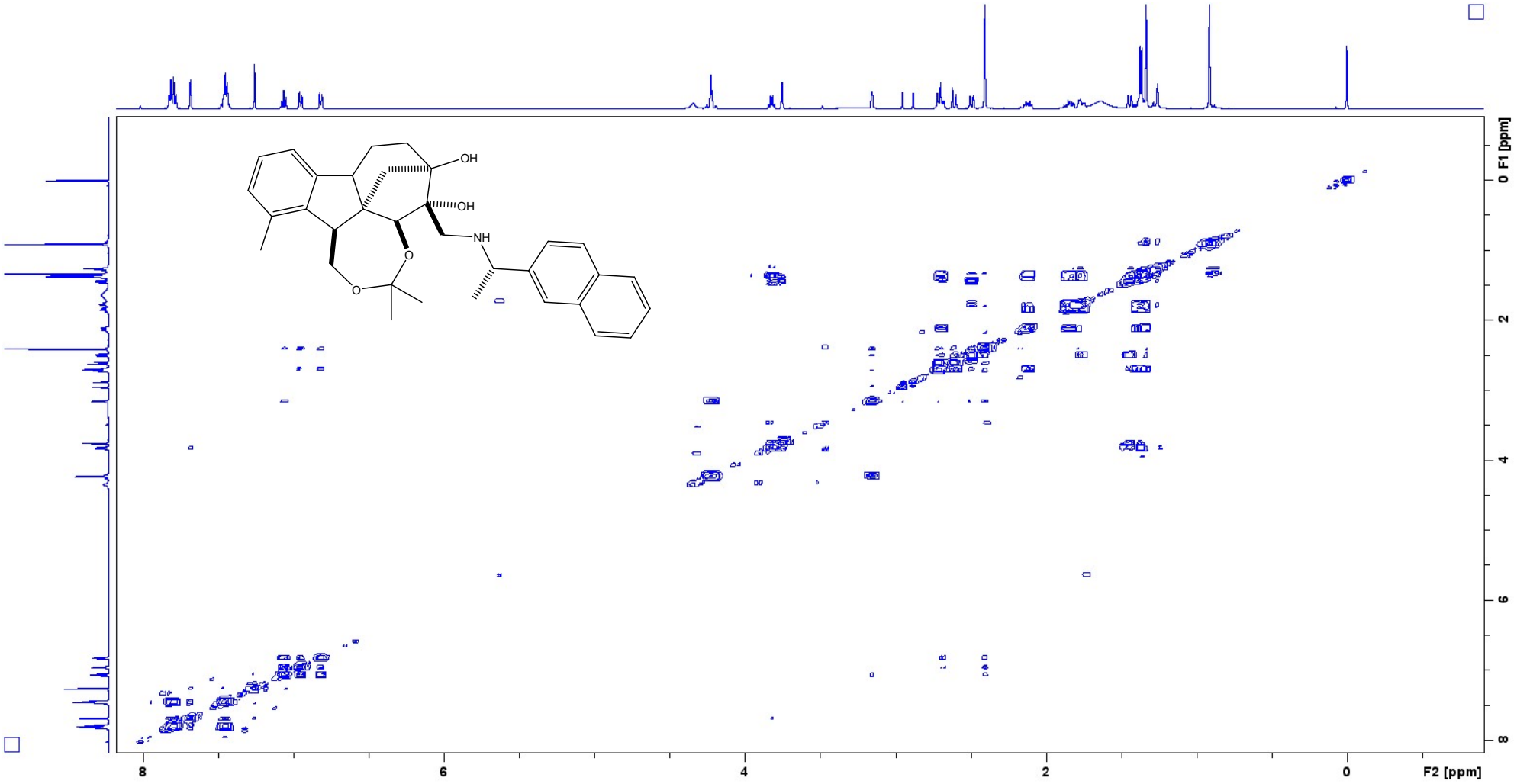
^{1}H-NMR (500 MHz) of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-((((*S*)-1-(naphthalen-2-yl)ethyl)amino)methyl)-4a,5,7,8,8a,12b-hexahydro-4a^{1},6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **13**



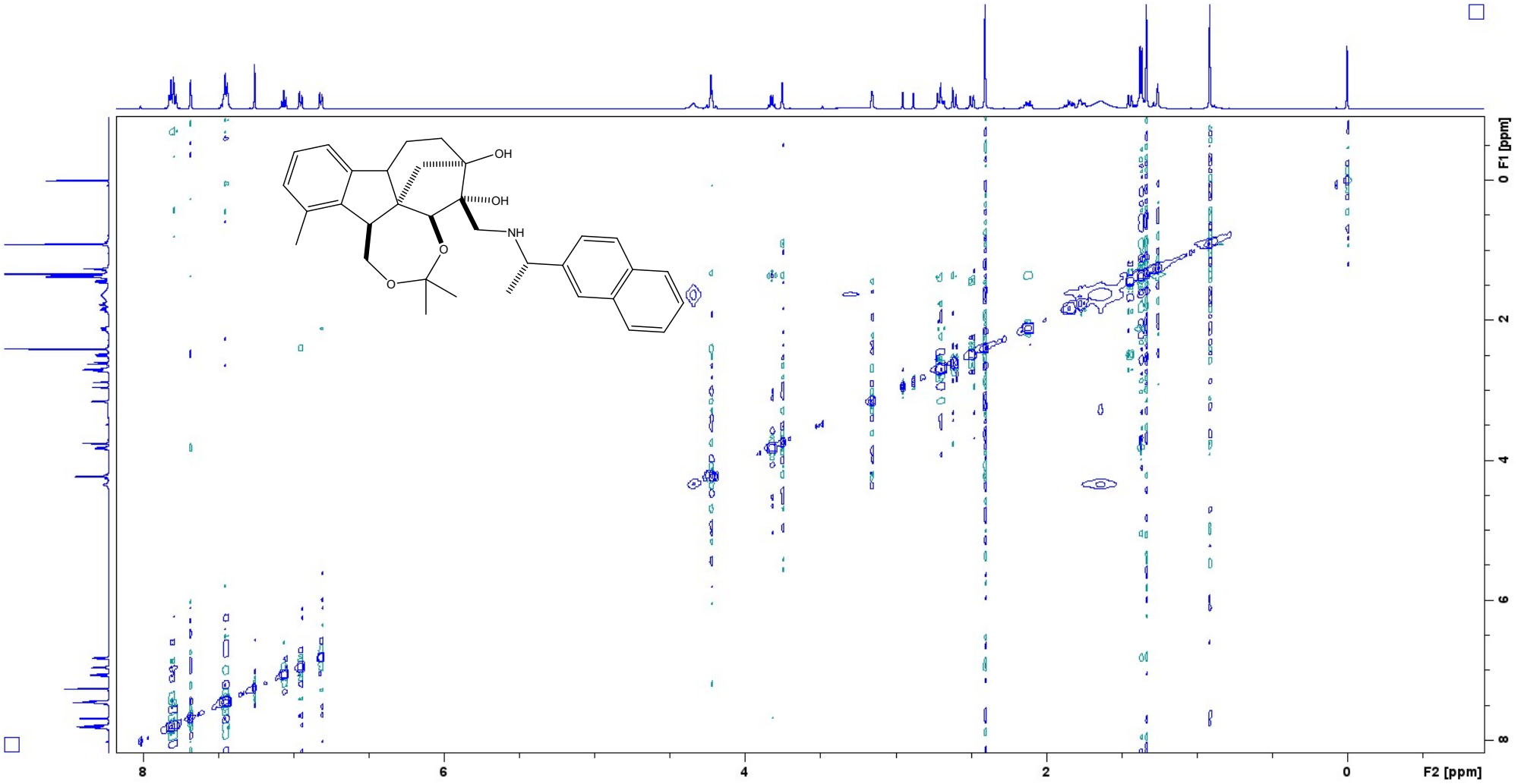
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-((((*S*)-1-(naphthalen-2-yl)ethyl)amino)methyl)-4a,5,7,8,8a,12b-hexahydro-4a^{1},6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **13**



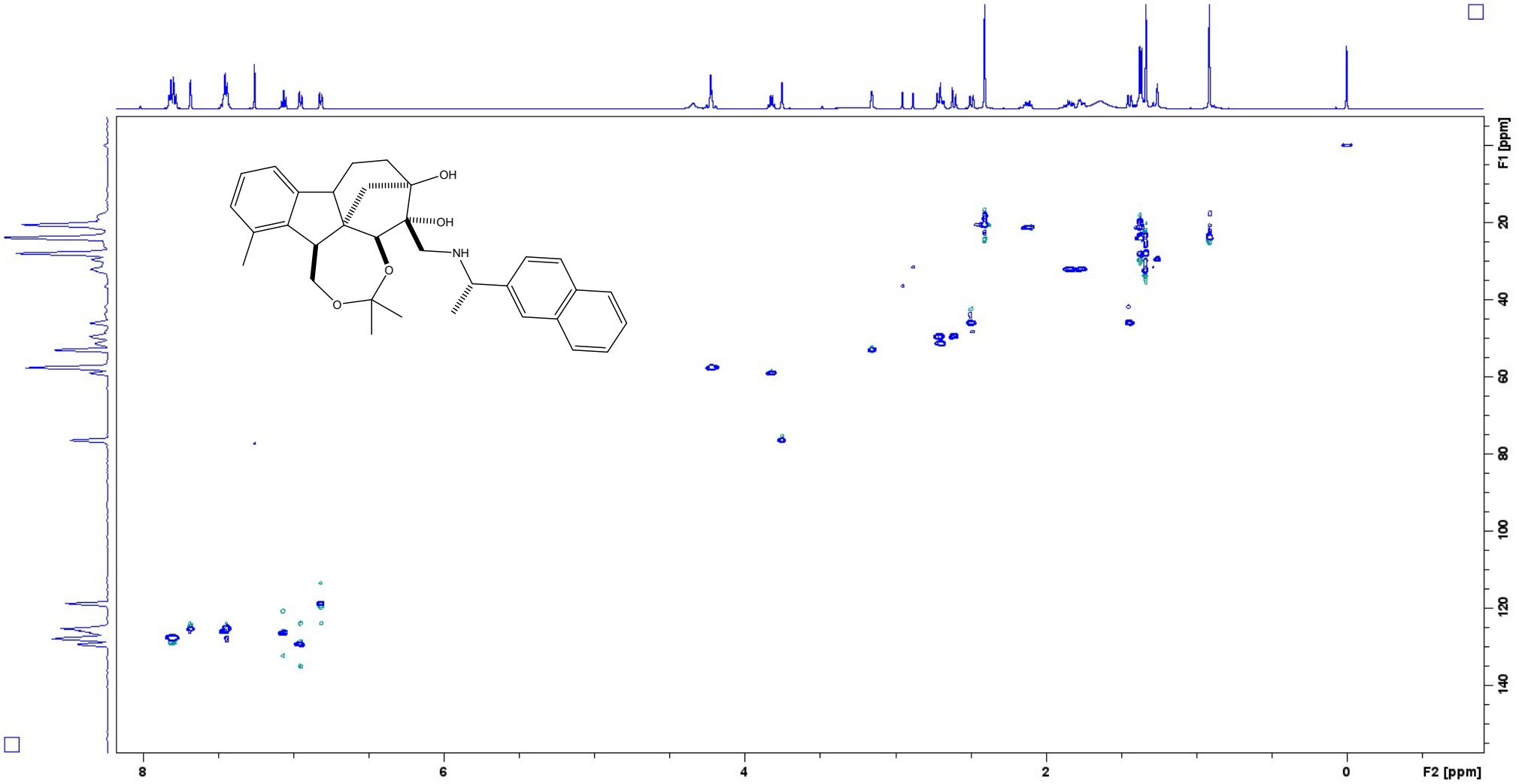
COSY of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-((((*S*)-1-(naphthalen-2-yl)ethyl)amino)methyl)-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **13**



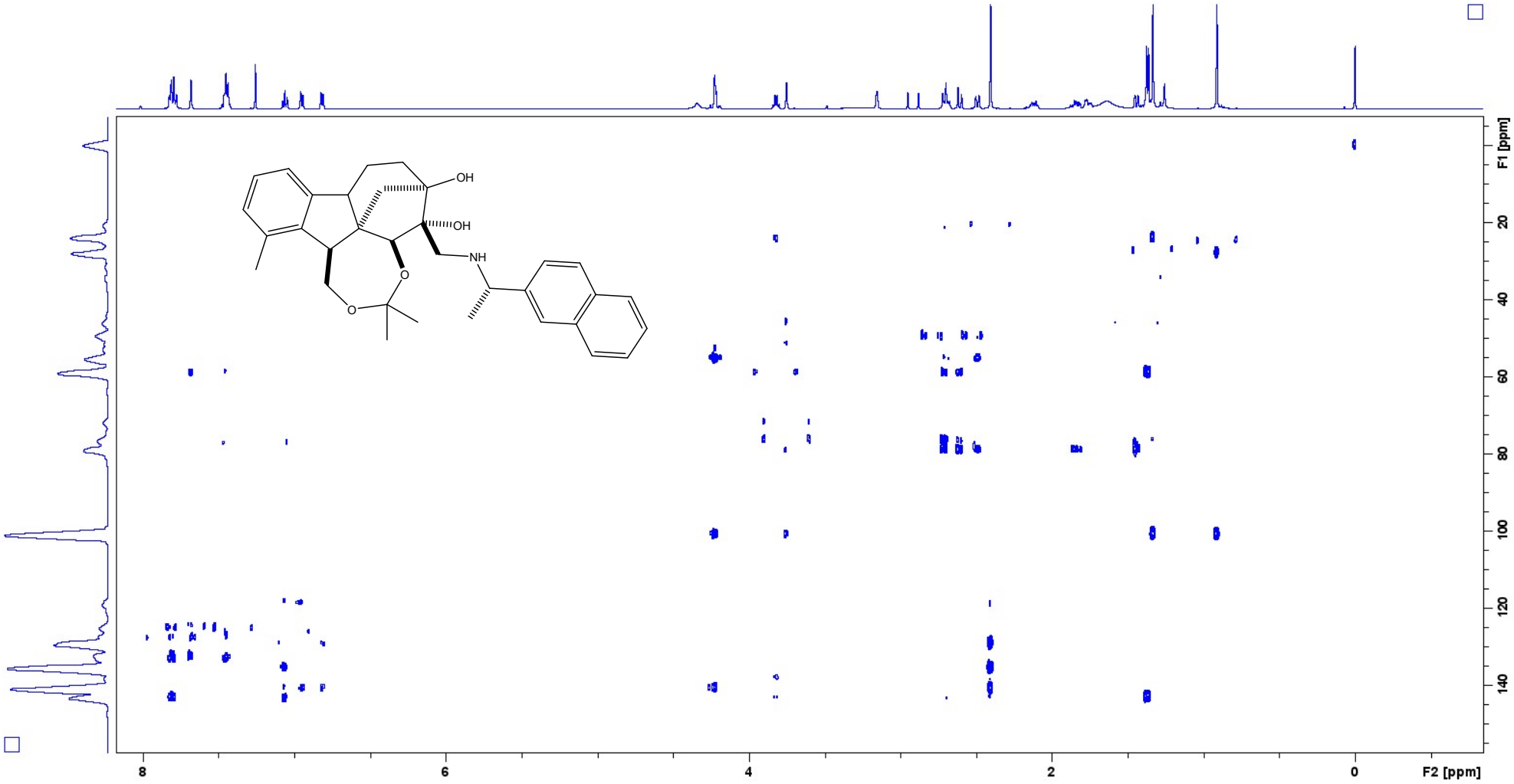
NOESY of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-((((*S*)-1-(naphthalen-2-yl)ethyl)amino)methyl)-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **13**



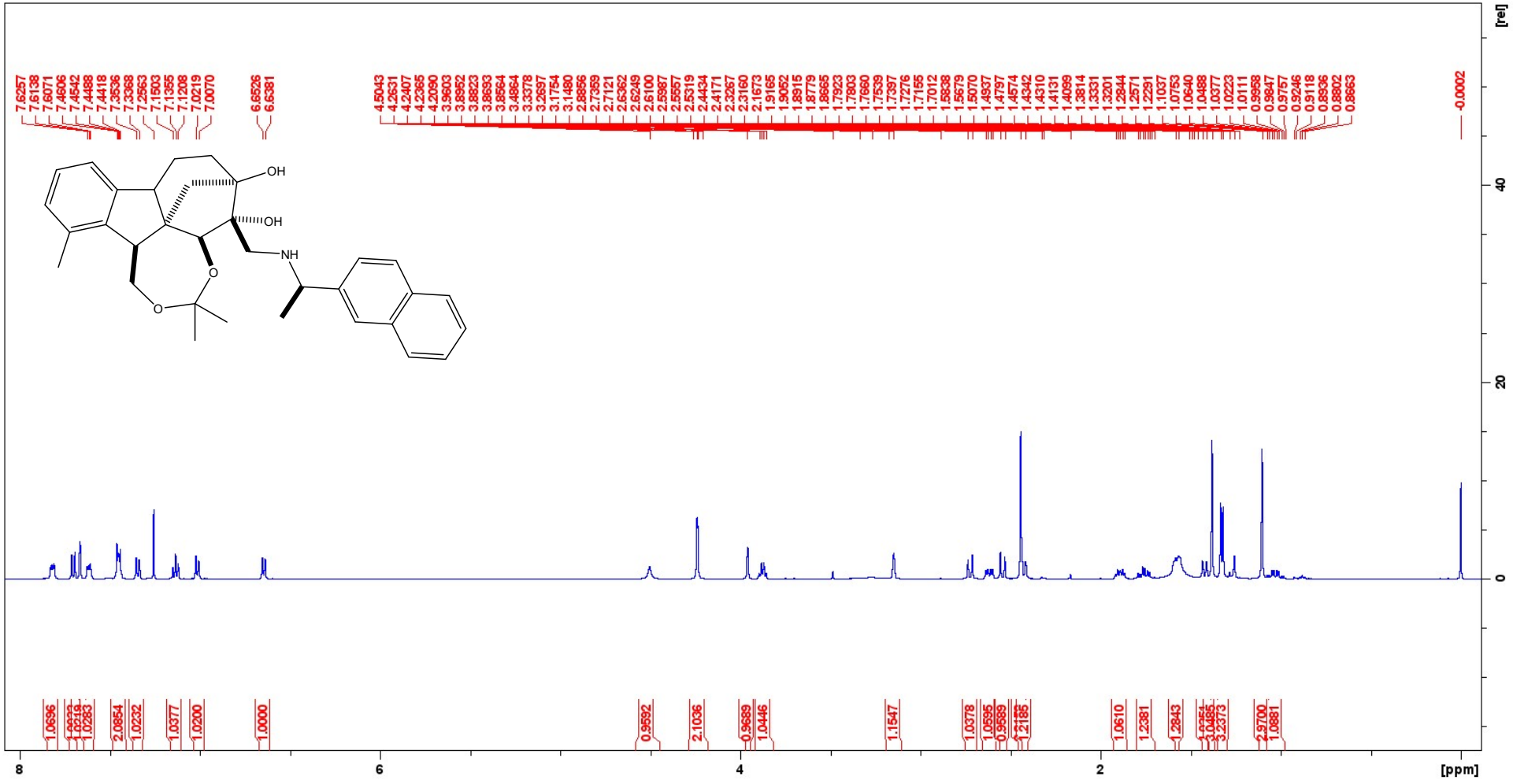
HSQC of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-((((*S*)-1-(naphthalen-2-yl)ethyl)amino)methyl)-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **13**



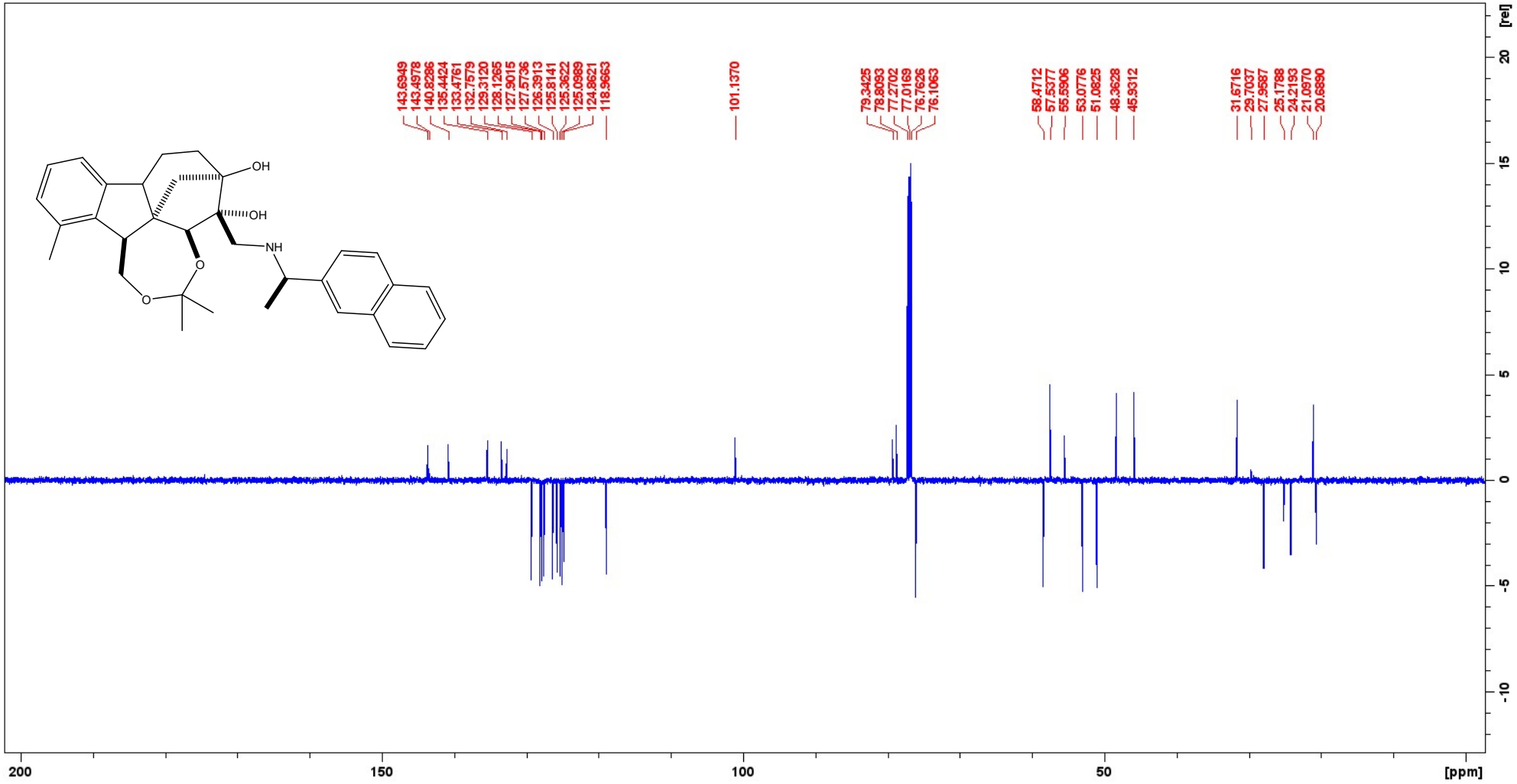
HMBC of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-((((*S*)-1-(naphthalen-2-yl)ethyl)amino)methyl)-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **13**



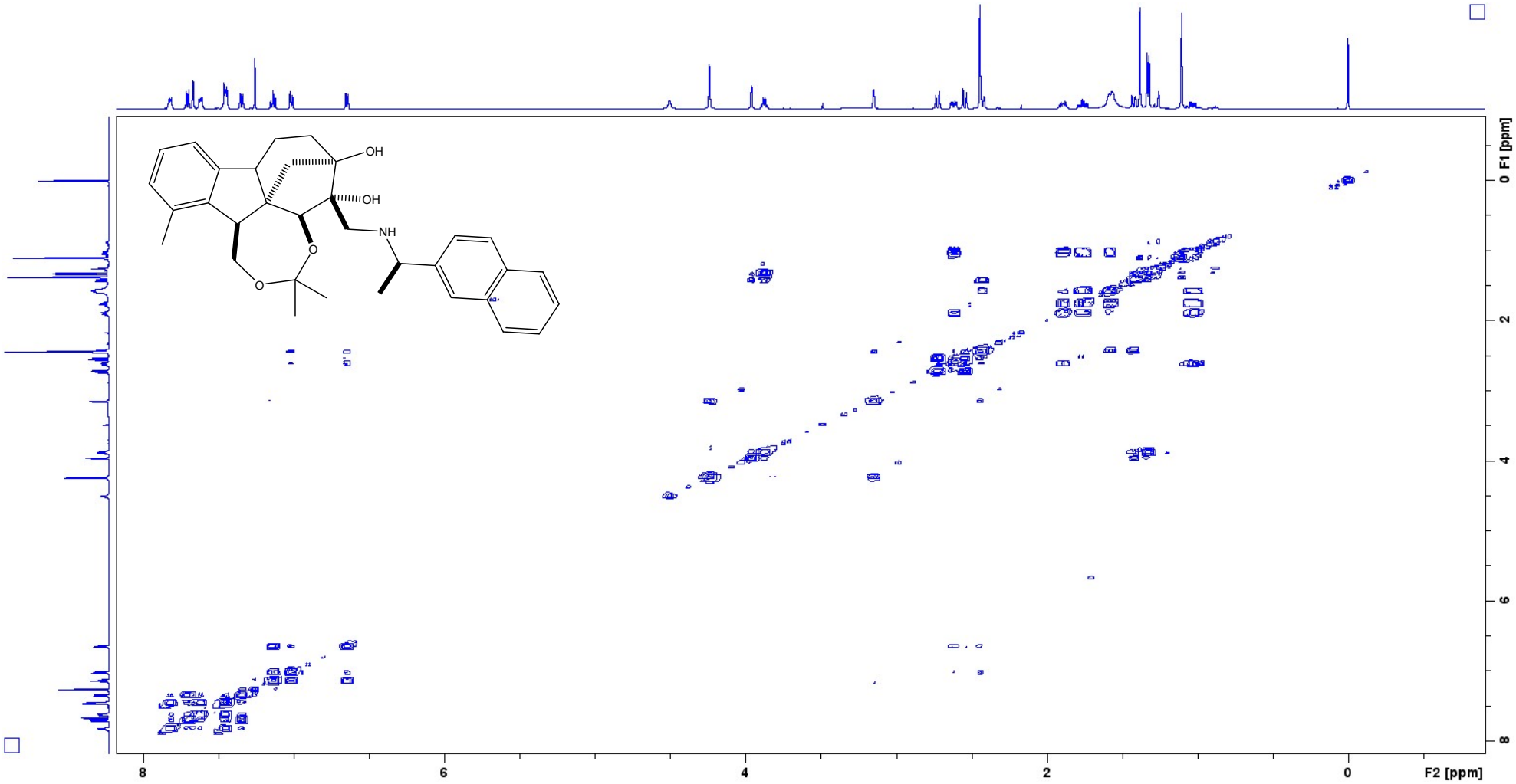
^{1}H-NMR (500 MHz) of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-((((*R*)-1-(naphthalen-2-yl)ethyl)amino)methyl)-4a,5,7,8,8a,12b-hexahydro-4a^{1},6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **14**



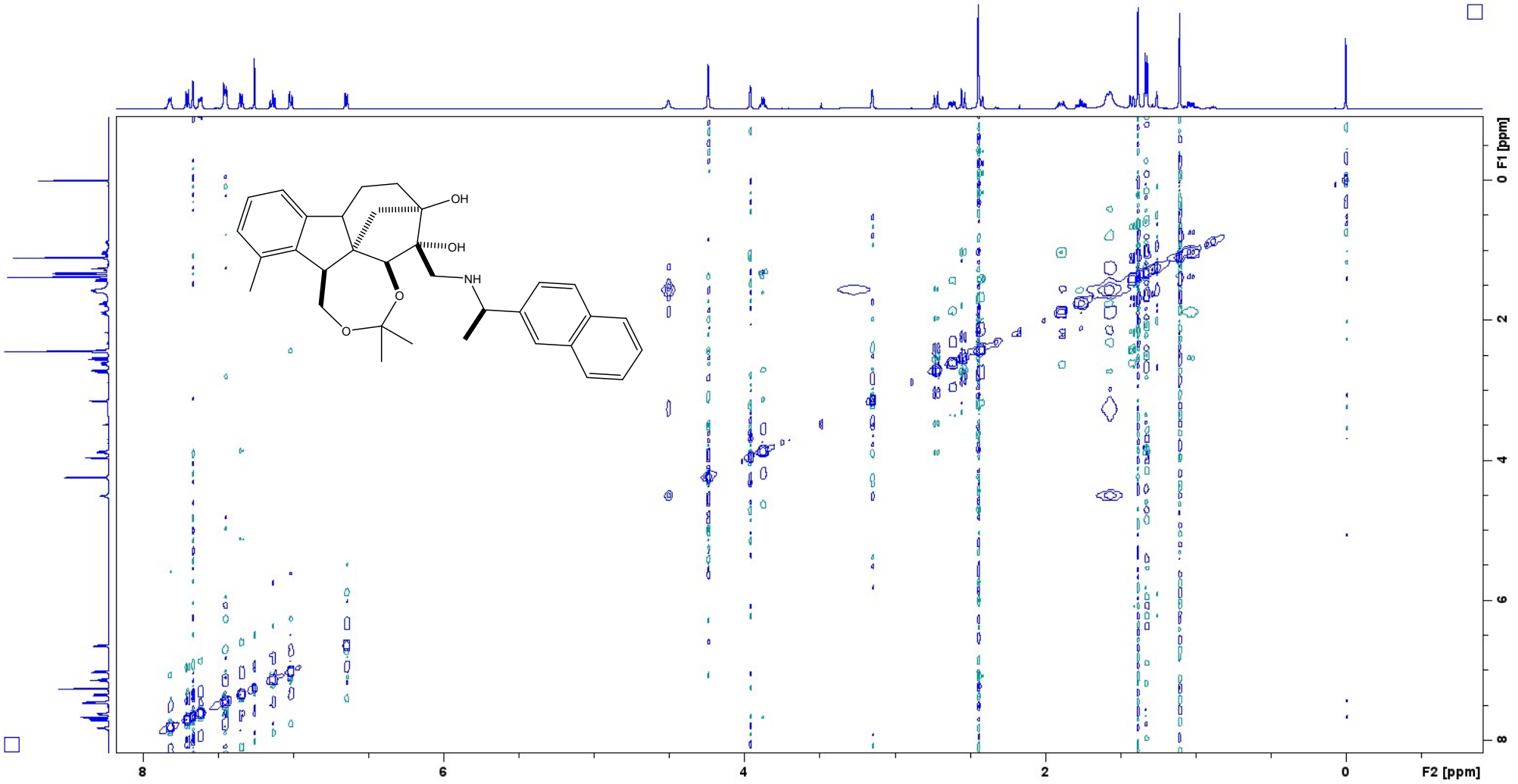
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-((((*R*)-1-(naphthalen-2-yl)ethyl)amino)methyl)-4a,5,7,8,8a,12b-hexahydro-4a^{1},6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **14**



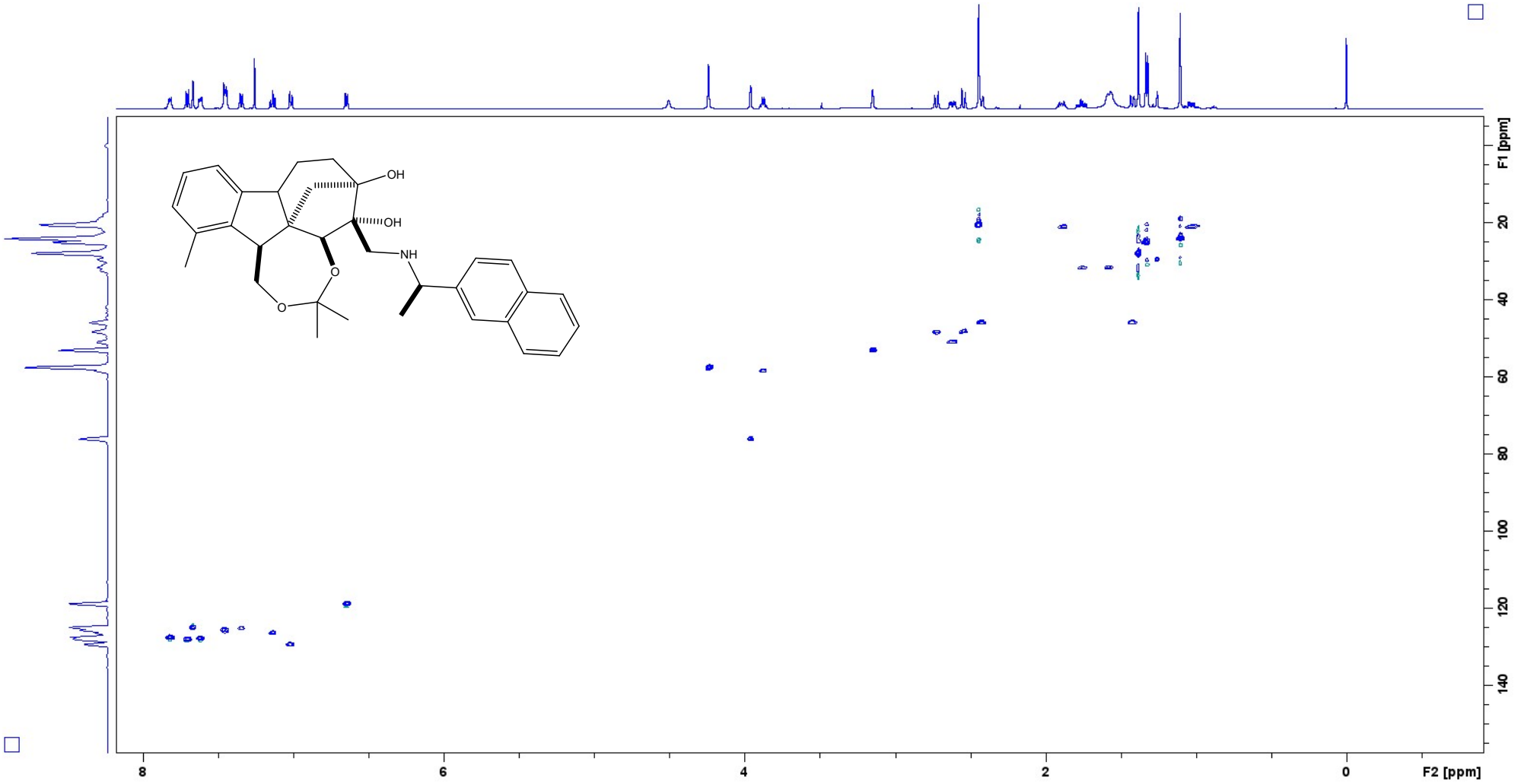
COSY of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-((((*R*)-1-(naphthalen-2-yl)ethyl)amino)methyl)-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **14**



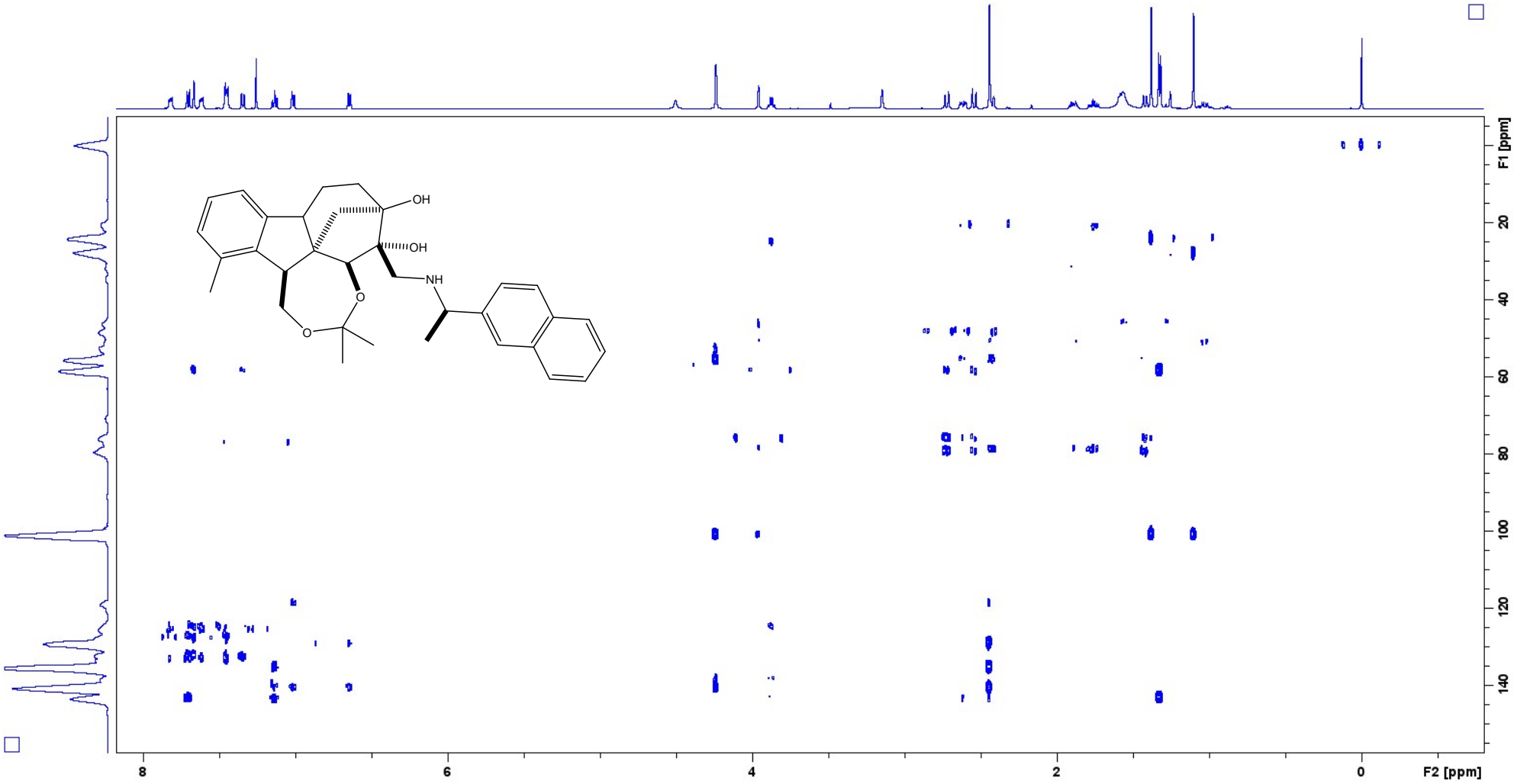
NOESY of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-((((*R*)-1-(naphthalen-2-yl)ethyl)amino)methyl)-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **14**



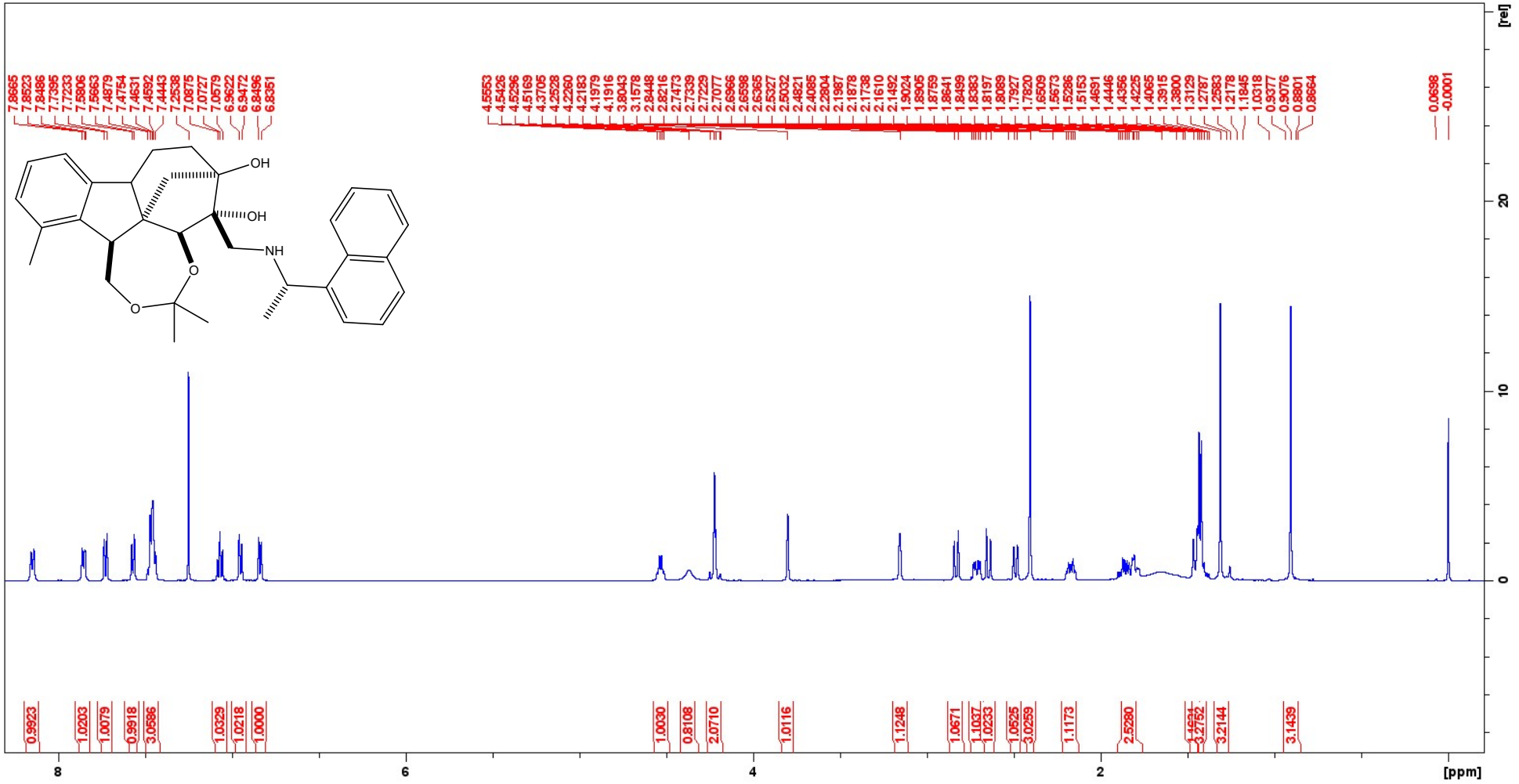
HSQC of (4a*S*,4a[1]*R*,5*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-((((*R*)-1-(naphthalen-2-yl)ethyl)amino)methyl)-4a,5,7,8,8a,12b-hexahydro-4a[1],6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **14**



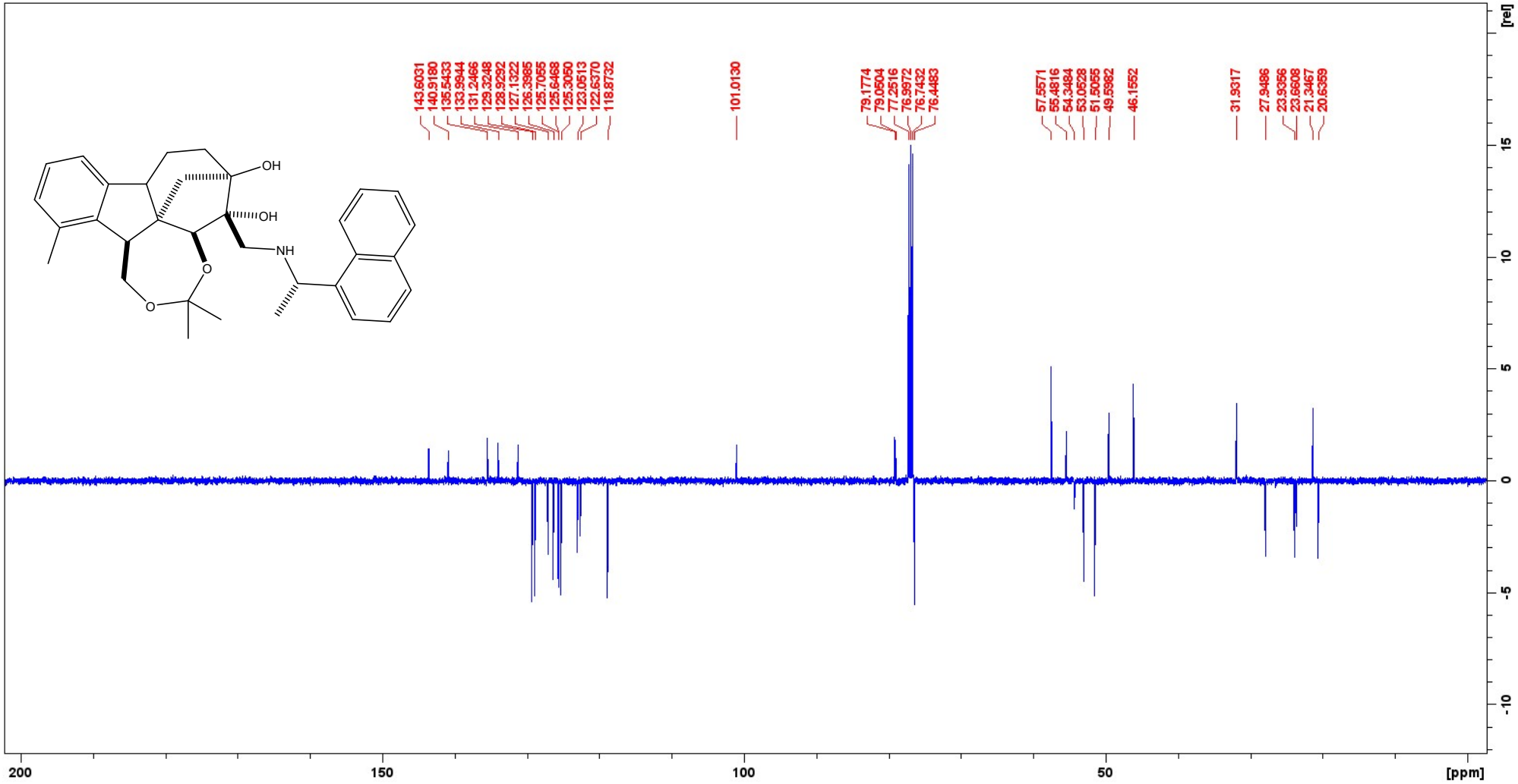
HMBC (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-((((*R*)-1-(naphthalen-2-yl)ethyl)amino)methyl)-4a,5,7,8,8a,12b-hexahydro-4a^{1},6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **14**



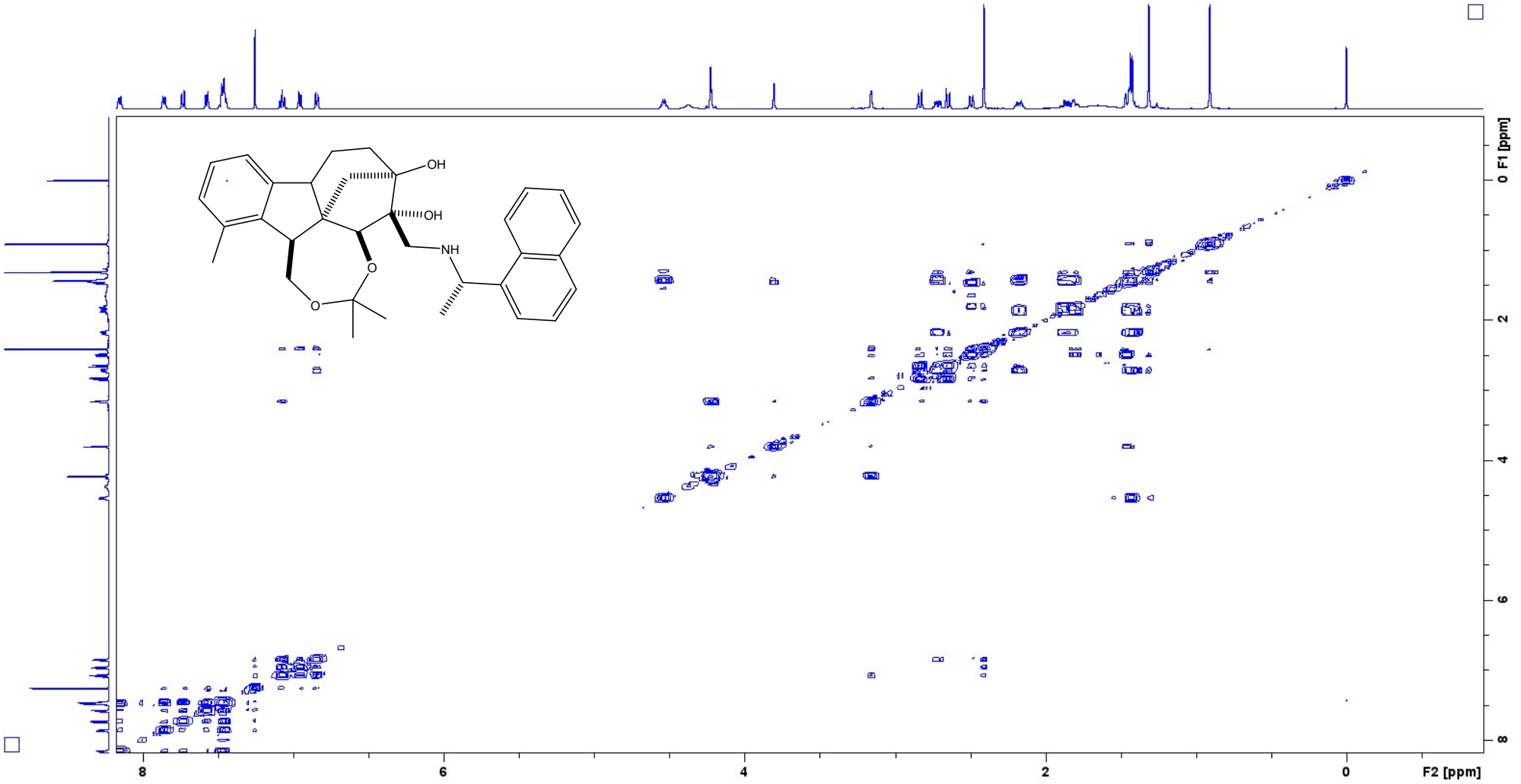
^{1}H-NMR (500 MHz) of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-((((*S*)-1-(naphthalen-1-yl)ethyl)amino)methyl)-4a,5,7,8,8a,12b-hexahydro-4a^{1},6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1H)-diol **15**



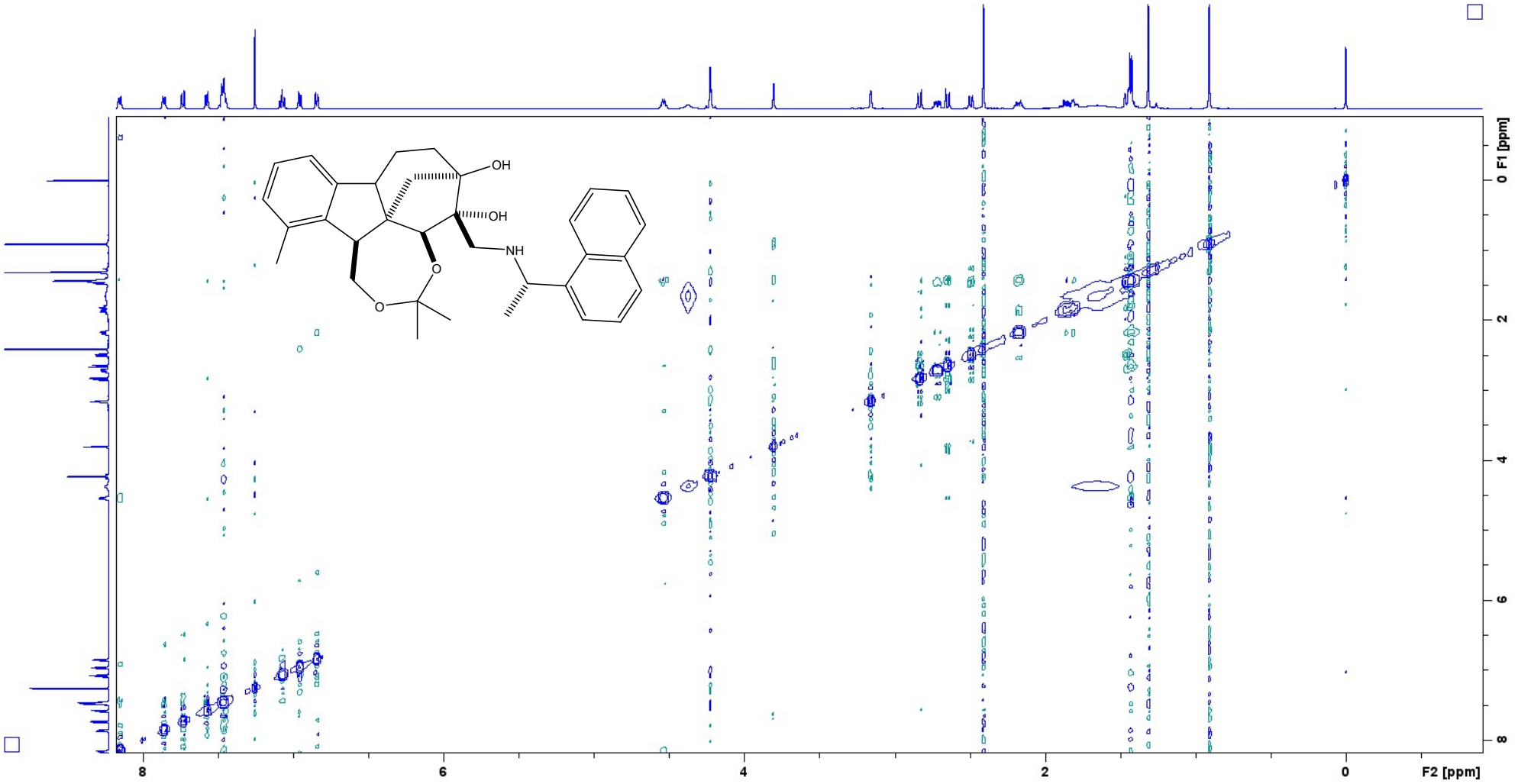
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-((((*S*)-1-(naphthalen-1-yl)ethyl)amino)methyl)-4a,5,7,8,8a,12b-hexahydro-4a^{1},6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1H)-diol **15**



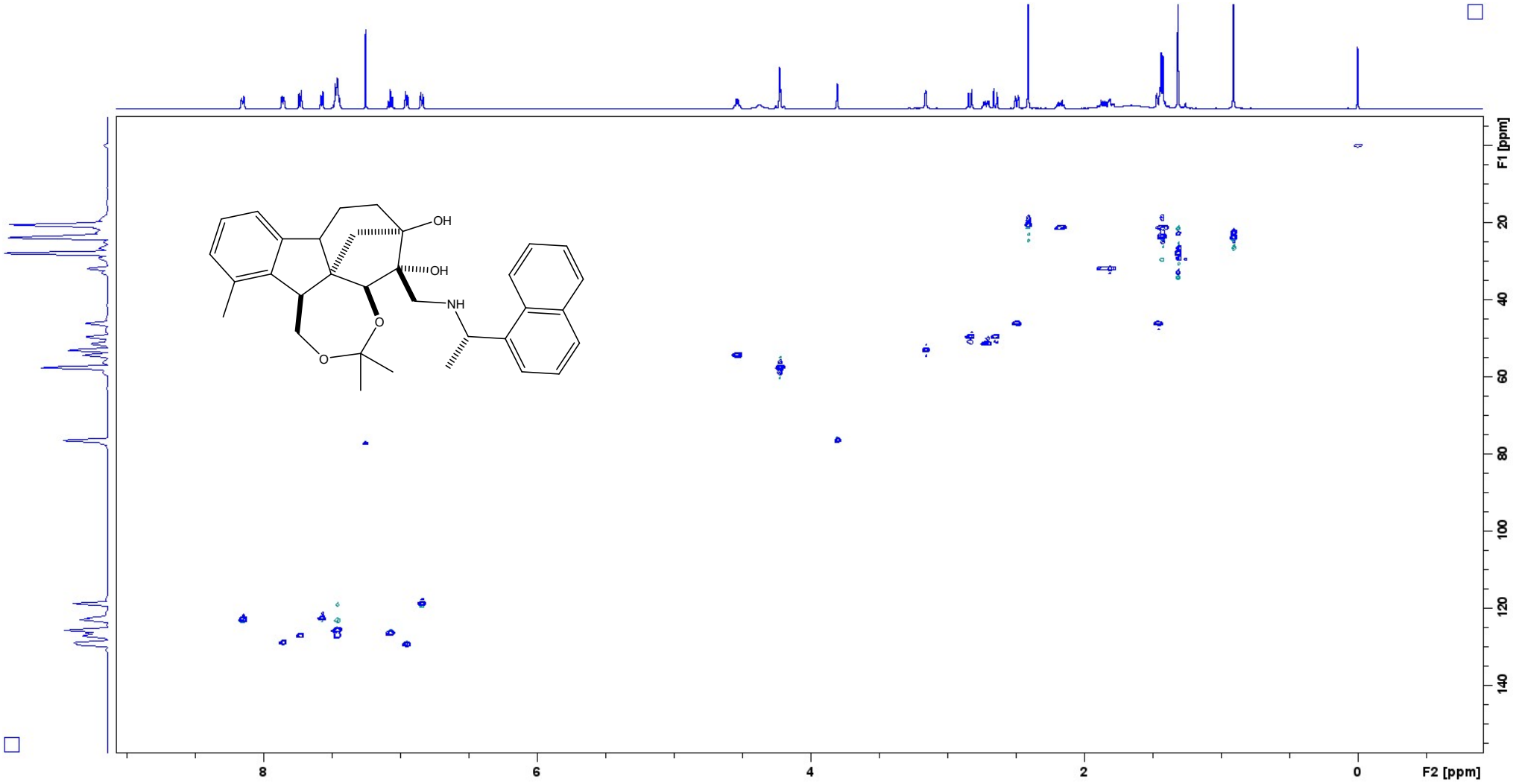
COSY of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-((((*S*)-1-(naphthalen-1-yl)ethyl)amino)methyl)-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1H)-diol **15**



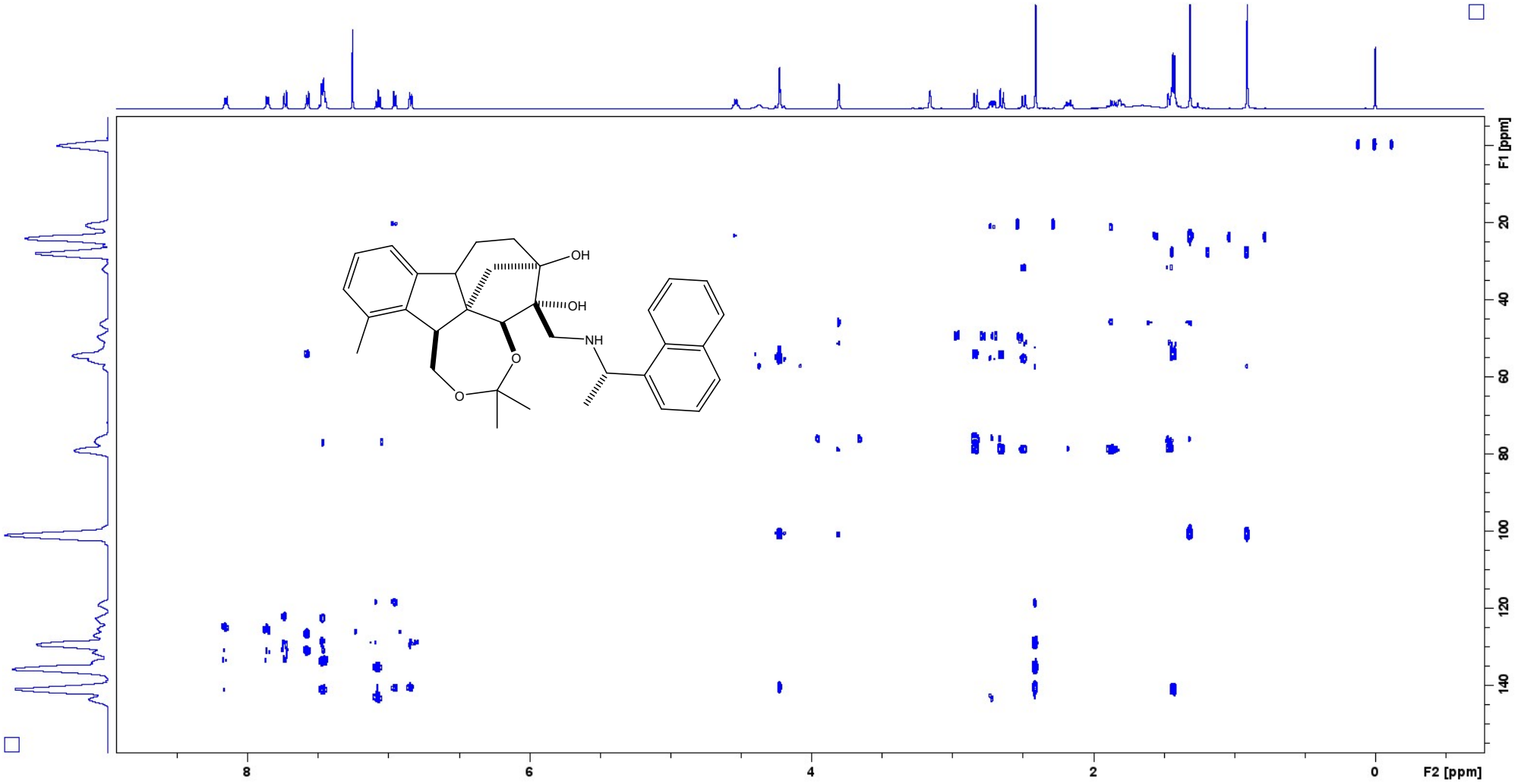
NOESY of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-((((*S*)-1-(naphthalen-1-yl)ethyl)amino)methyl)-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1H)-diol **15**



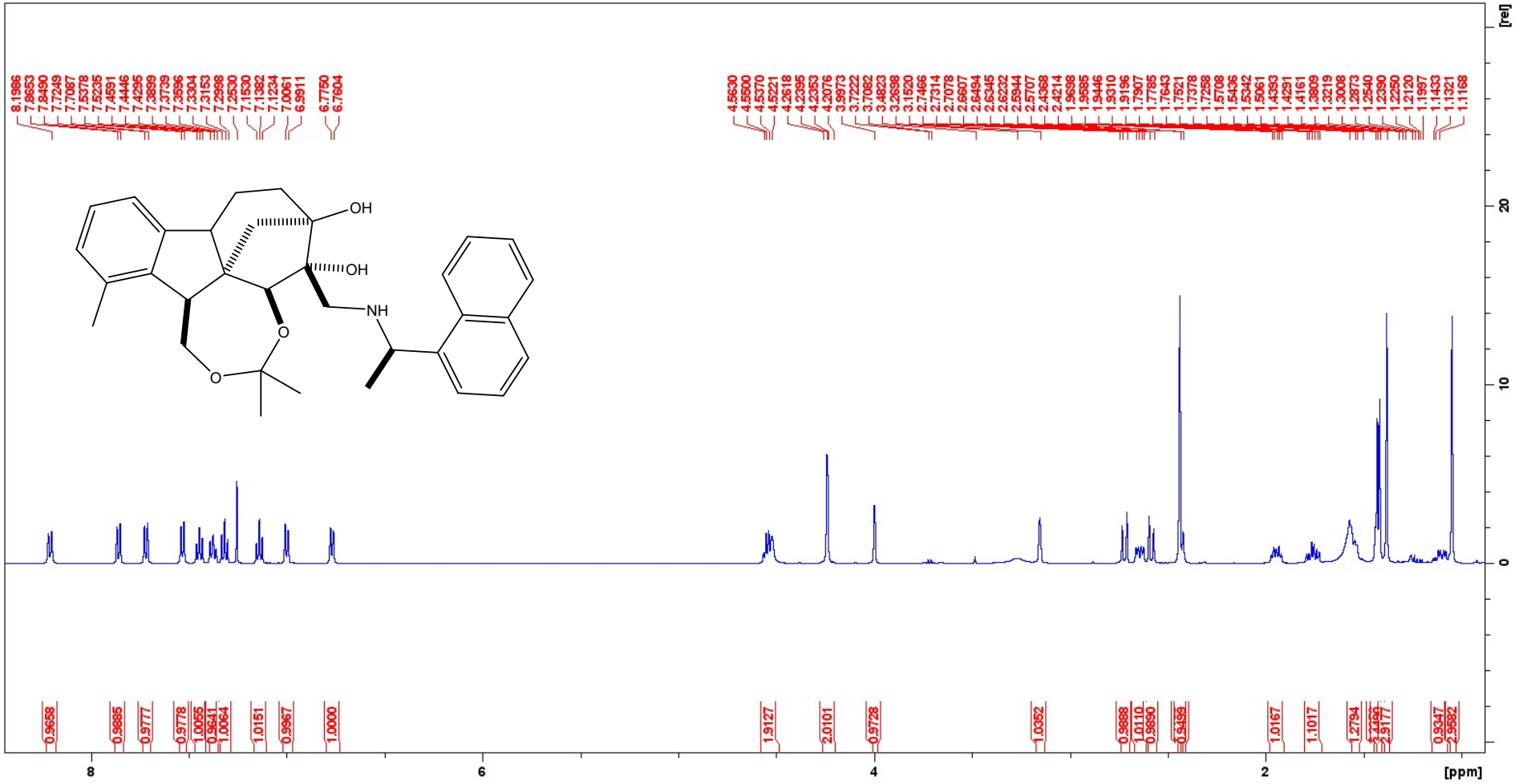
HSQC of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-((((*S*)-1-(naphthalen-1-yl)ethyl)amino)methyl)-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1H)-diol **15**



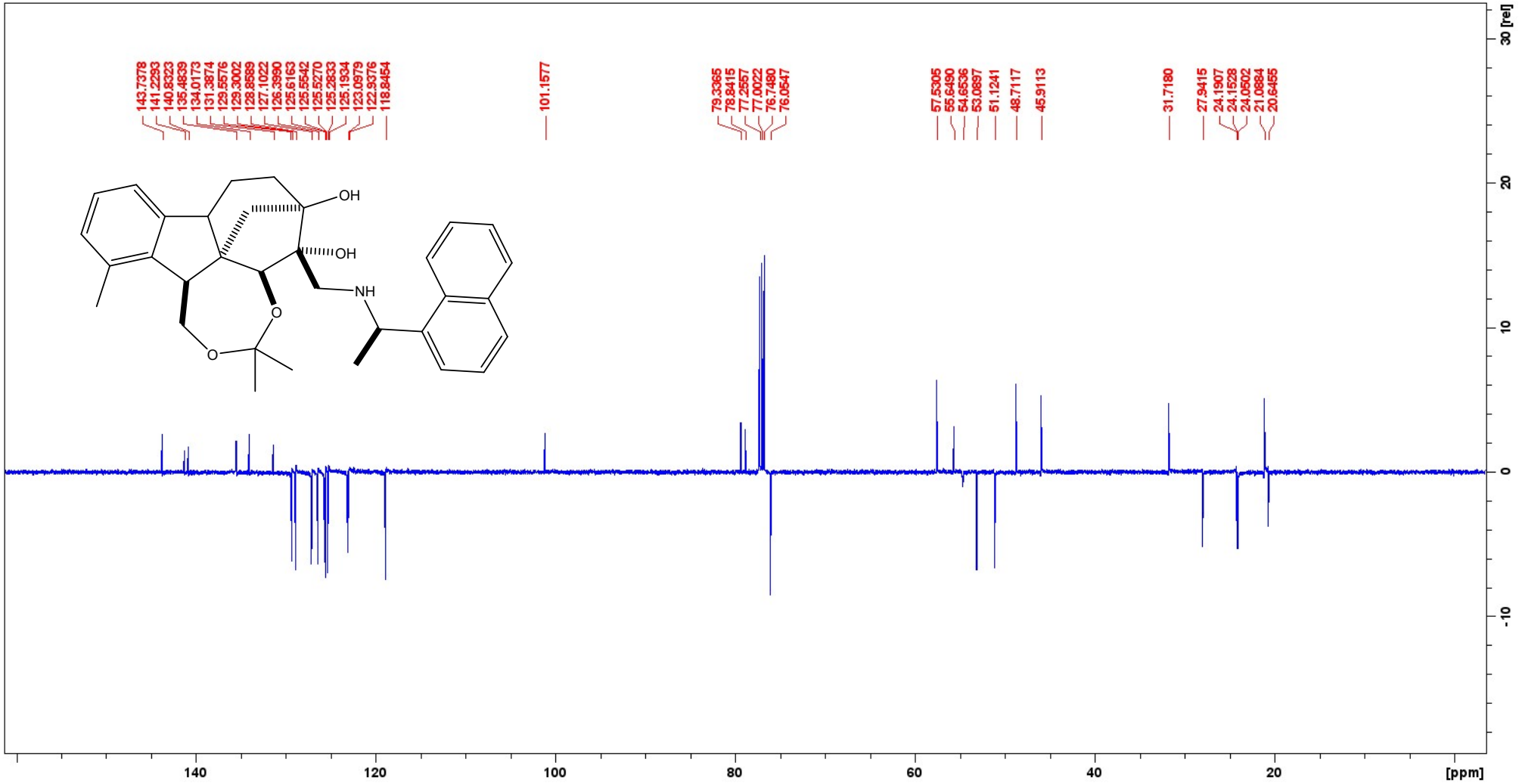
HMBC of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-((((*S*)-1-(naphthalen-1-yl)ethyl)amino)methyl)-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1H)-diol **15**



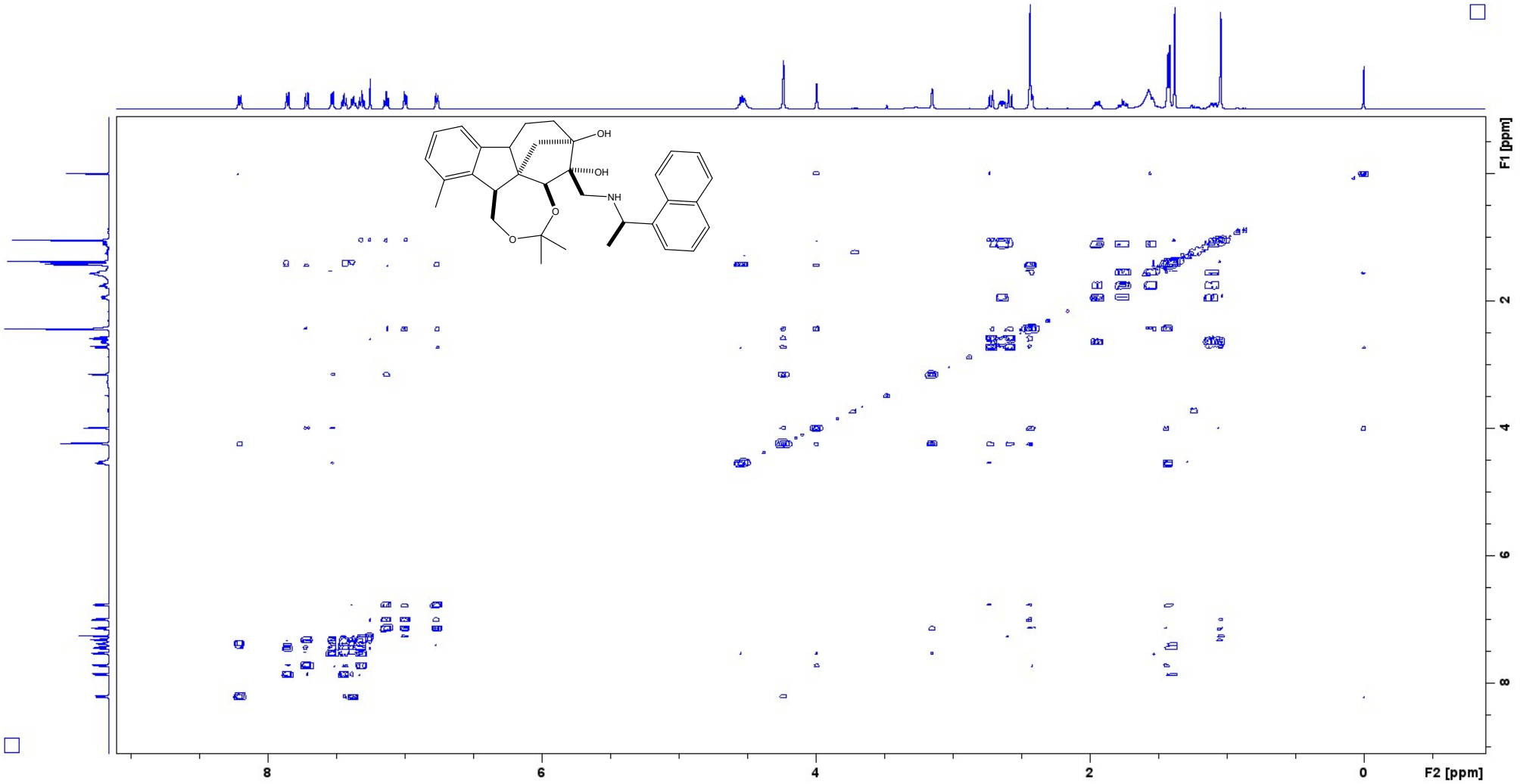
^{1}H-NMR (500 MHz) of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-((((*R*)-1-(naphthalen-1-yl)ethyl)amino)methyl)-4a,5,7,8,8a,12b-hexahydro-4a^{1},6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **16**



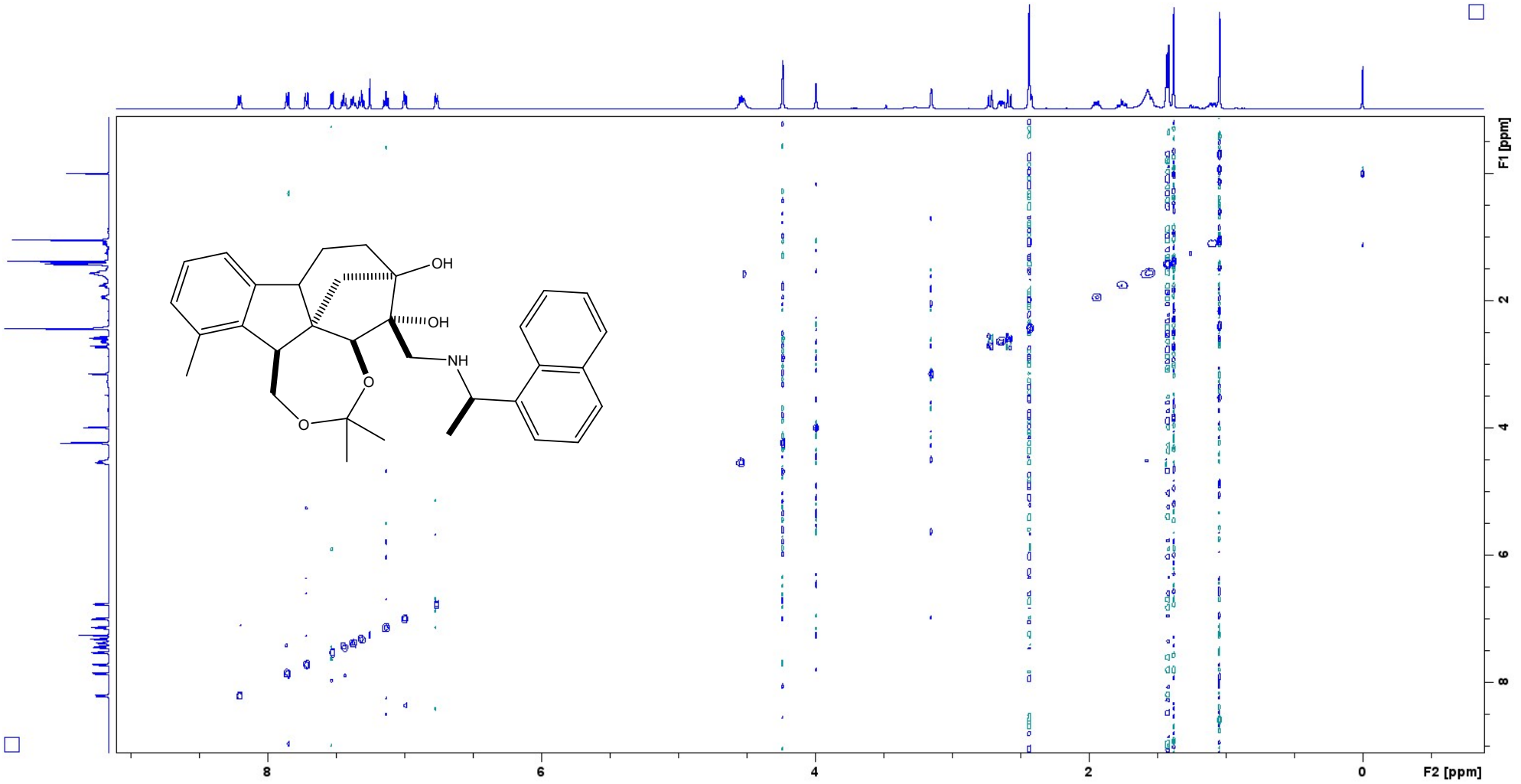
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-((((*R*)-1-(naphthalen-1-yl)ethyl)amino)methyl)-4a,5,7,8,8a,12b-hexahydro-4a^{1},6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **16**



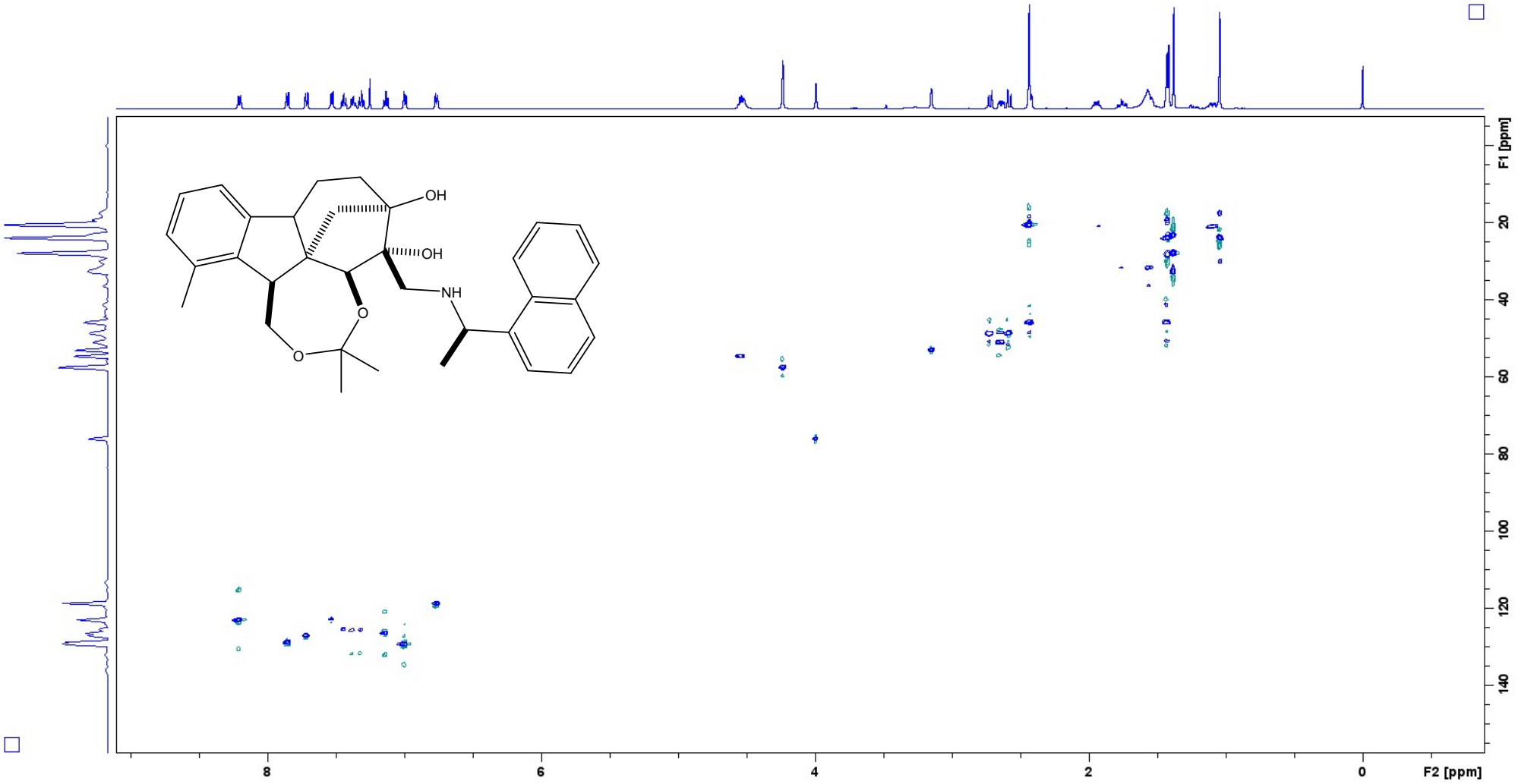
COSY of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-((((*R*)-1-(naphthalen-1-yl)ethyl)amino)methyl)-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **16**



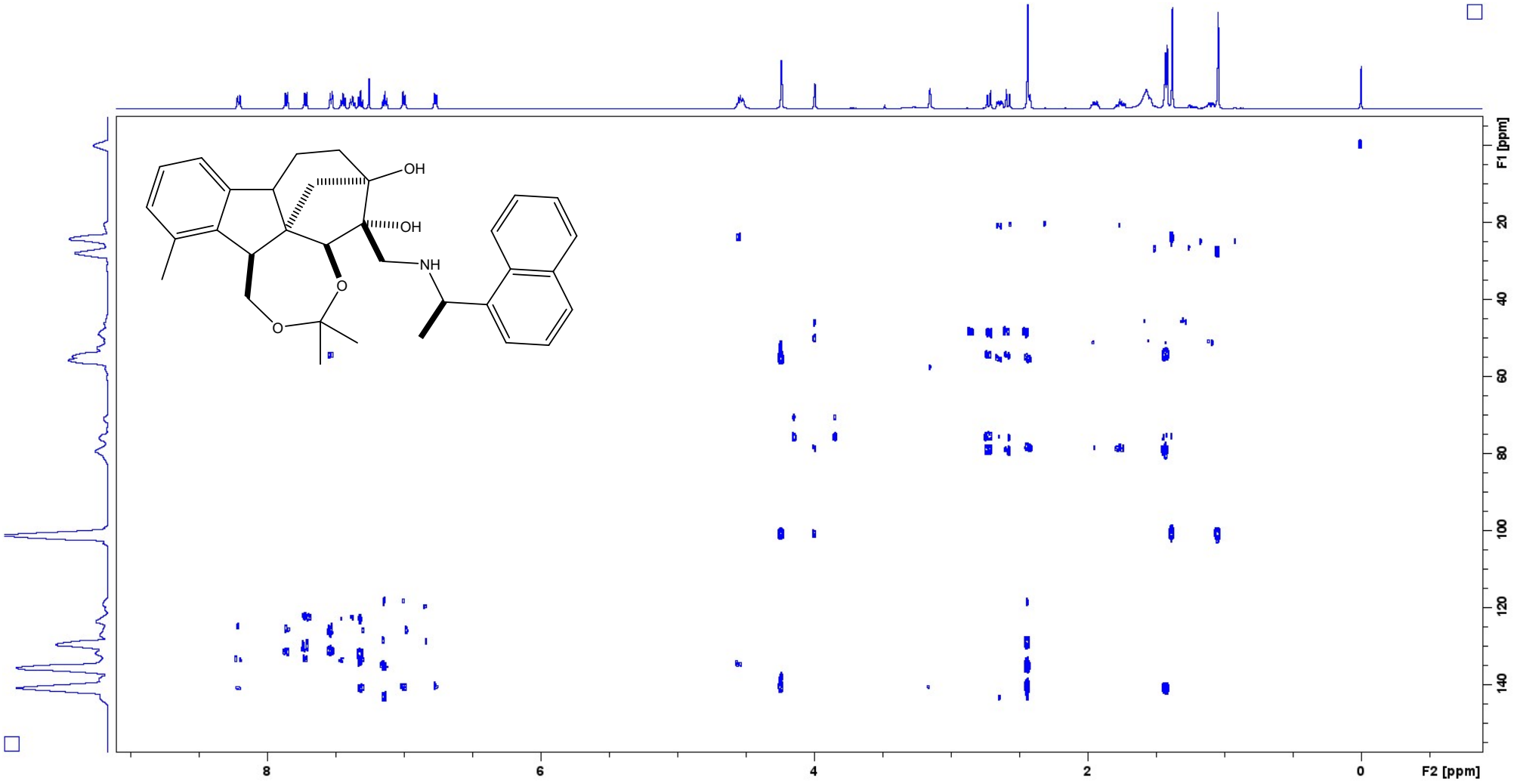
NOESY of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-((((*R*)-1-(naphthalen-1-yl)ethyl)amino)methyl)-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **16**



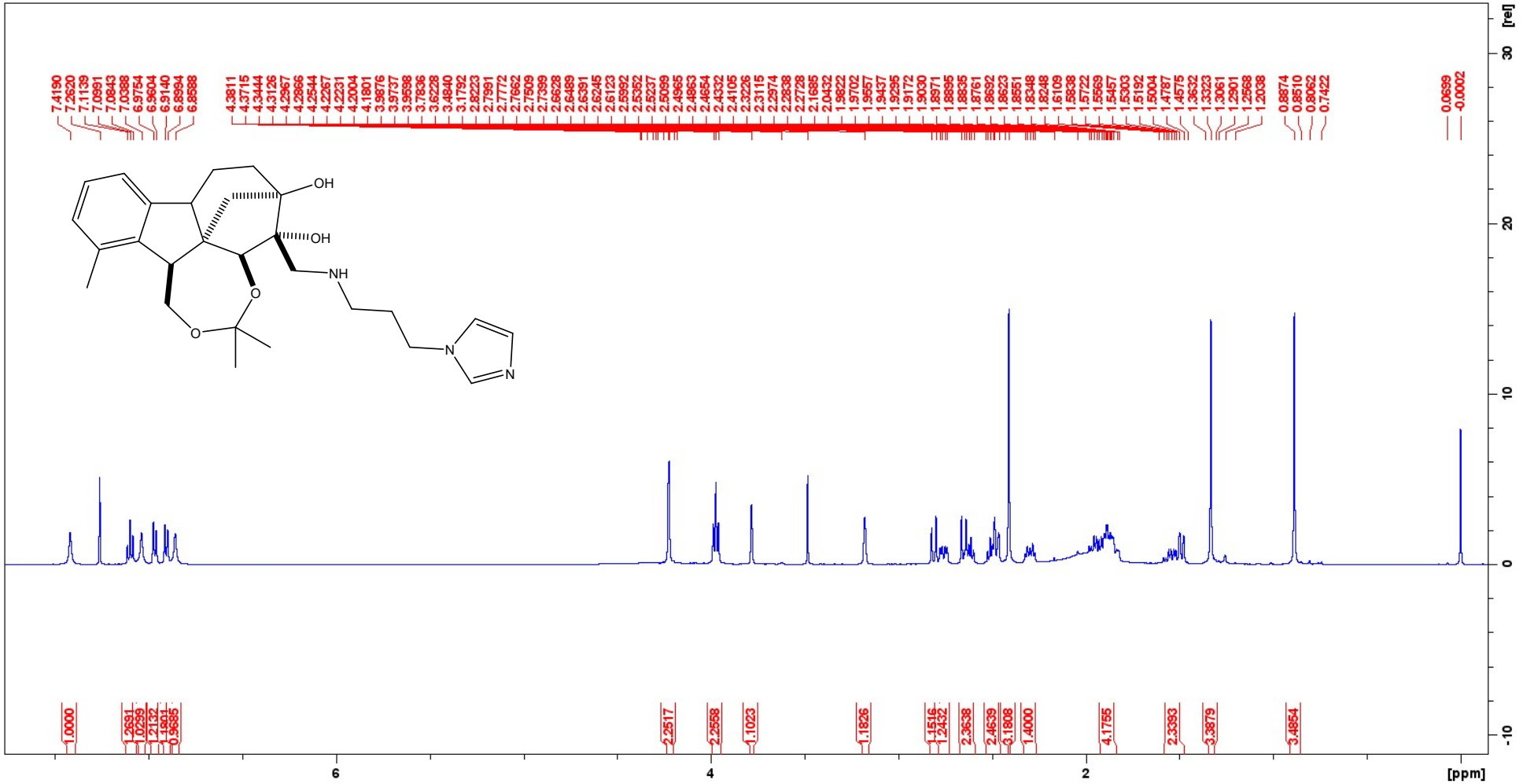
HSQC of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-((((*R*)-1-(naphthalen-1-yl)ethyl)amino)methyl)-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **16**



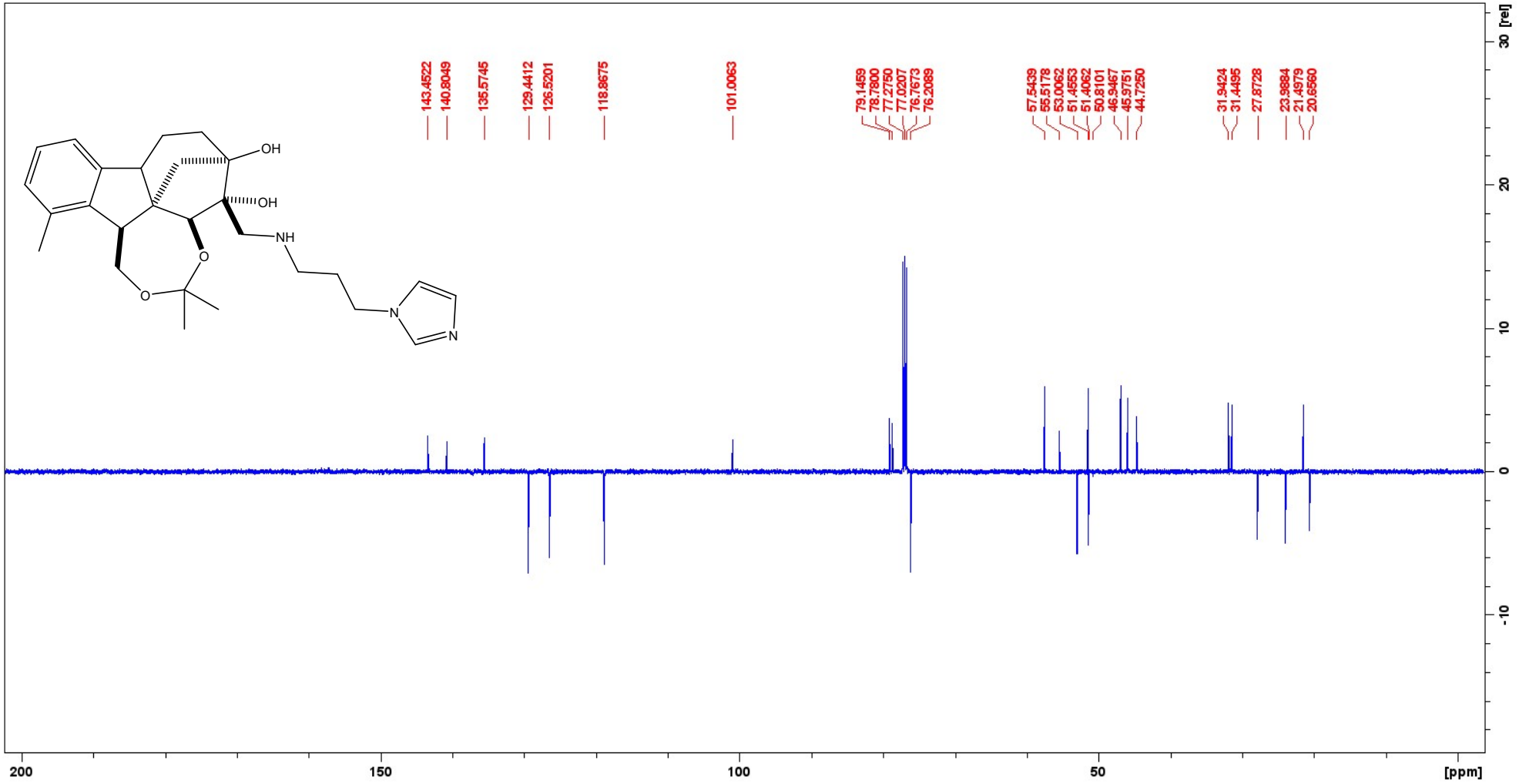
HMBC of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-3,3,12-Trimethyl-5-((((*R*)-1-(naphthalen-1-yl)ethyl)amino)methyl)-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **16**



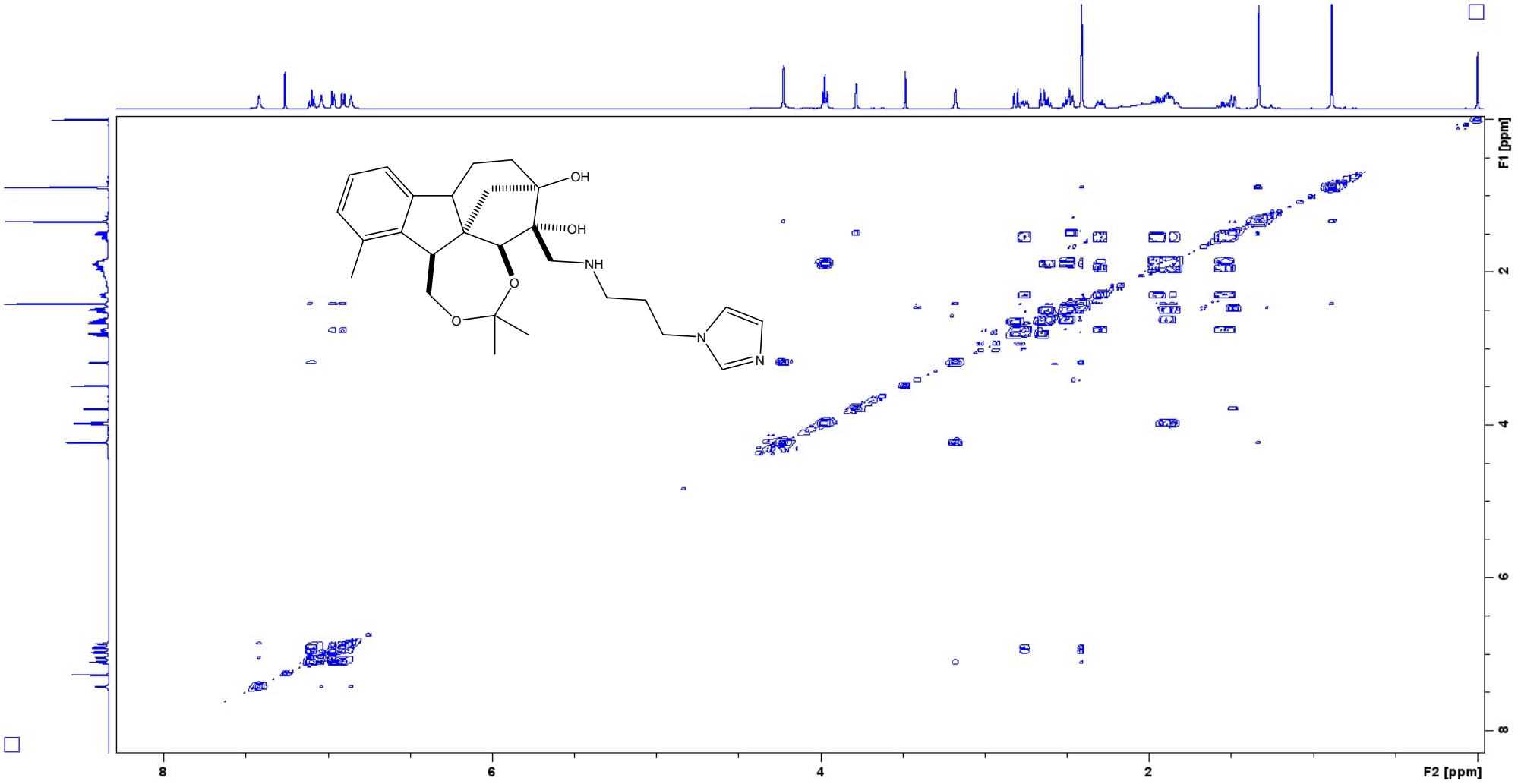
^{1}H-NMR (500 MHz) of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-5-(((3-(1*H*-Imidazol-1-yl)propyl)amino)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^{1},6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **17**



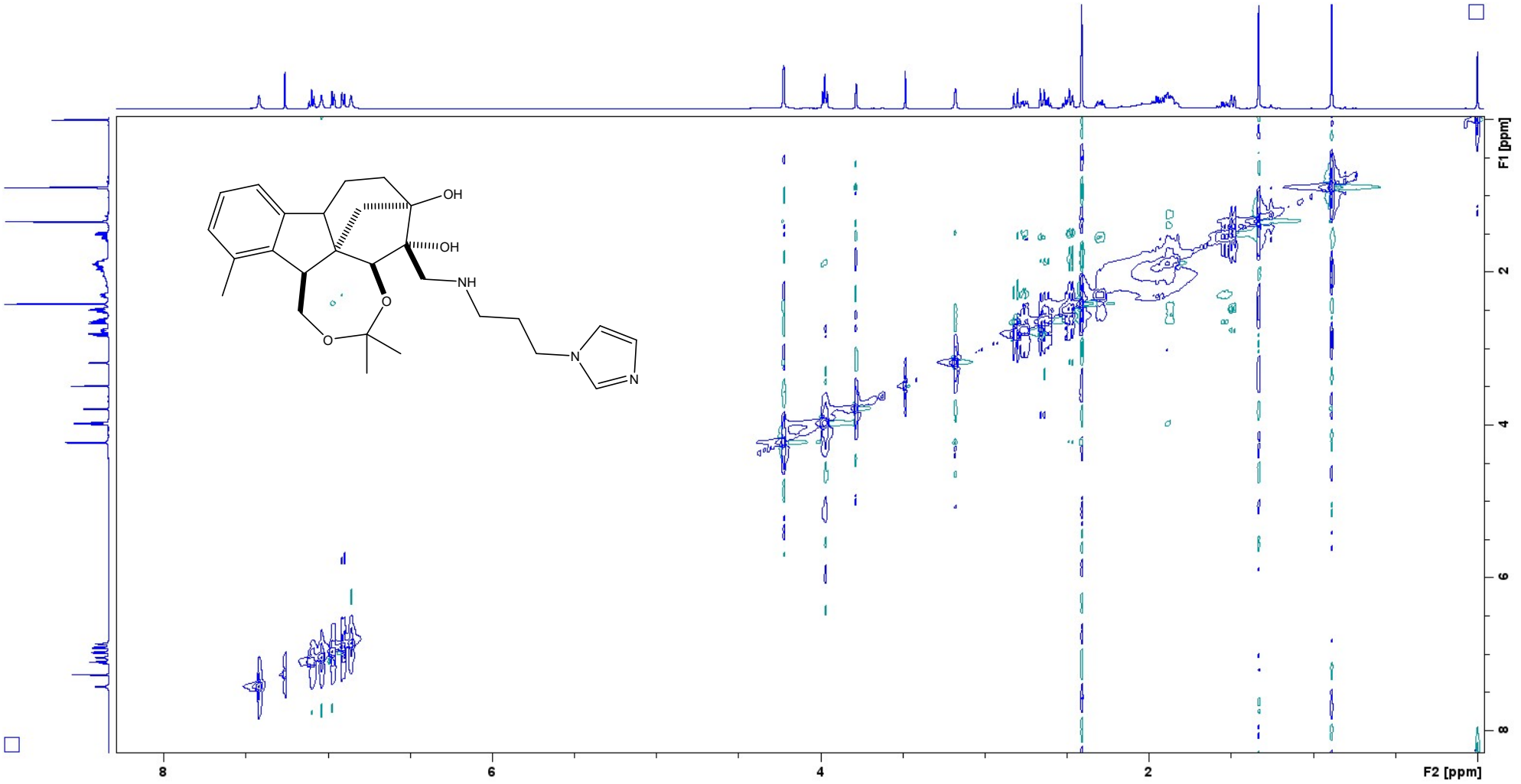
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-5-(((3-(1*H*-Imidazol-1-yl)propyl)amino)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^{1},6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **17**



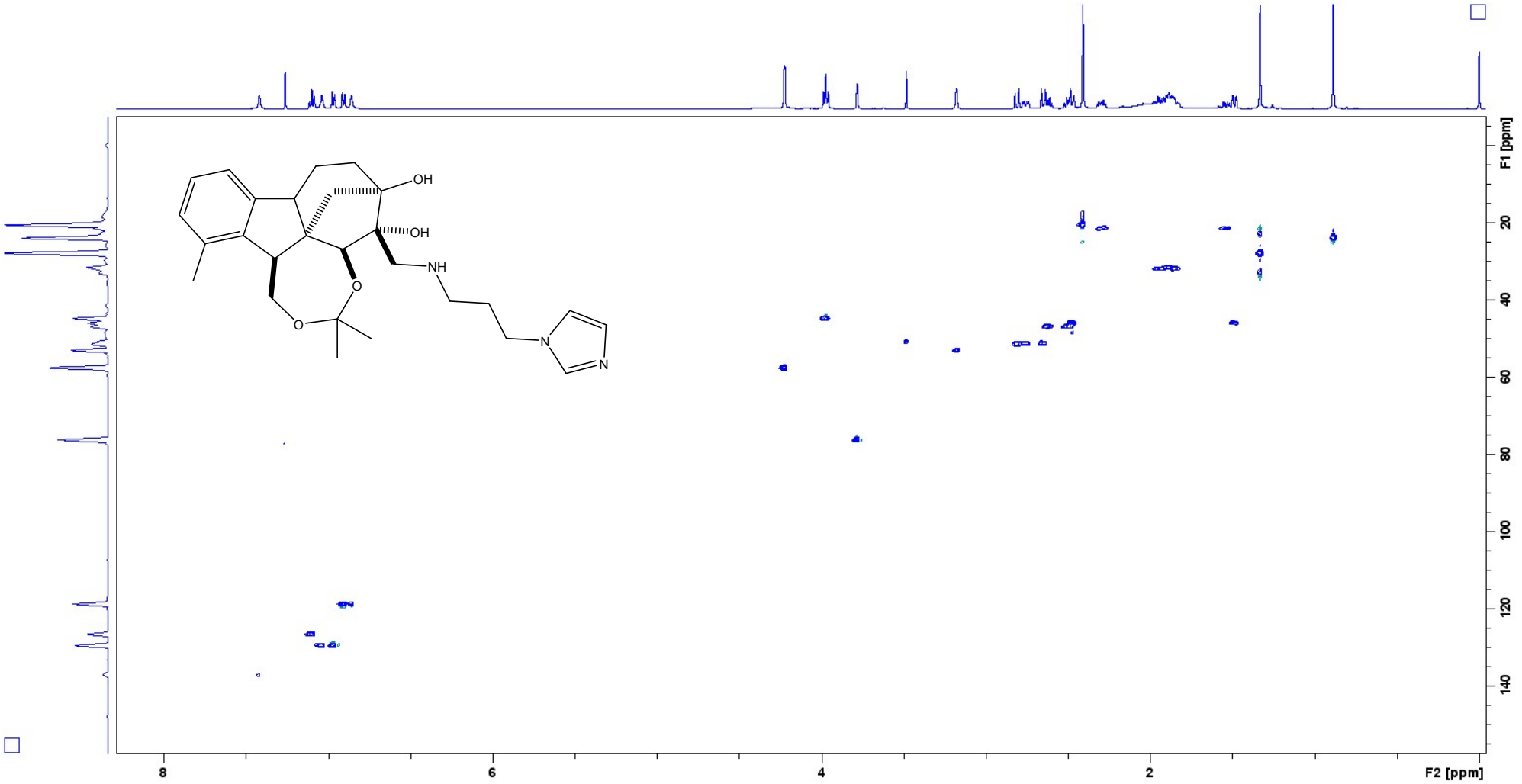
COSY of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-5-(((3-(1*H*-Imidazol-1-yl)propyl)amino)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **17**



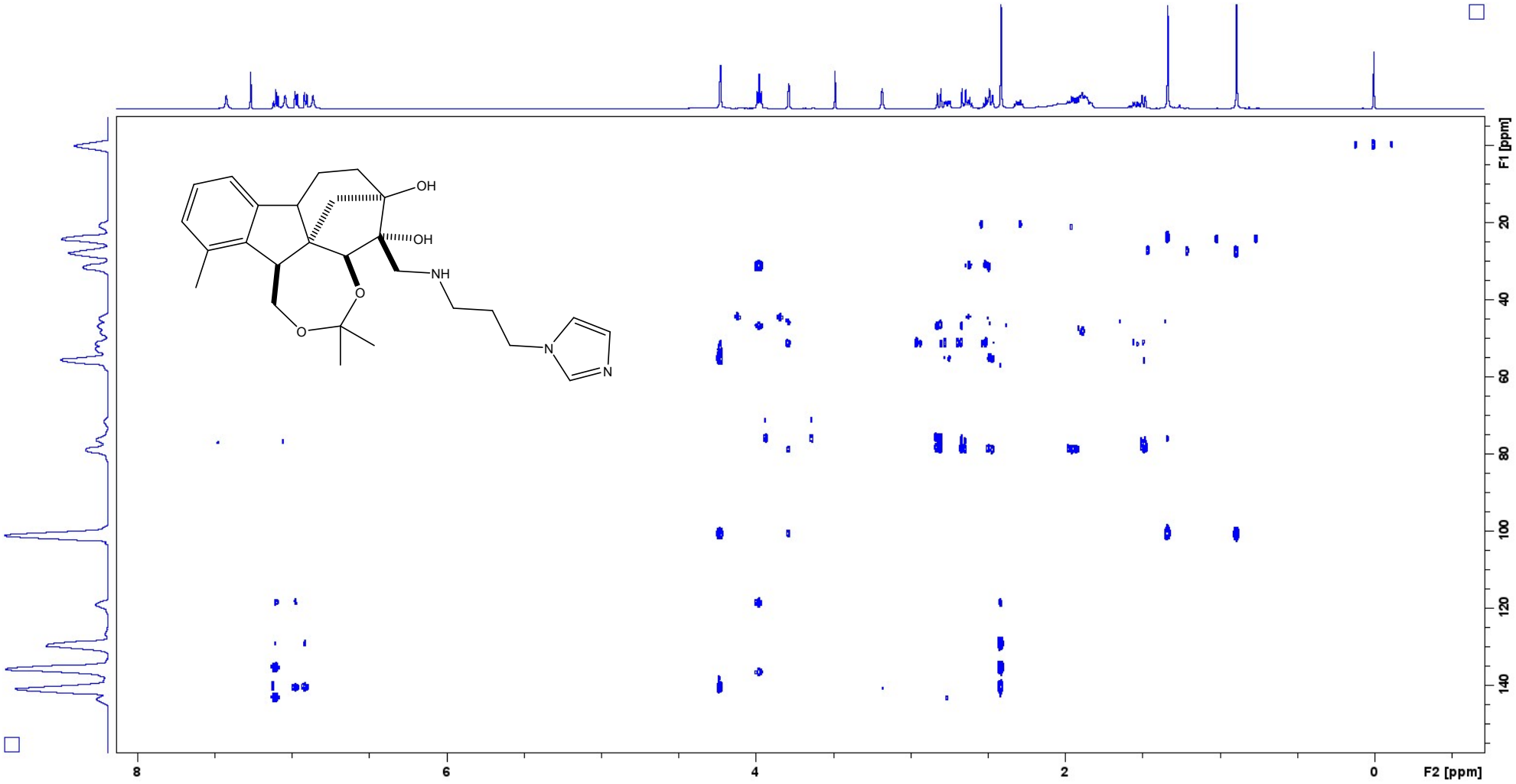
NOESY of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-5-(((3-(1*H*-Imidazol-1-yl)propyl)amino)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **17**



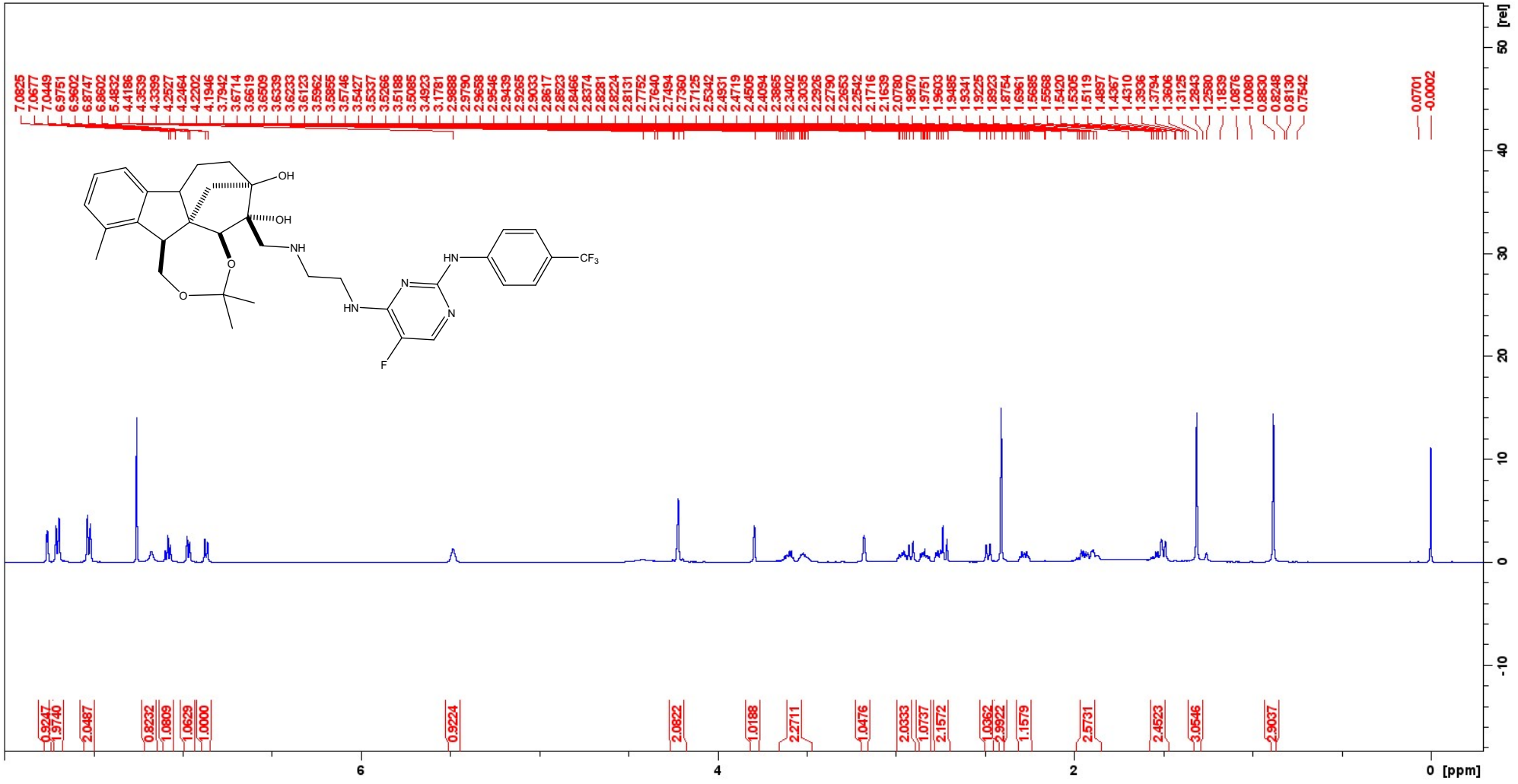
HSQC of (4a*S*,4a[1]*R*,5*R*,6*S*,12b*S*)-5-(((3-(1*H*-Imidazol-1-yl)propyl)amino)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a[1],6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **17**



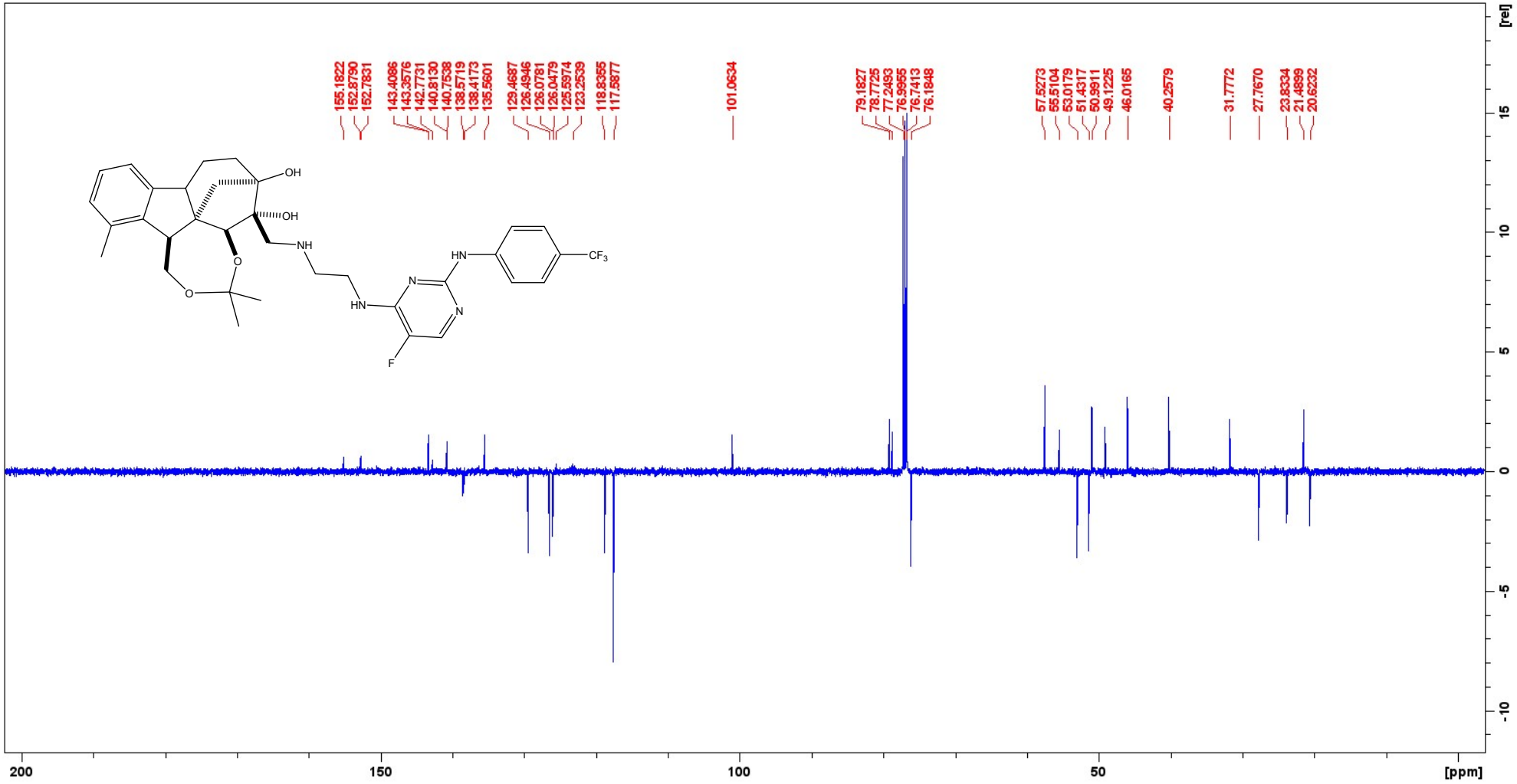
HMBC of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-5-(((3-(1*H*-Imidazol-1-yl)propyl)amino)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **17**



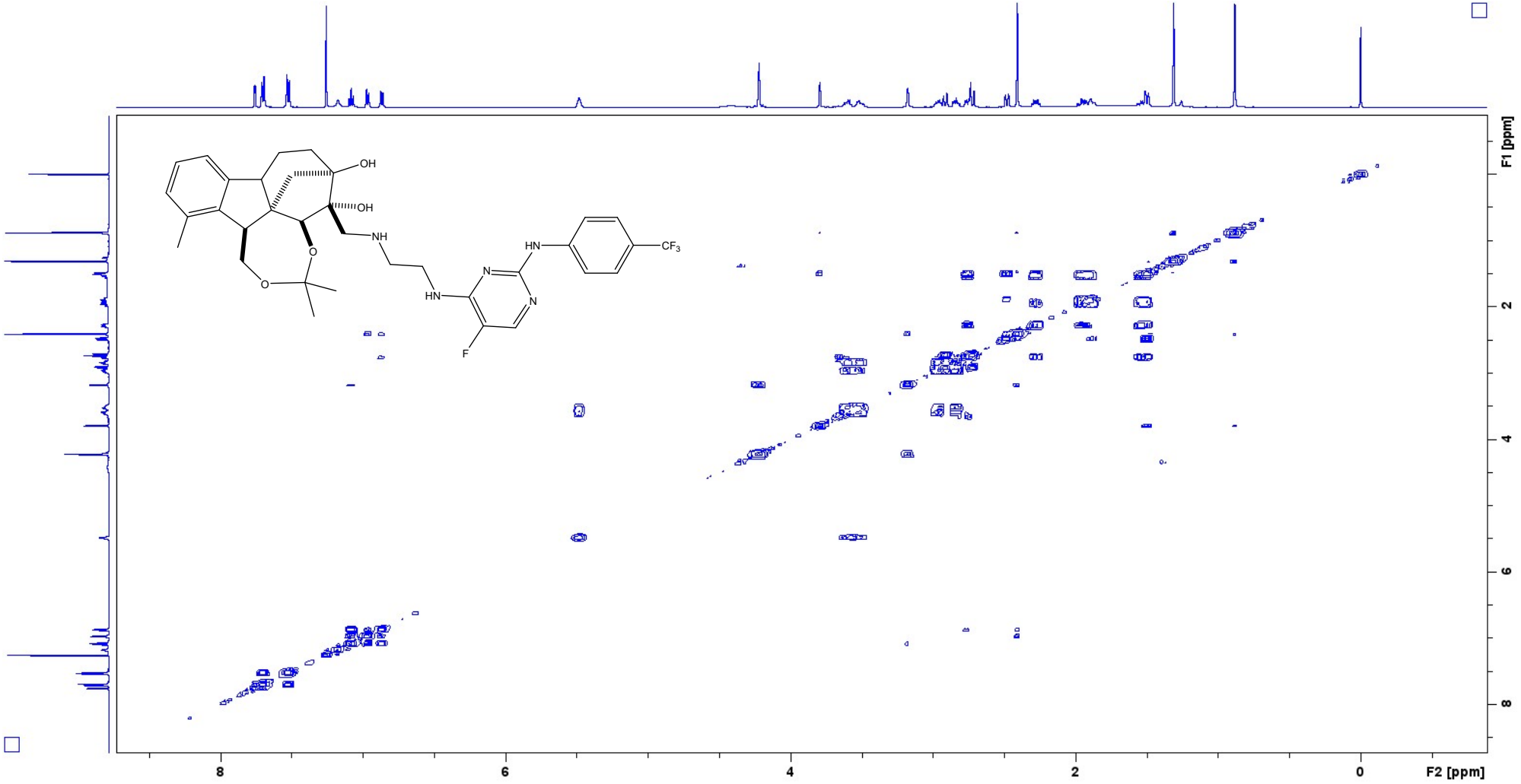
^{1}H-NMR (500 MHz) of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-5-(((2-((5-Fluoro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)ethyl)amino)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^{1},6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **18**



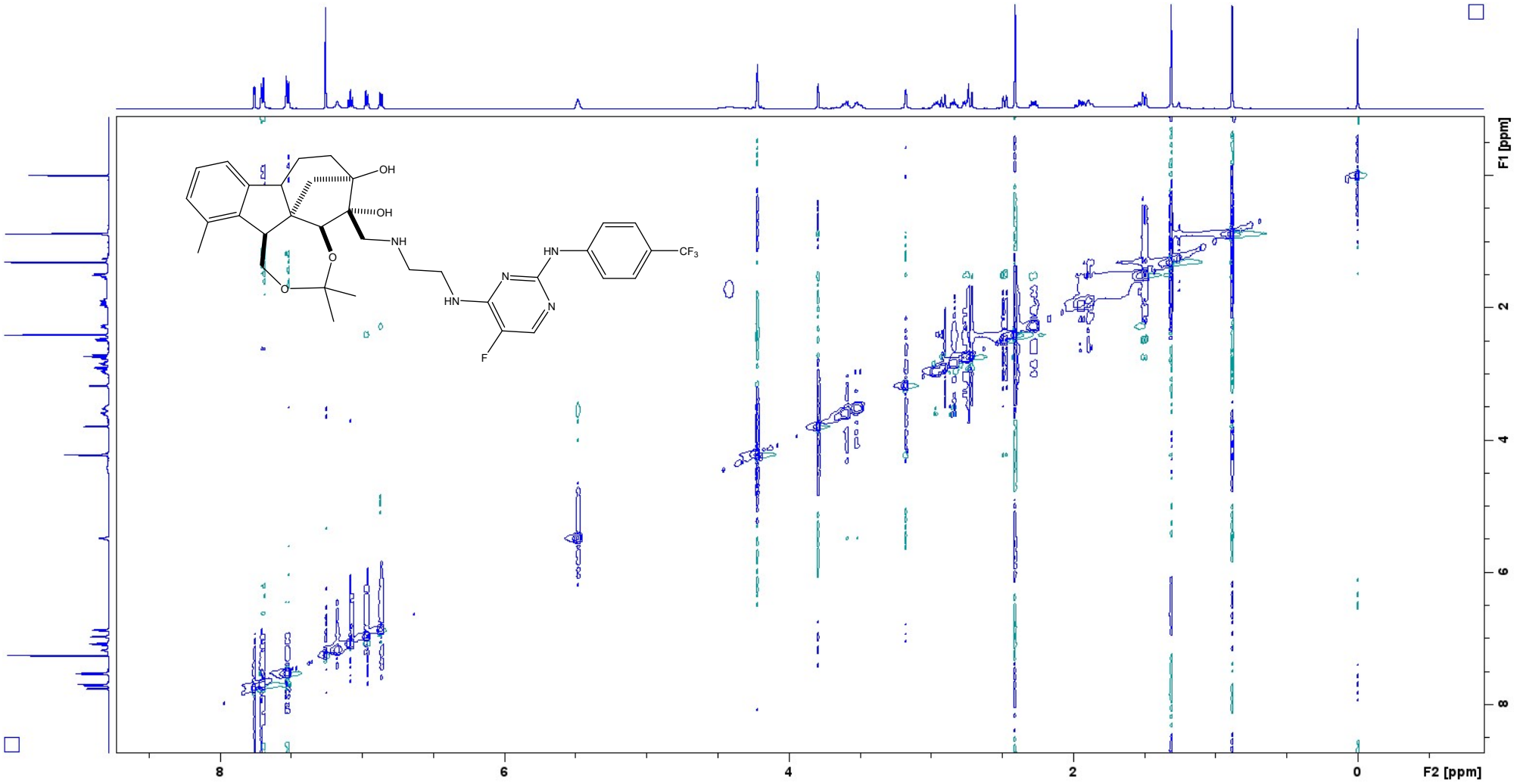
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-5-(((2-((5-Fluoro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)ethyl)amino)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^{1},6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **18**



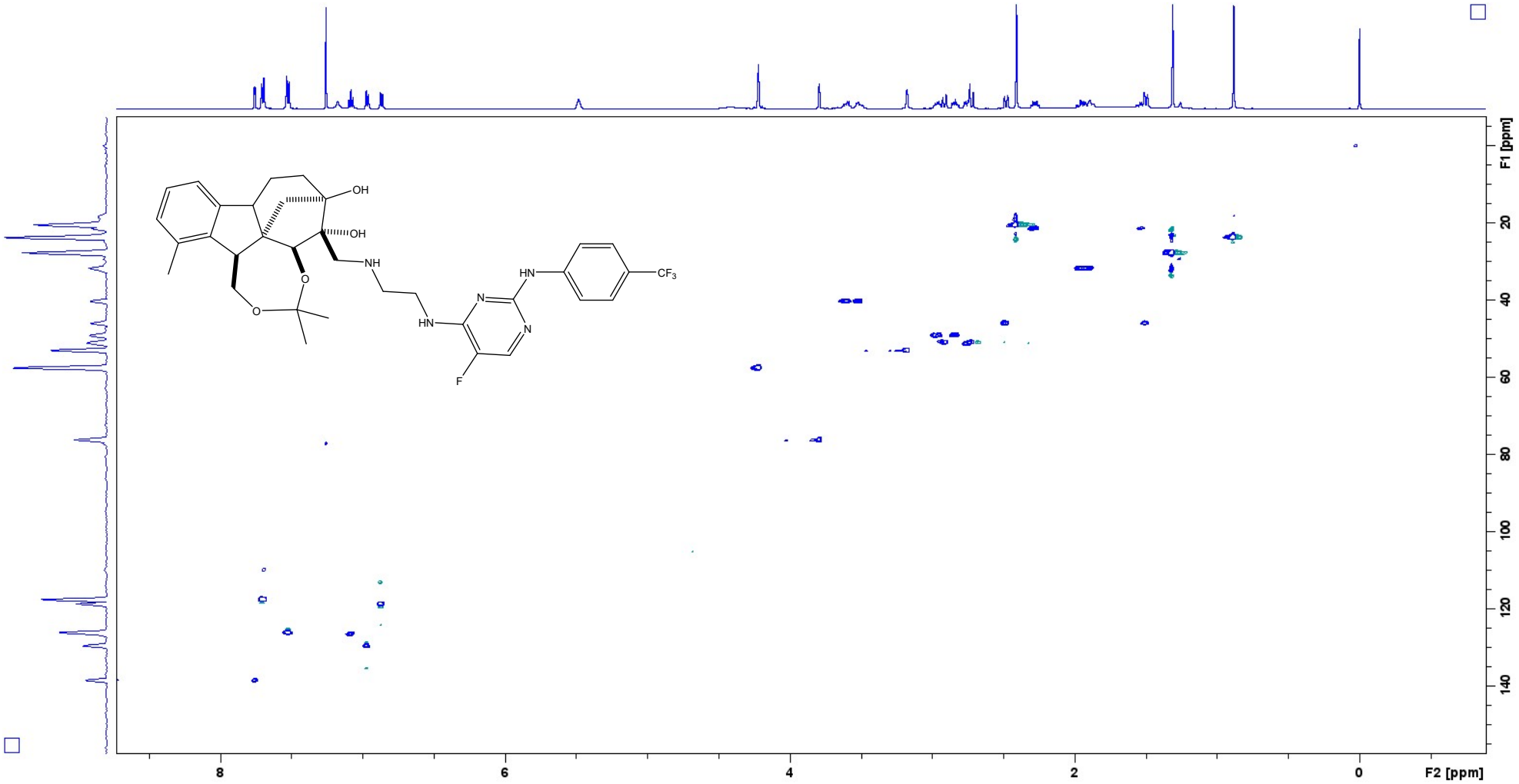
COSY of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-5-(((2-((5-Fluoro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)ethyl)amino)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^{1},6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **18**



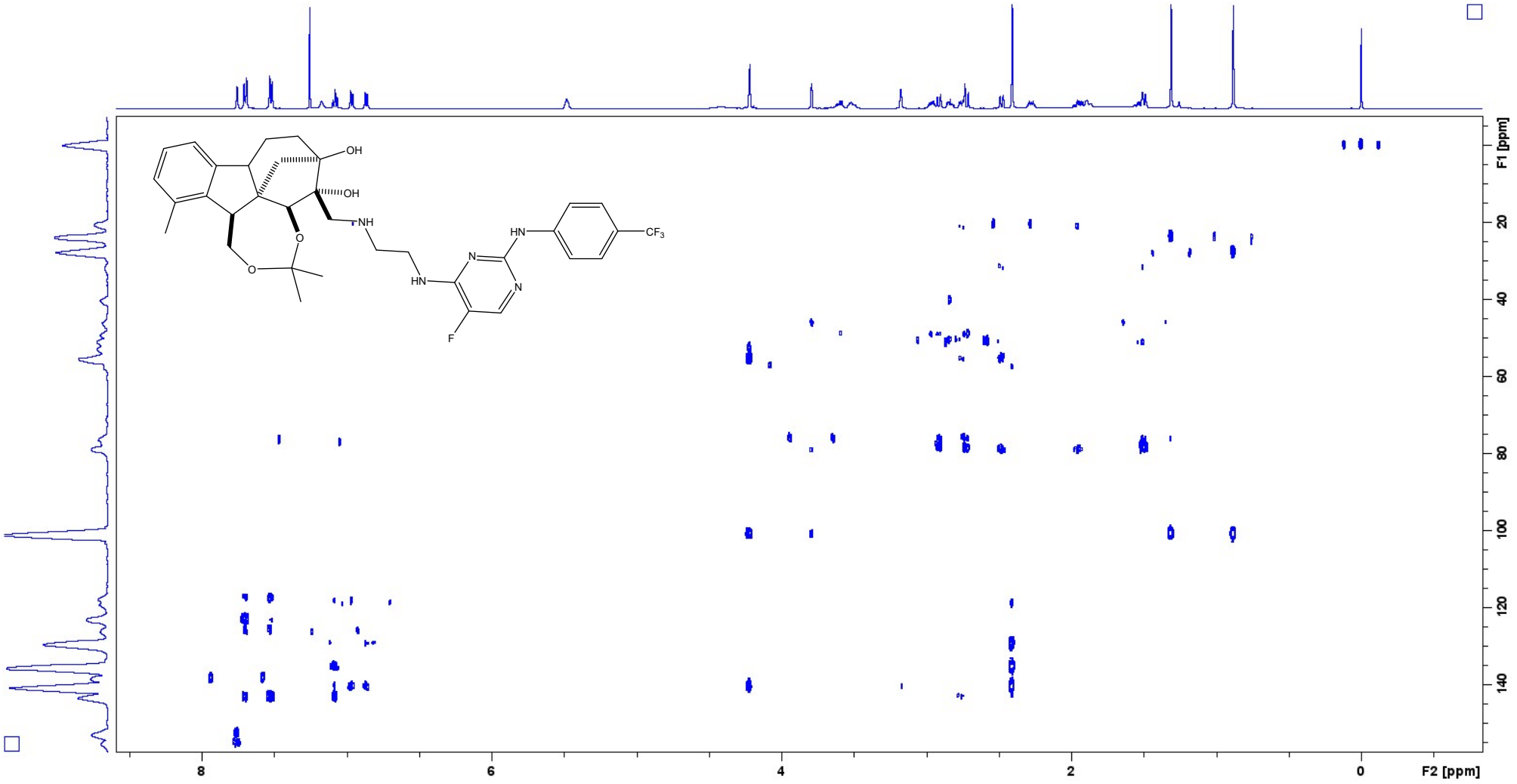
NOESY of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-5-(((2-((5-Fluoro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)ethyl)amino)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **18**



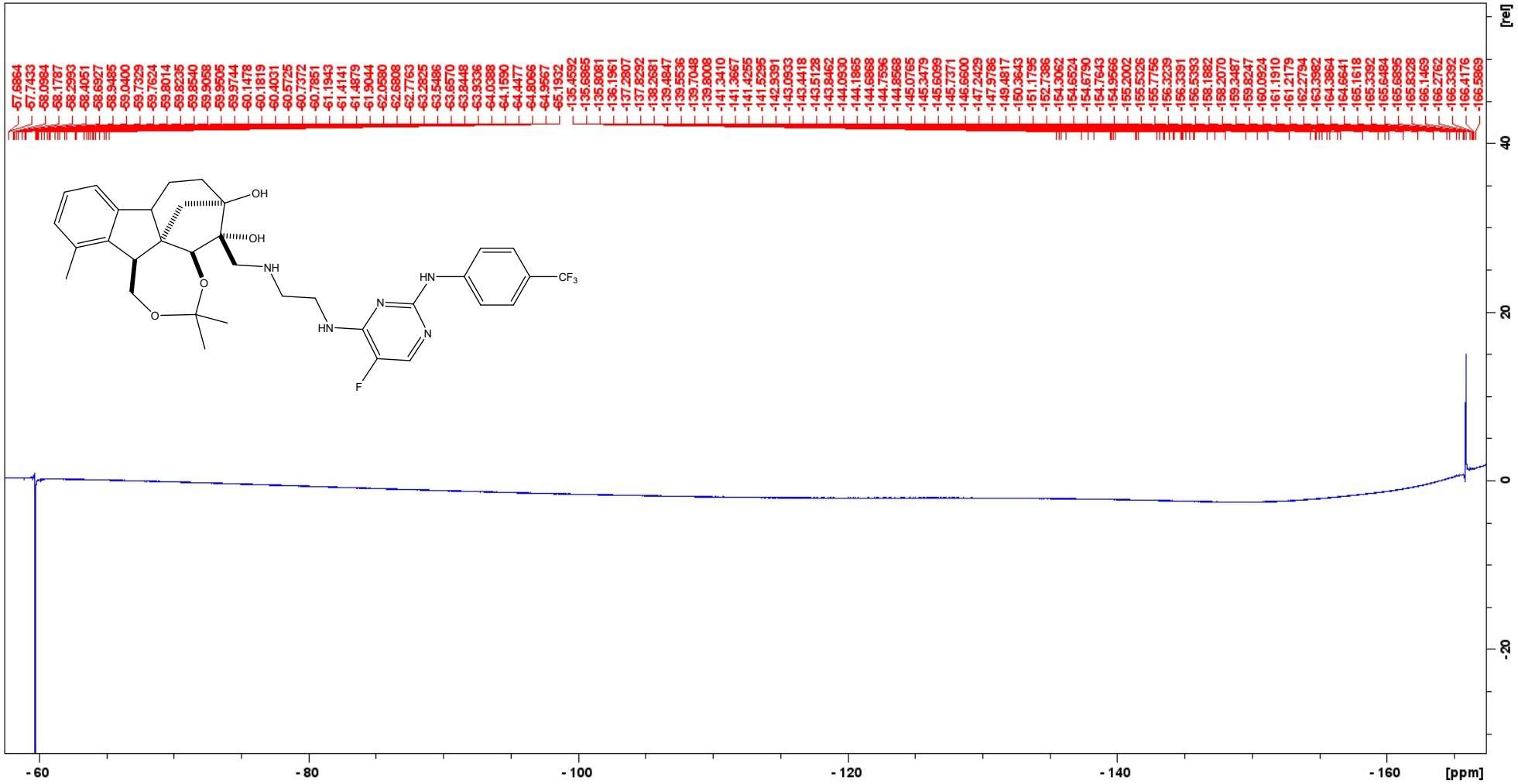
HSQC of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-5-(((2-((5-Fluoro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)ethyl)amino)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **18**



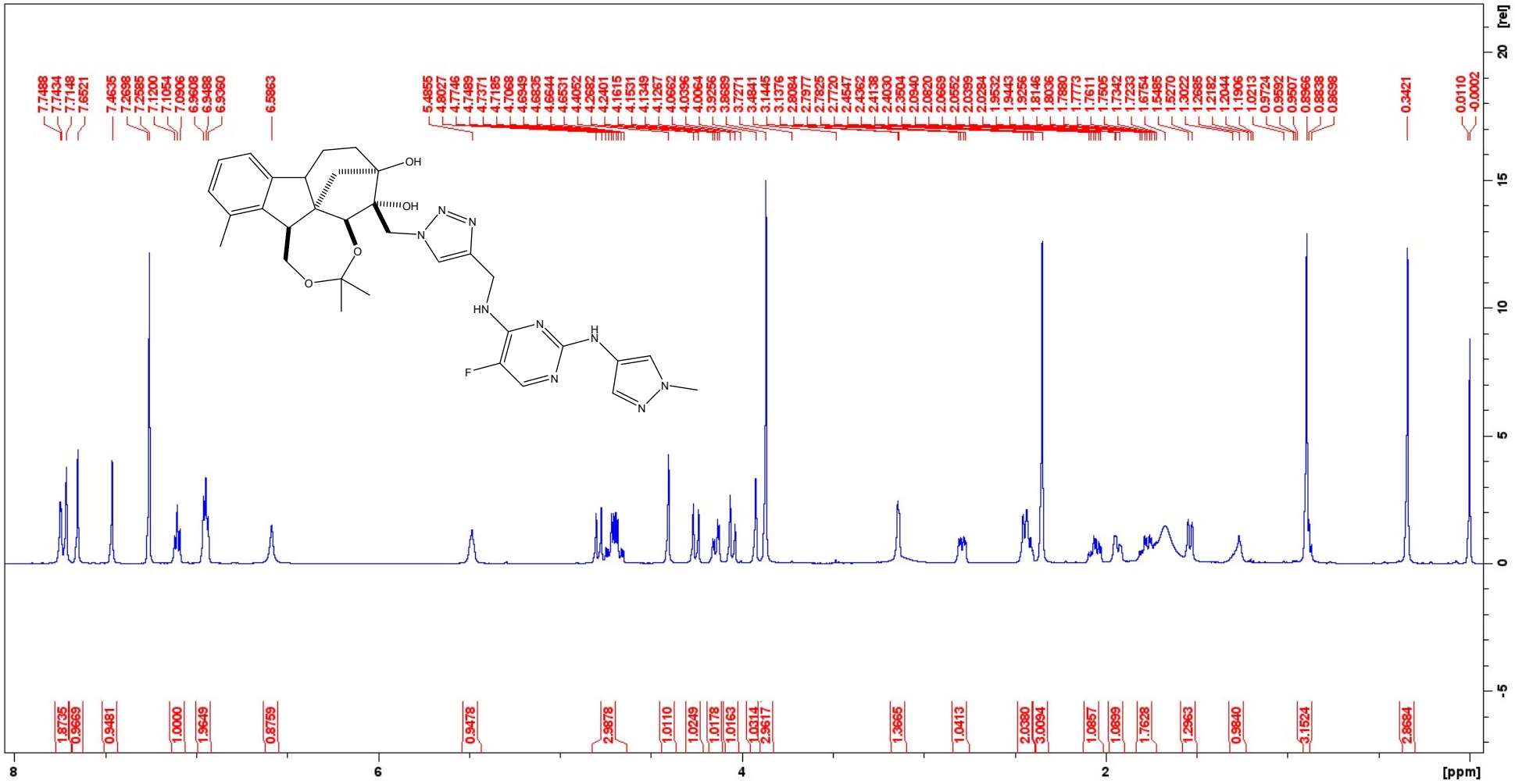
HMBC of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-5-(((2-((5-Fluoro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)ethyl)amino)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^1,6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **18**



^{19}F *J*-MOD NMR (470 MHz) of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-5-(((2-((5-Fluoro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)ethyl)amino)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a^{1},6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepine-5,6(1*H*)-diol **18**

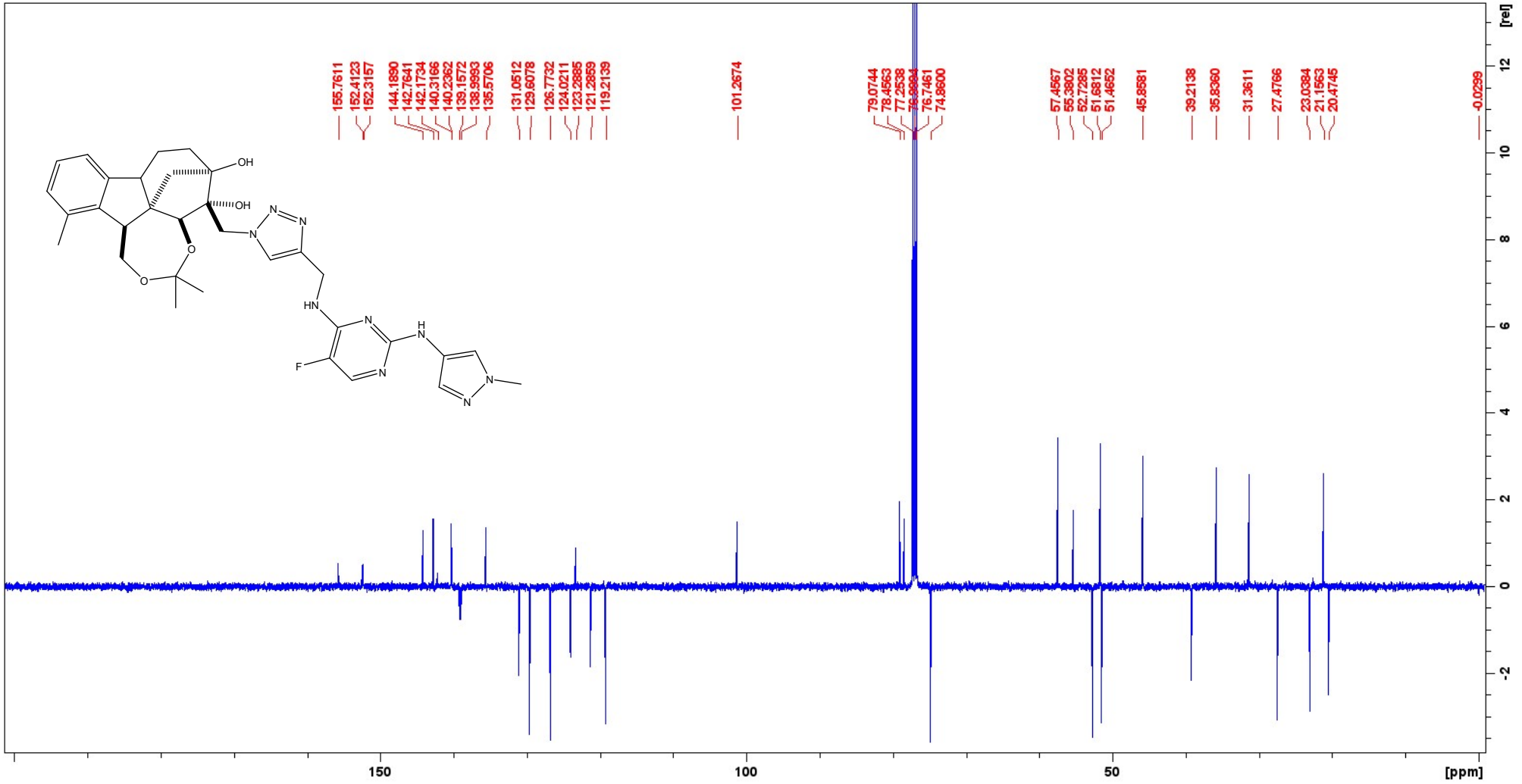


^{1}H-NMR (500 MHz) of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-5-((4-(((5-Fluoro-2-((1-methyl-1H-pyrazol-4-yl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-*de*][1,3]dioxepine-5,6(1*H*)-diol **30**

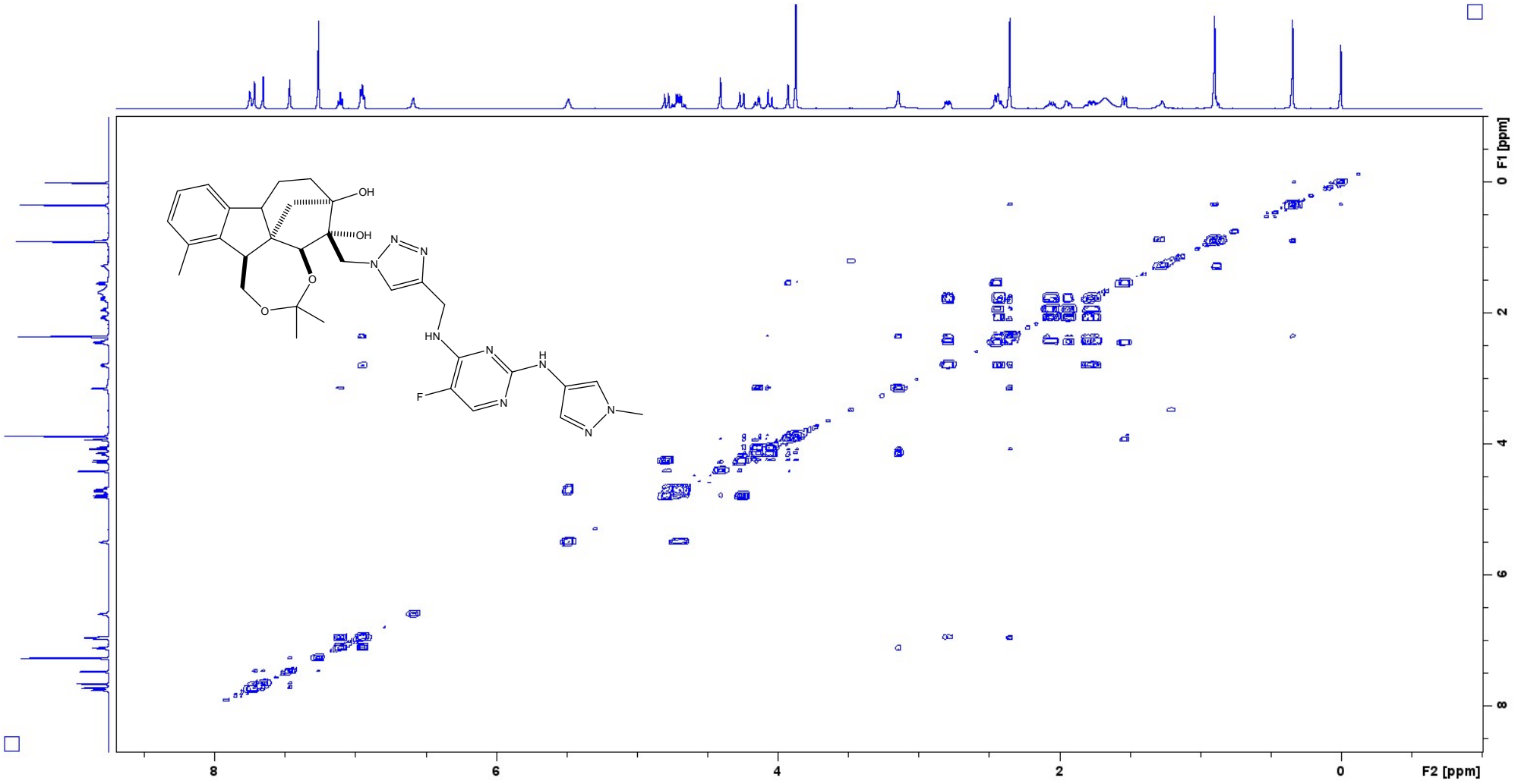


$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of (4a*S*,4a[1]*R*,5*R*,6*S*,12b*S*)-5-((4-(((5-Fluoro-2-((1-methyl-1H-pyrazol-4-yl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-*de*][1,3]dioxepine-5,6(1*H*)-diol

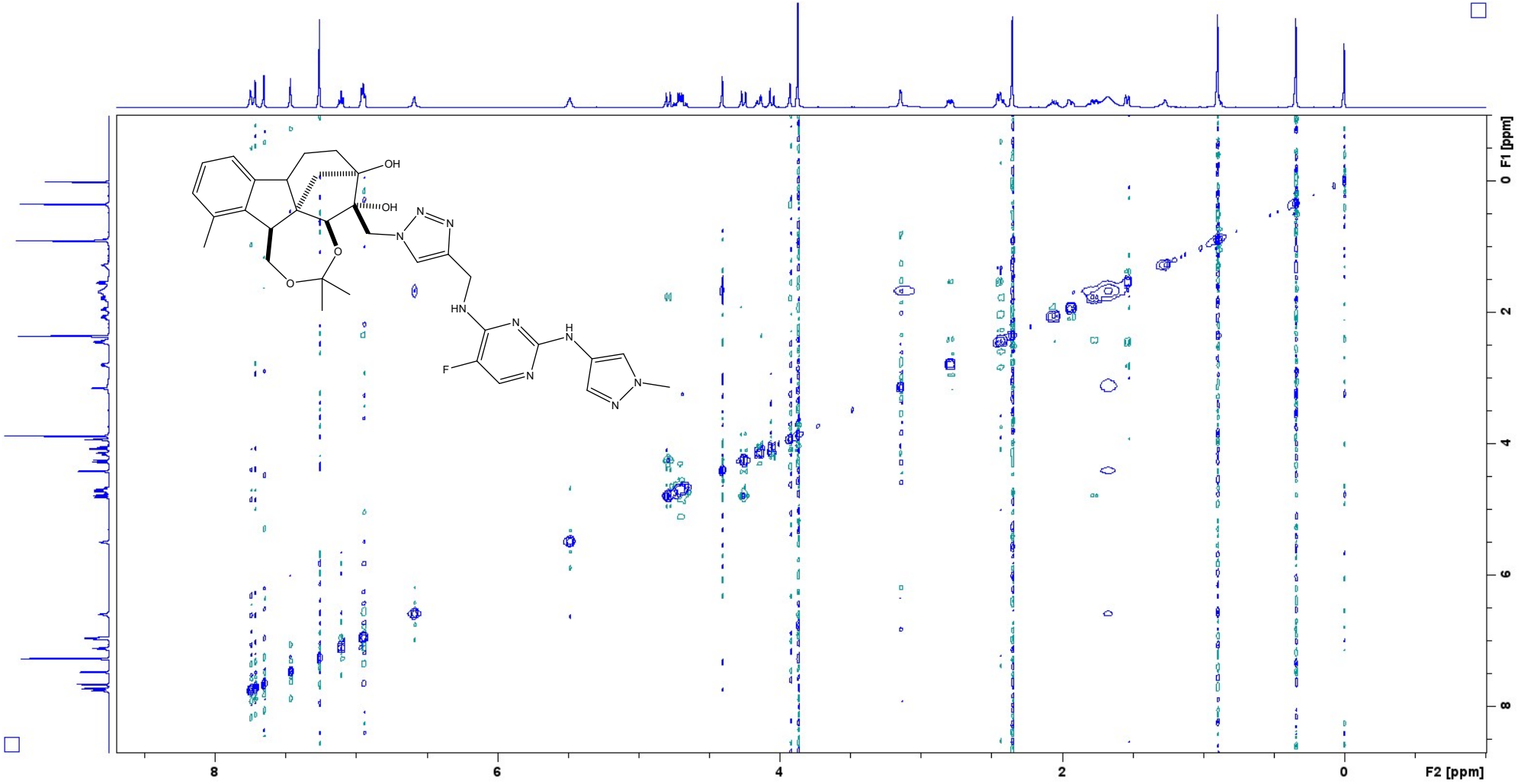
30



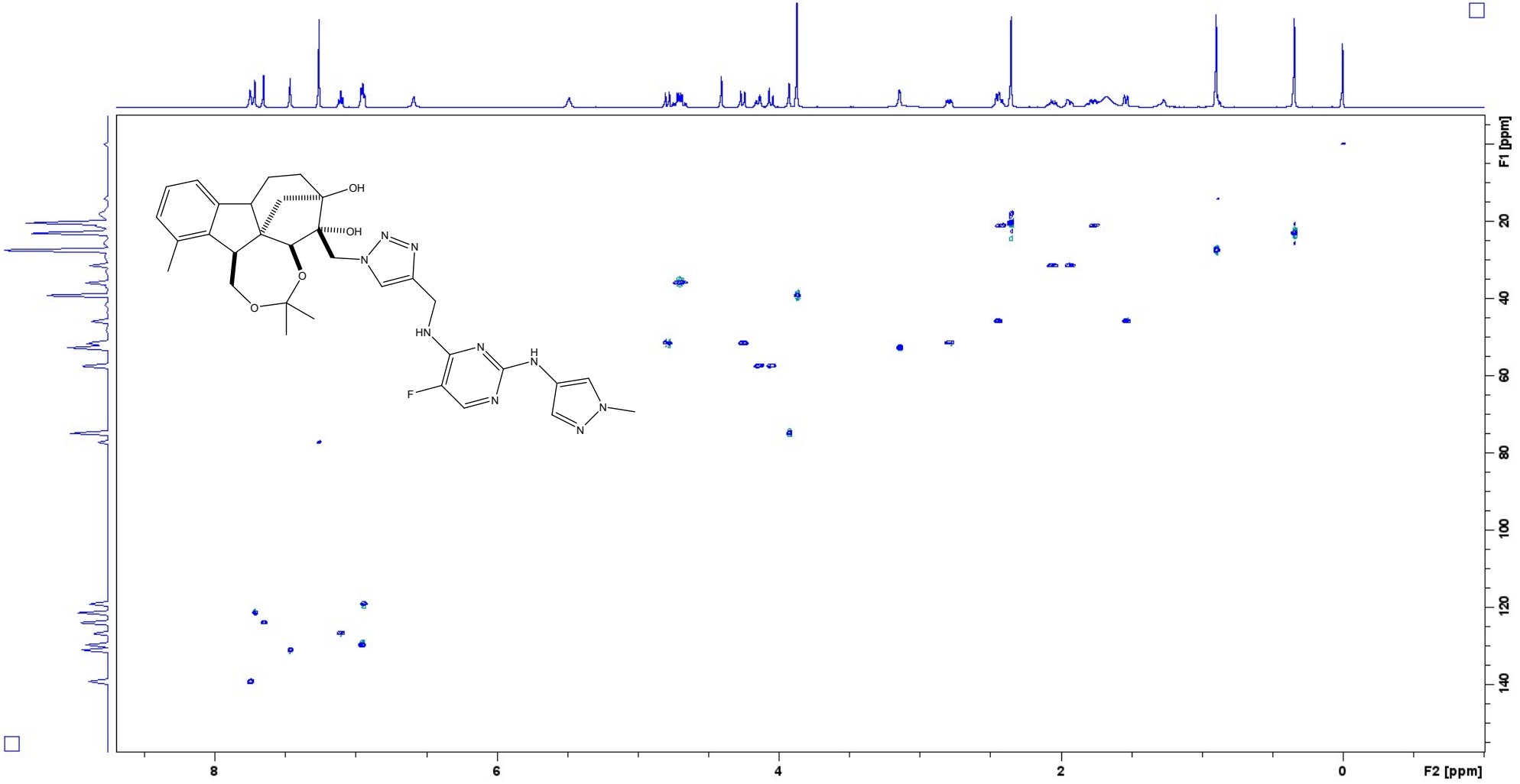
COSY of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-5-((4-(((5-Fluoro-2-((1-methyl-1H-pyrazol-4-yl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-*de*][1,3]dioxepine-5,6(1*H*)-diol **30**



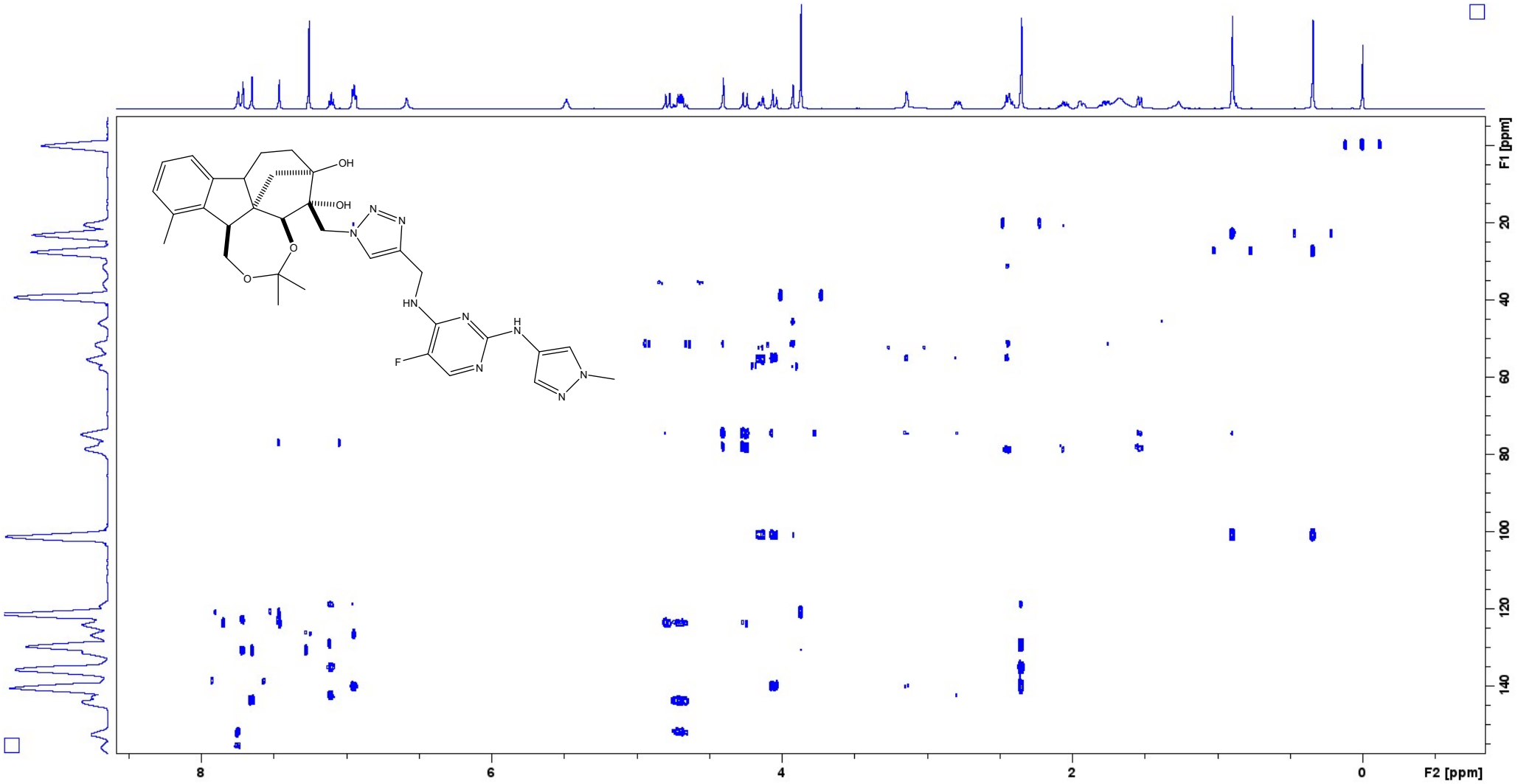
NOESY of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-5-((4-(((5-Fluoro-2-((1-methyl-1H-pyrazol-4-yl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-*de*][1,3]dioxepine-5,6(1*H*)-diol **30**



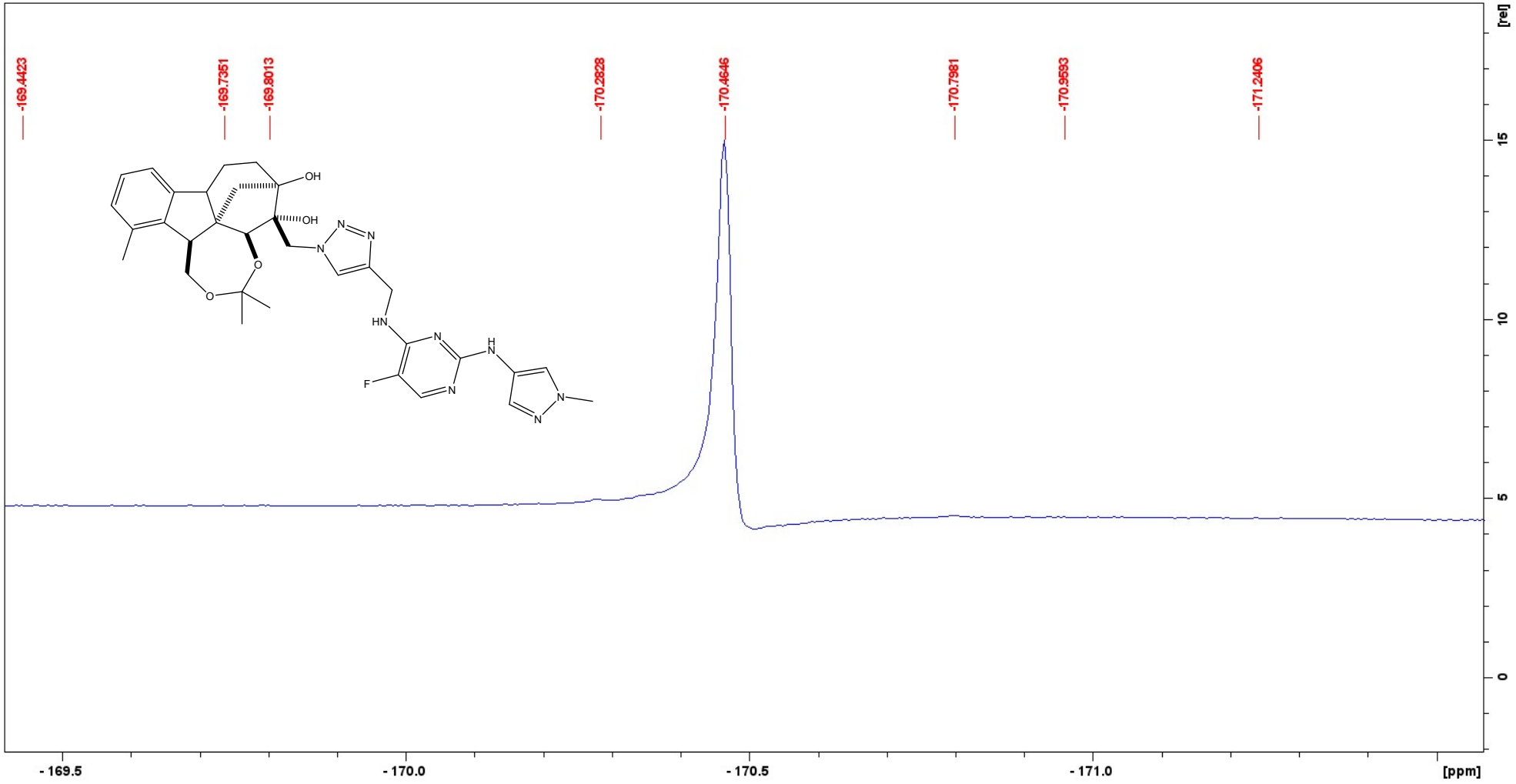
HSQC of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-5-((4-(((5-Fluoro-2-((1-methyl-1H-pyrazol-4-yl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-*de*][1,3]dioxepine-5,6(1*H*)-diol **30**



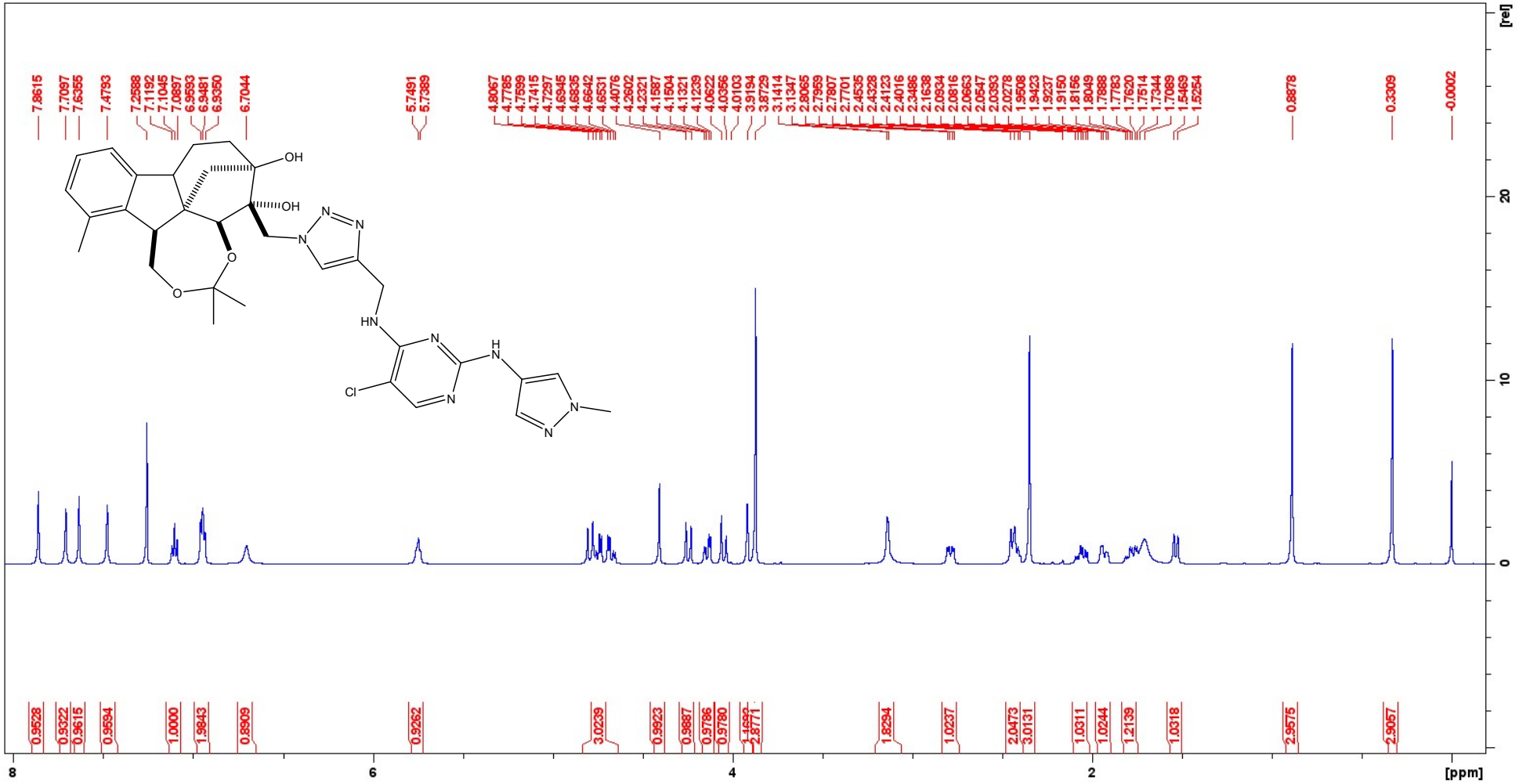
HMBC of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-5-((4-(((5-Fluoro-2-((1-methyl-1H-pyrazol-4-yl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-*de*][1,3]dioxepine-5,6(1*H*)-diol **30**



^{19}F *J*-MOD NMR (470 MHz) of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-5-((4-(((5-Fluoro-2-((1-methyl-1H-pyrazol-4-yl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-*de*][1,3]dioxepine-5,6(1*H*)-diol **30**

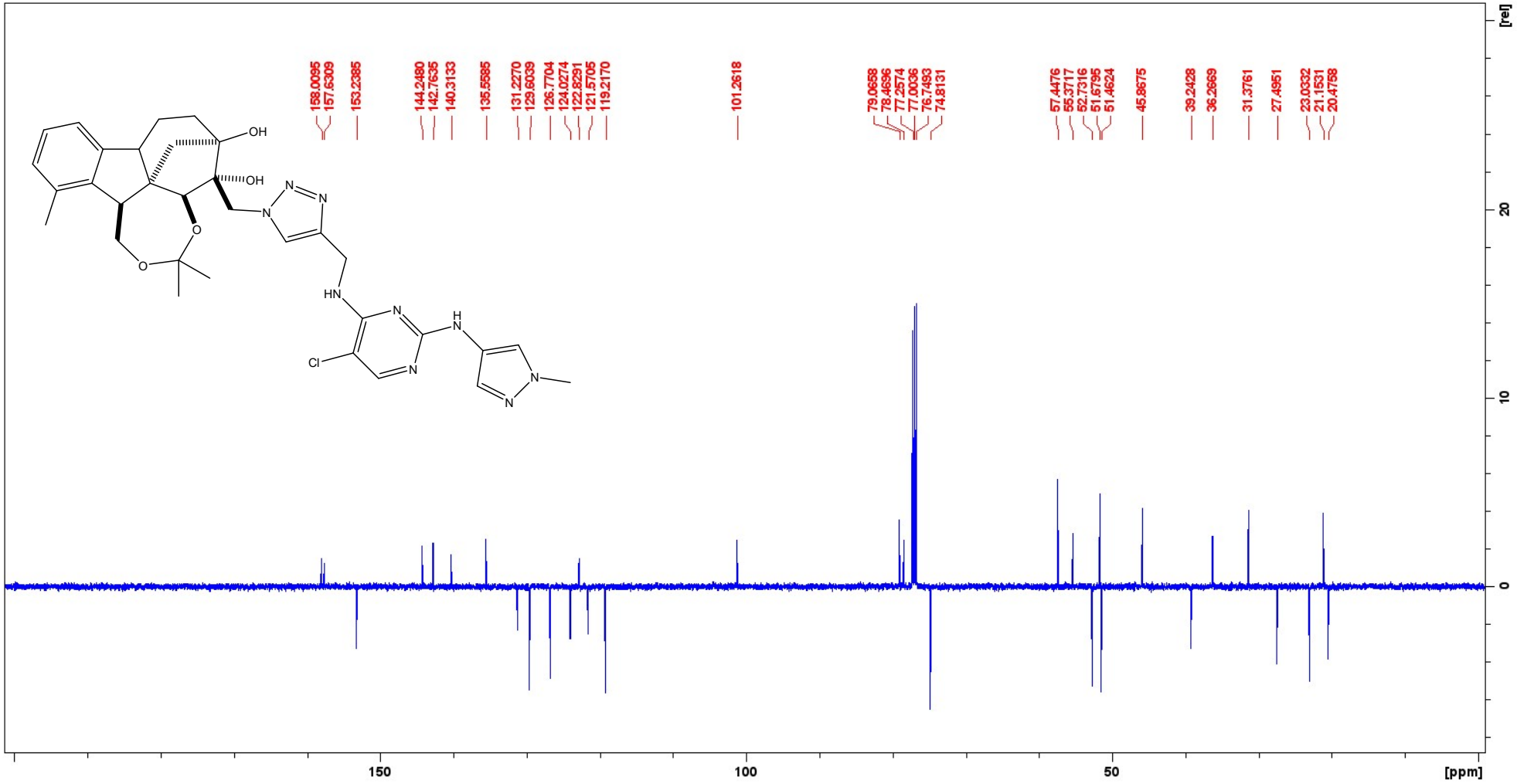


^{1}H-NMR (500 MHz) of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-5-((4-(((5-Chloro-2-((1-methyl-1*H*-pyrazol-4-yl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-*de*][1,3]dioxepine-5,6(1*H*)-diol **31**

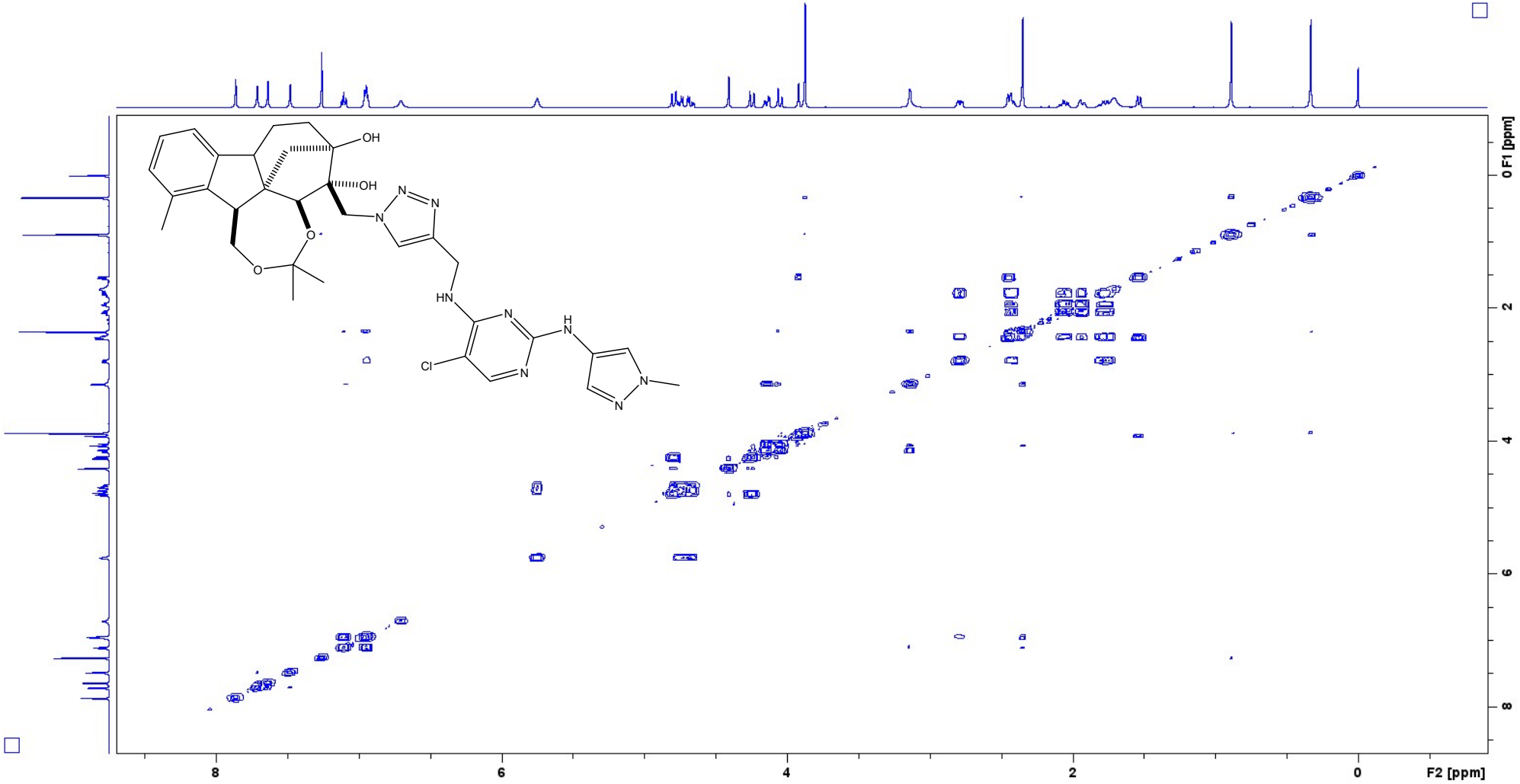


^{13}C{1H} *J*-MOD NMR (125 MHz) of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-5-((4-(((5-Chloro-2-((1-methyl-1*H*-pyrazol-4-yl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-*de*][1,3]dioxepine-5,6(1*H*)-diol

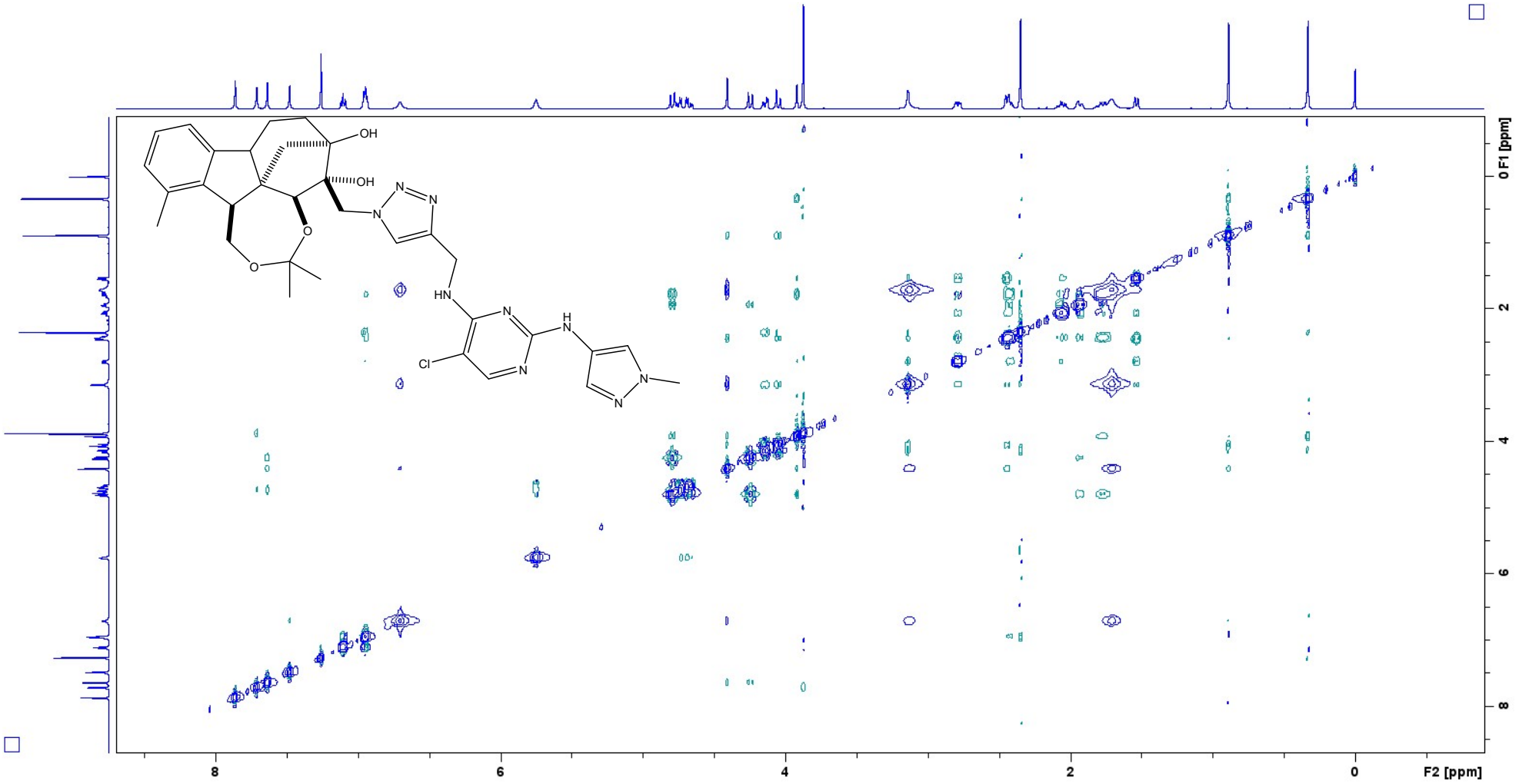
31



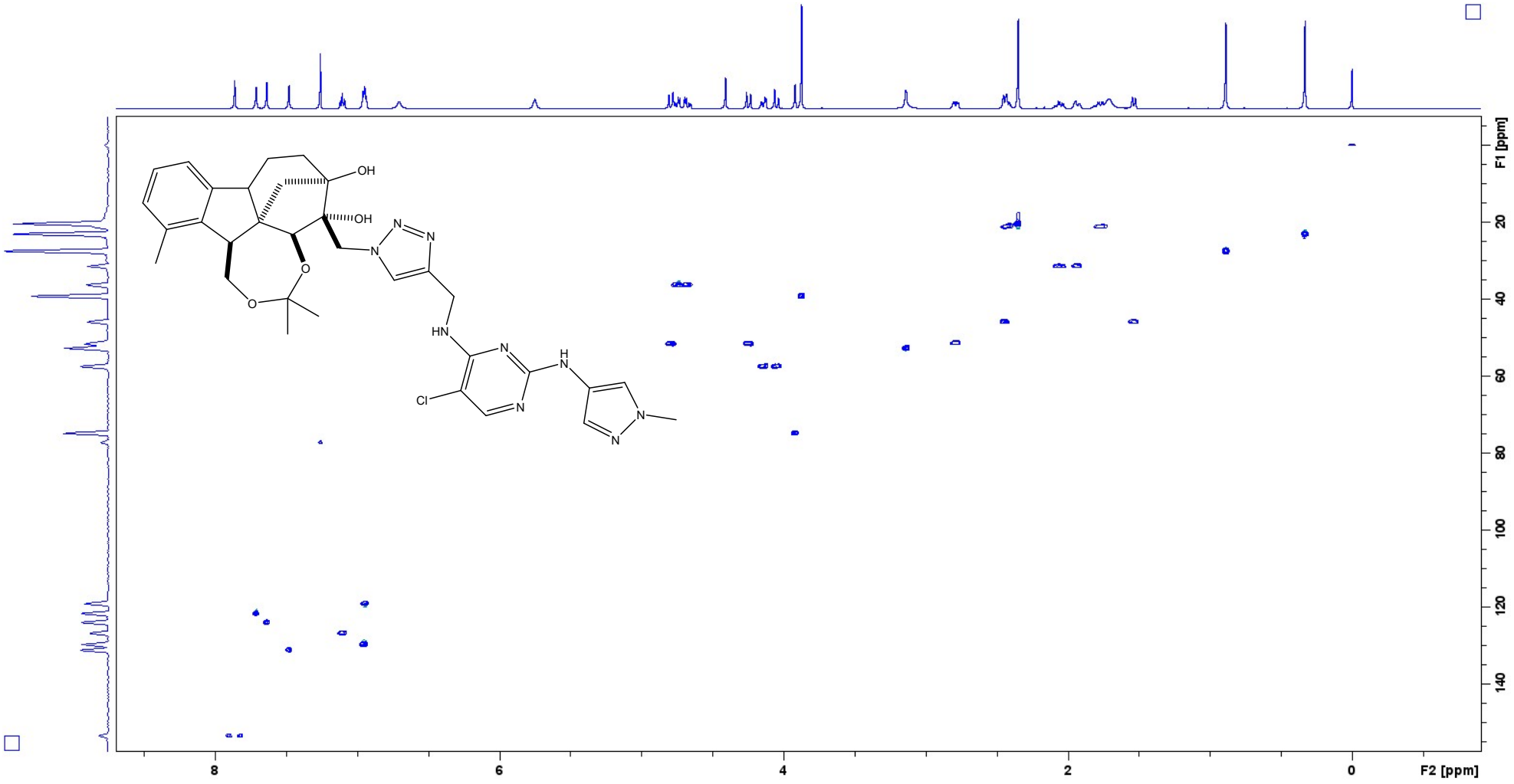
COSY of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-5-((4-(((5-Chloro-2-((1-methyl-1*H*-pyrazol-4-yl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-*de*][1,3]dioxepine-5,6(1*H*)-diol **31**



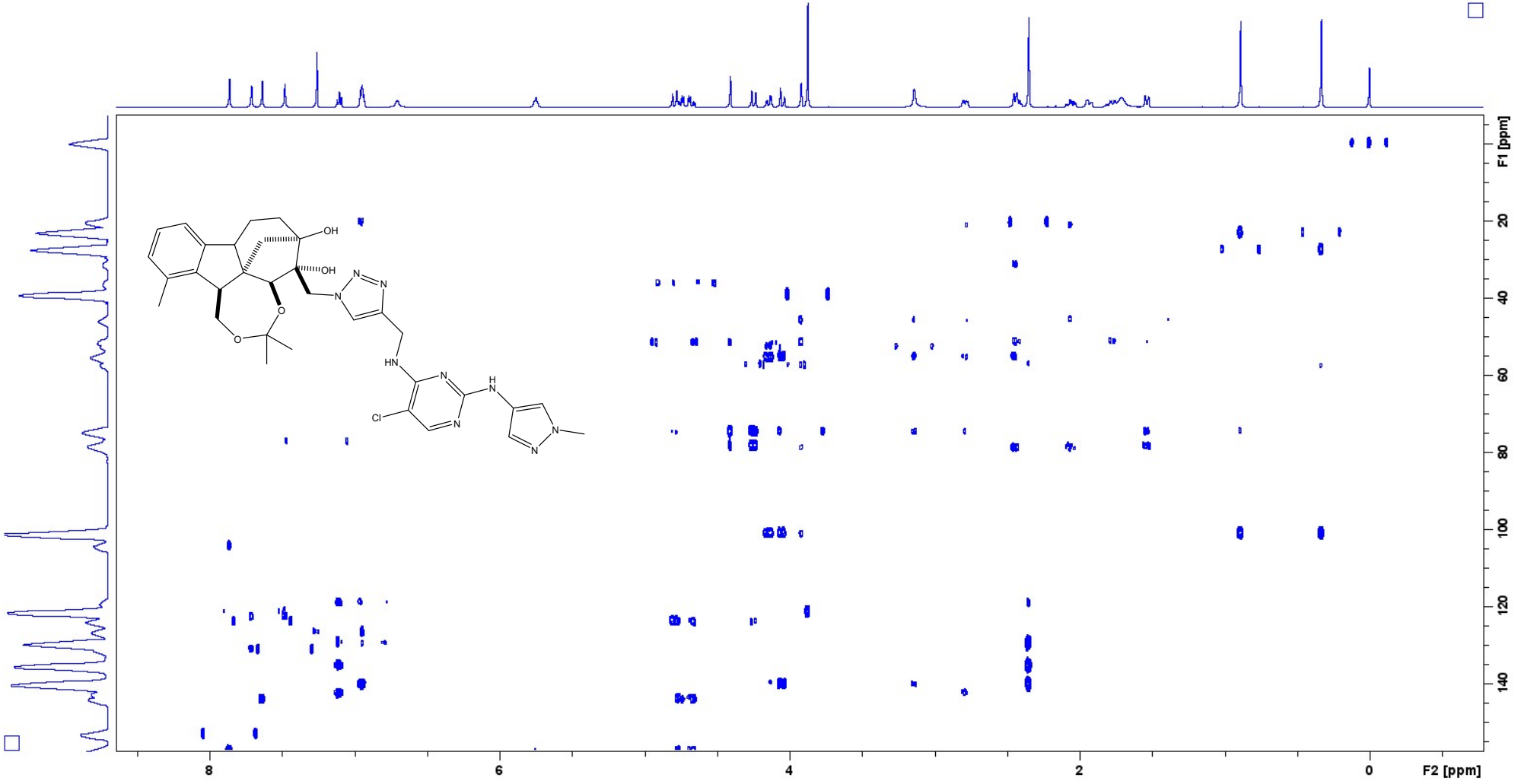
NOESY of (4a*S*,4a[1]*R*,5*R*,6*S*,12b*S*)-5-((4-(((5-Chloro-2-((1-methyl-1*H*-pyrazol-4-yl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-*de*][1,3]dioxepine-5,6(1*H*)-diol **31**



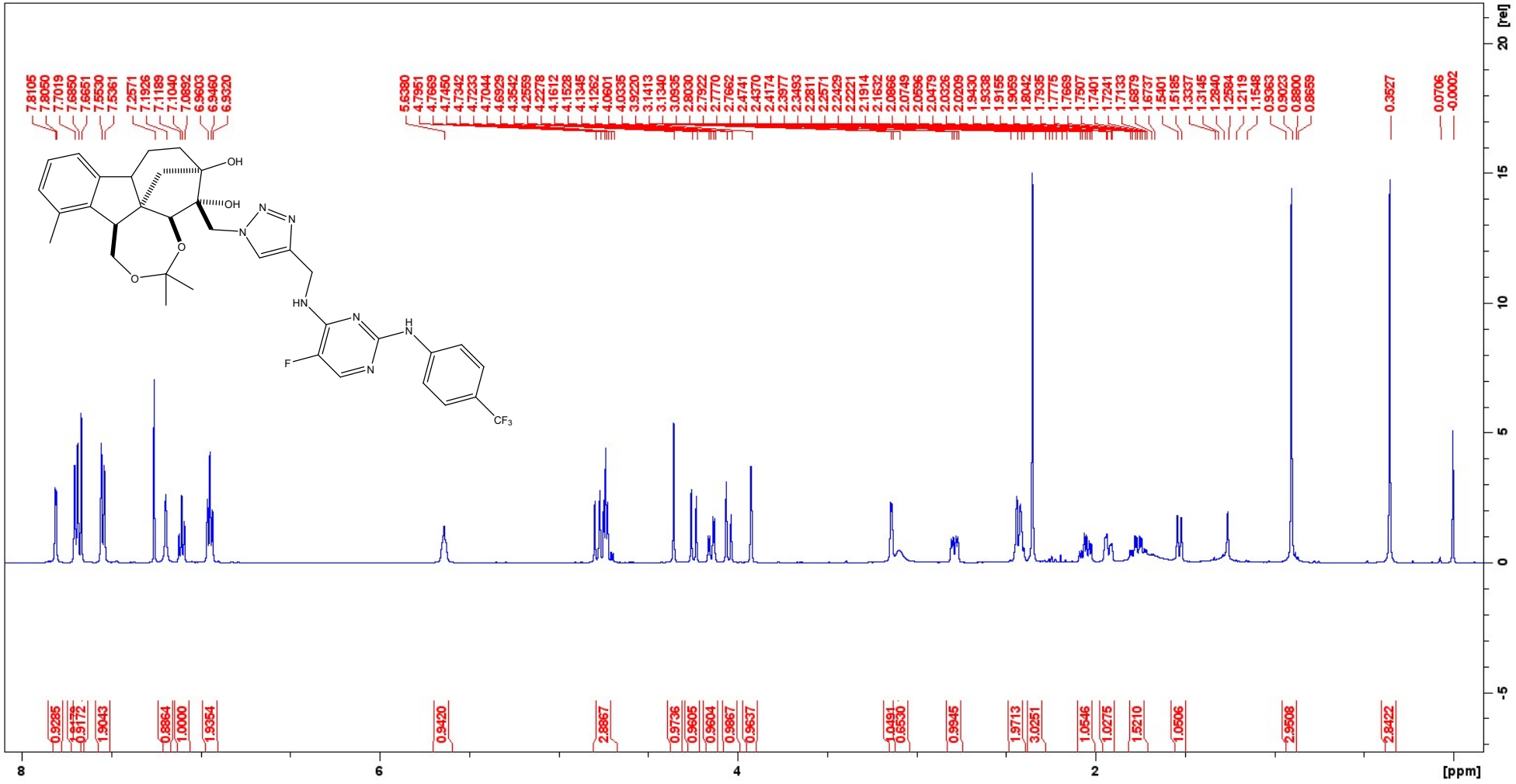
HSQC of (4a*S*,4a[1]*R*,5*R*,6*S*,12b*S*)-5-((4-(((5-Chloro-2-((1-methyl-1*H*-pyrazol-4-yl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-*de*][1,3]dioxepine-5,6(1*H*)-diol **31**



HMBC of (4a*S*,4a[1]*R*,5*R*,6*S*,12b*S*)-5-((4-(((5-Chloro-2-((1-methyl-1*H*-pyrazol-4-yl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-*de*][1,3]dioxepine-5,6(1*H*)-diol **31**

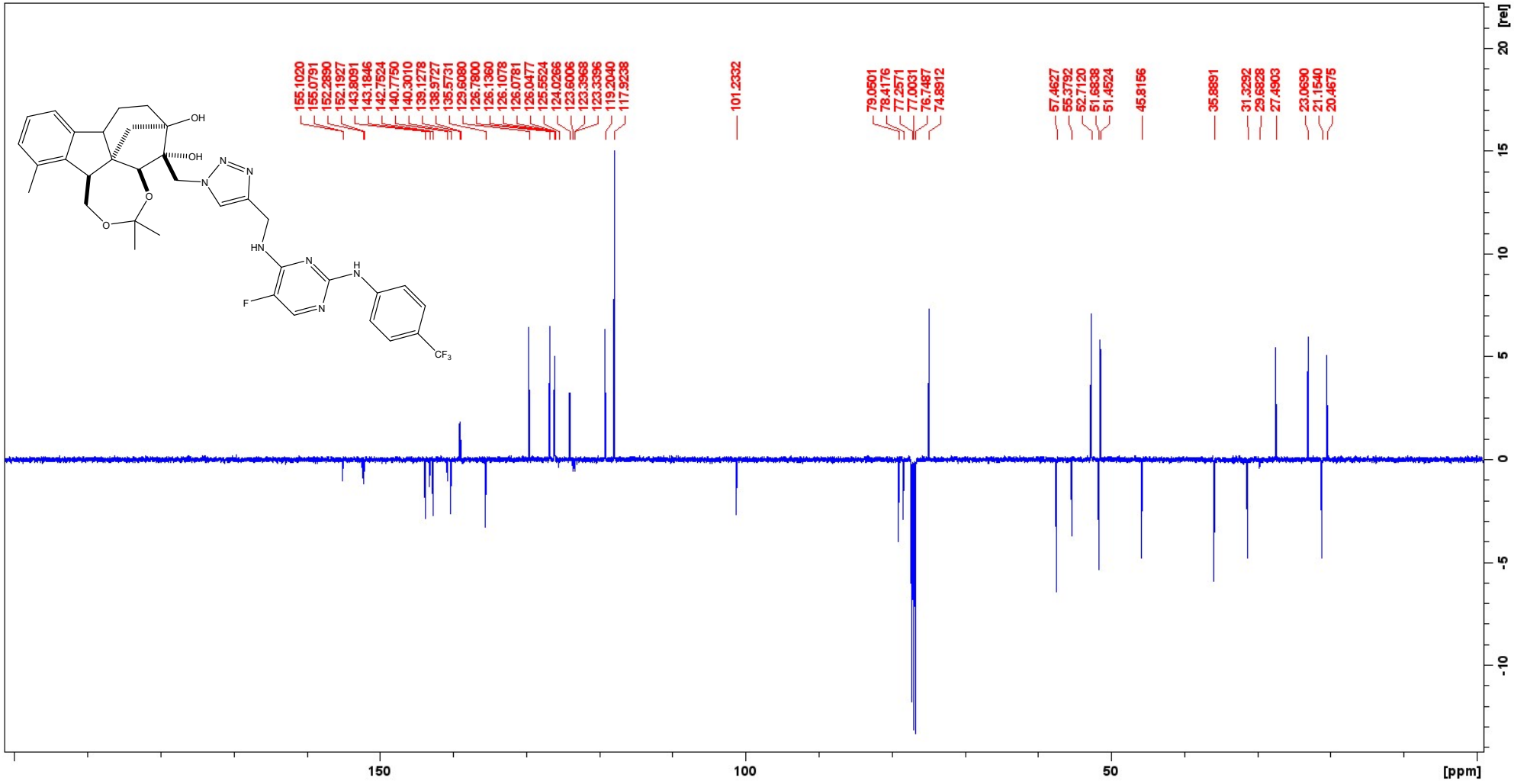


^{1}H-NMR (500 MHz) of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-5-((4-(((5-Fluoro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-*de*][1,3]dioxepine-5,6(1*H*)-diol **32**

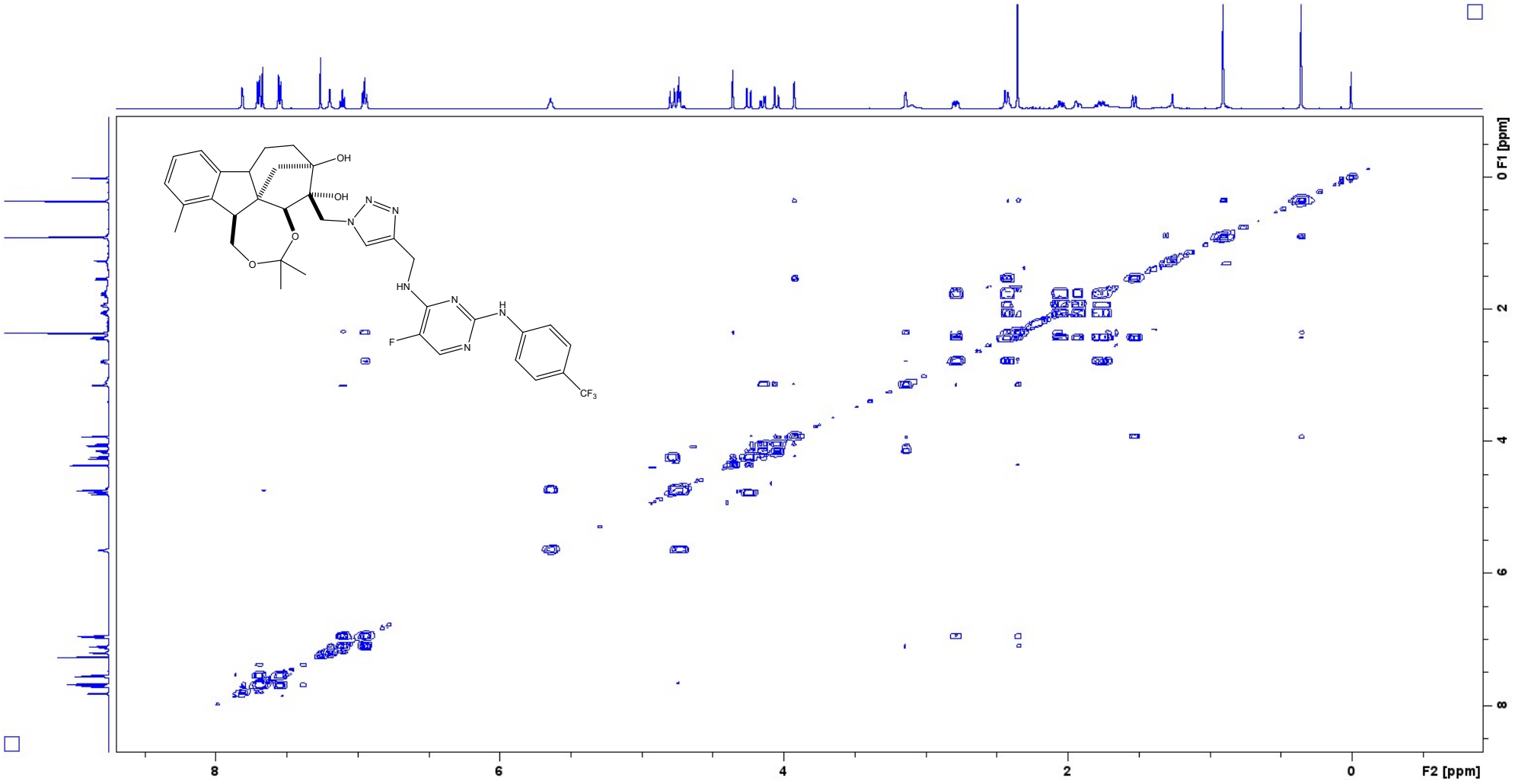


^{13}C{1H} *J*-MOD NMR (125 MHz) of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-5-((4-(((5-Fluoro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-*de*][1,3]dioxepine-5,6(1*H*)-diol

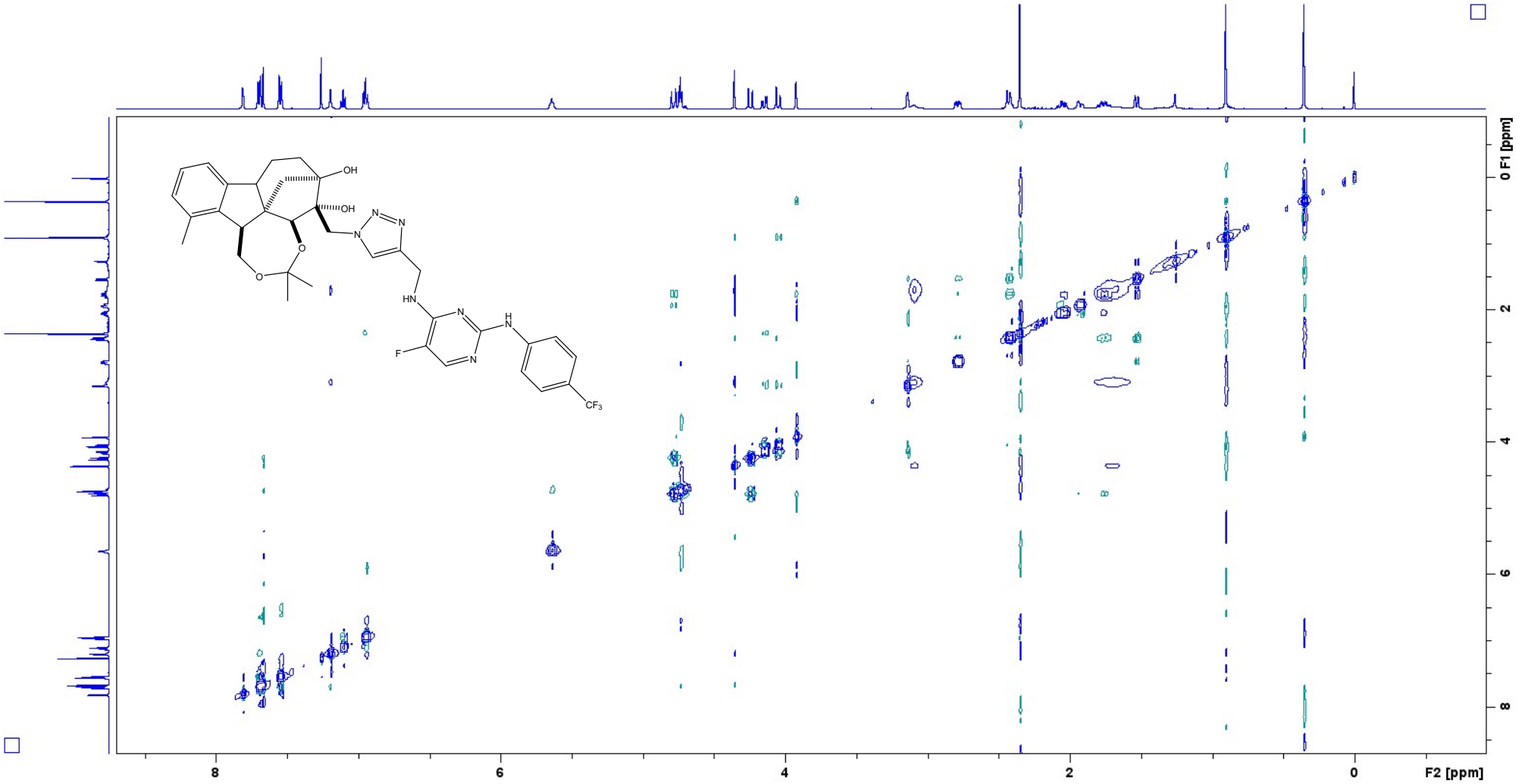
32



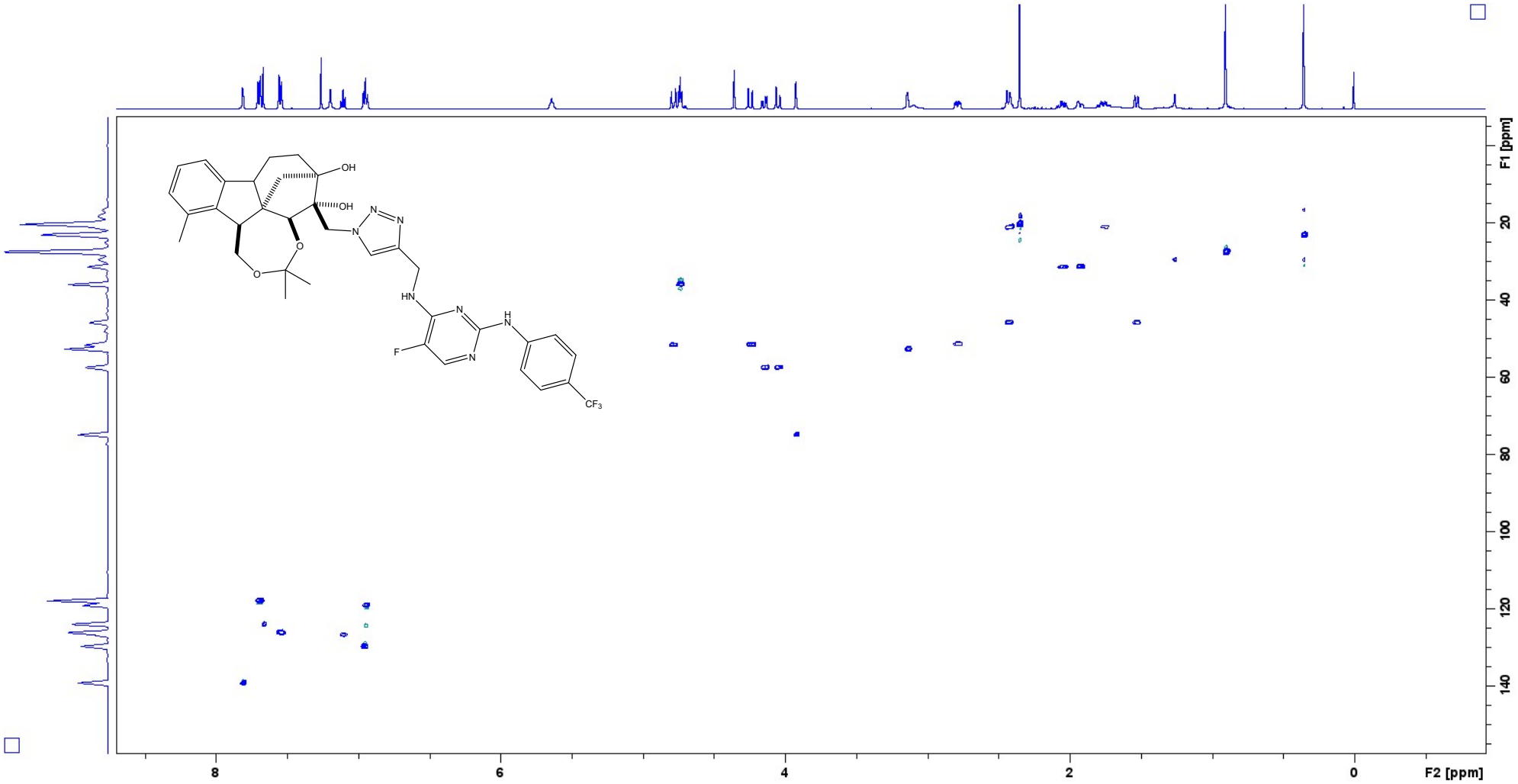
COSY of (4a*S*,4a[1]*R*,5*R*,6*S*,12b*S*)-5-((4-(((5-Fluoro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-*de*][1,3]dioxepine-5,6(1*H*)-diol **32**



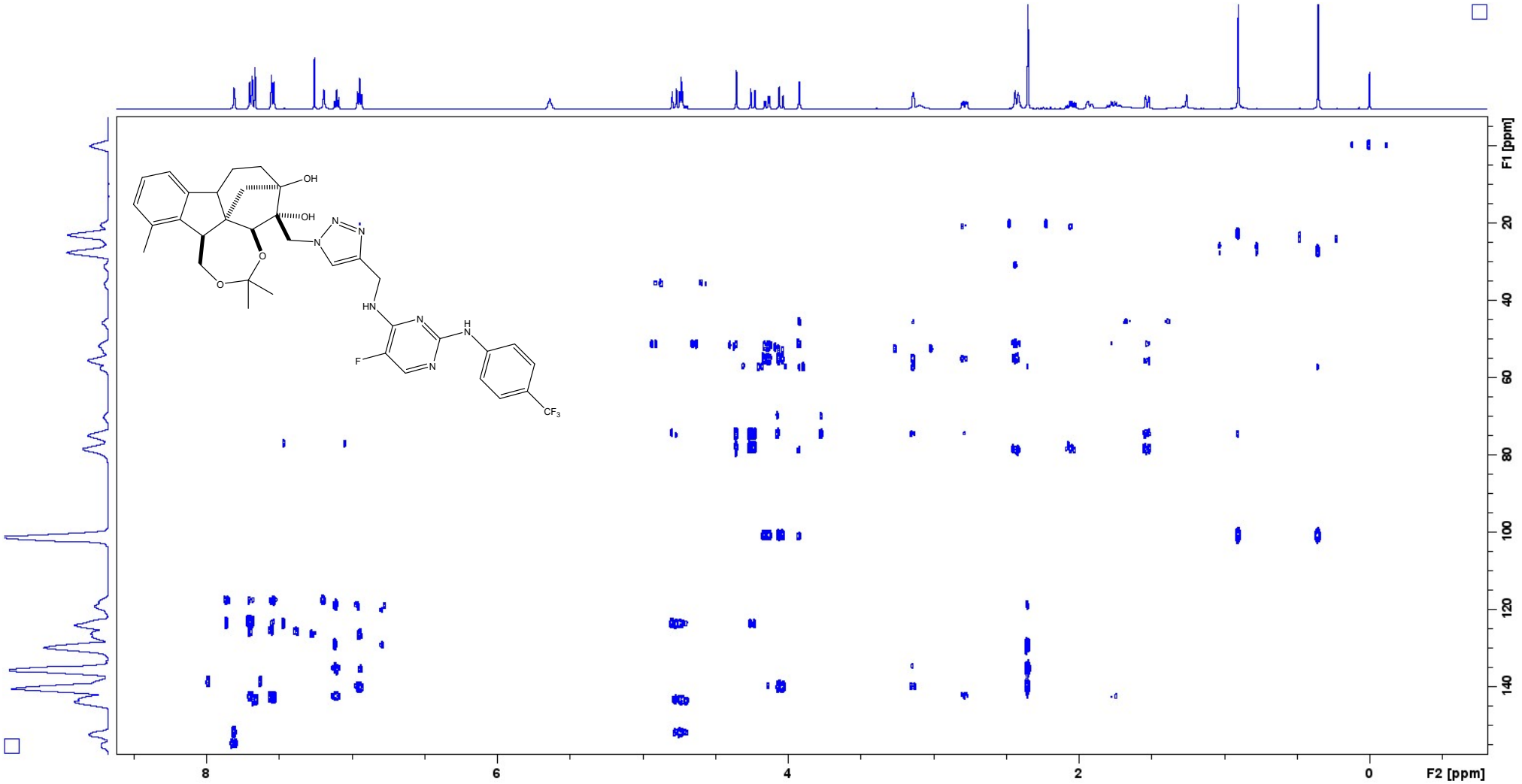
NOESY of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-5-((4-(((5-Fluoro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-*de*][1,3]dioxepine-5,6(1*H*)-diol **32**



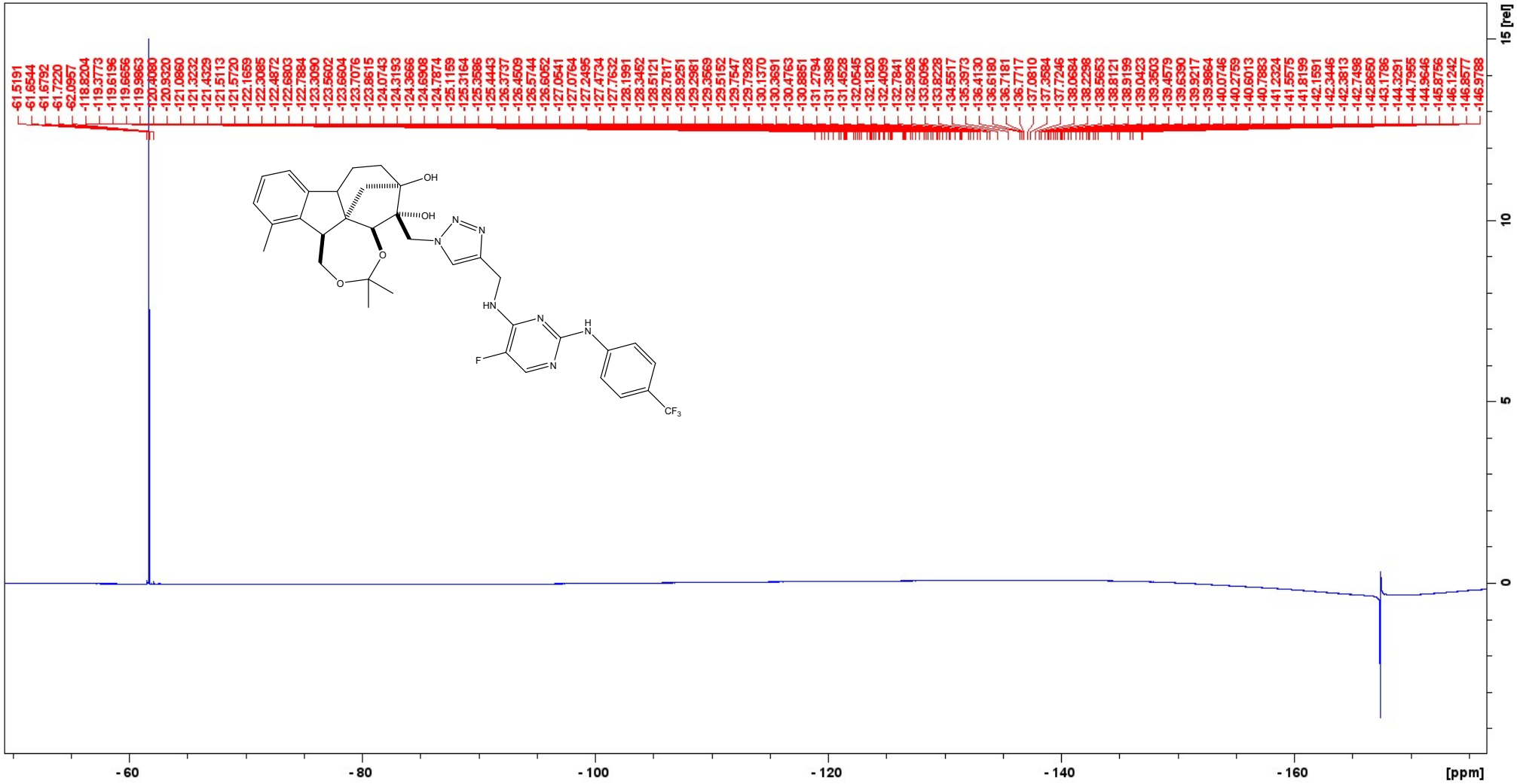
HSQC of (4a*S*,4a[1]*R*,5*R*,6*S*,12b*S*)-5-((4-(((5-Fluoro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-*de*][1,3]dioxepine-5,6(1*H*)-diol **32**



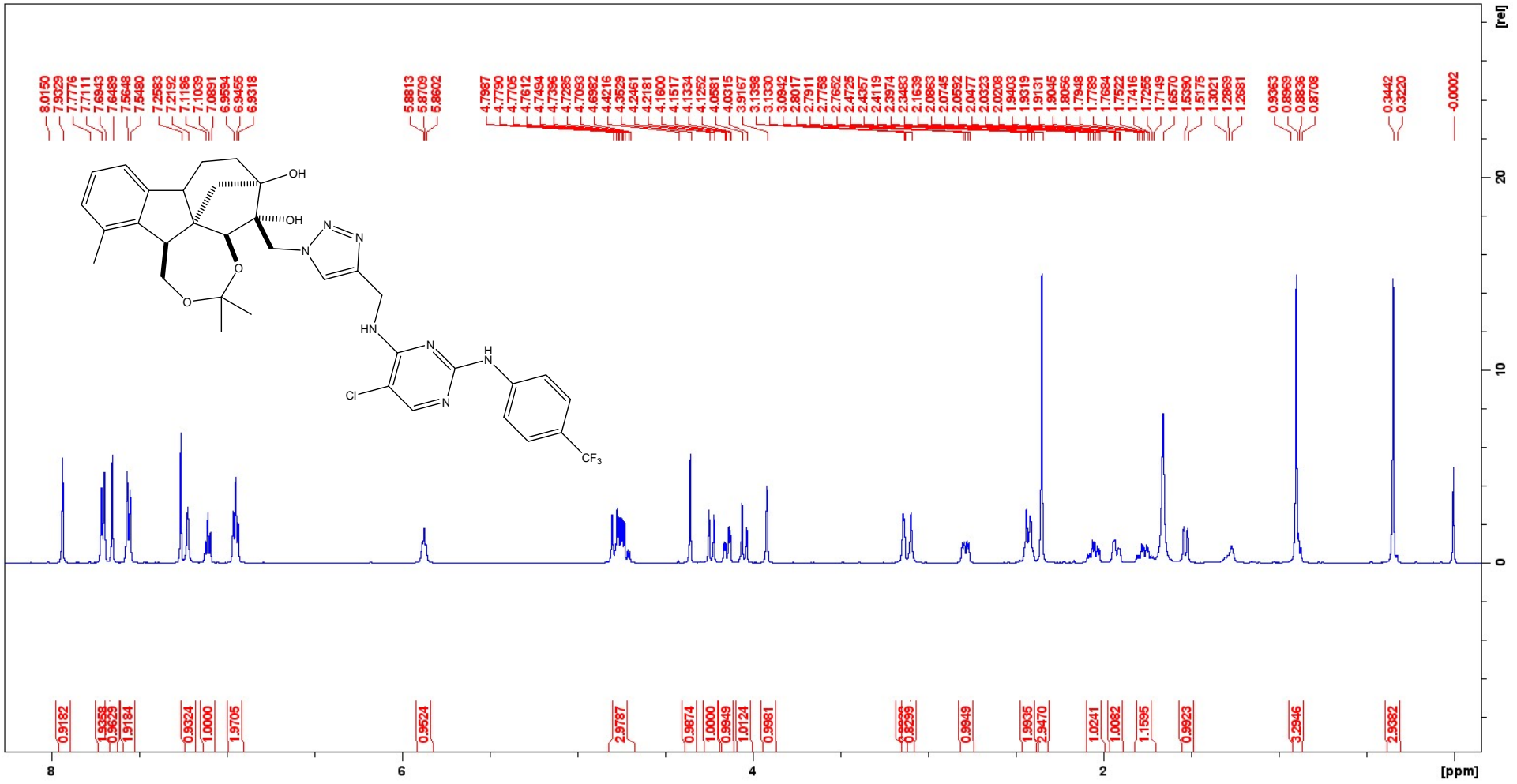
HMBC of (4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-5-((4-(((5-Fluoro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-*de*][1,3]dioxepine-5,6(1*H*)-diol **32**



^{19}F *J*-MOD NMR (470 MHz) of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-5-((4-(((5-Fluoro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-*de*][1,3]dioxepine-5,6(1*H*)-diol **32**

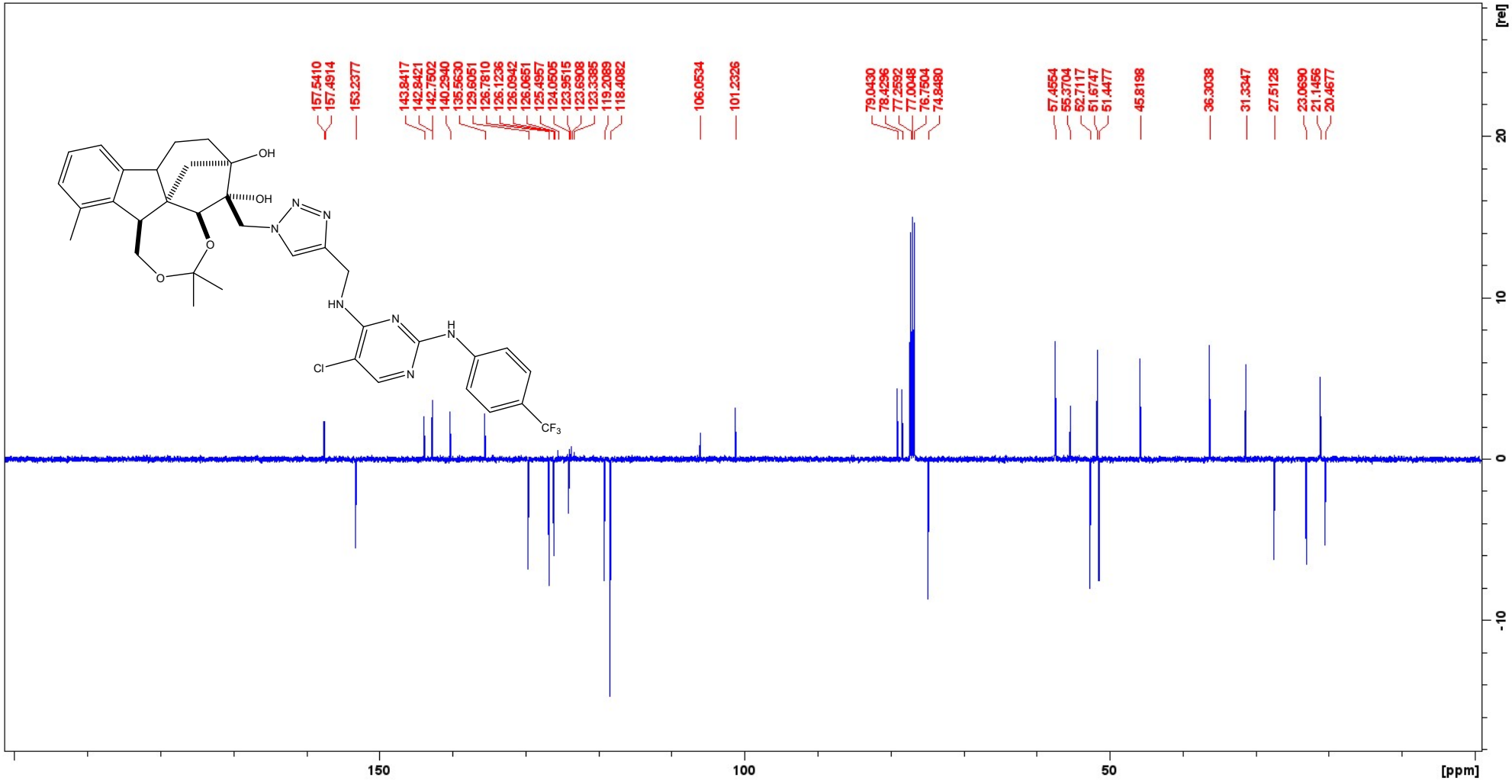


^{1}H-NMR (500 MHz) of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-5-((4-(((5-Chloro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-*de*][1,3]dioxepine-5,6(1*H*)-diol **33**

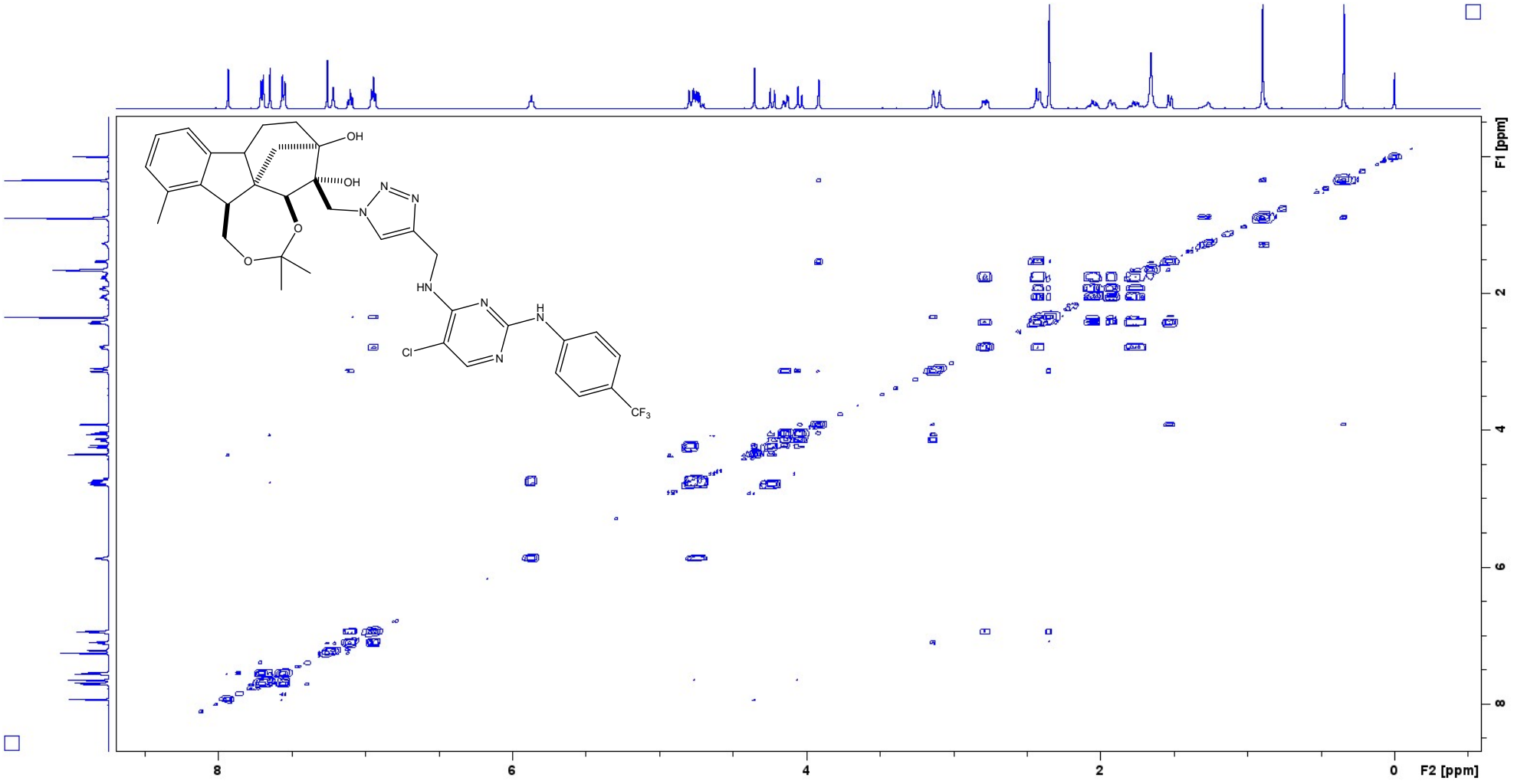


$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-5-((4-(((5-Chloro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-*de*][1,3]dioxepine-5,6(1*H*)-diol

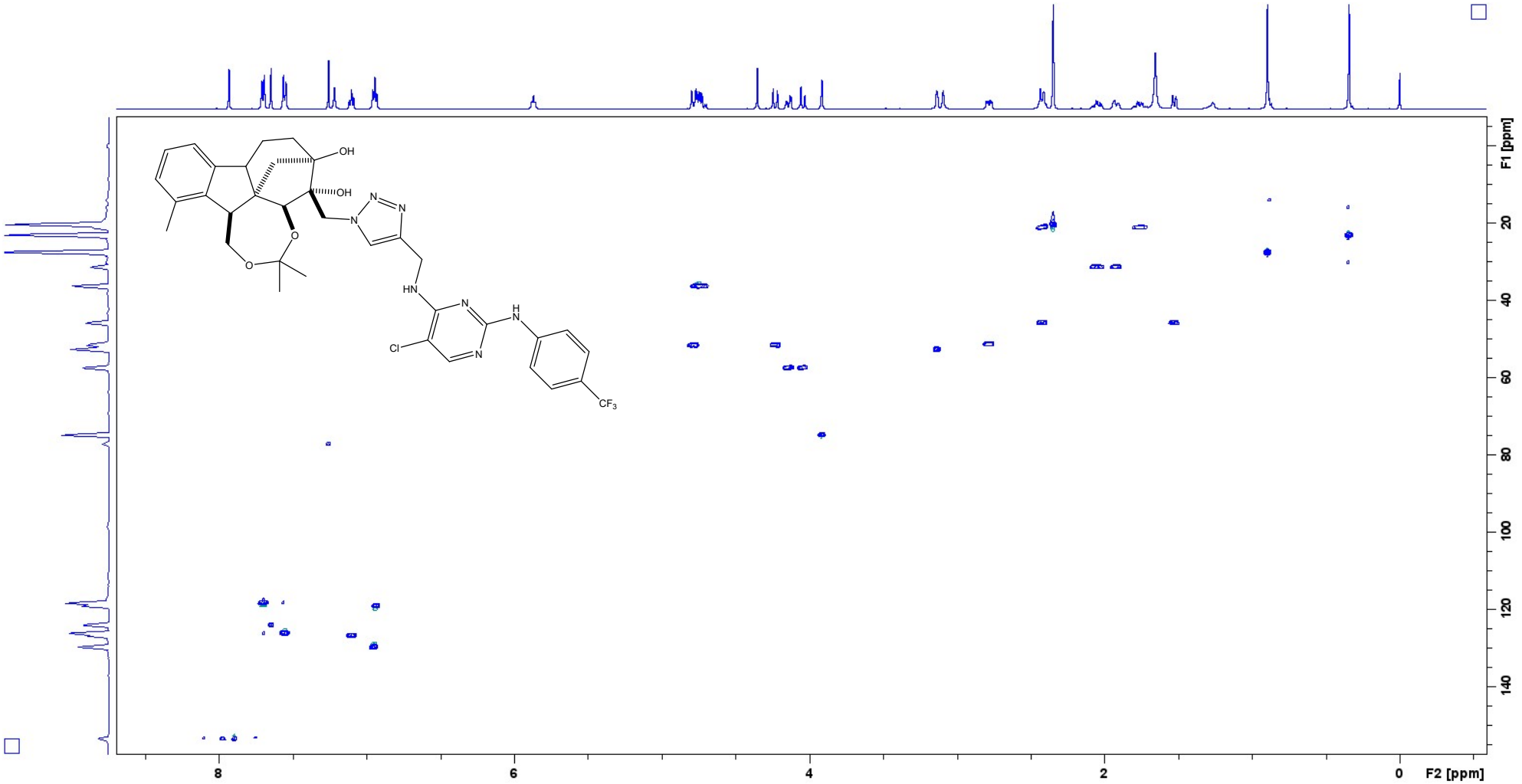
33



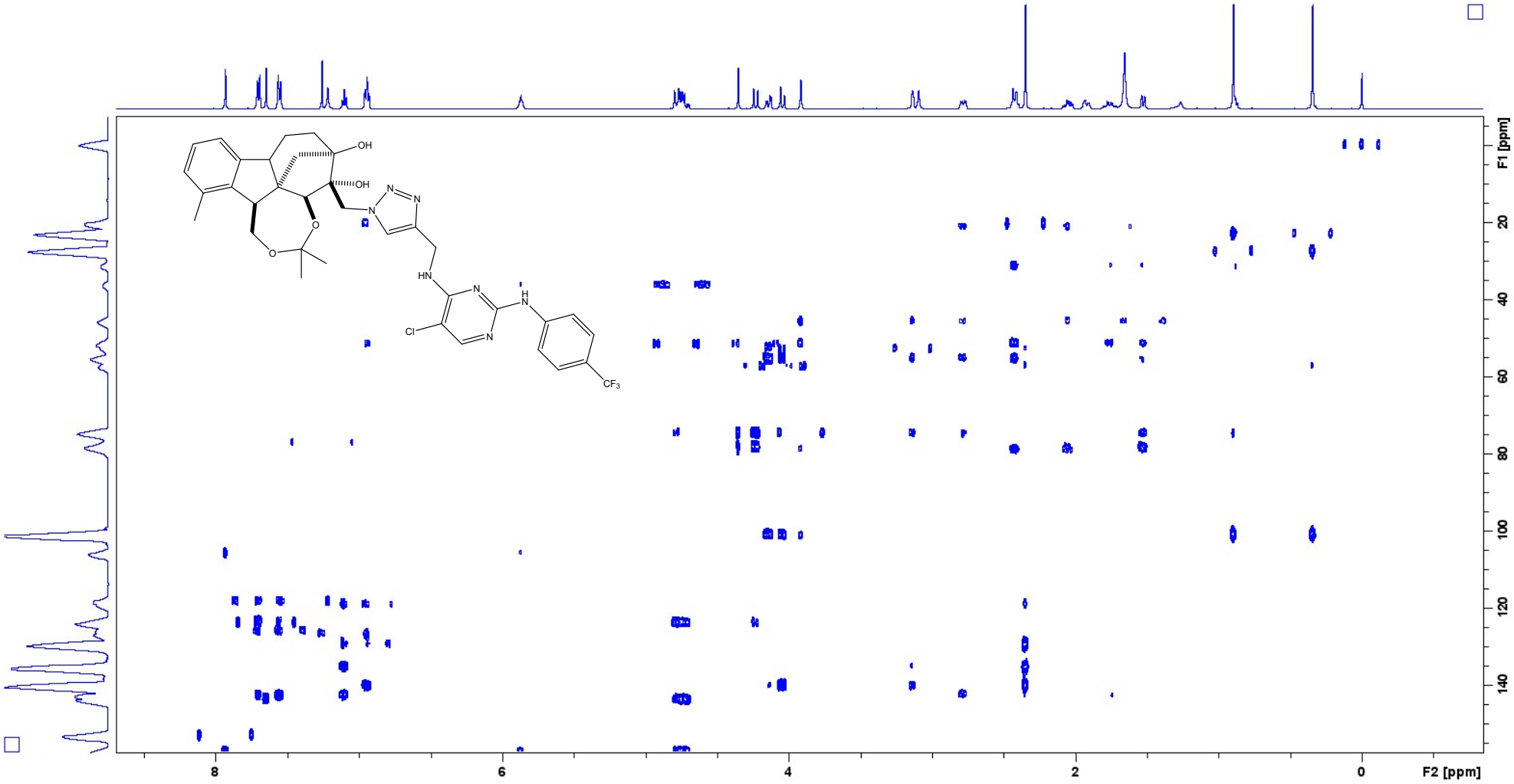
COSY of (4a*S*,4a[1]*R*,5*R*,6*S*,12b*S*)-5-((4-(((5-Chloro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-*de*][1,3]dioxepine-5,6(1*H*)-diol **33**



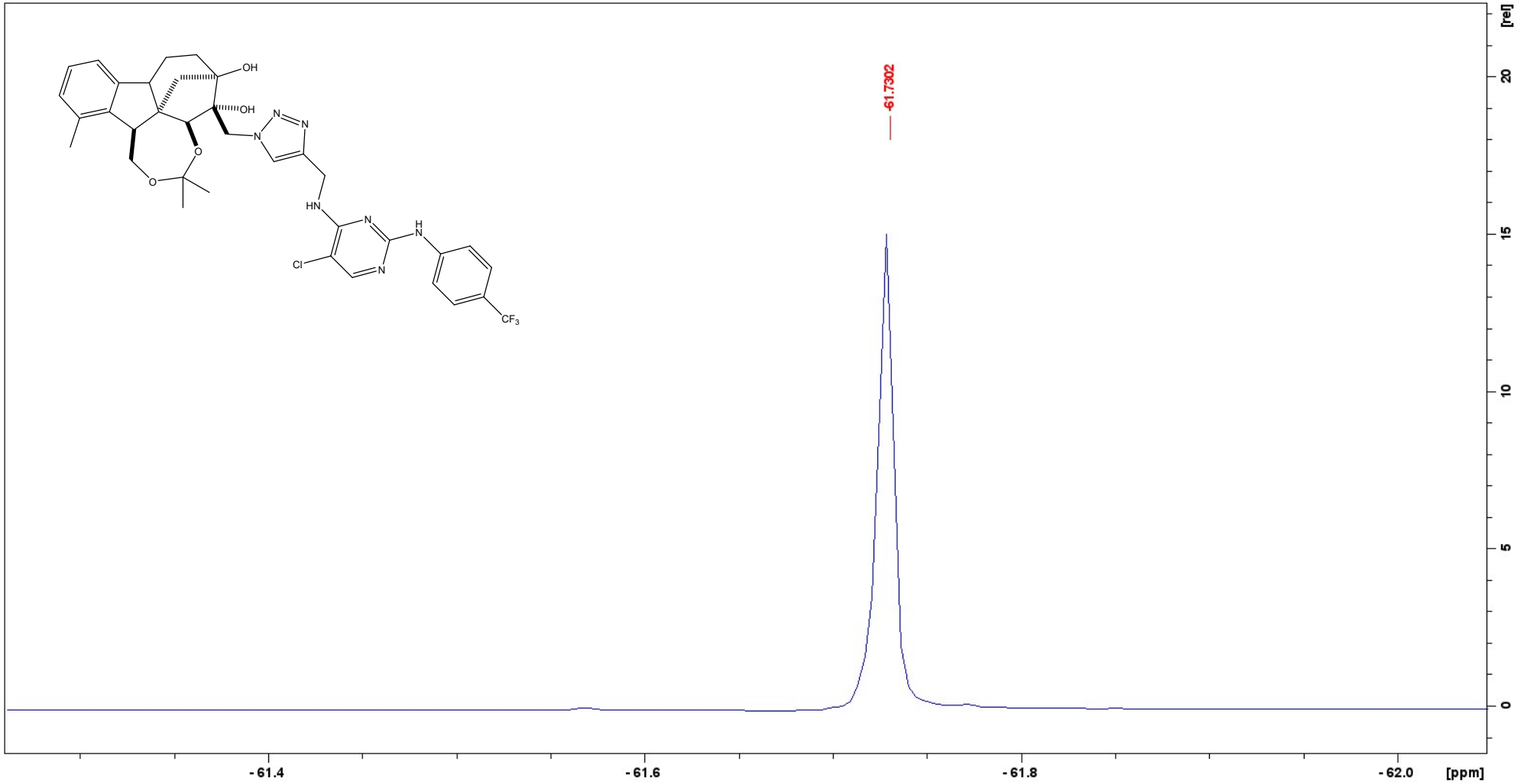
HSQC of (4a*S*,4a[1]*R*,5*R*,6*S*,12b*S*)-5-((4-(((5-Chloro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-*de*][1,3]dioxepine-5,6(1*H*)-diol **33**



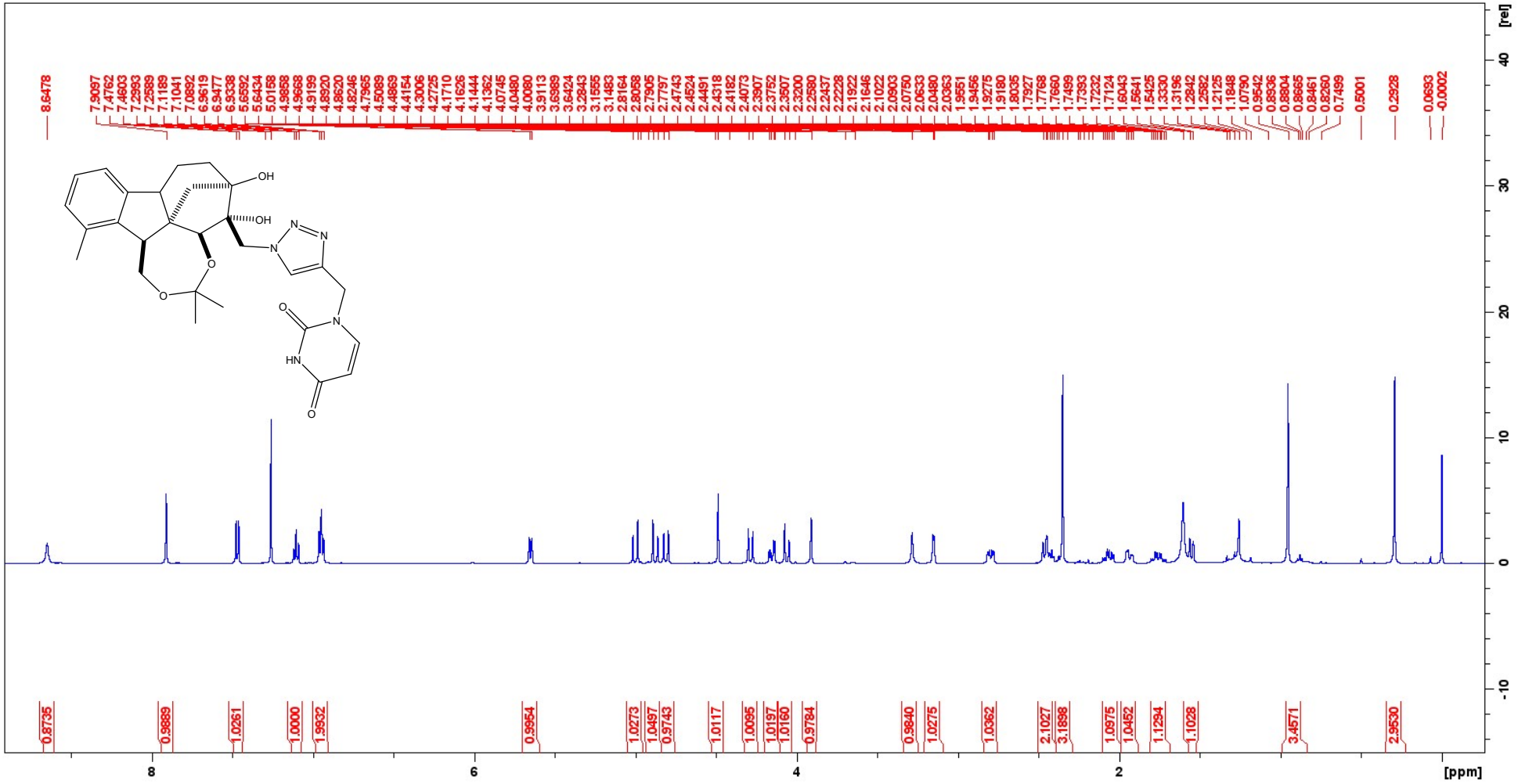
HMBC of (4a*S*,4a[1]*R*,5*R*,6*S*,12b*S*)-5-((4-(((5-Chloro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-*de*][1,3]dioxepine-5,6(1*H*)-diol **33**



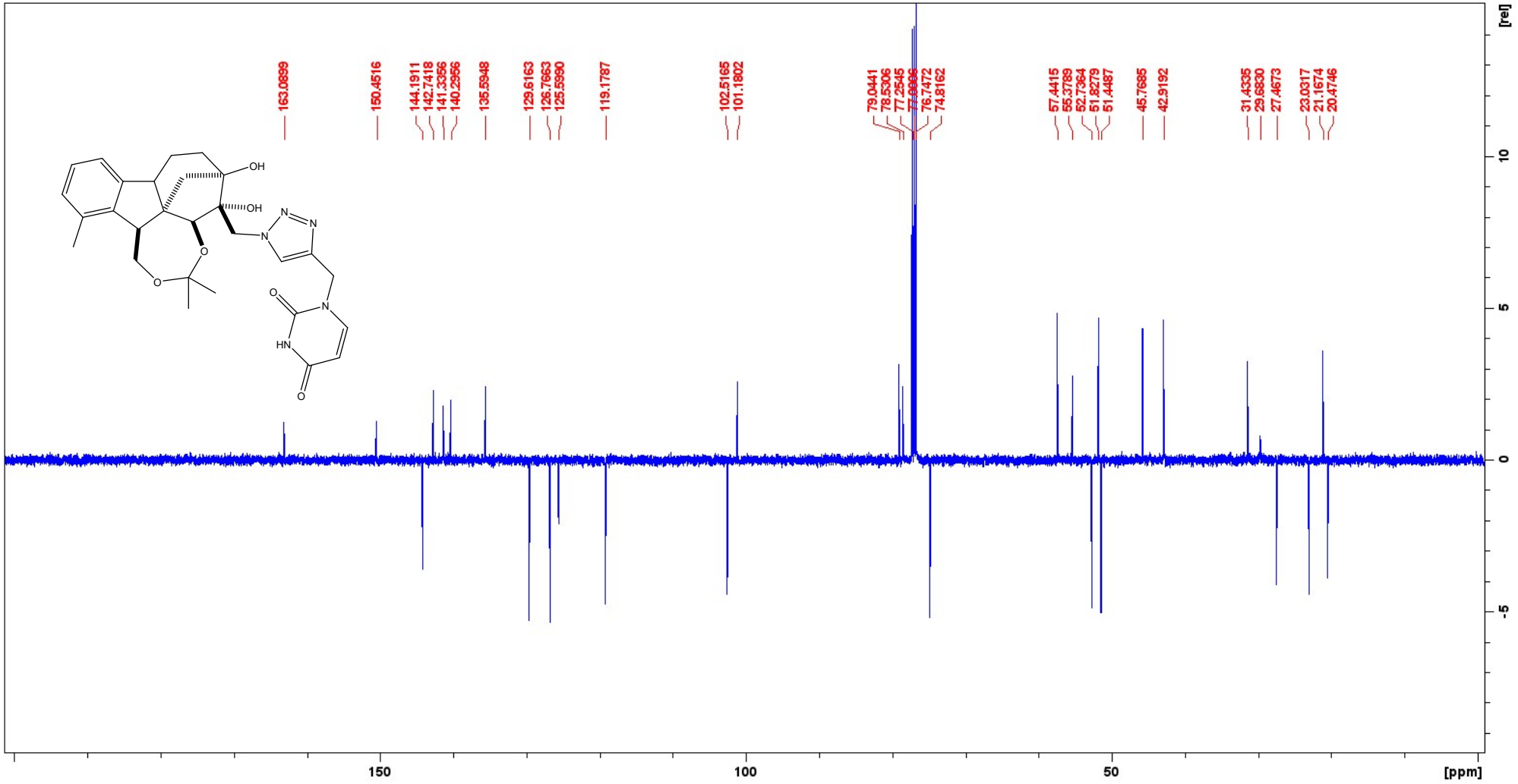
^{19}F *J*-MOD NMR (470 MHz) of (4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-5-((4-(((5-Chloro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-3,3,12-trimethyl-4a,5,7,8,8a,12b-hexahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-*de*][1,3]dioxepine-5,6(1*H*)-diol **33**



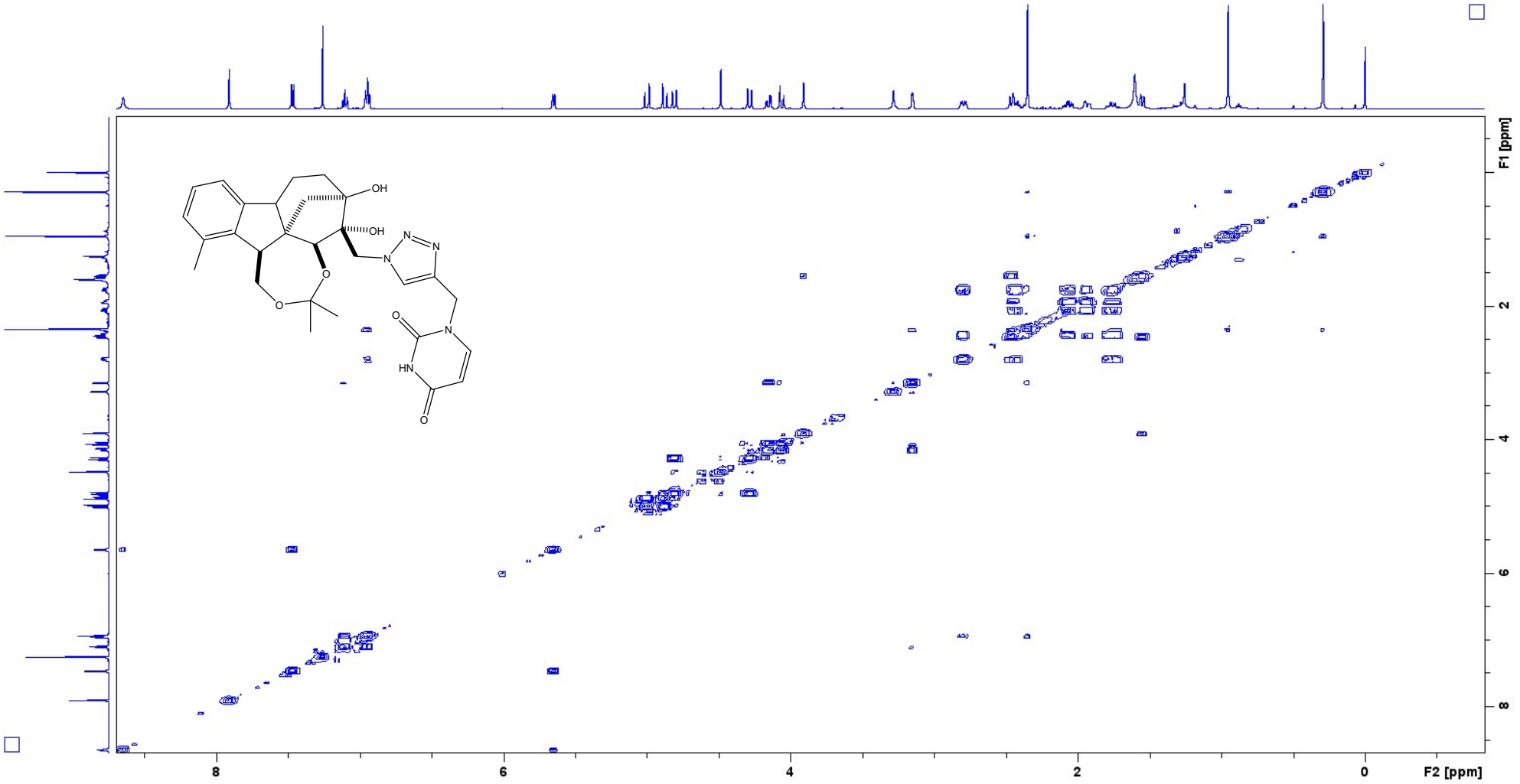
^{1}H-NMR (500 MHz) of 1-((1-(((4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-5,6-Dihydroxy-3,3,12-trimethyl-1,4a,5,6,7,8,8a,12b-octahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-*de*][1,3]dioxepin-5-yl)methyl)-1*H*-1,2,3-triazol-4-yl)methyl)pyrimidine-2,4(1*H*,3*H*)-dione **34**



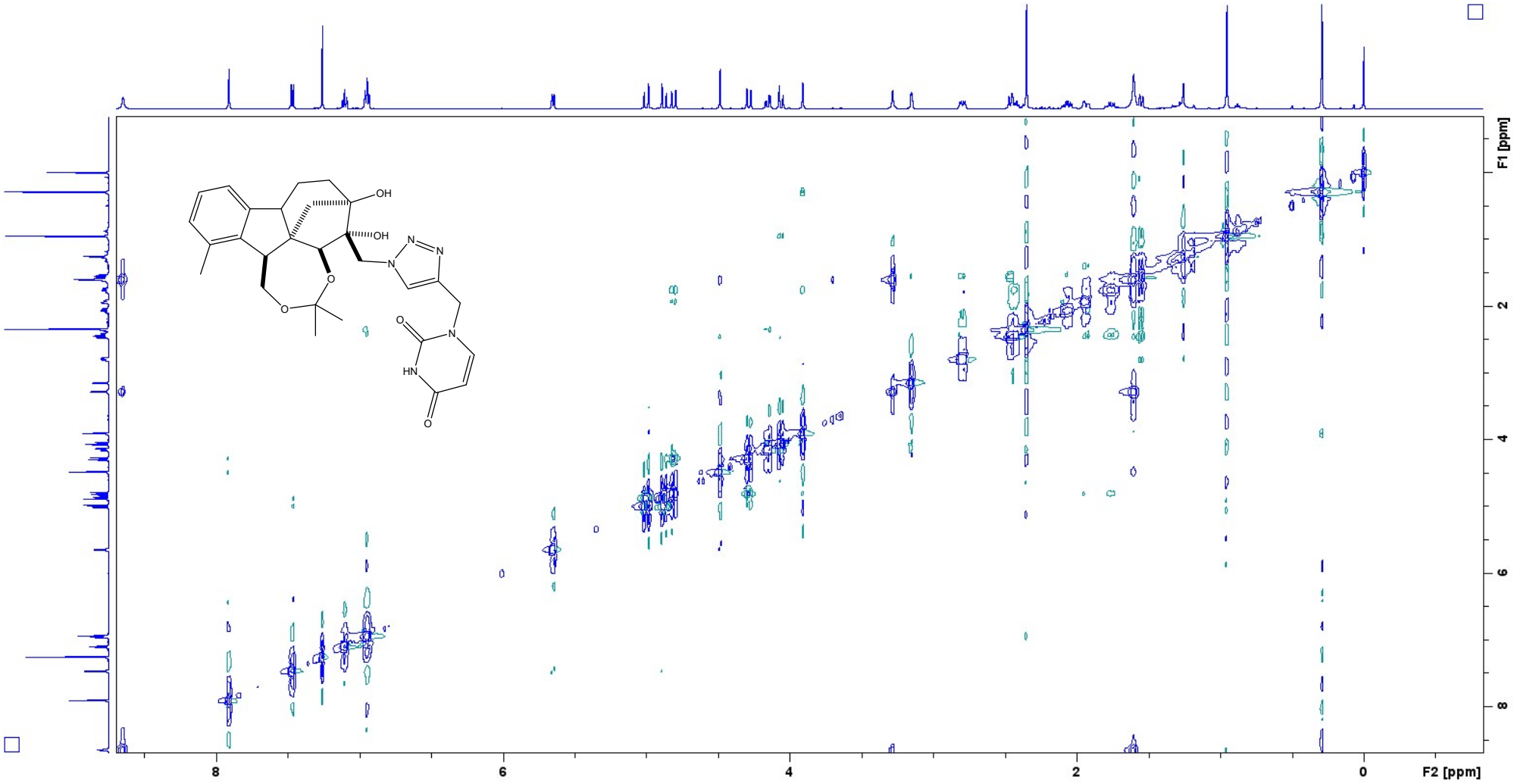
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of 1-((1-(((4a*S*,4a^{1}*R*,5*R*,6*S*,12b*S*)-5,6-Dihydroxy-3,3,12-trimethyl-1,4a,5,6,7,8,8a,12b-octahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-*de*][1,3]dioxepin-5-yl)methyl)-1*H*-1,2,3-triazol-4-yl)methyl)pyrimidine-2,4(1*H*,3*H*)-dione **34**



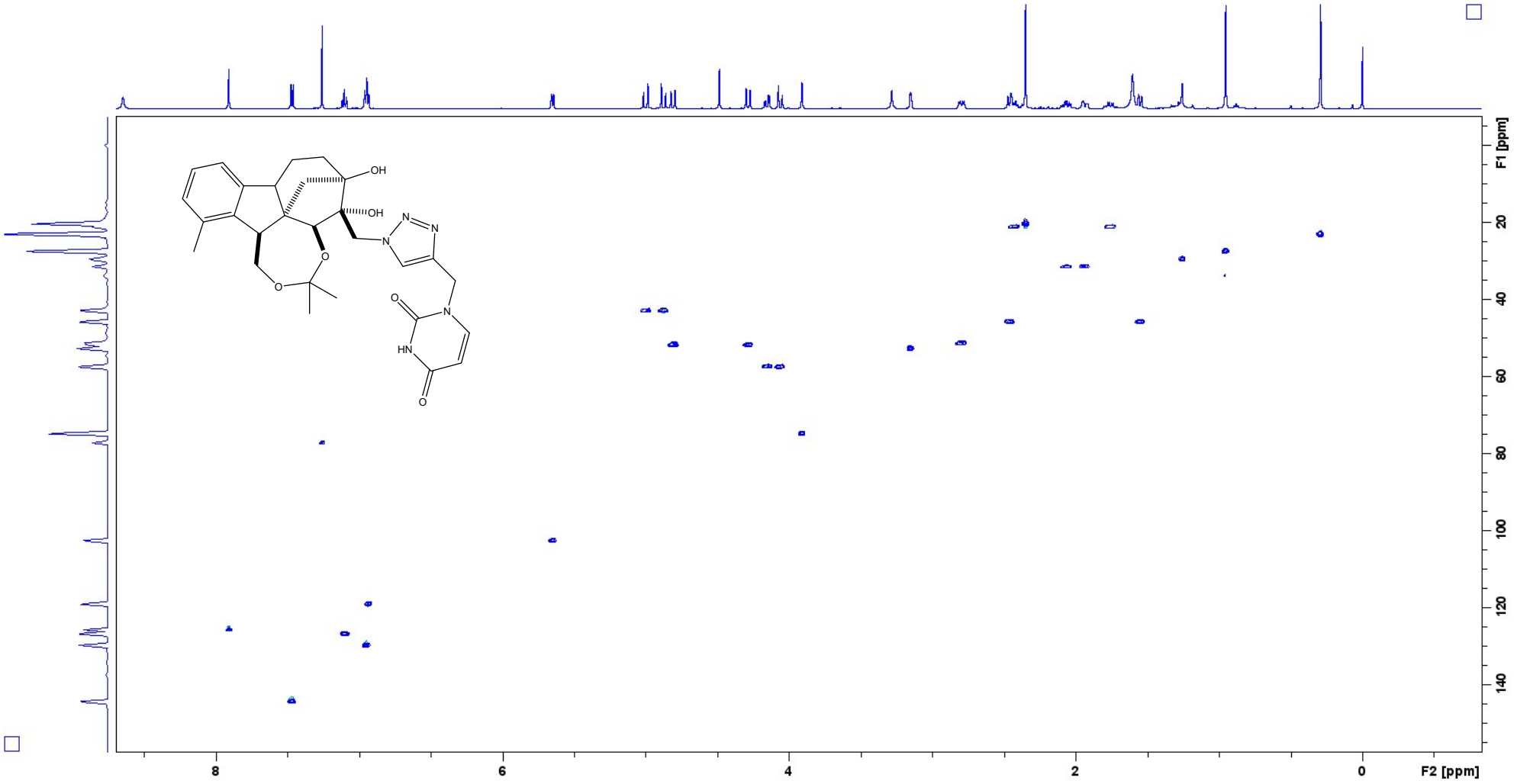
COSY of 1-((1-(((4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-5,6-Dihydroxy-3,3,12-trimethyl-1,4a,5,6,7,8,8a,12b-octahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-*de*][1,3]dioxepin-5-yl)methyl)-1*H*-1,2,3-triazol-4-yl)methyl)pyrimidine-2,4(1*H*,3*H*)-dione **34**



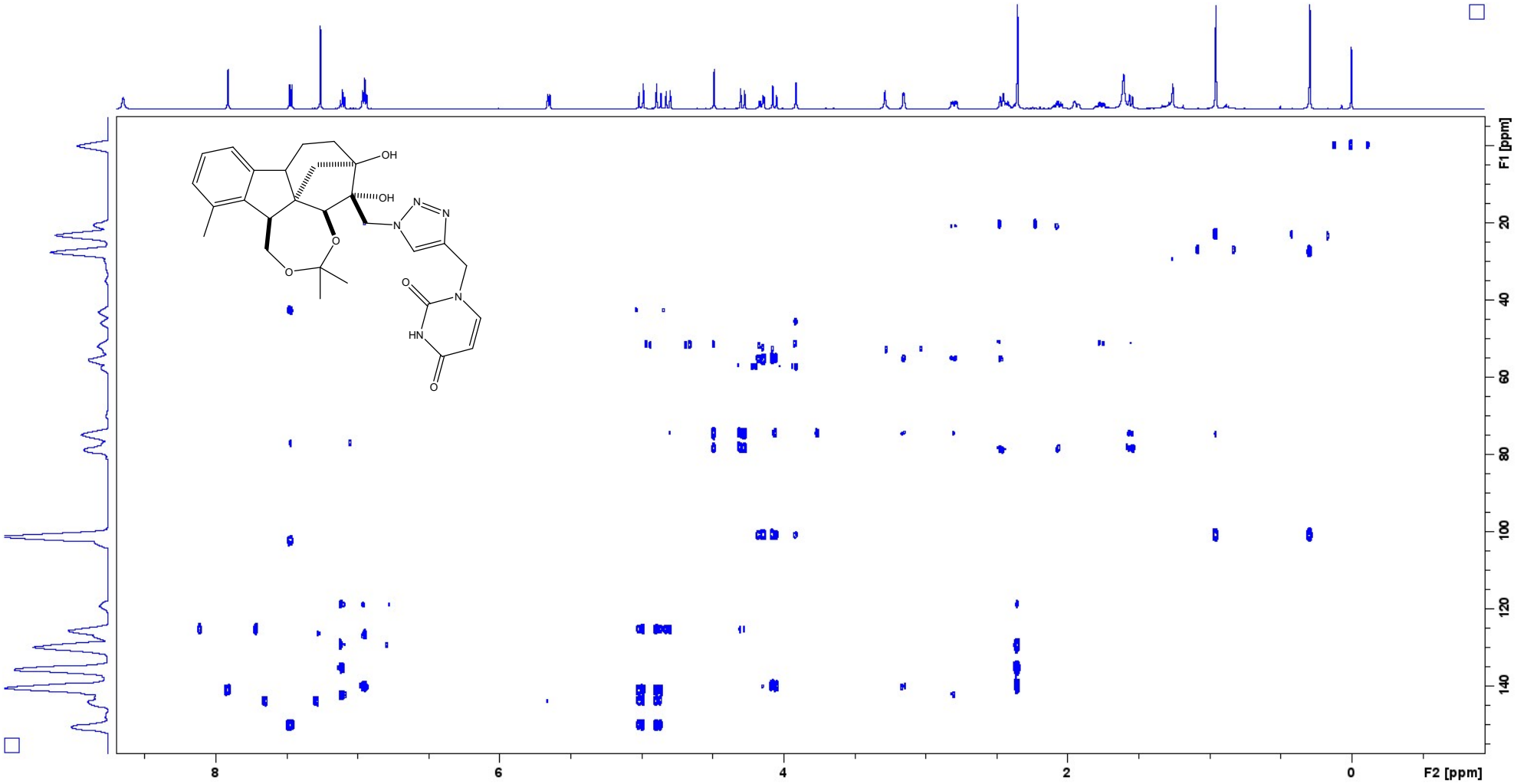
NOESY of 1-((1-(((4a*S*,4a^1*R*,5*R*,6*S*,12b*S*)-5,6-Dihydroxy-3,3,12-trimethyl-1,4a,5,6,7,8,8a,12b-octahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-*de*][1,3]dioxepin-5-yl)methyl)-1*H*-1,2,3-triazol-4-yl)methyl)pyrimidine-2,4(1*H*,3*H*)-dione **34**



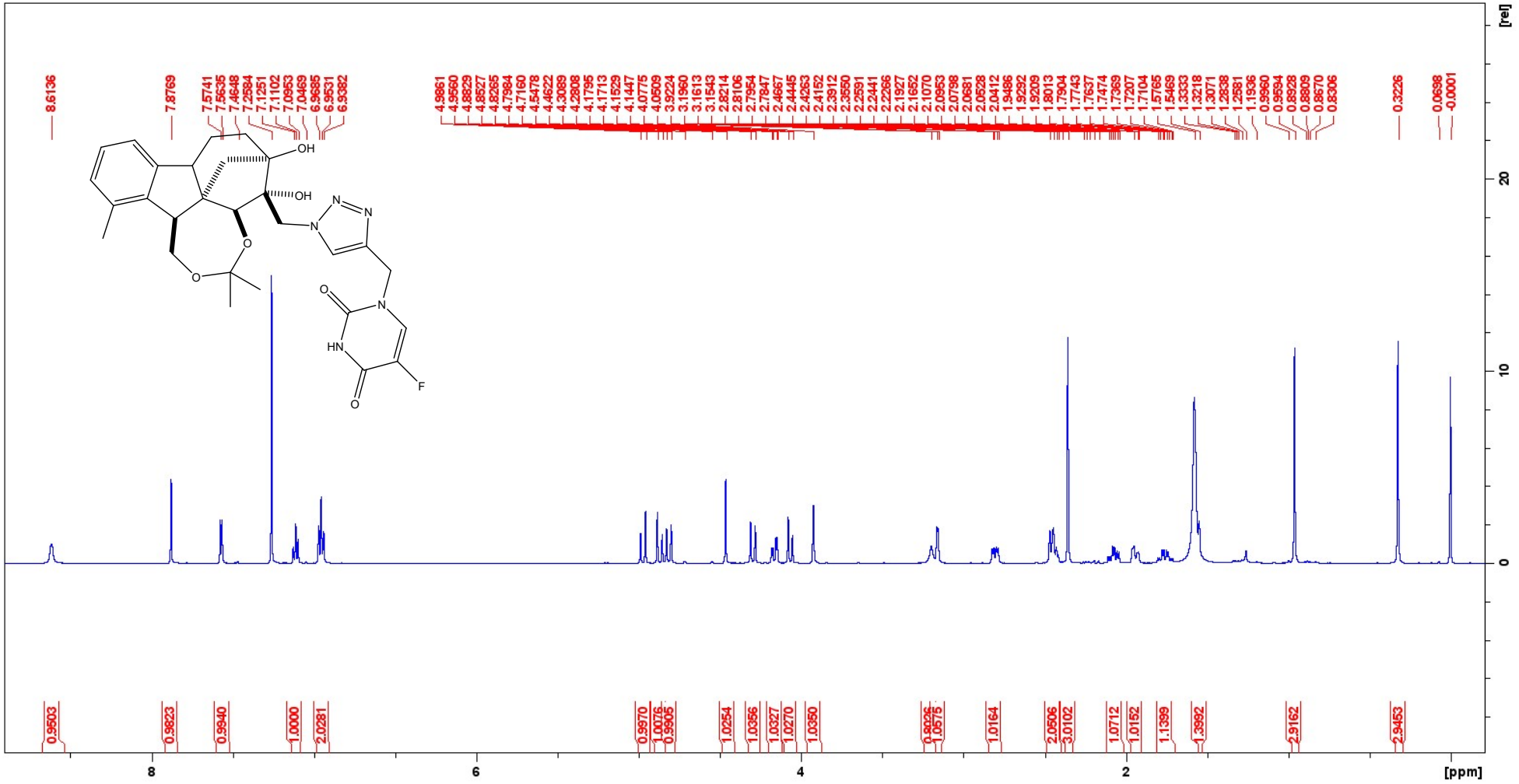
HSQC of 1-((1-(((4a*S*,4a[1]*R*,5*R*,6*S*,12b*S*)-5,6-Dihydroxy-3,3,12-trimethyl-1,4a,5,6,7,8,8a,12b-octahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-*de*][1,3]dioxepin-5-yl)methyl)-1*H*-1,2,3-triazol-4-yl)methyl)pyrimidine-2,4(1*H*,3*H*)-dione **34**



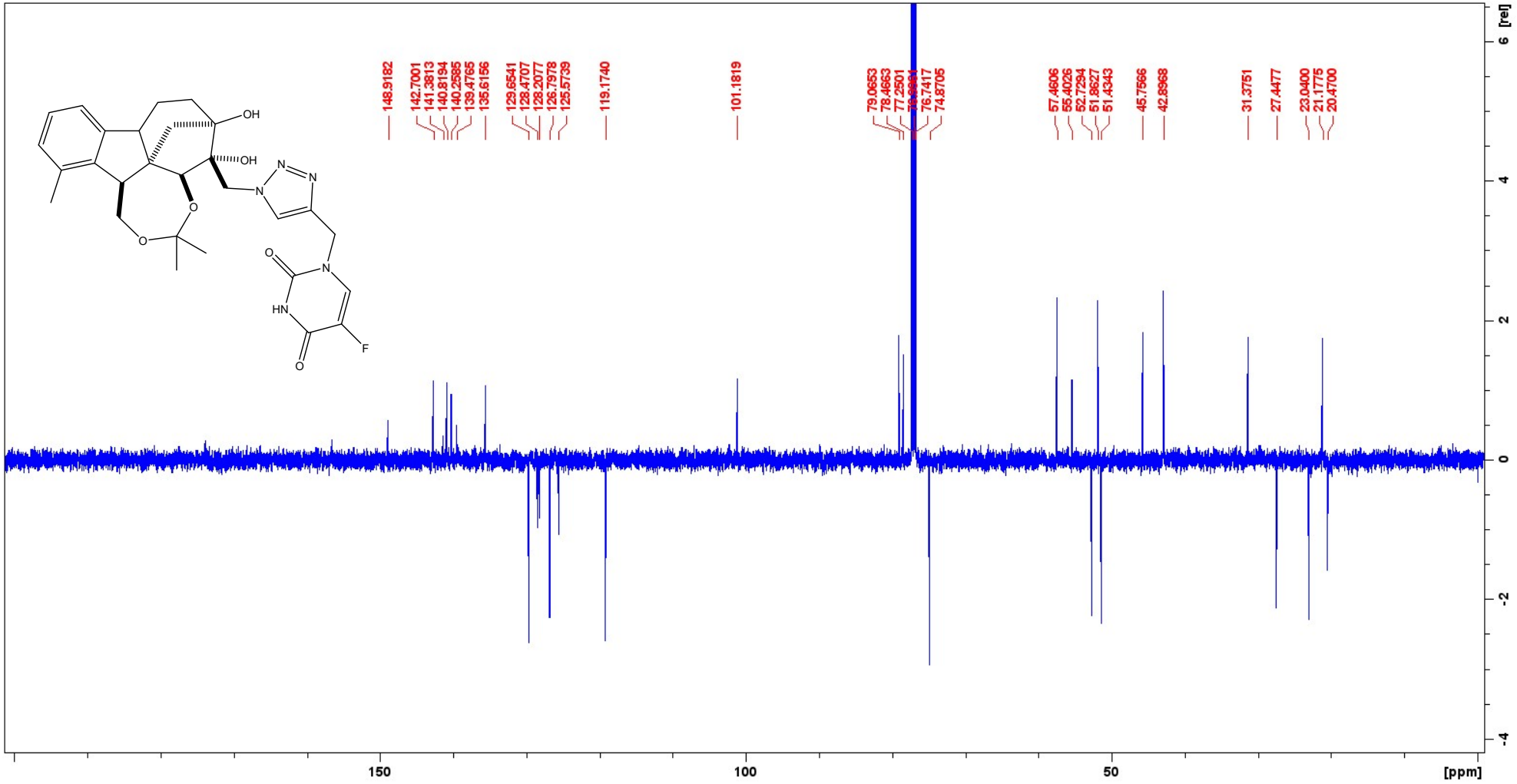
HMBC of 1-((1-(((4a*S*,4a[1]*R*,5*R*,6*S*,12b*S*)-5,6-Dihydroxy-3,3,12-trimethyl-1,4a,5,6,7,8,8a,12b-octahydro-4a1,6-methanobenzo[2,3]azuleno[8,1-*de*][1,3]dioxepin-5-yl)methyl)-1*H*-1,2,3-triazol-4-yl)methyl)pyrimidine-2,4(1*H*,3*H*)-dione **34**



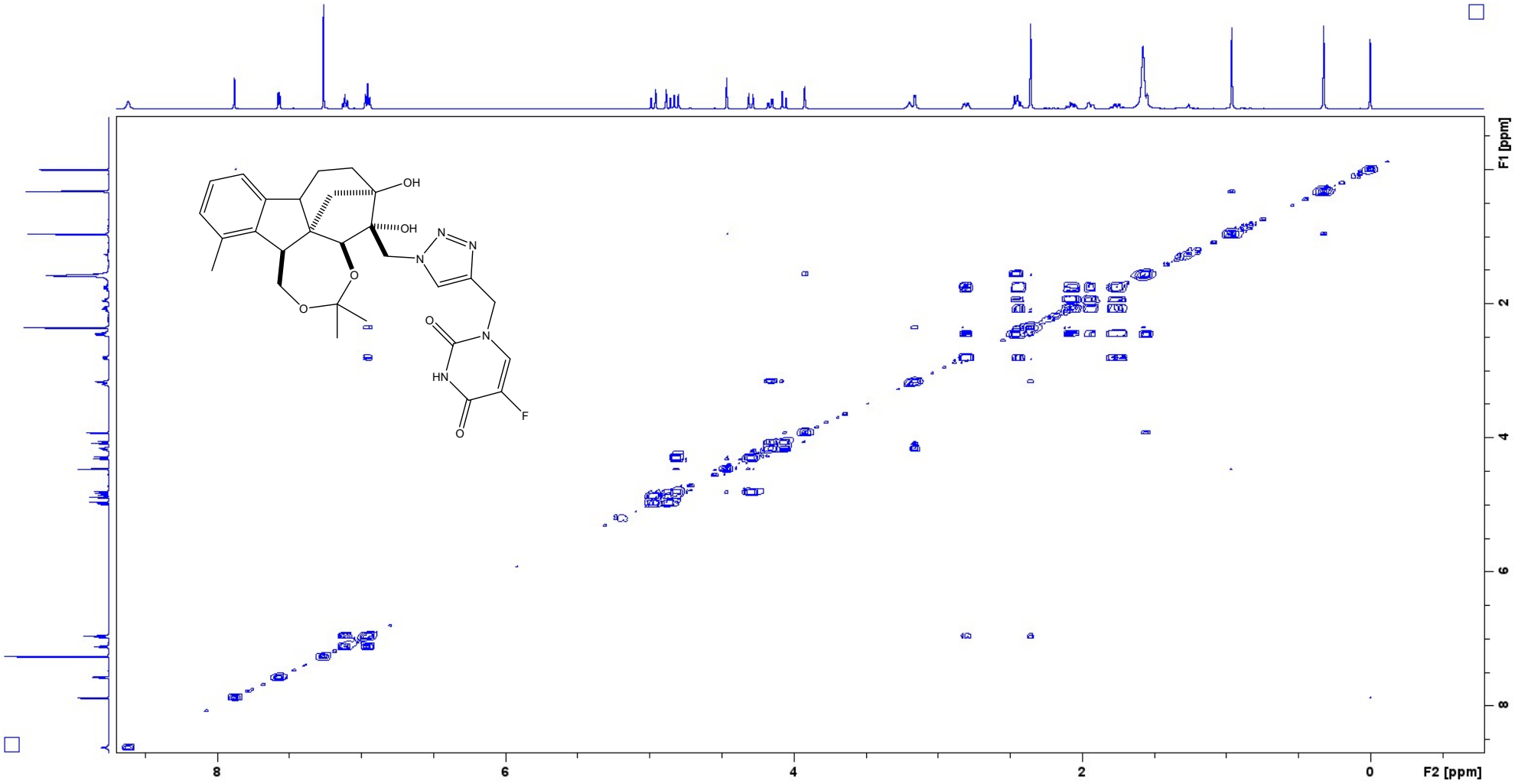
^{1}H-NMR (500 MHz) of 1,4a,5,6,7,8,8a,12b-octahydro-4a^{1},6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepin-5-yl)methyl)-1*H*-1,2,3-triazol-4-yl)methyl)-5-fluoropyrimidine-2,4(1*H*,3*H*)-dione **35**



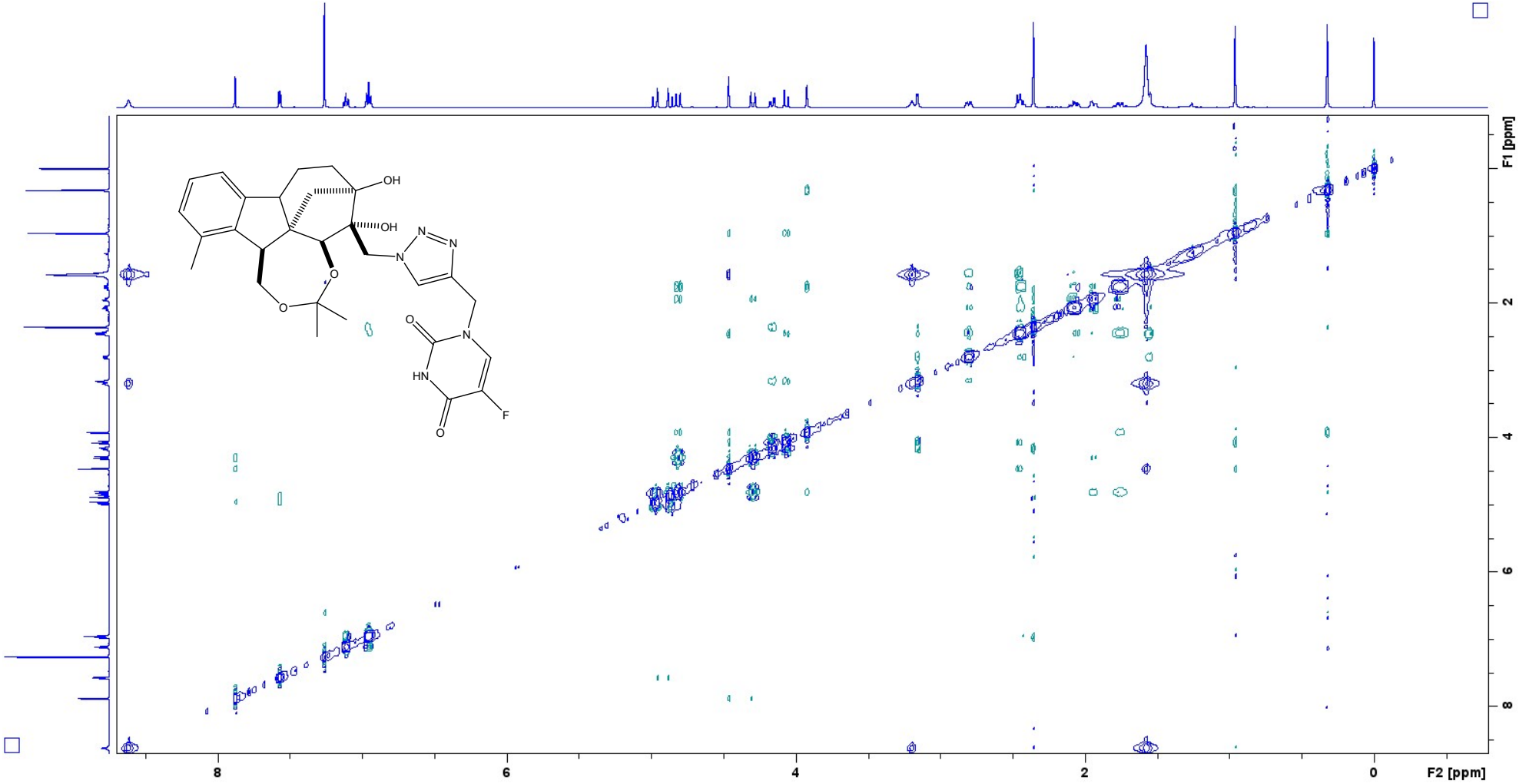
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of 1,4a,5,6,7,8,8a,12b-octahydro-4a[1],6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepin-5-yl)methyl)-1*H*-1,2,3-triazol-4-yl)methyl)-5-fluoropyrimidine-2,4(1*H*,3*H*)-dione **35**



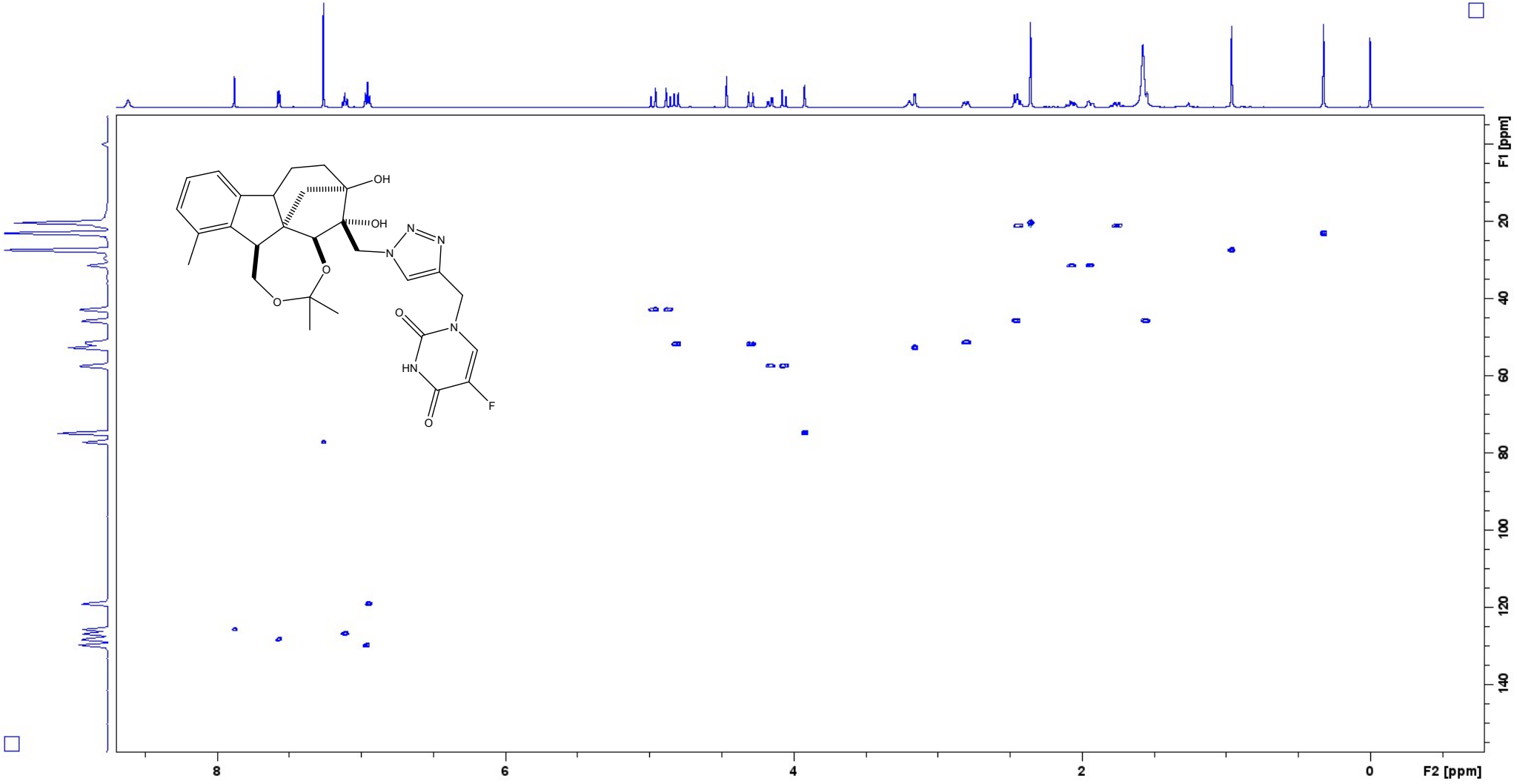
COSY of 1,4a,5,6,7,8,8a,12b-octahydro-4a[1],6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepin-5-yl)methyl)-1*H*-1,2,3-triazol-4-yl)methyl)-5-fluoropyrimidine-2,4(1*H*,3*H*)-dione **35**



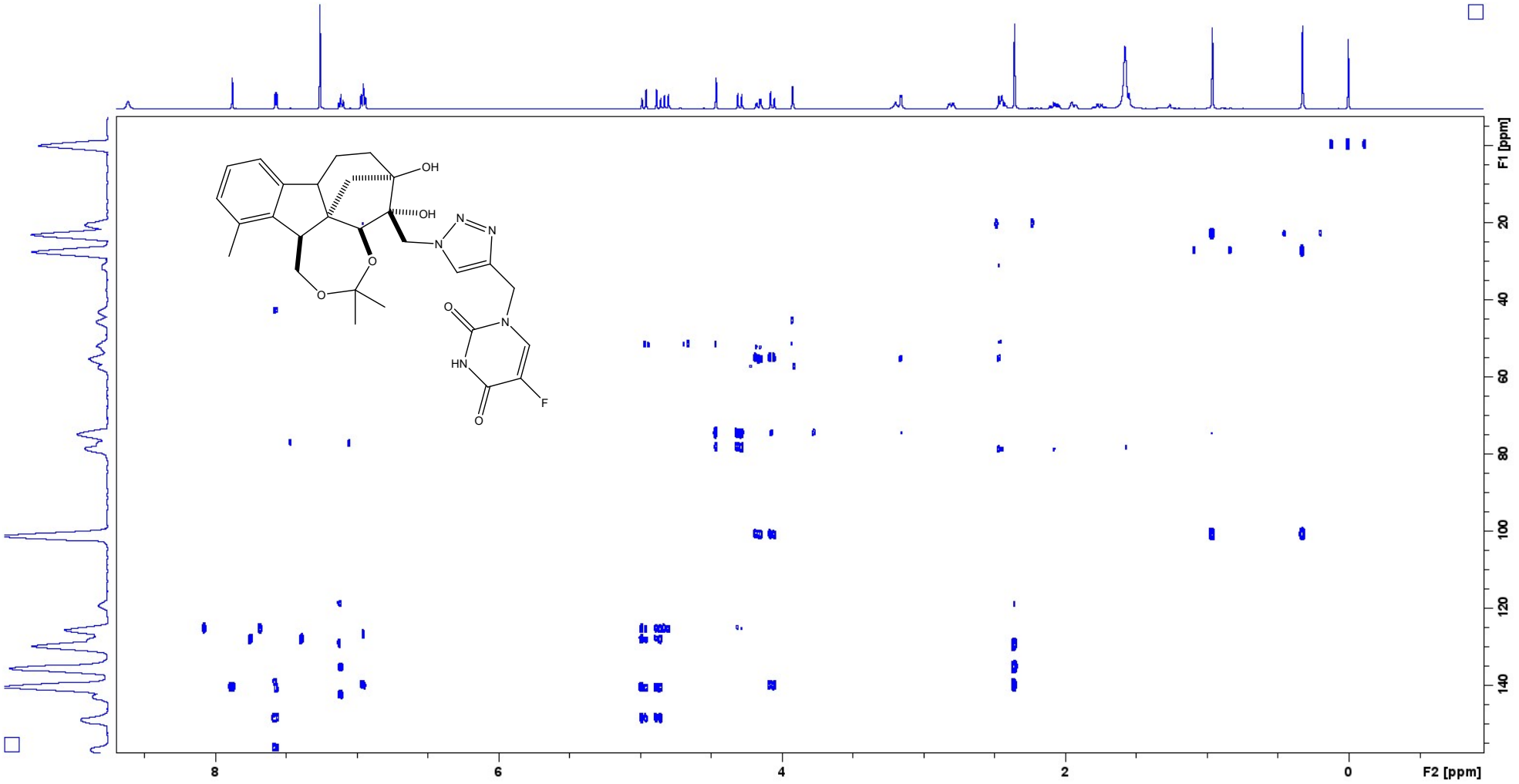
NOESY of 1,4a,5,6,7,8,8a,12b-octahydro-4a[1],6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepin-5-yl)methyl)-1*H*-1,2,3-triazol-4-yl)methyl)-5-fluoropyrimidine-2,4(1*H*,3*H*)-dione **35**



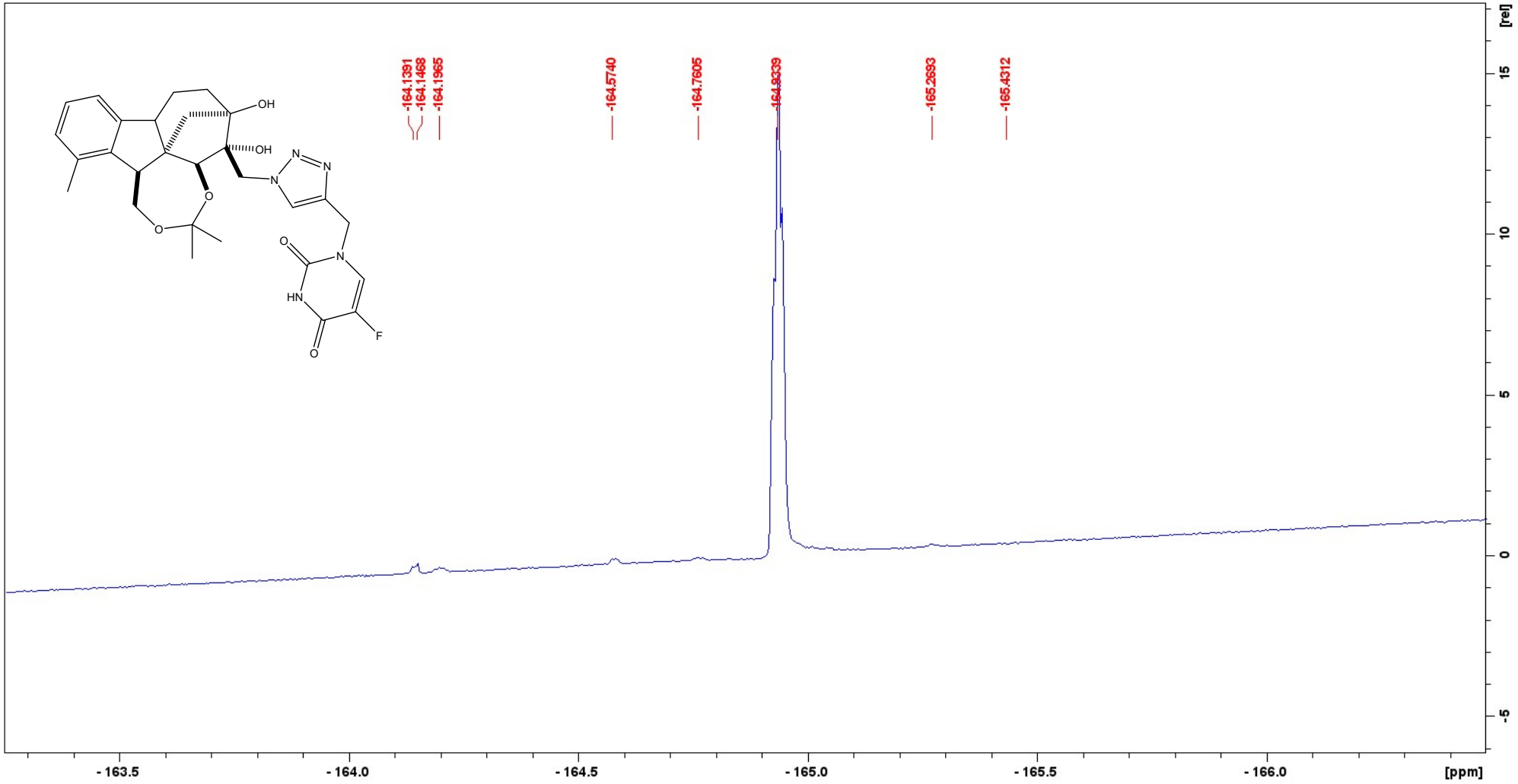
HSQC of 1,4a,5,6,7,8,8a,12b-octahydro-4a[1],6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepin-5-yl)methyl)-1*H*-1,2,3-triazol-4-yl)methyl)-5-fluoropyrimidine-2,4(1*H*,3*H*)-dione **35**



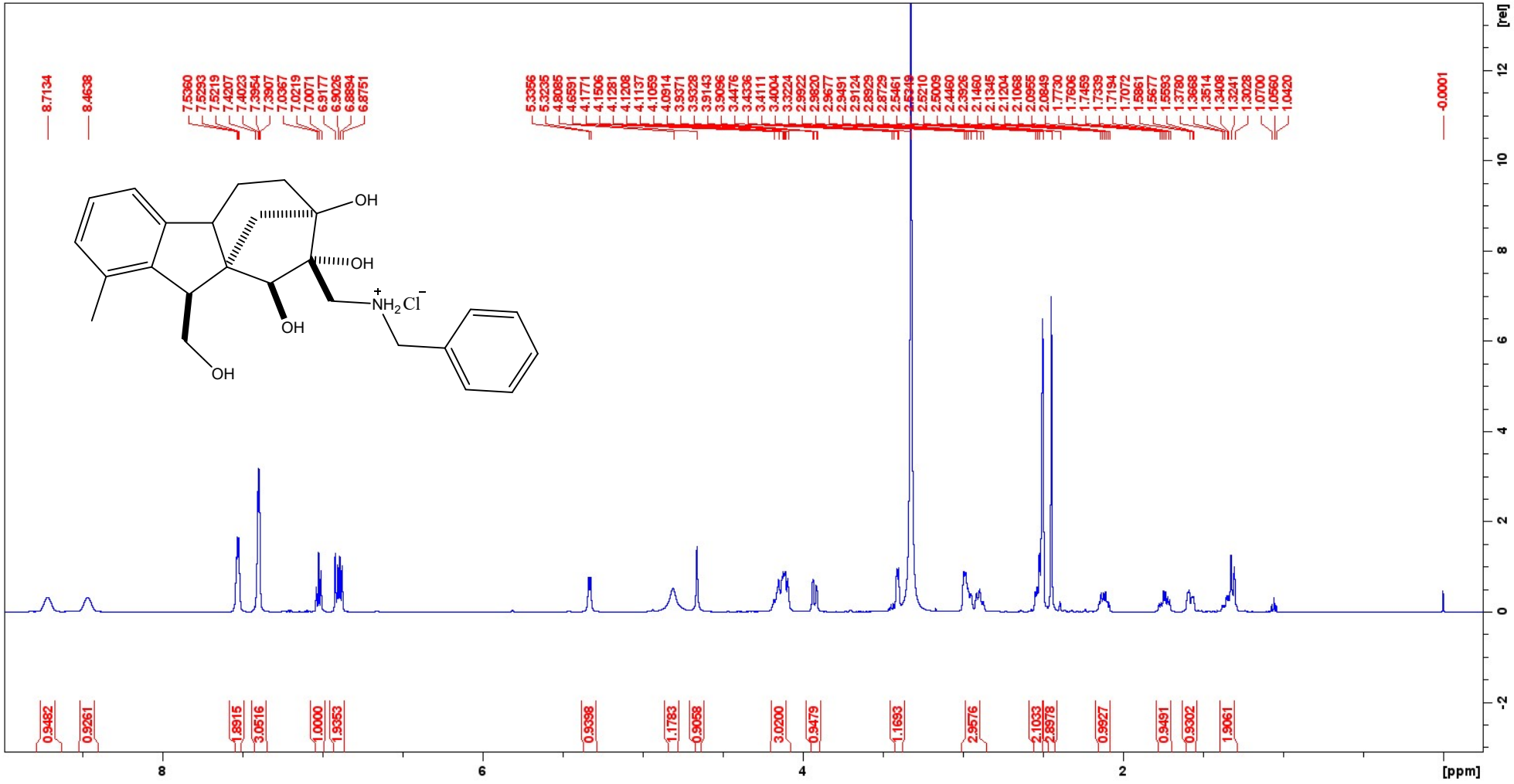
HMBC of 1,4a,5,6,7,8,8a,12b-octahydro-4a[1],6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepin-5-yl)methyl)-1*H*-1,2,3-triazol-4-yl)methyl)-5-fluoropyrimidine-2,4(1*H*,3*H*)-dione **35**



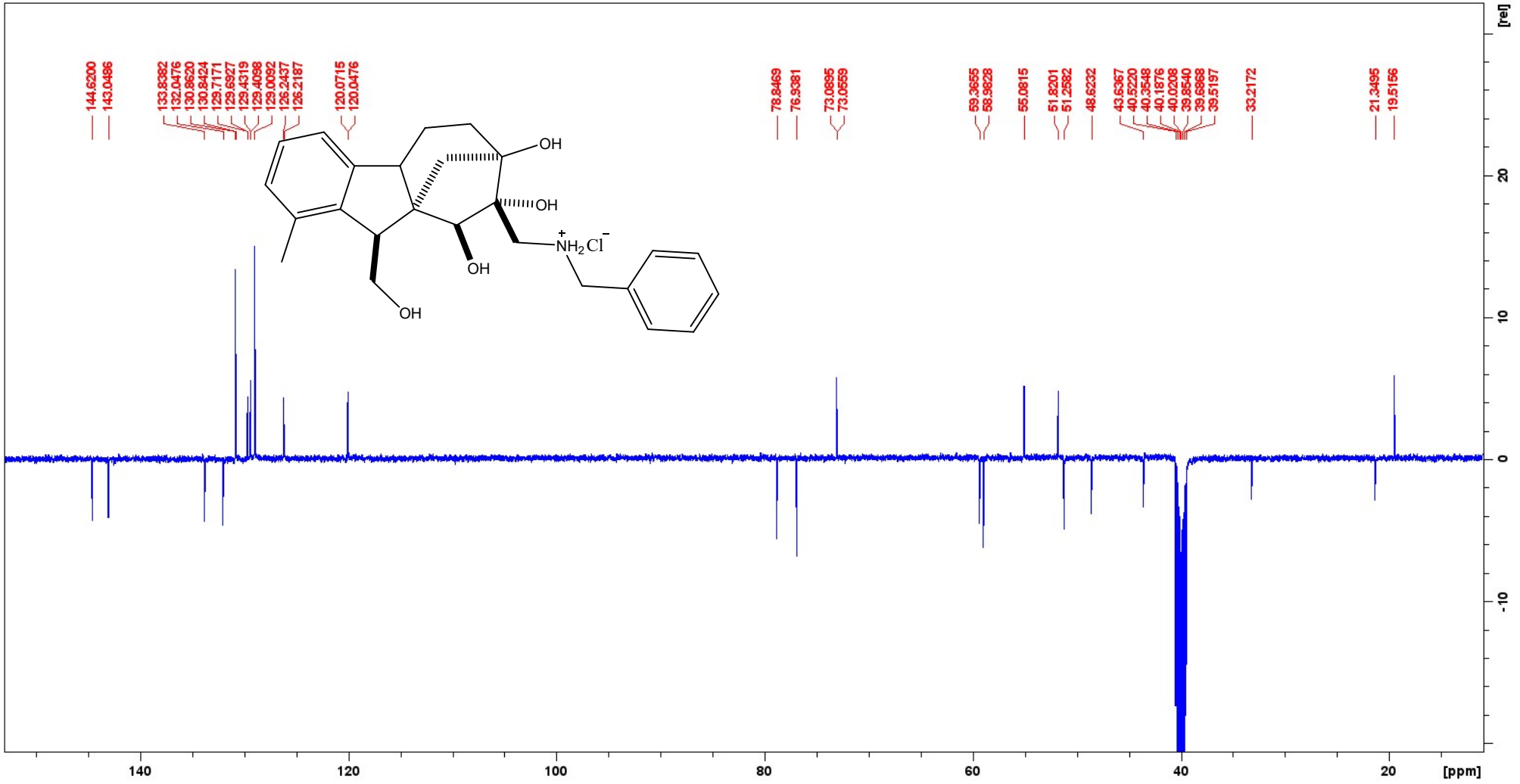
^{19}F *J*-MOD NMR (470 MHz) of 1,4a,5,6,7,8,8a,12b-octahydro-4a[1],6-methanobenzo[2,3]azuleno[8,1-de][1,3]dioxepin-5-yl)methyl)-1*H*-1,2,3-triazol-4-yl)methyl)-5-fluoropyrimidine-2,4(1*H*,3*H*)-dione **35**



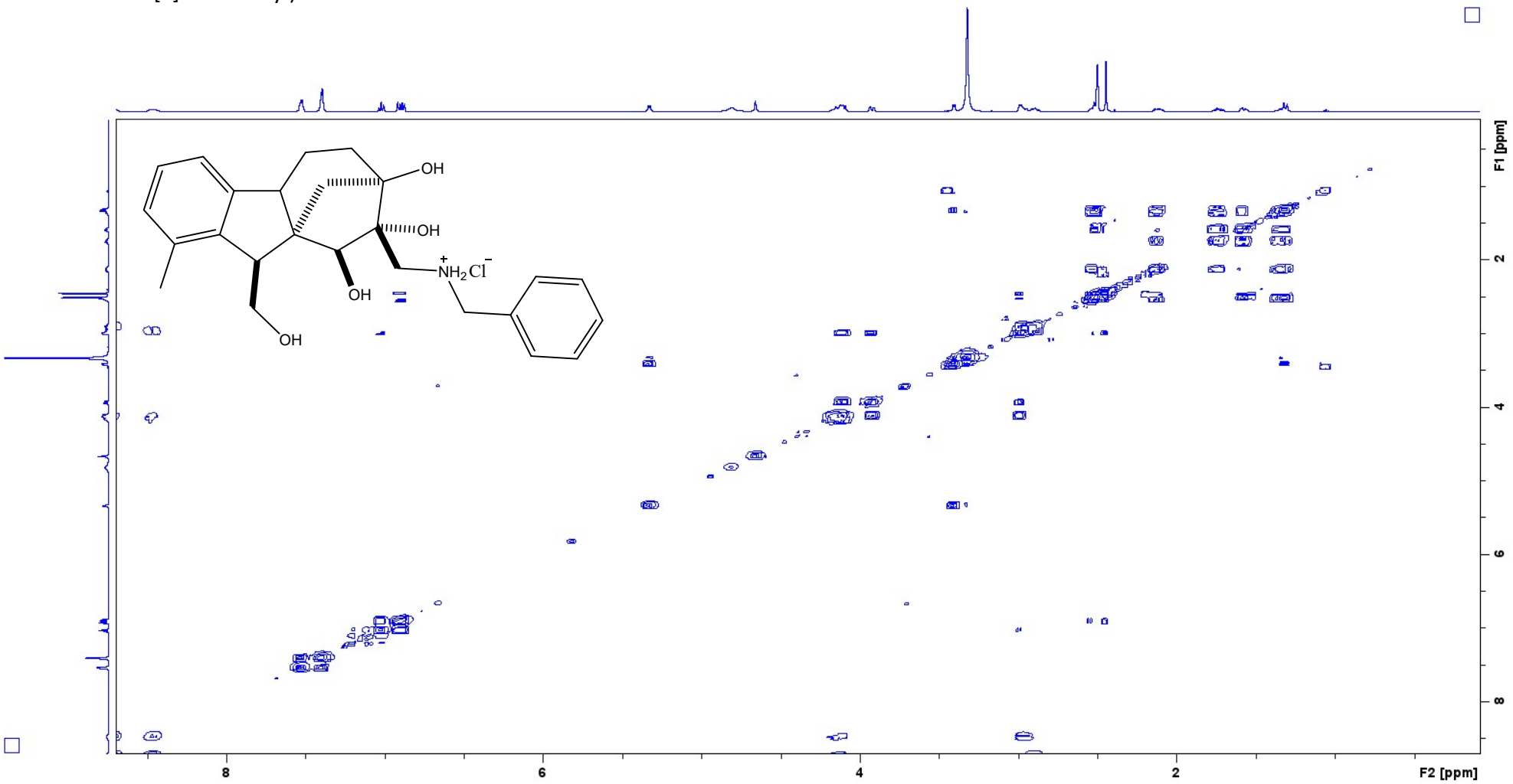
^{1}H-NMR (500 MHz) of *N*-Benzyl-1-((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methanaminium chloride **19**



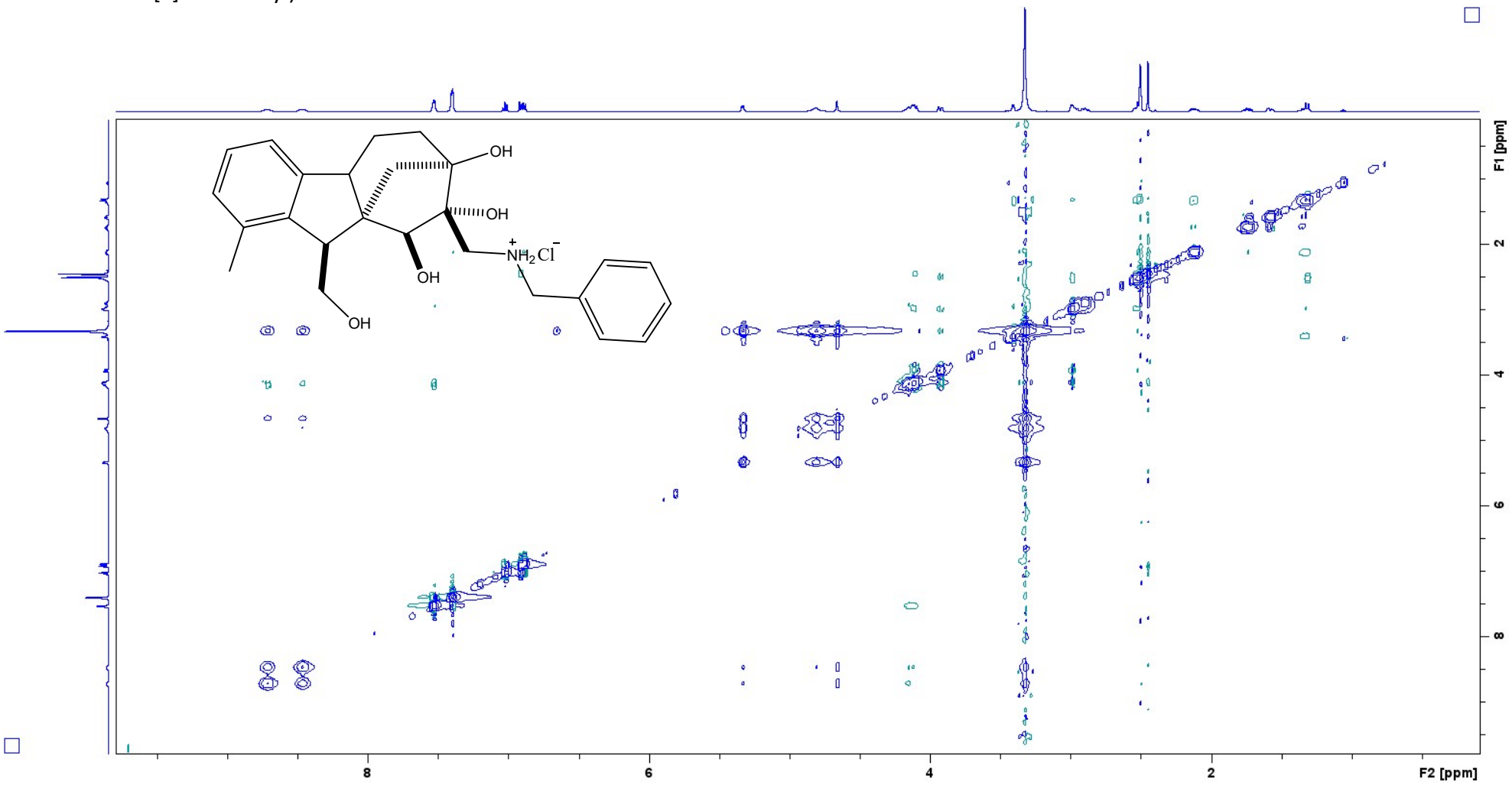
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of *N*-Benzyl-1-((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methanaminium chloride **19**



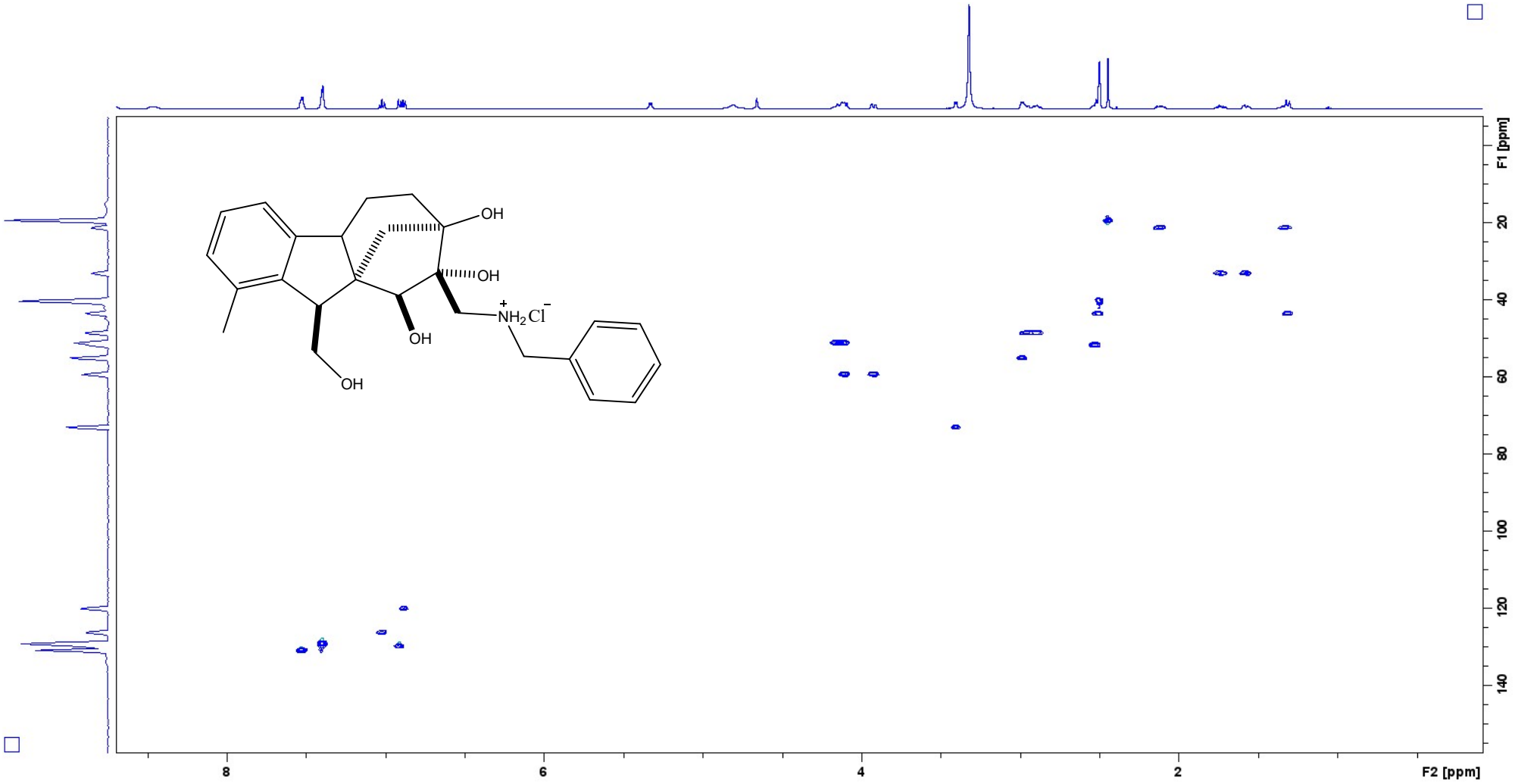
COSY of *N*-Benzyl-1-((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methanaminium chloride **19**



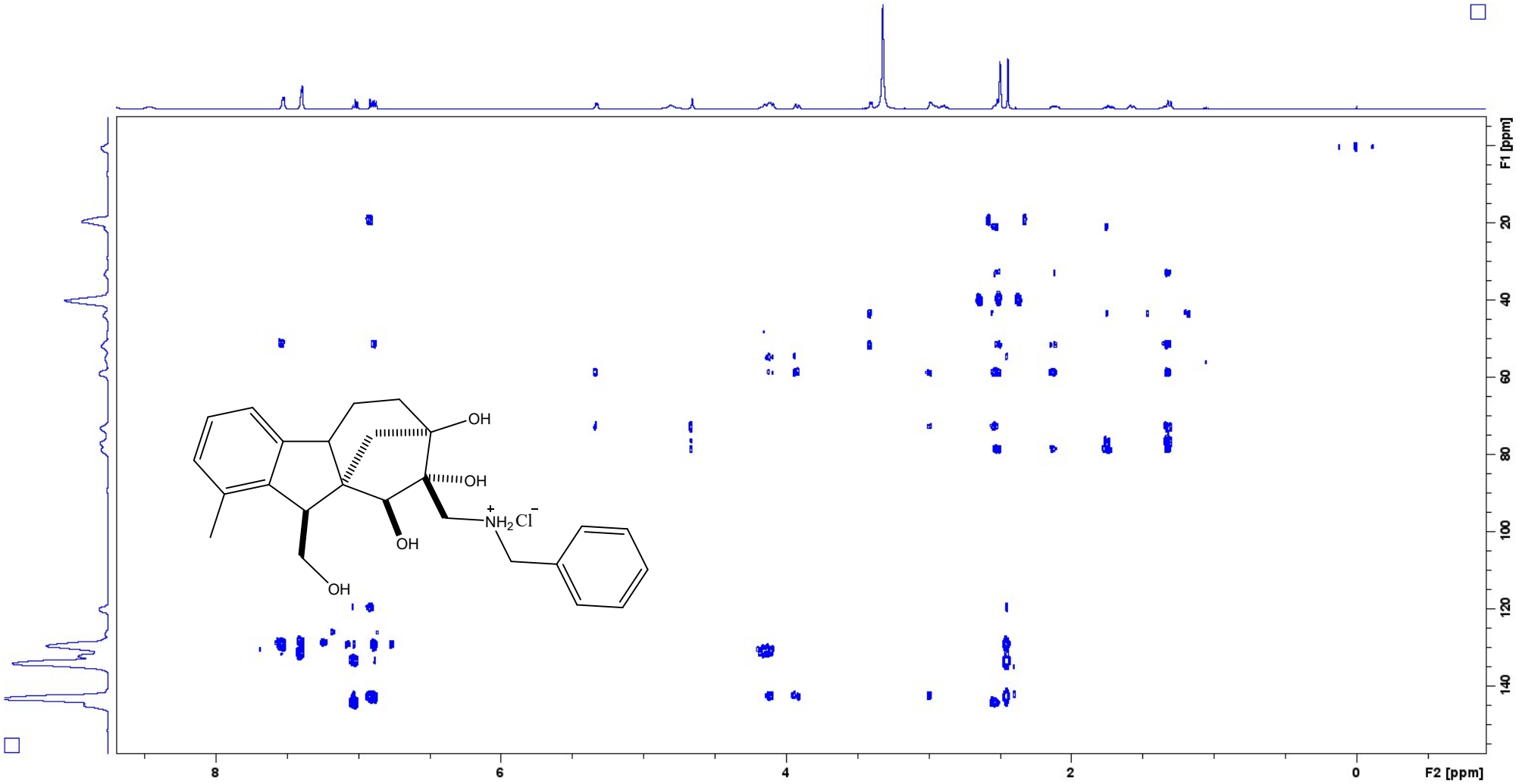
NOESY of *N*-Benzyl-1-((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methanaminium chloride **19**



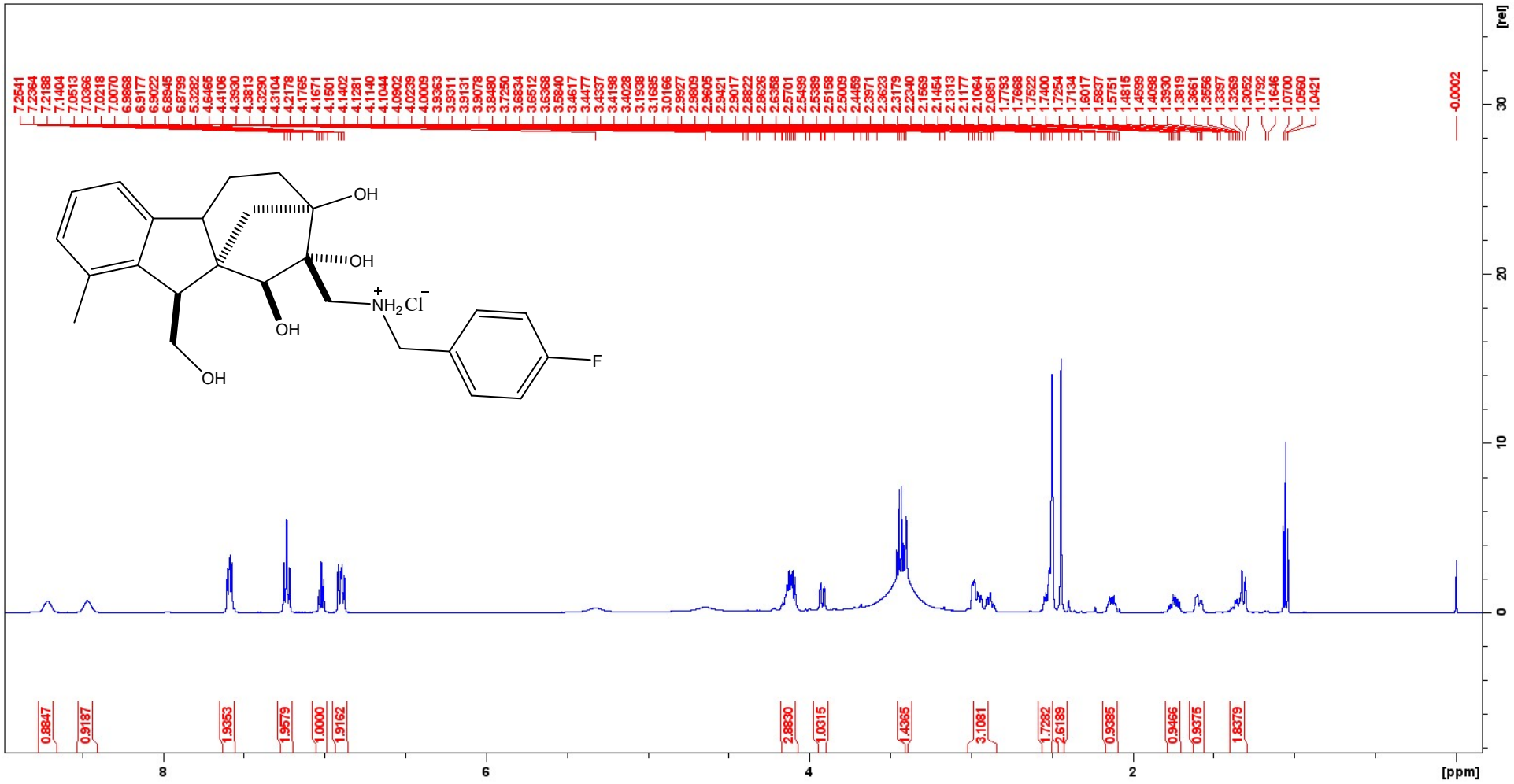
HSQC of *N*-Benzyl-1-((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methanaminium chloride **19**



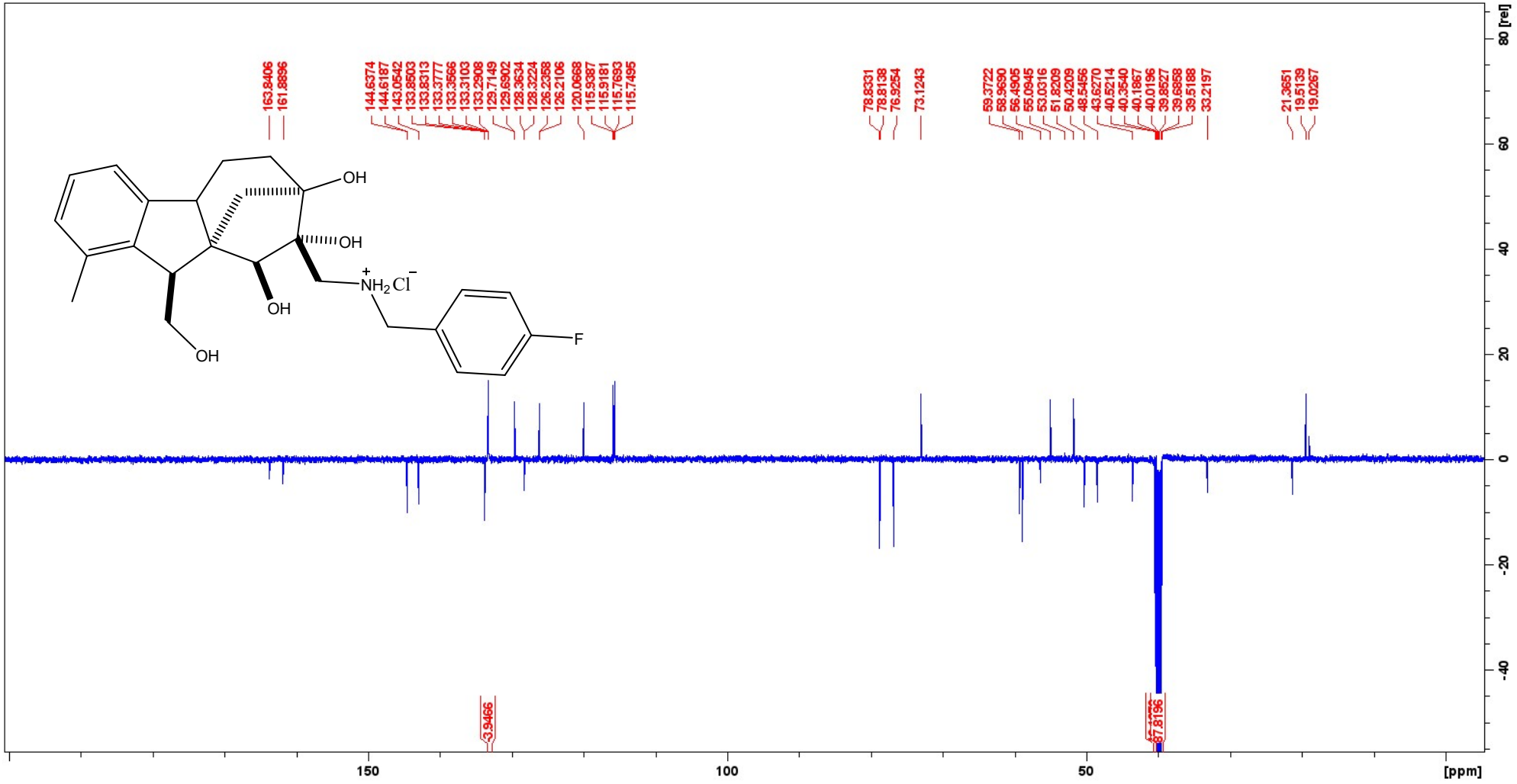
HMBC of *N*-Benzyl-1-((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methanaminium chloride **19**



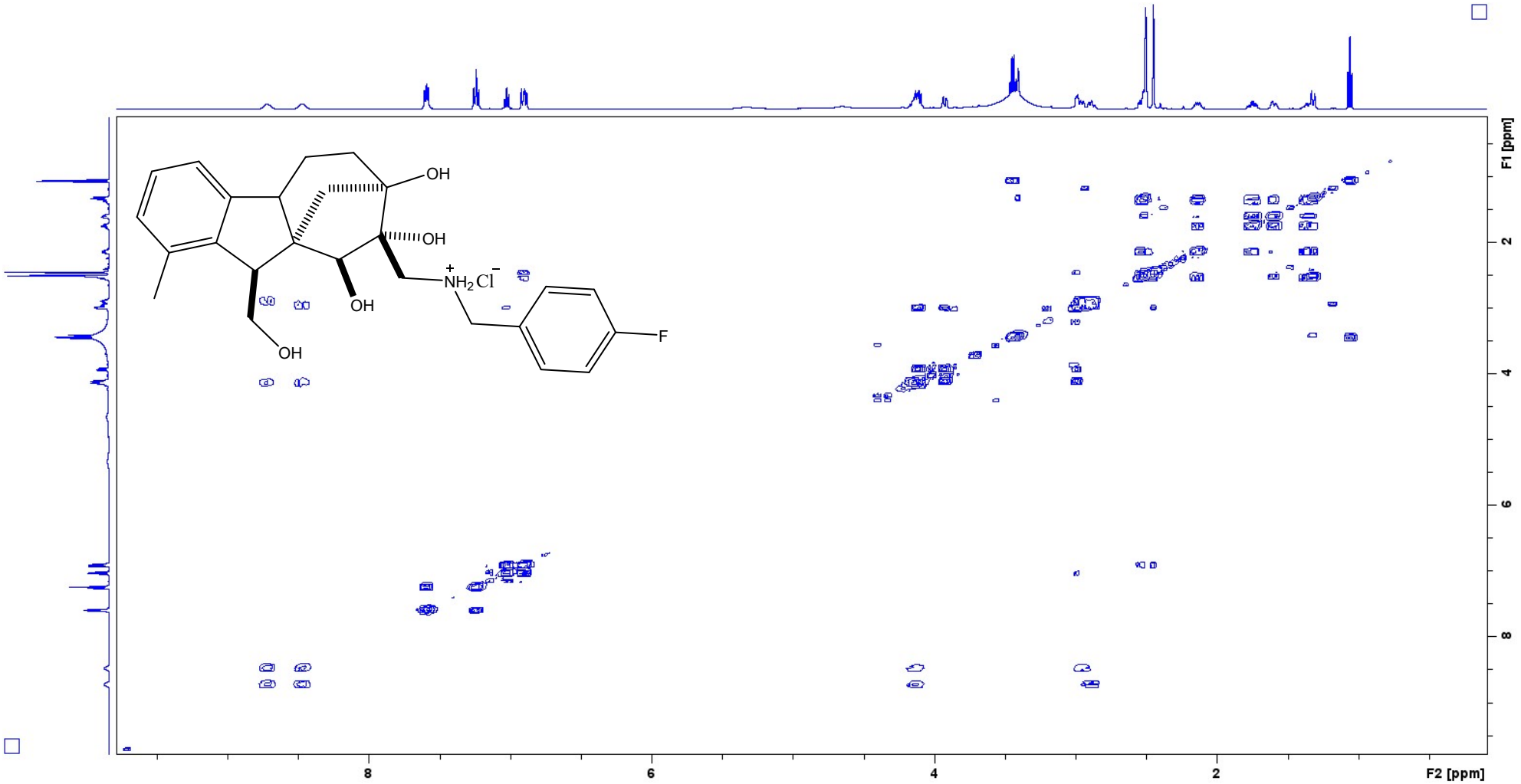
^{1}H-NMR (500 MHz) of *N*-(4-Fluorobenzyl)-1-((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methanaminium **20**



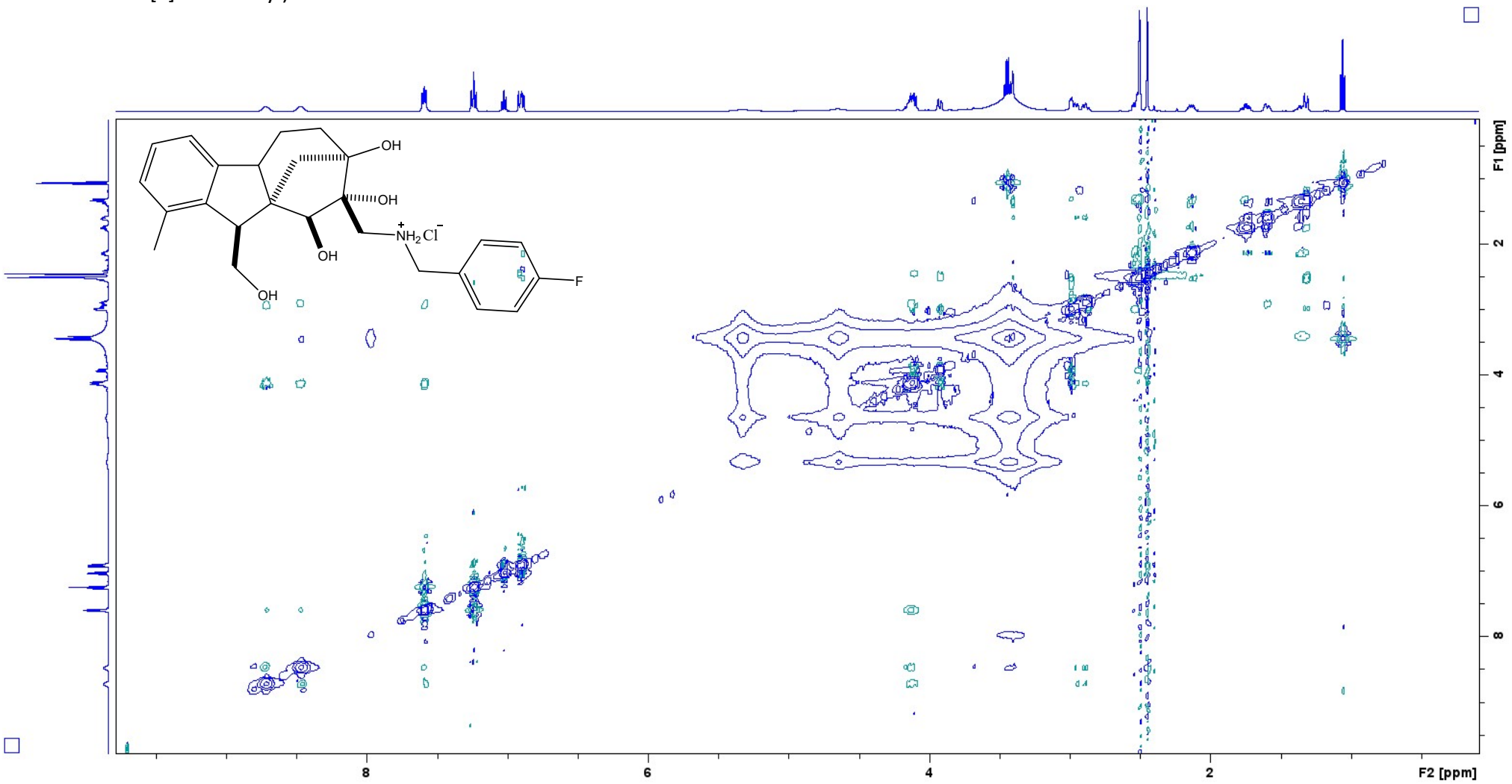
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of *N*-(4-Fluorobenzyl)-1-((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methanaminium **20**



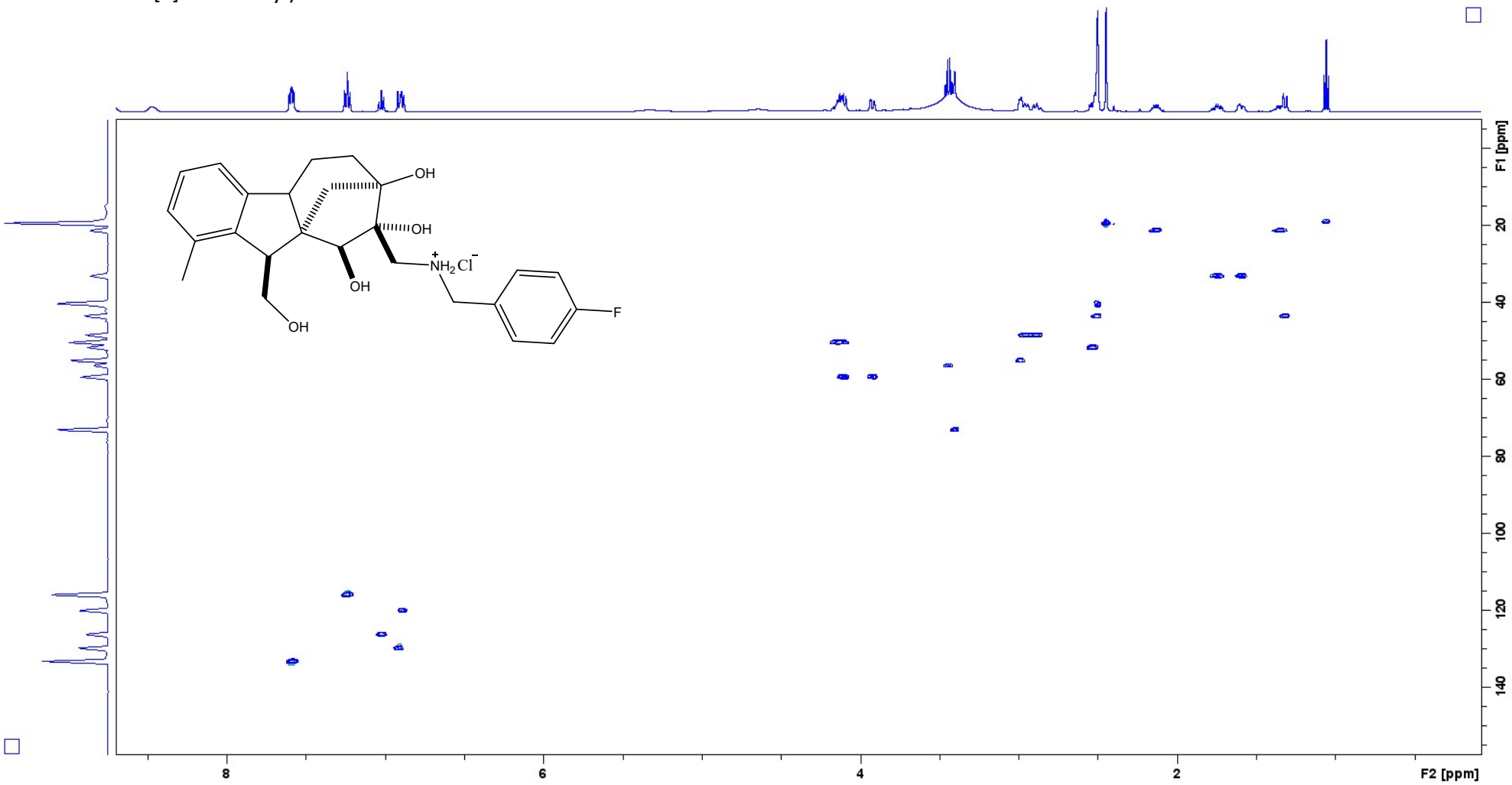
CSOY of *N*-(4-Fluorobenzyl)-1-((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methanaminium **20**



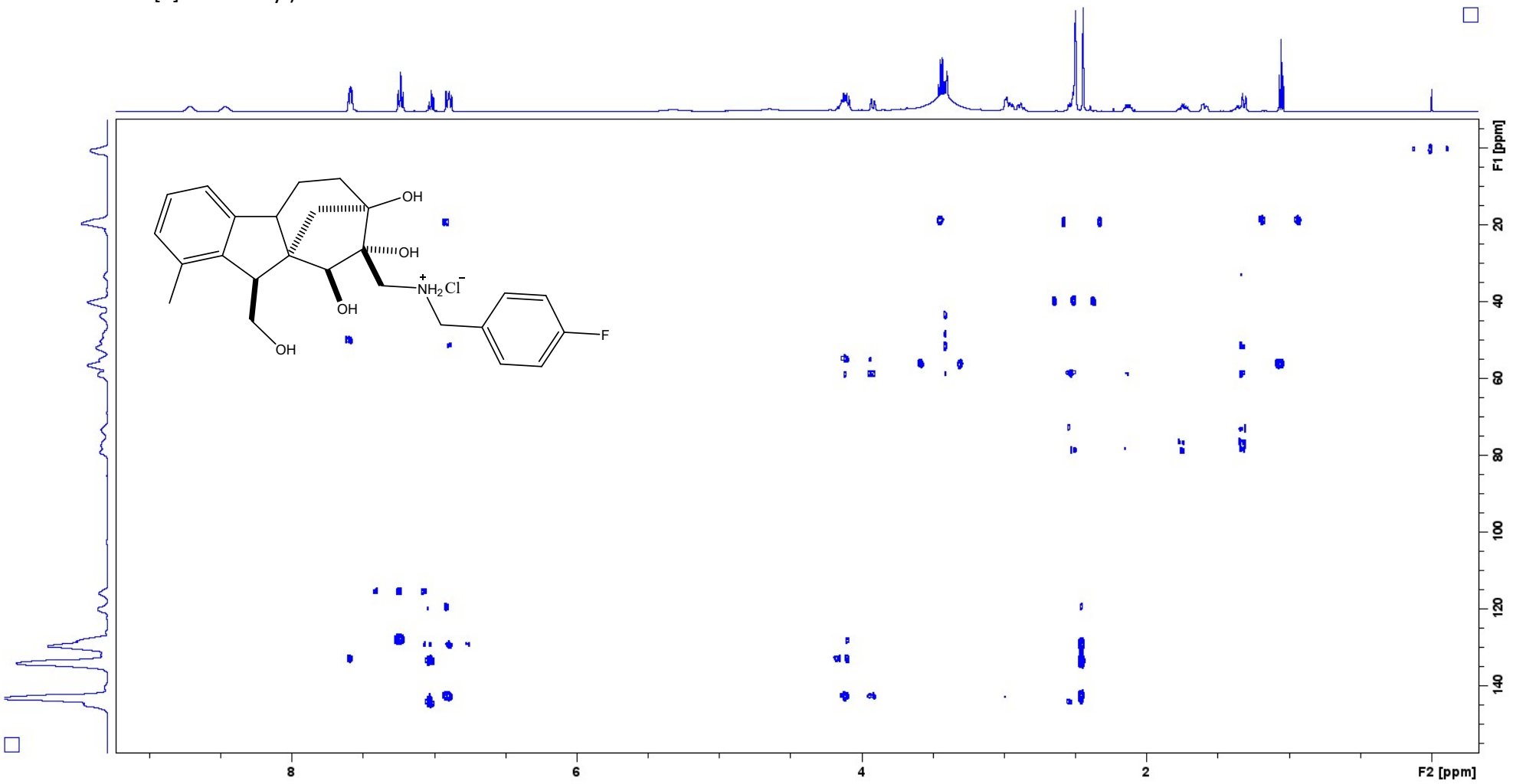
NOESY of *N*-(4-Fluorobenzyl)-1-((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methanaminium **20**



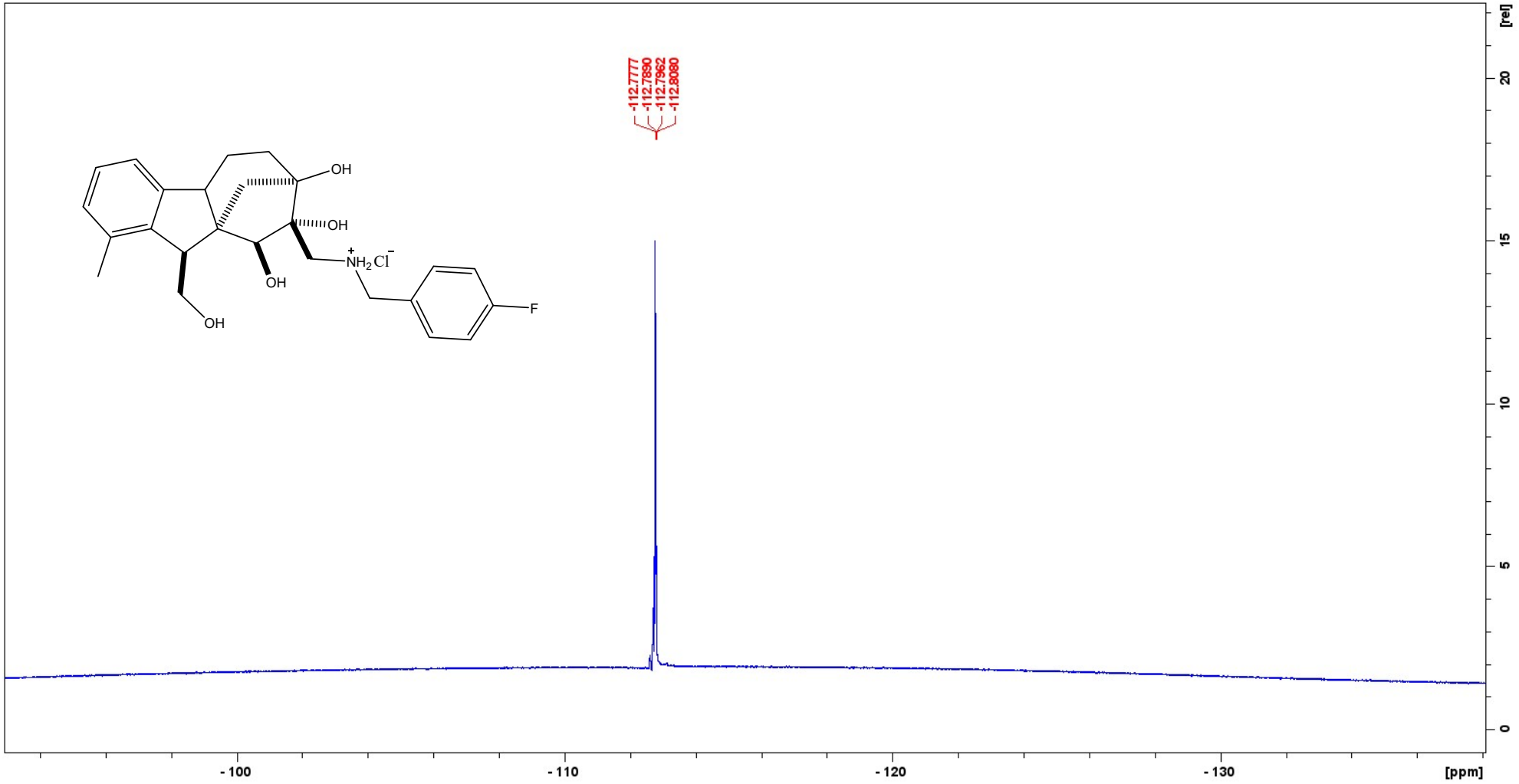
HSQC of *N*-(4-Fluorobenzyl)-1-((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methanaminium **20**



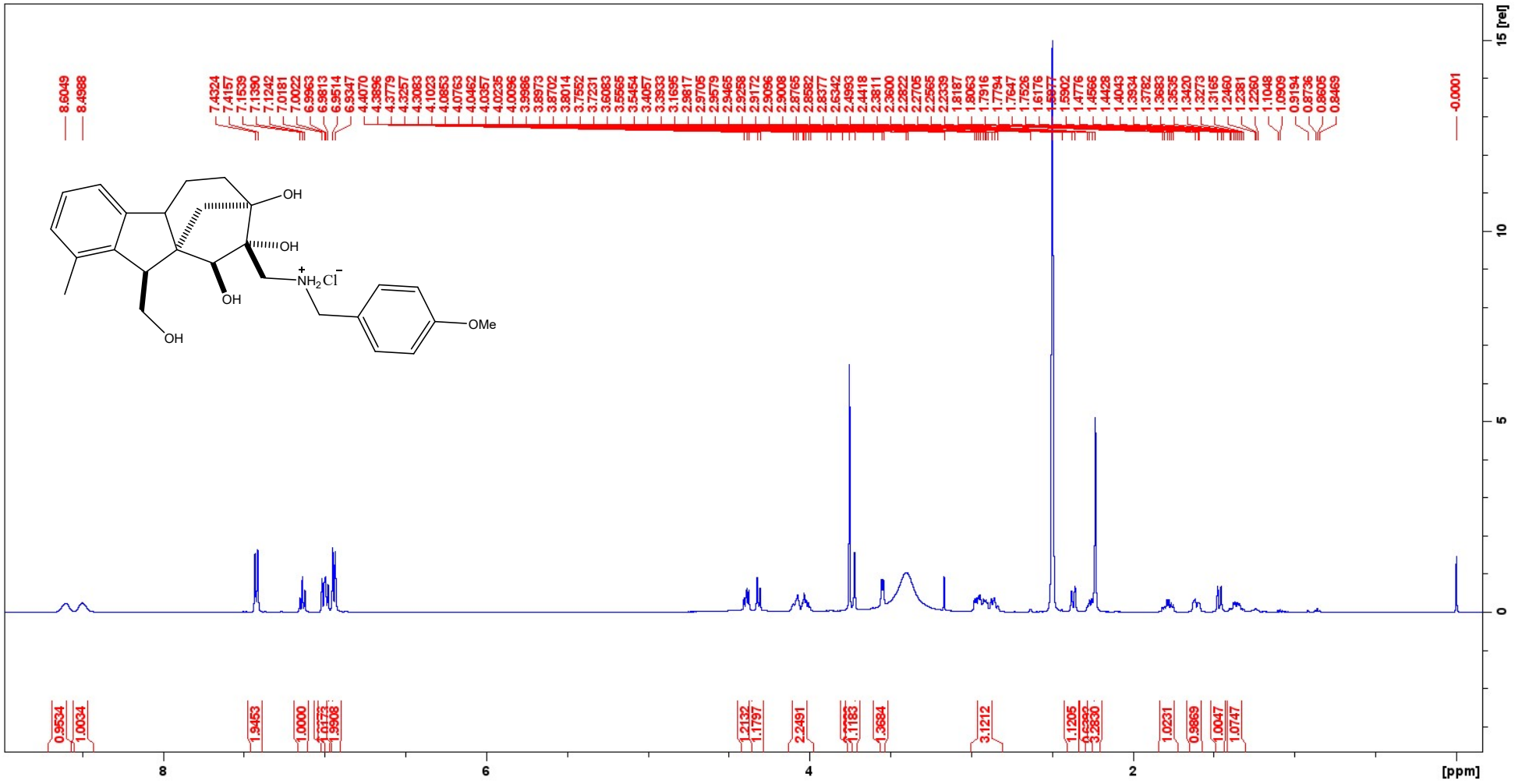
HMBC of *N*-(4-Fluorobenzyl)-1-((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methanaminium **20**



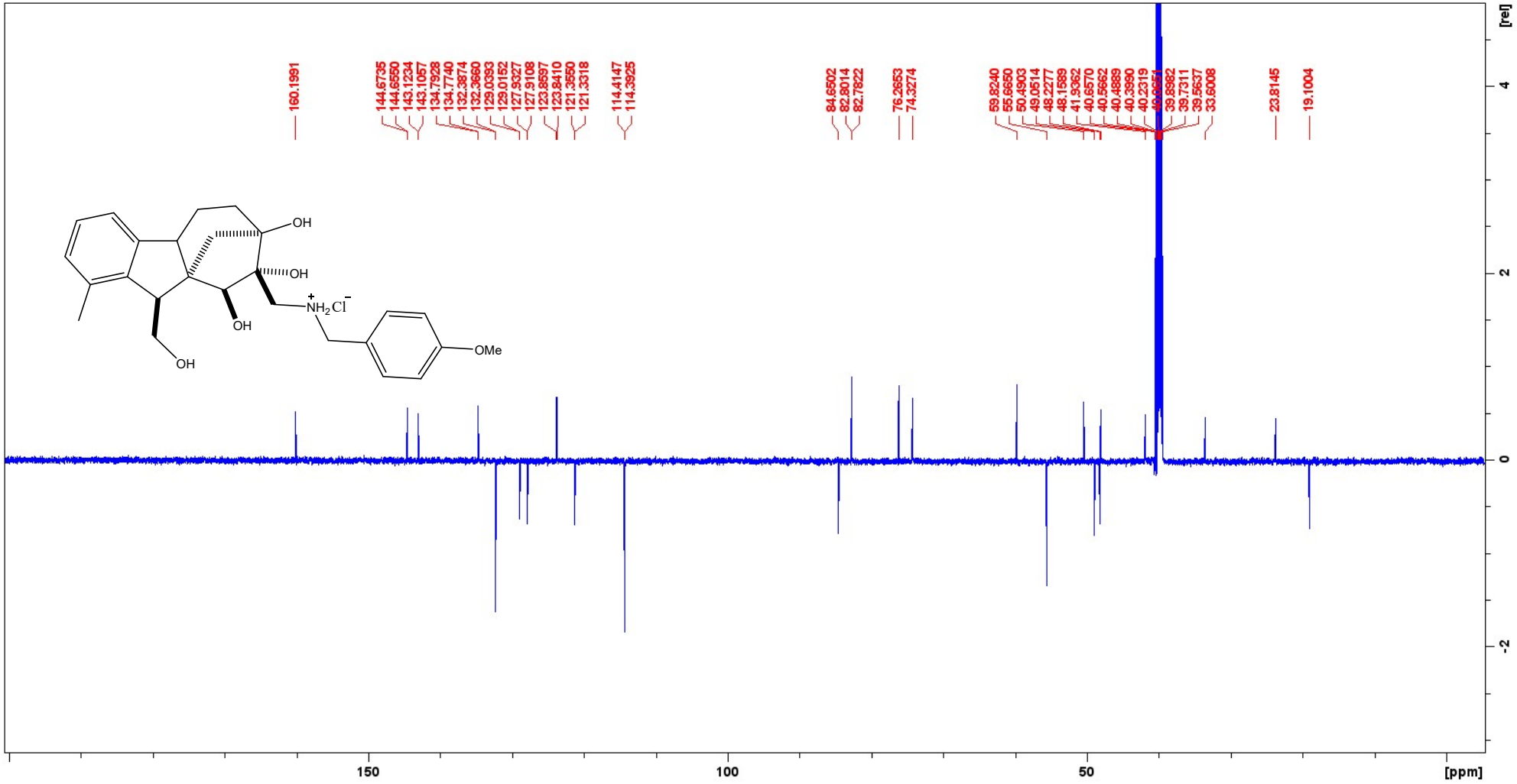
^{19}F *J*-MOD NMR (470 MHz) of *N*-(4-Fluorobenzyl)-1-((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methanaminium **20**



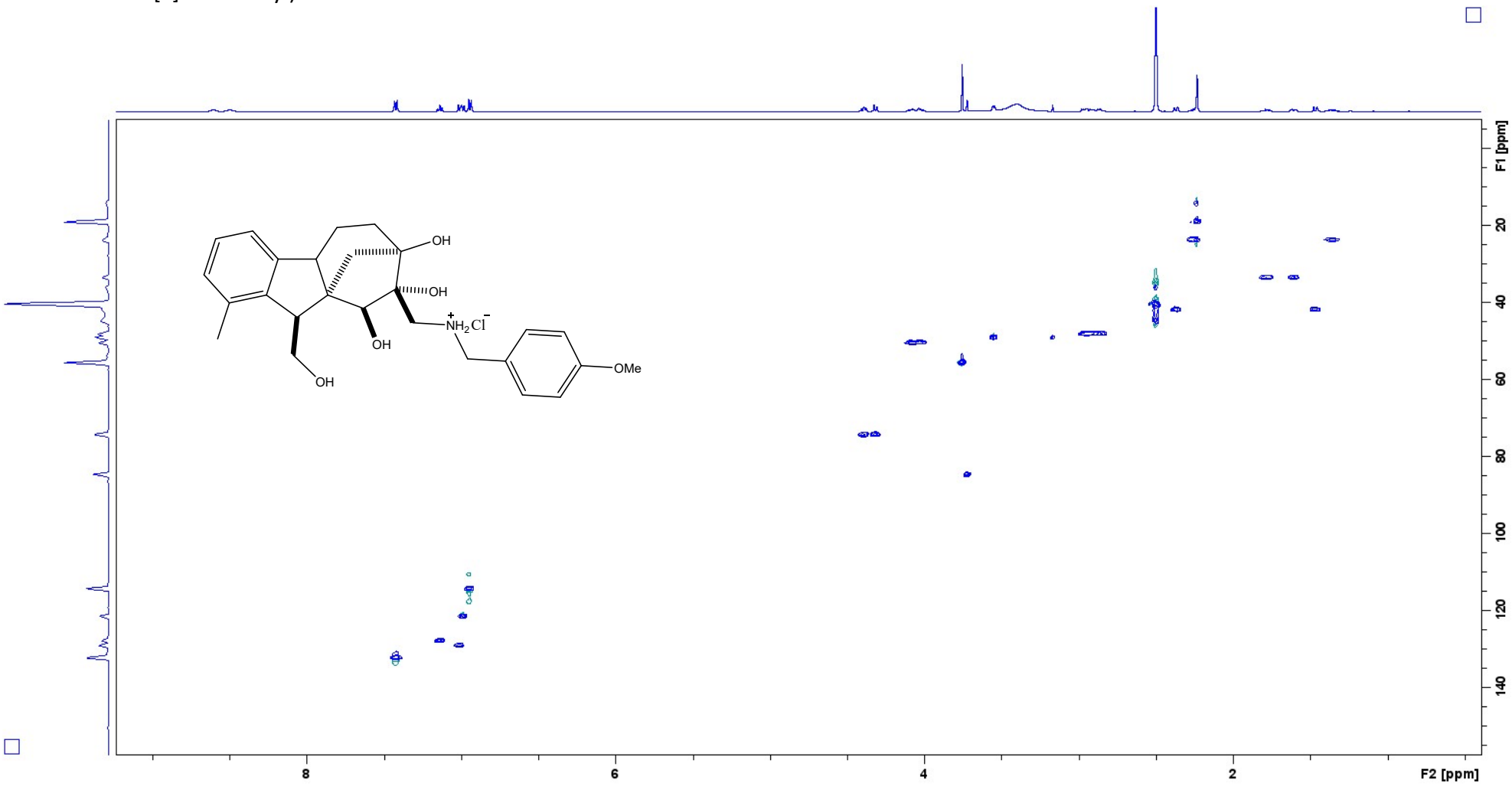
^{1}H-NMR (500 MHz) of *N*-(4-Methoxybenzyl)-1-((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methanaminium chloride **21**



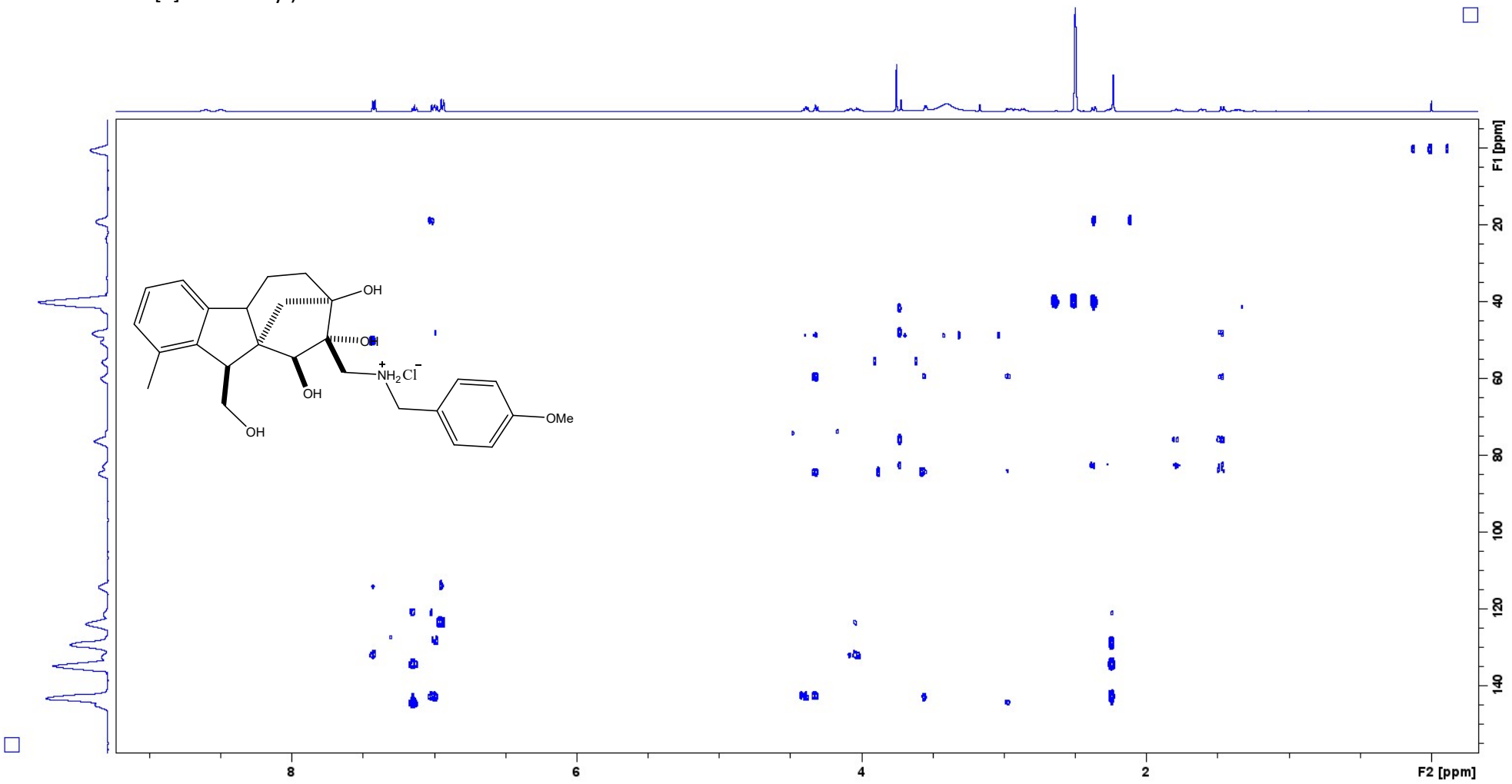
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of *N*-(4-Methoxybenzyl)-1-((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methanaminium chloride **21**



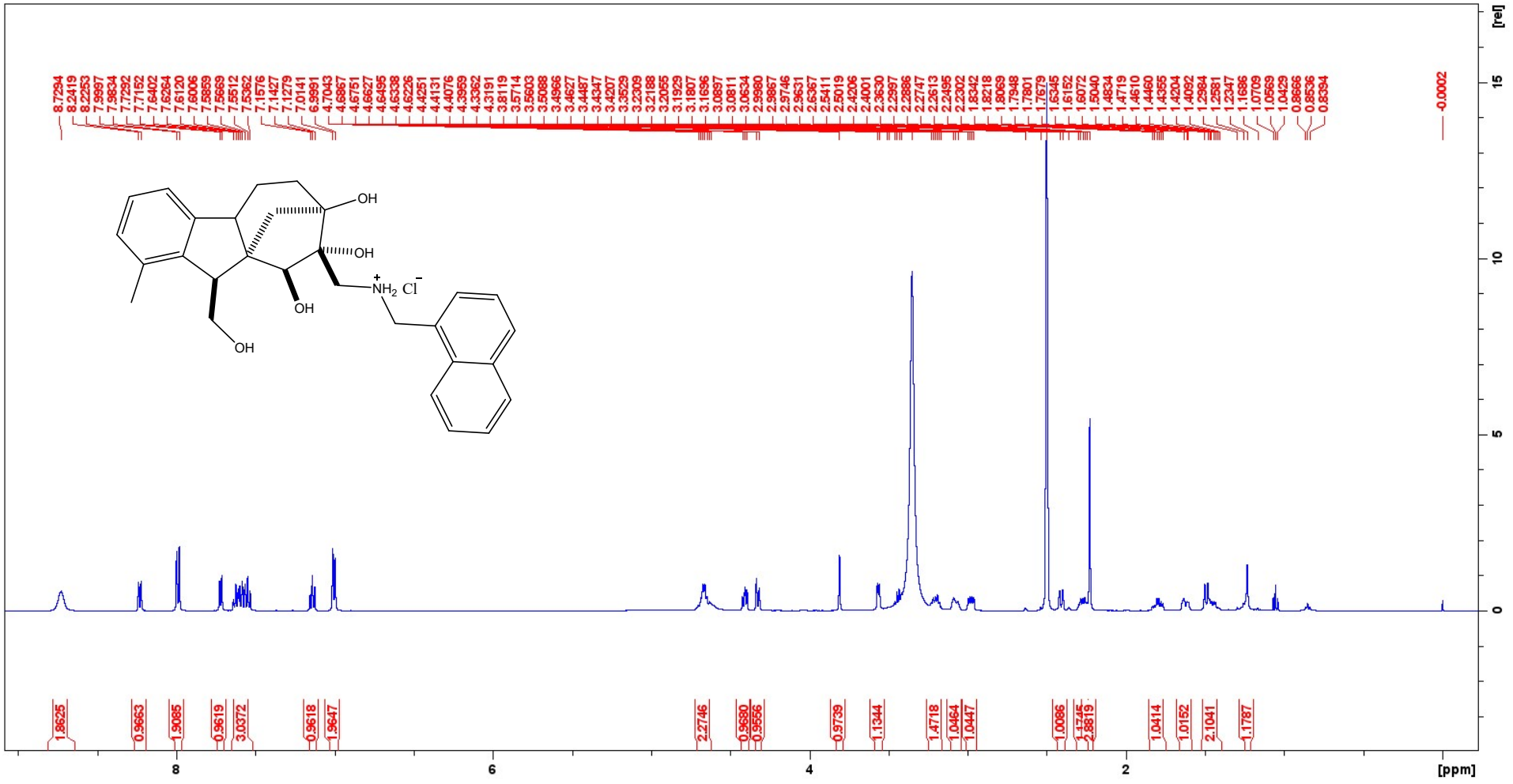
HSQC of *N*-(4-Methoxybenzyl)-1-((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methanaminium chloride **21**



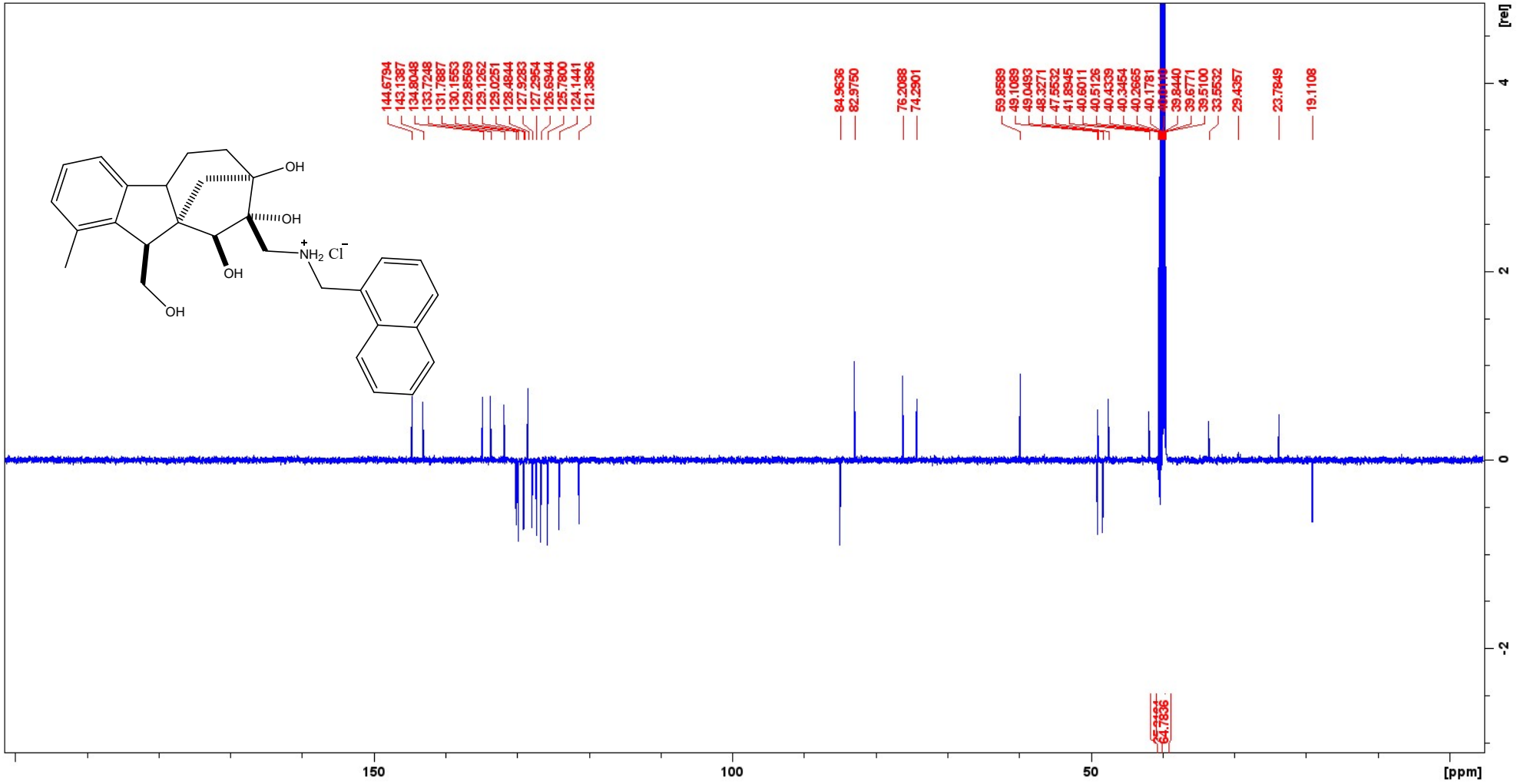
HMBC of *N*-(4-Methoxybenzyl)-1-((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methanaminium chloride **21**



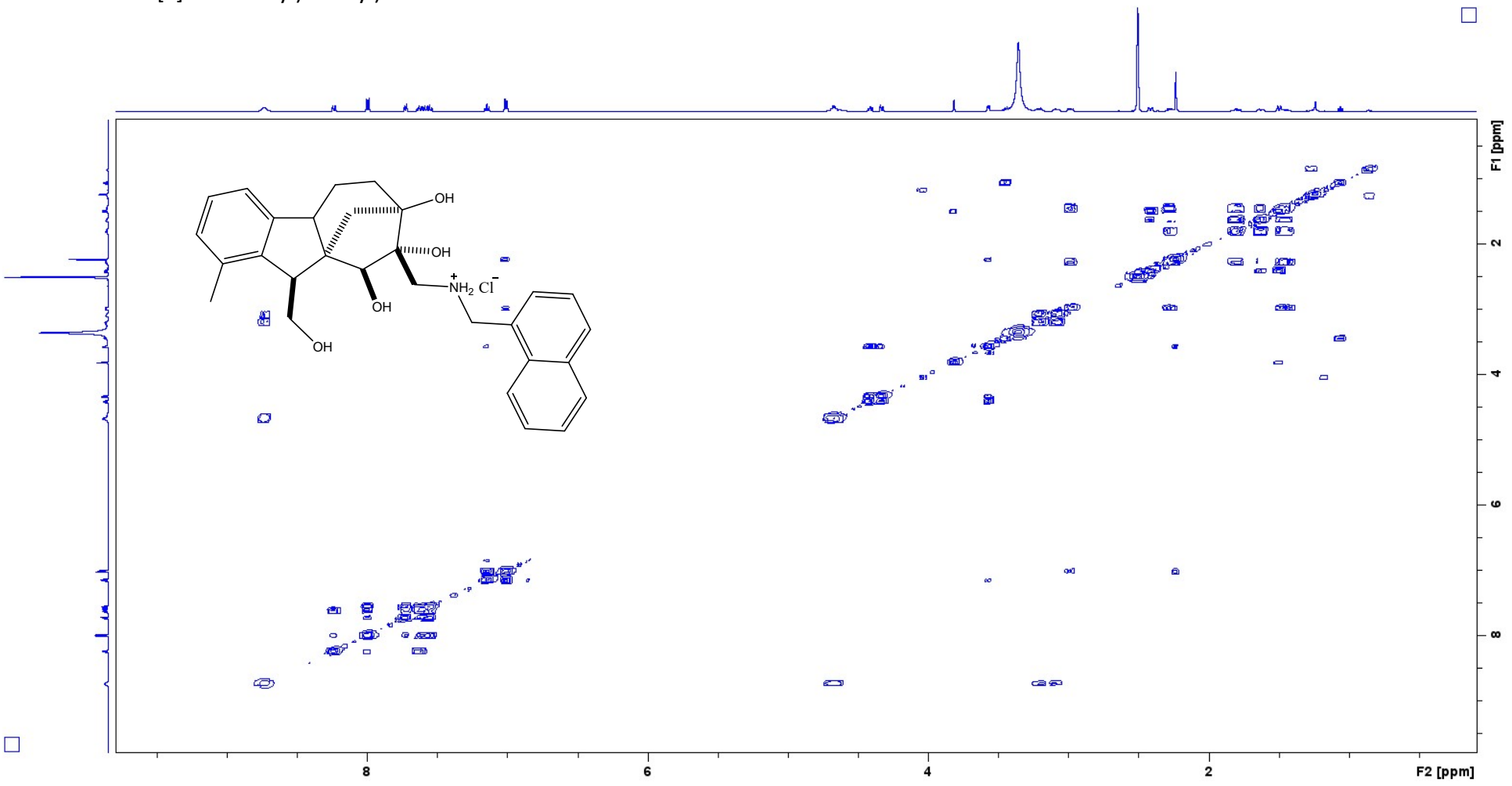
^{1}H-NMR (500 MHz) of 1-(Naphthalen-1-yl)-*N*-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)methanaminium chloride **22**



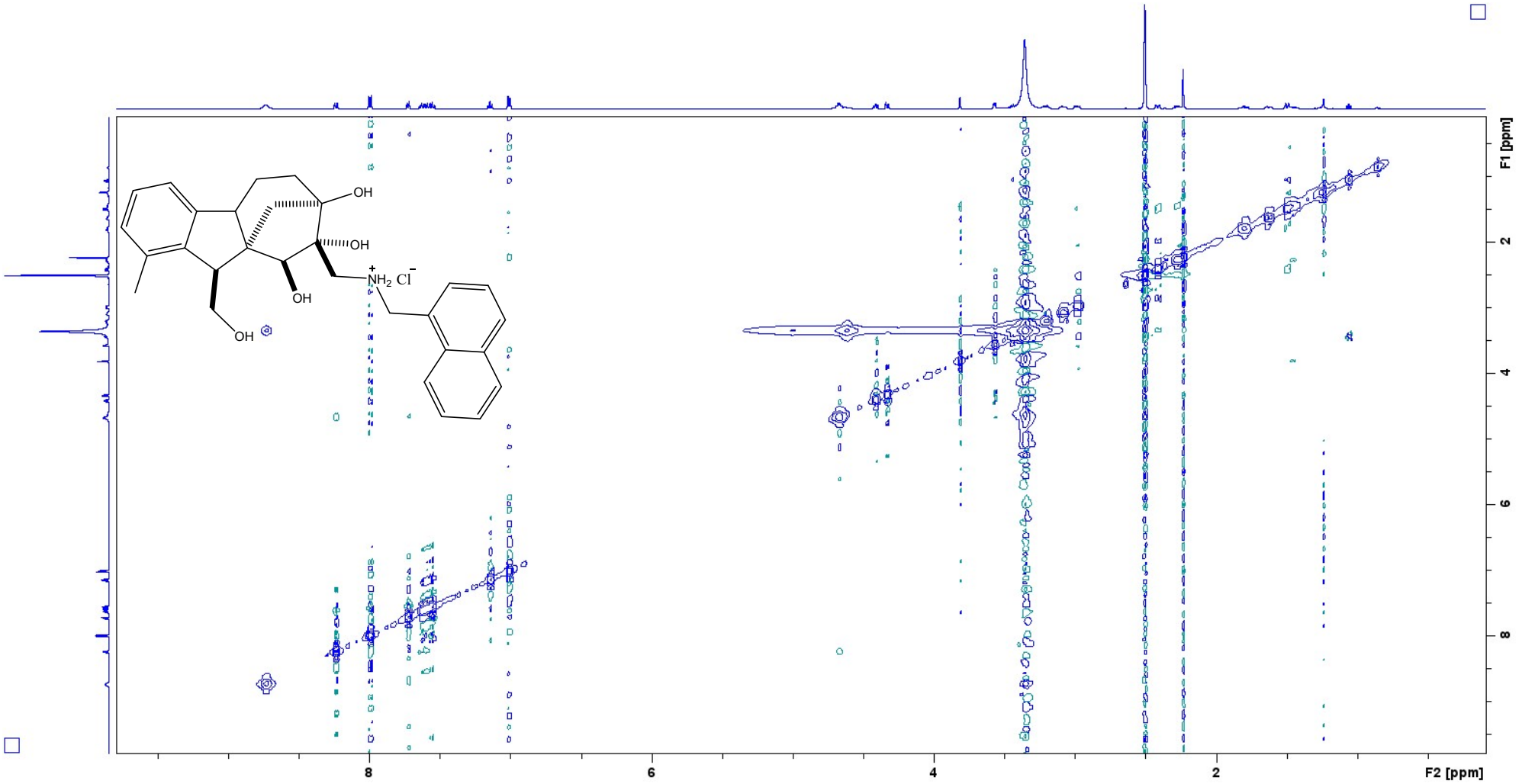
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of 1-(Naphthalen-1-yl)-*N*-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)methanaminium chloride **22**



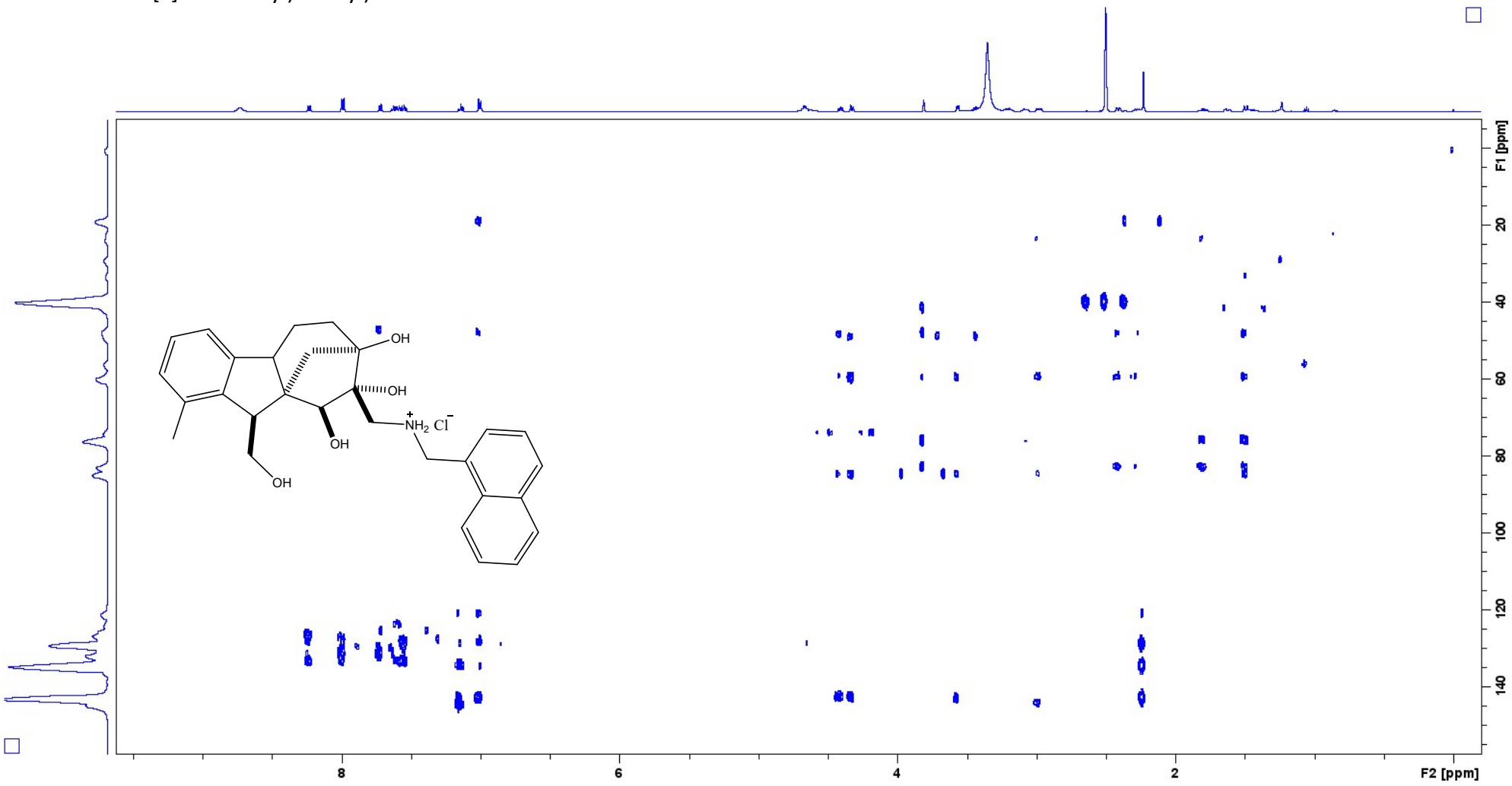
COSY of 1-(Naphthalen-1-yl)-*N*-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)methanaminium chloride **22**



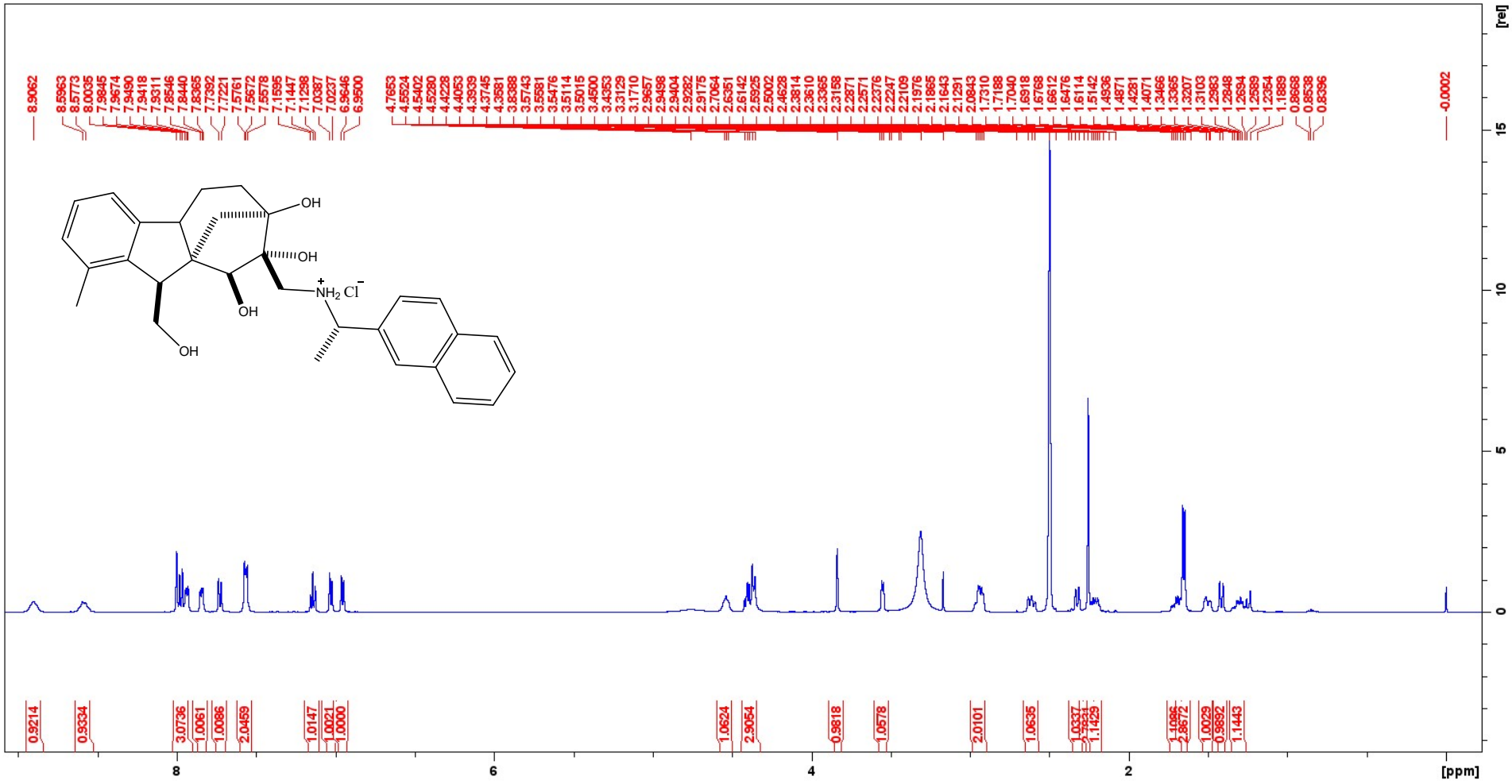
NOESY of 1-(Naphthalen-1-yl)-*N*-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)methanaminium chloride **22**



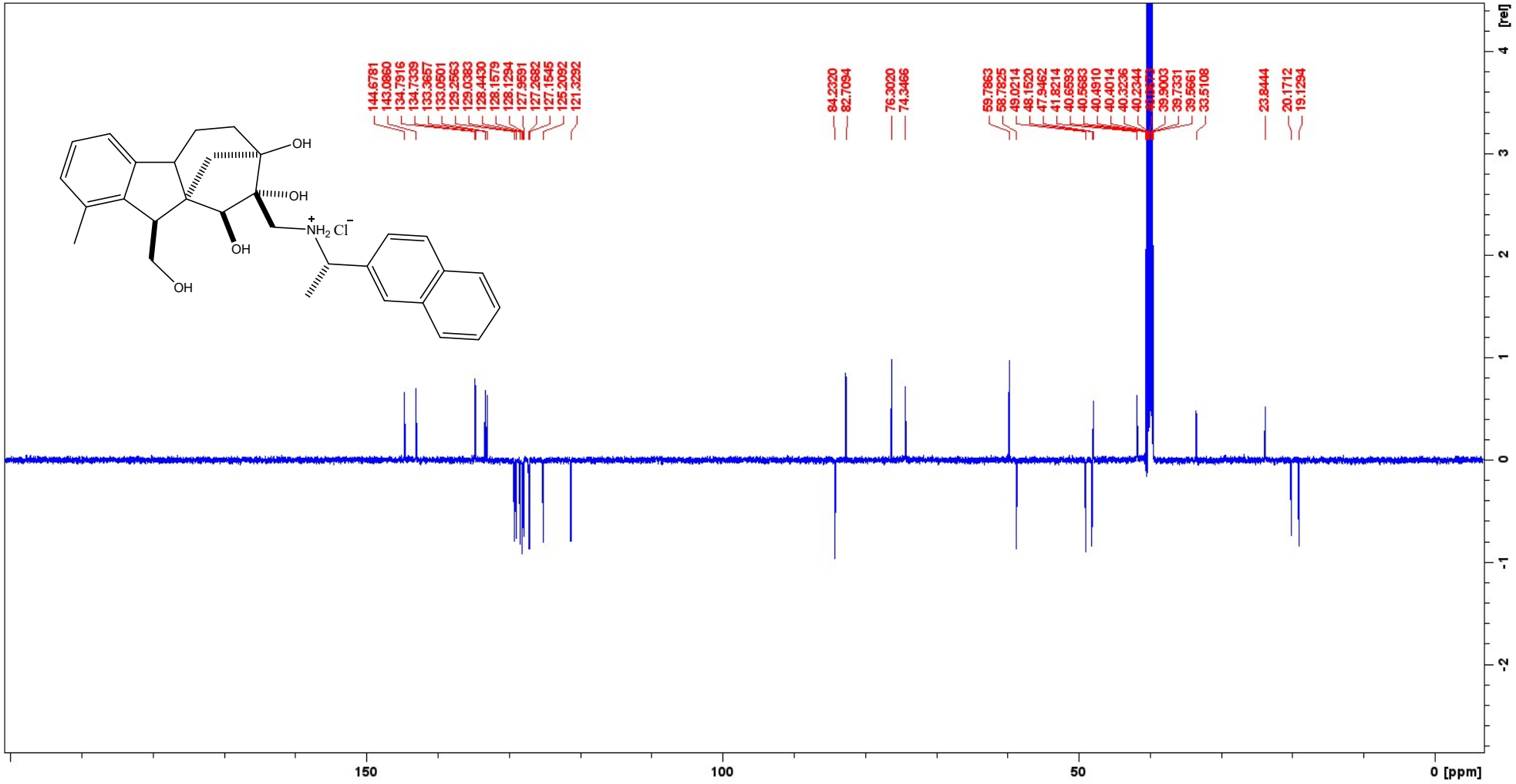
HMBC of 1-(Naphthalen-1-yl)-*N*-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)methanaminium chloride **22**



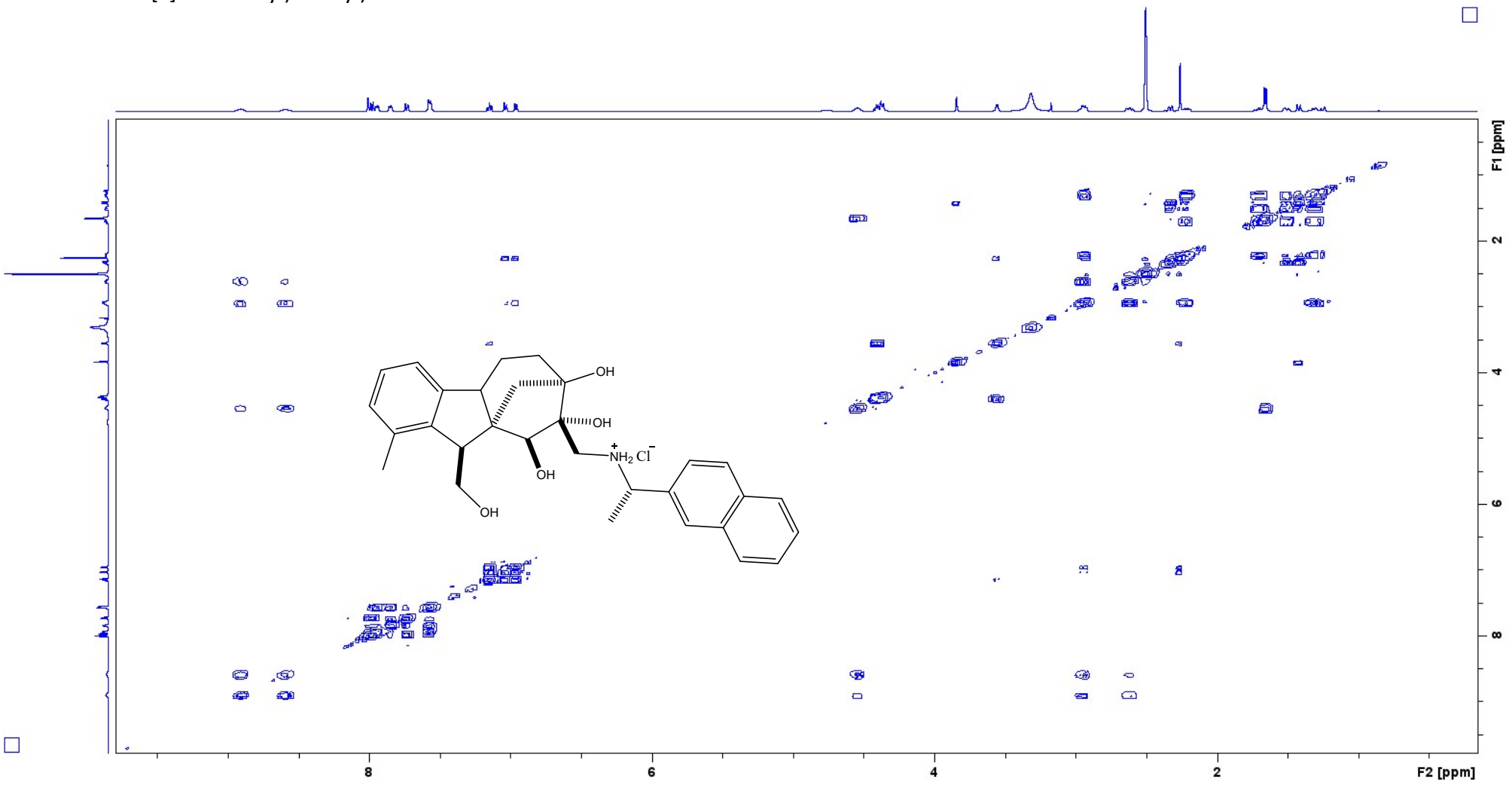
^{1}H-NMR (500 MHz) of (1*S*)-1-(Naphthalen-2-yl)-*N*-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)ethan-1-aminium chloride **23**



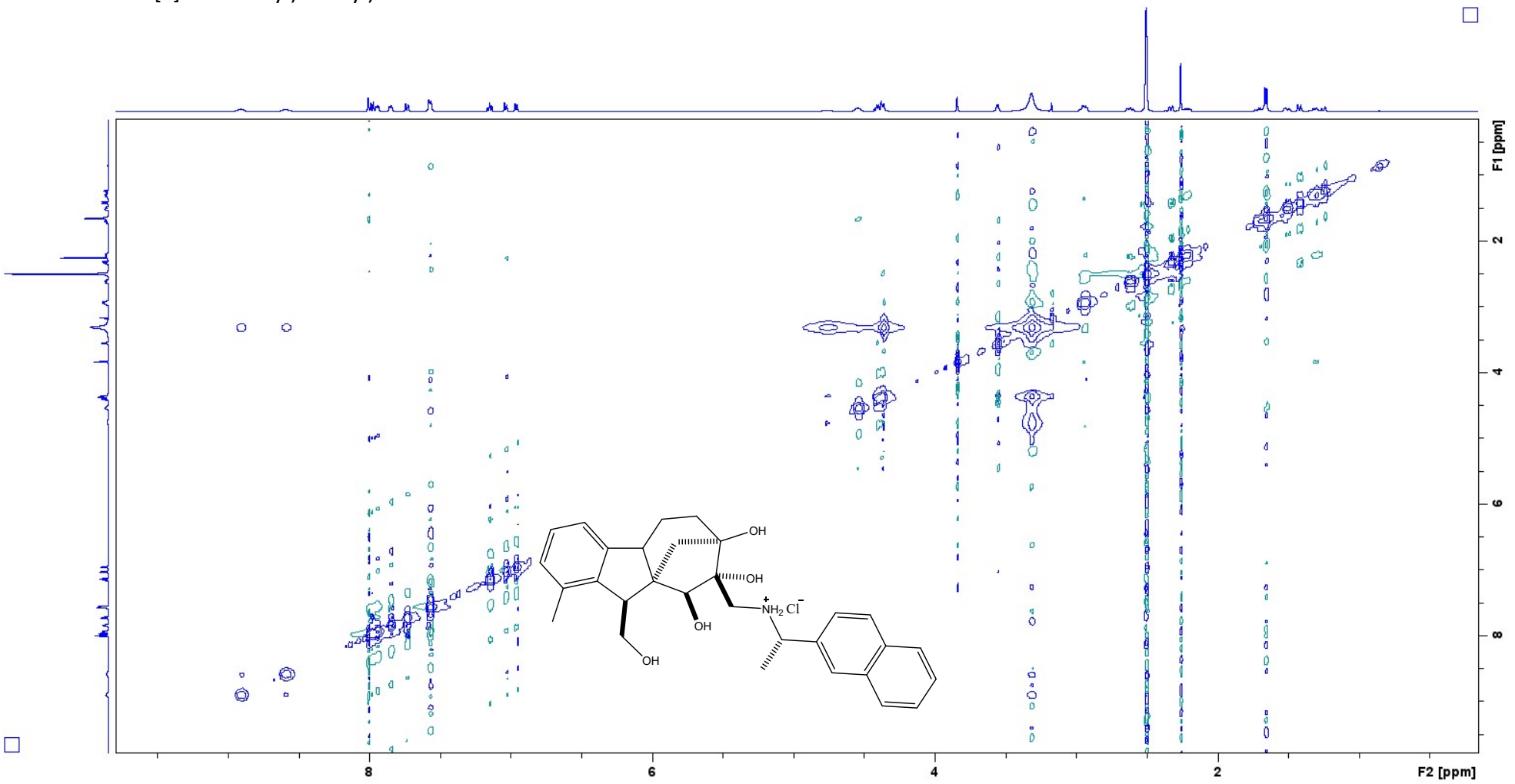
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of (1*S*)-1-(Naphthalen-2-yl)-*N*-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)ethan-1-aminium chloride **23**



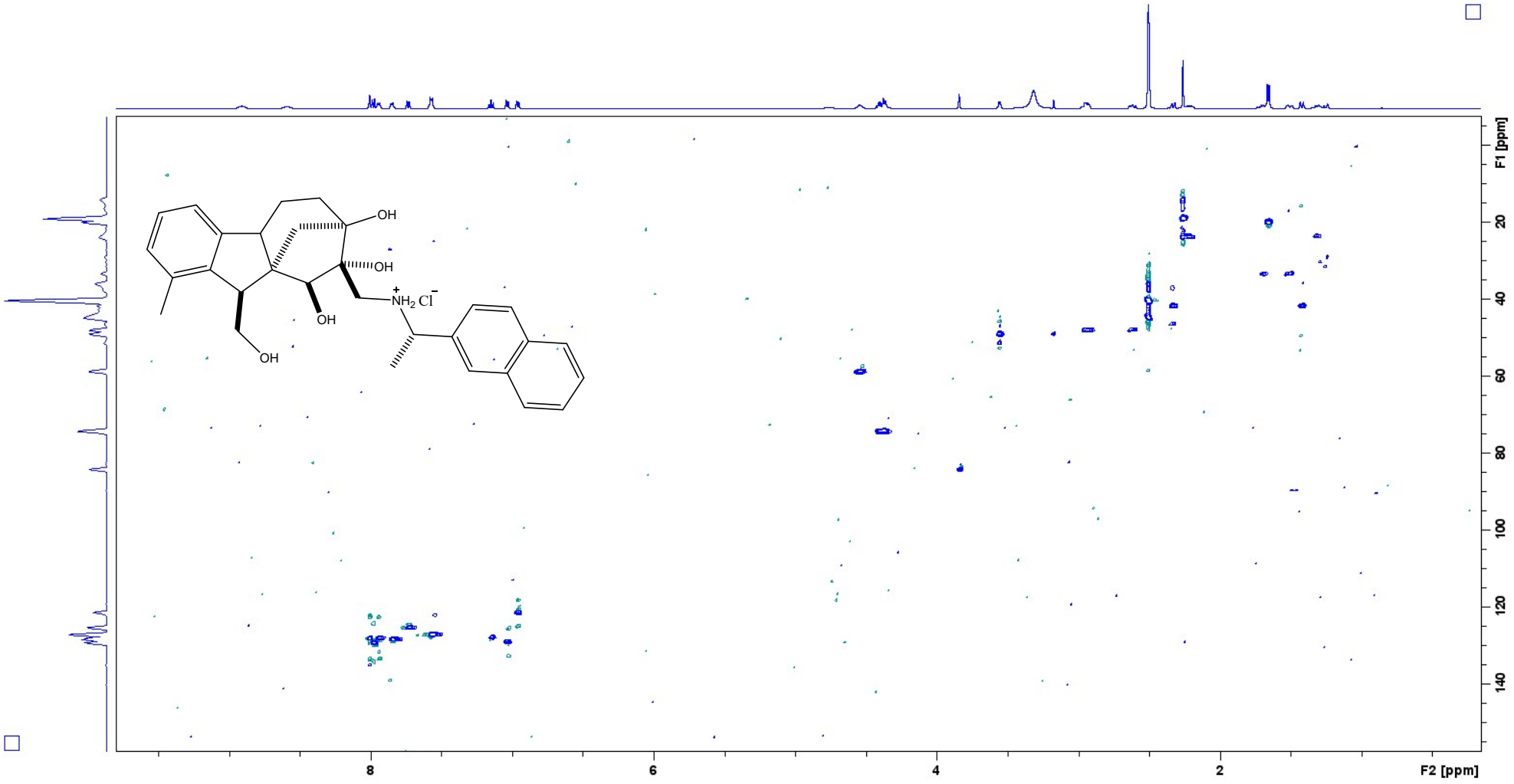
COSY of (1*S*)-1-(Naphthalen-2-yl)-*N*-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)ethan-1-aminium chloride **23**



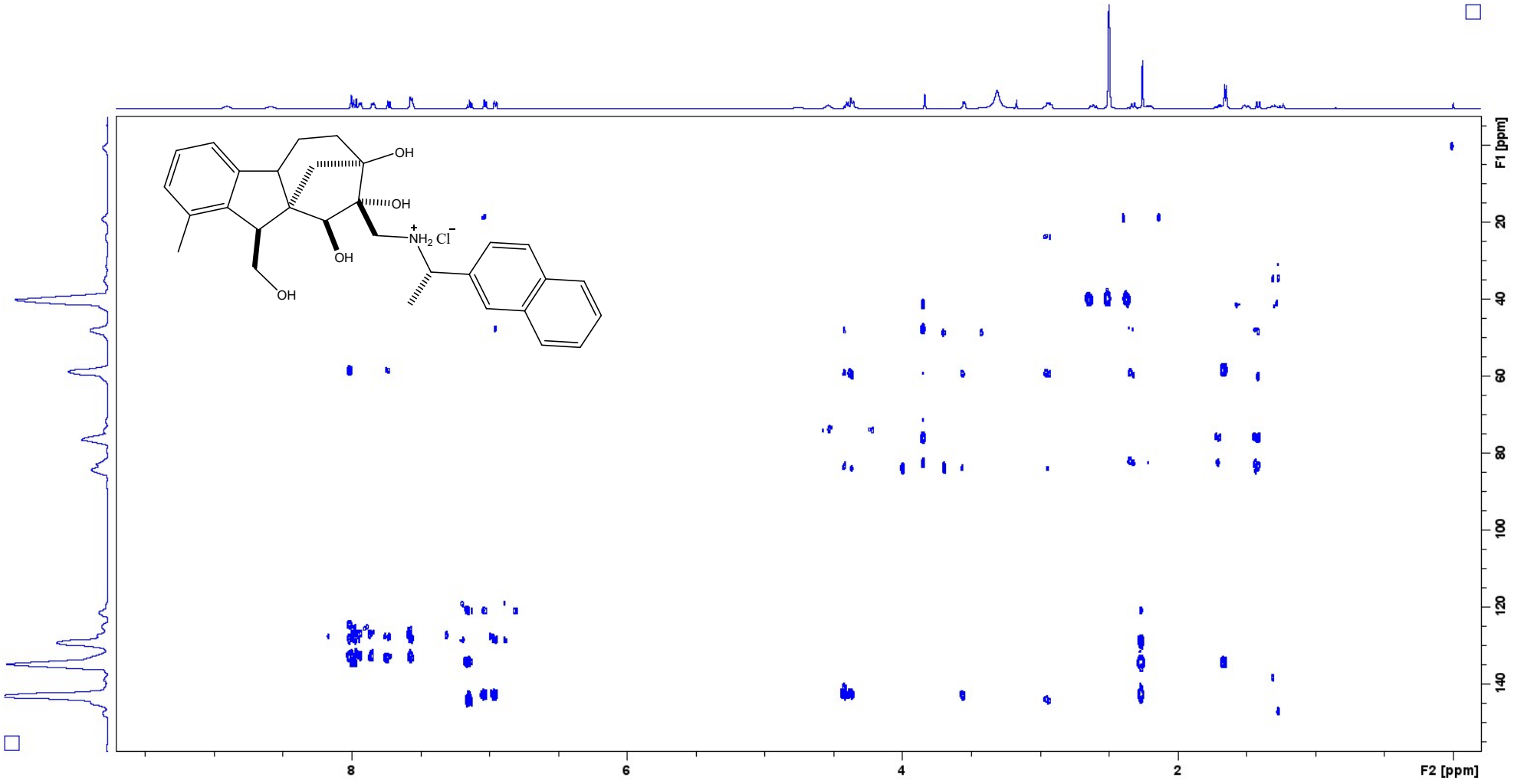
NOESY of (1*S*)-1-(Naphthalen-2-yl)-*N*-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)ethan-1-aminium chloride **23**



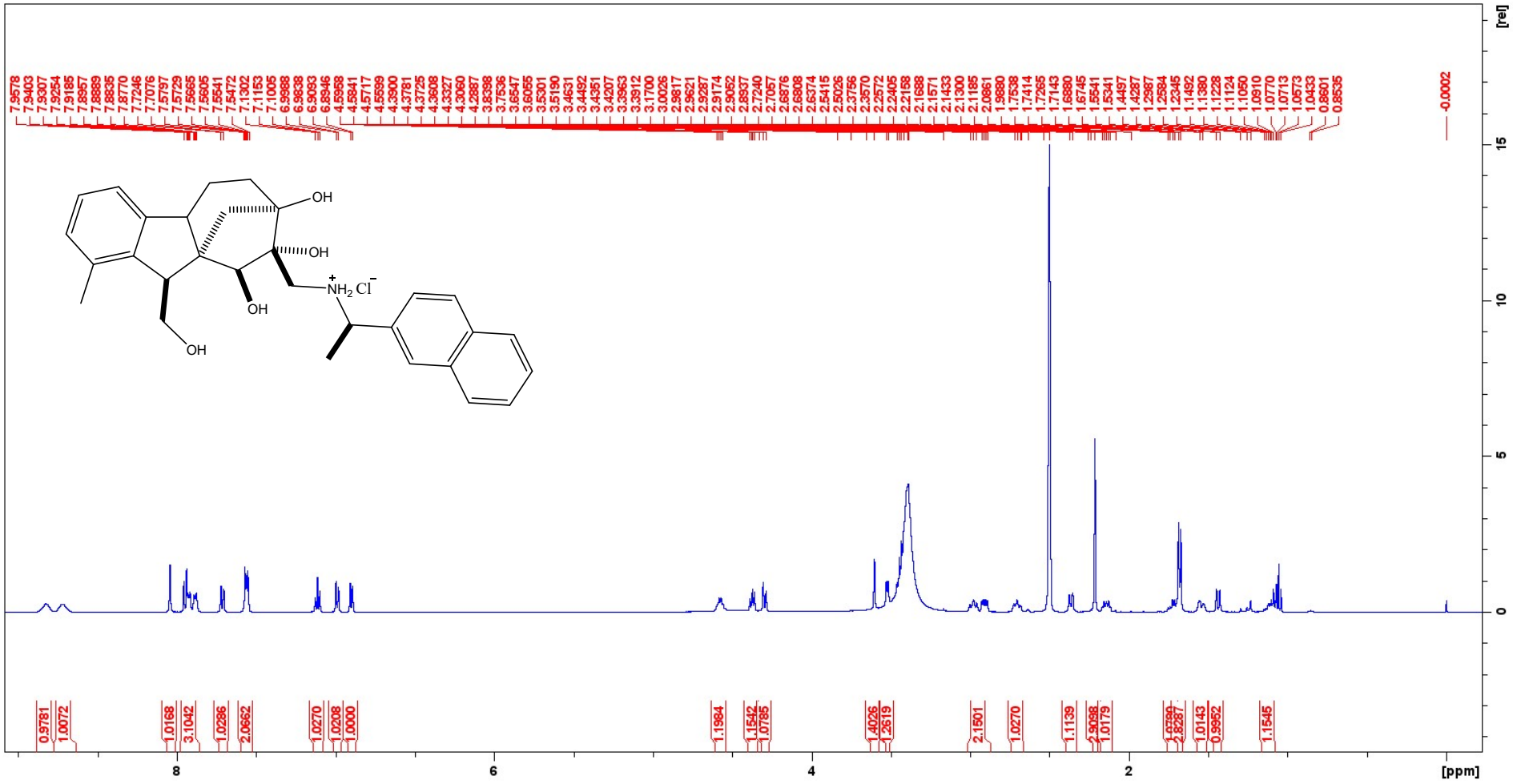
HSQC of (1*S*)-1-(Naphthalen-2-yl)-*N*-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)ethan-1-aminium chloride **23**



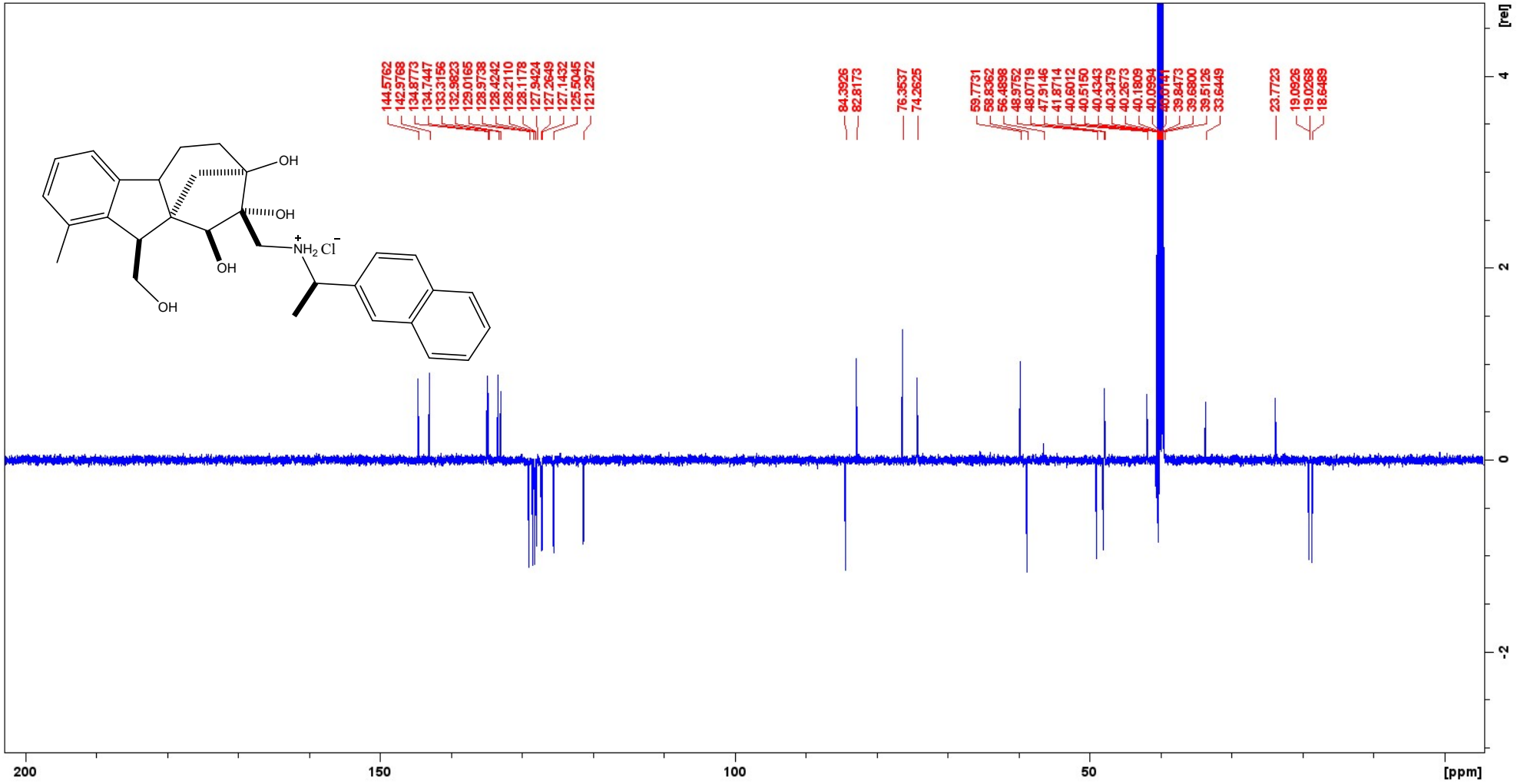
HMBC of (1*S*)-1-(Naphthalen-2-yl)-*N*-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)ethan-1-aminium chloride **23**



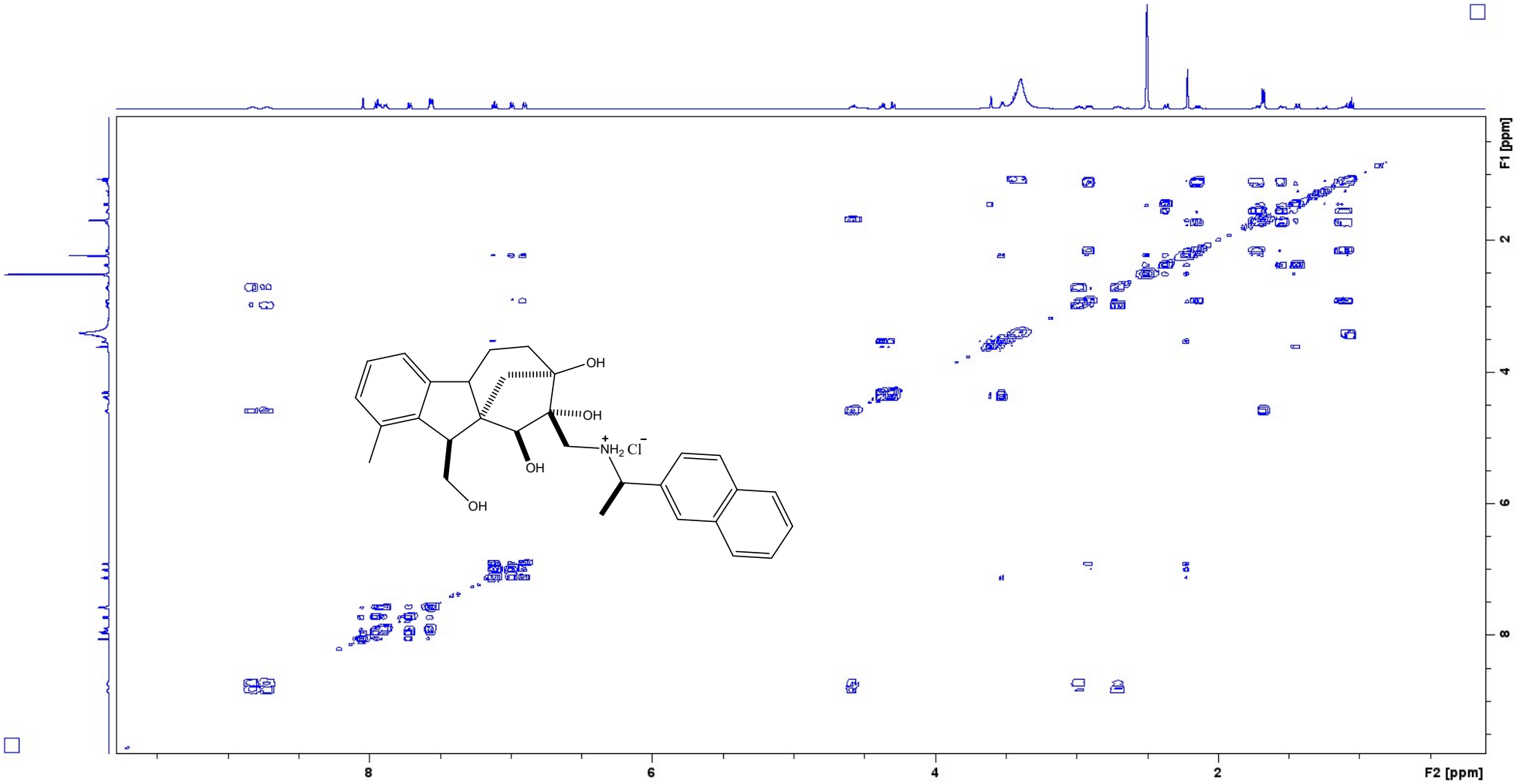
^{1}H-NMR (500 MHz) of (1*R*)-1-(Naphthalen-2-yl)-*N*-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)ethan-1-aminium chloride **24**



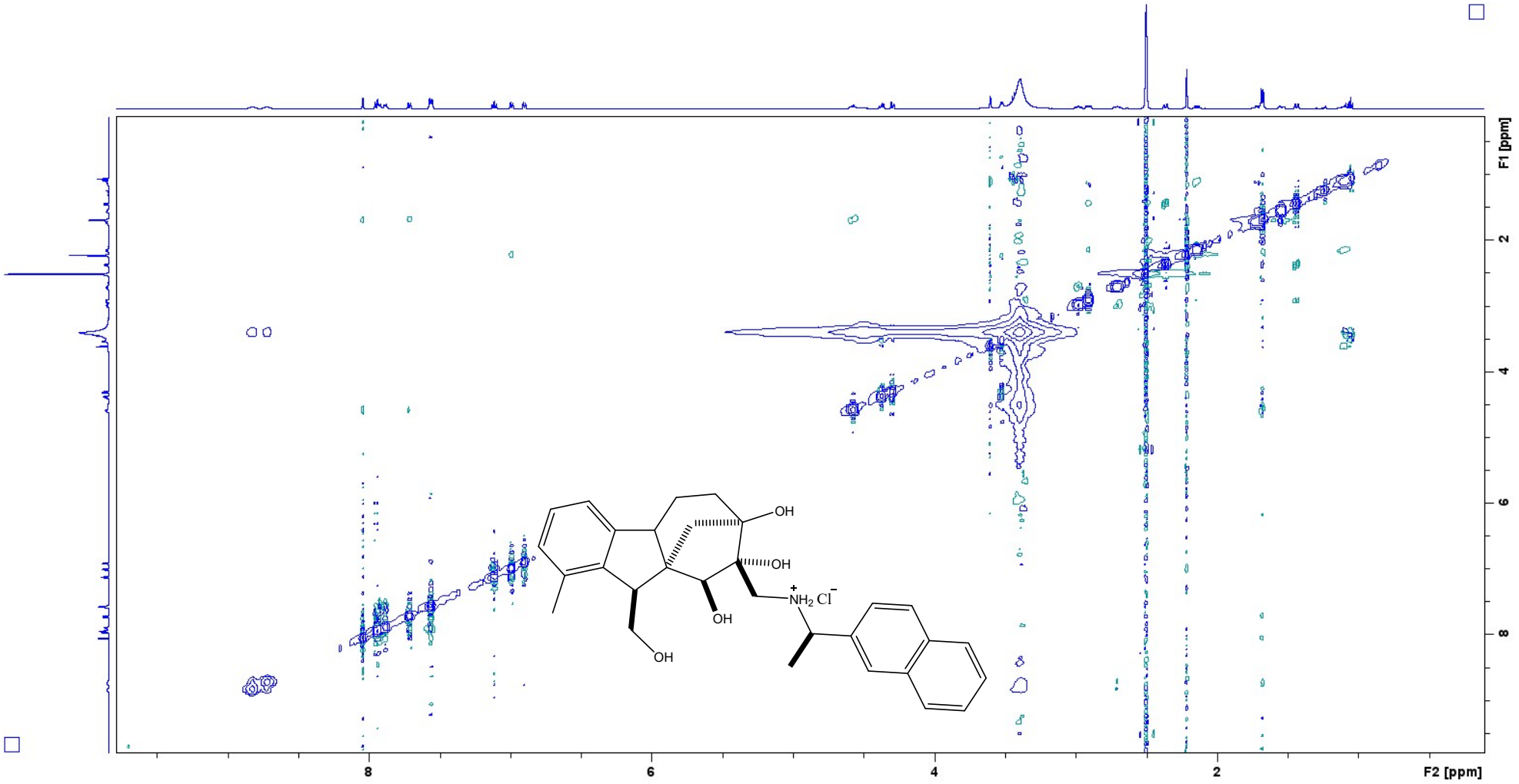
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of (1*R*)-1-(Naphthalen-2-yl)-*N*-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)ethan-1-aminium chloride **24**



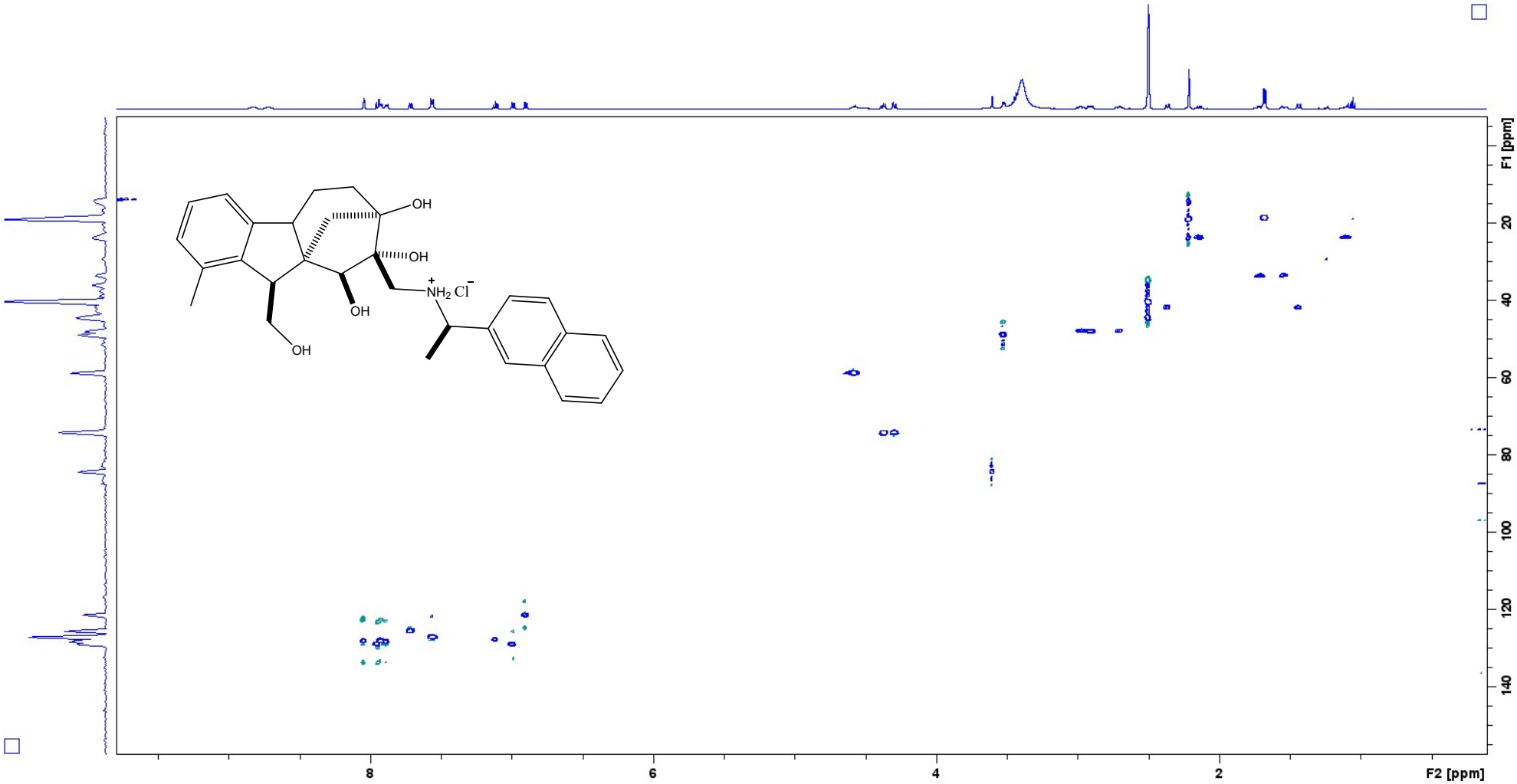
COSY of (1*R*)-1-(Naphthalen-2-yl)-*N*-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)ethan-1-aminium chloride **24**



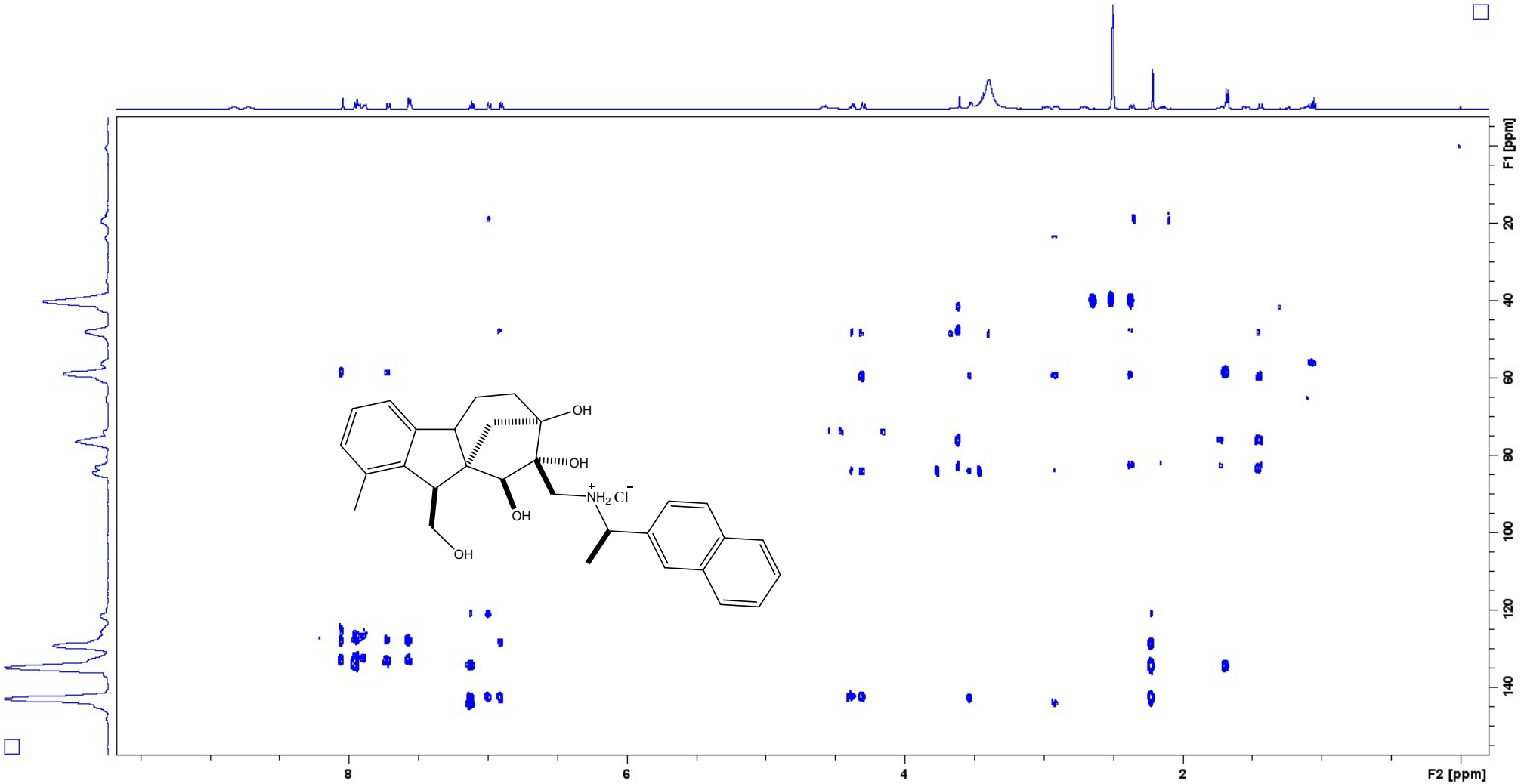
NOESY of (1*R*)-1-(Naphthalen-2-yl)-*N*-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)ethan-1-aminium chloride **24**



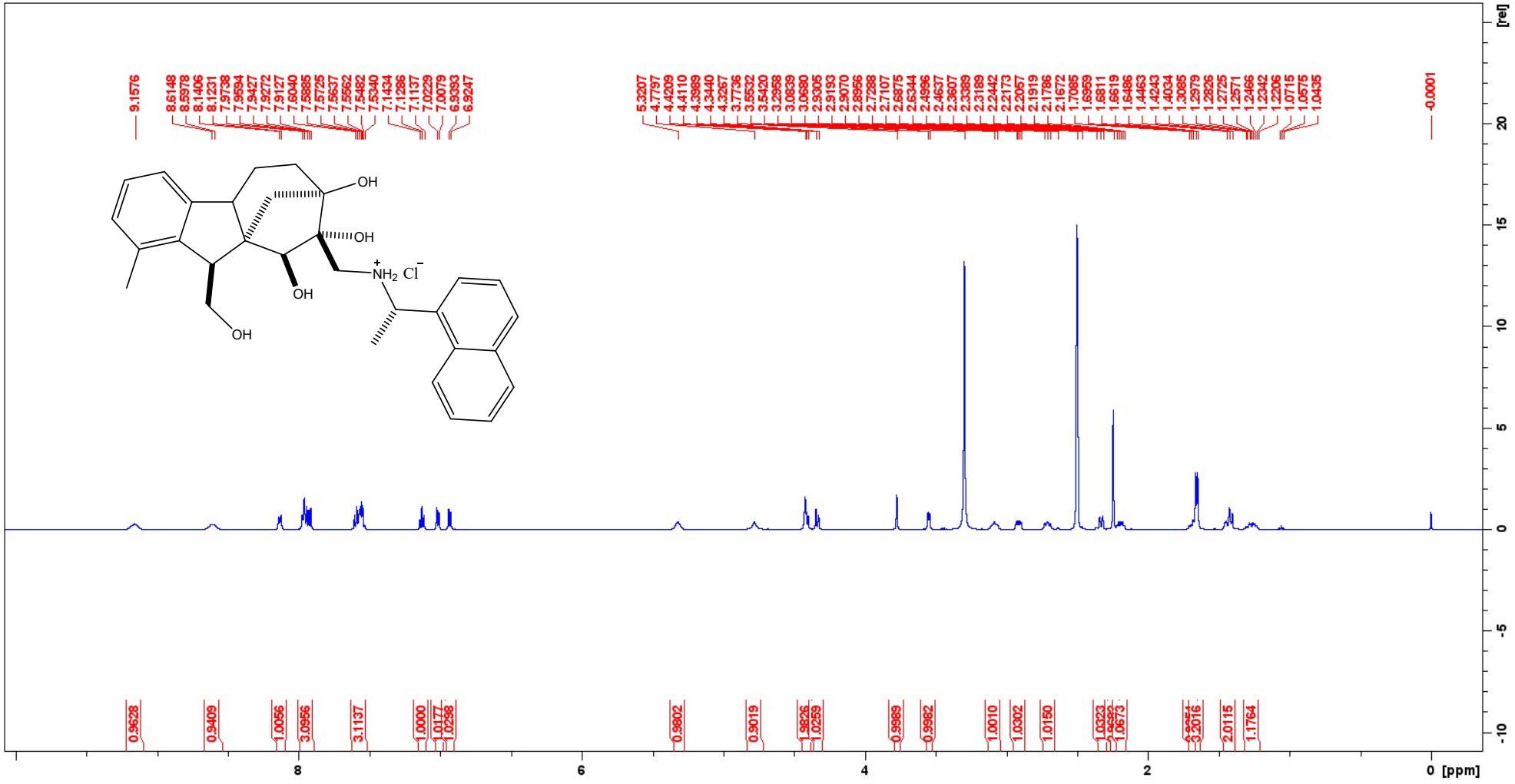
HSQC of (1*R*)-1-(Naphthalen-2-yl)-*N*-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)ethan-1-aminium chloride **24**



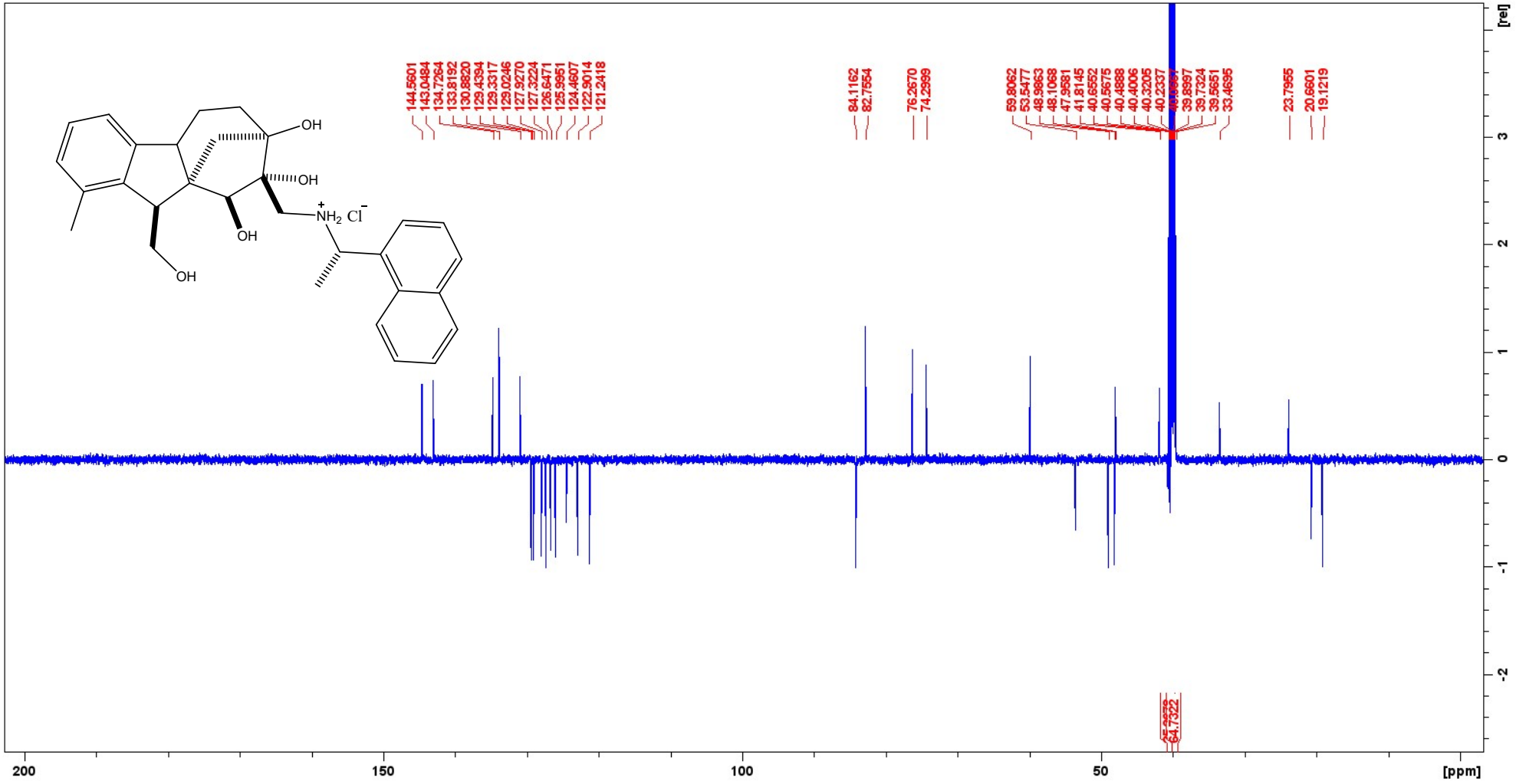
HMBC of (1*R*)-1-(Naphthalen-2-yl)-*N*-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)ethan-1-aminium chloride **24**



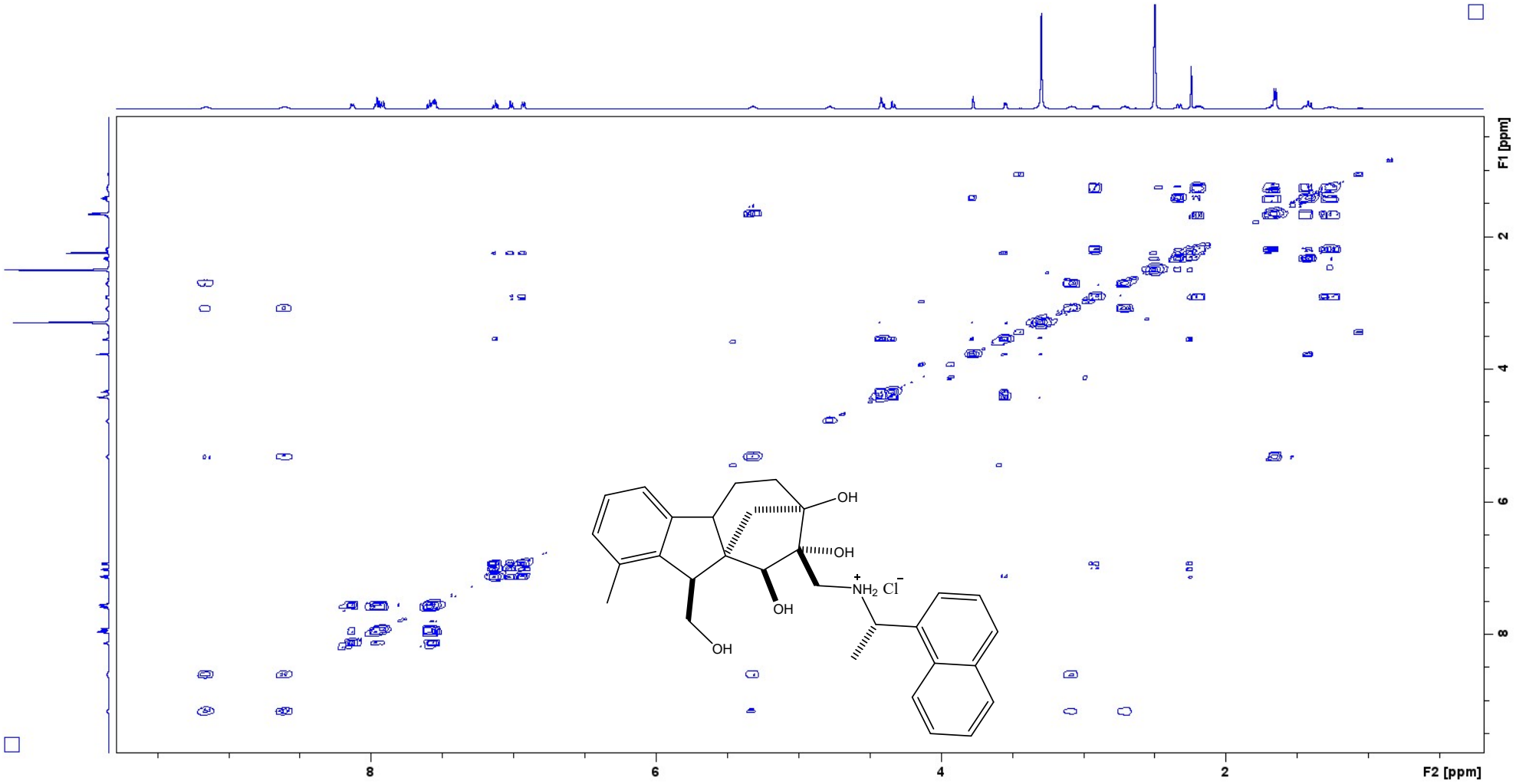
^{1}H-NMR (500 MHz) of (1*S*)-1-(Naphthalen-1-yl)-*N*-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)ethan-1-aminium chloride **25**



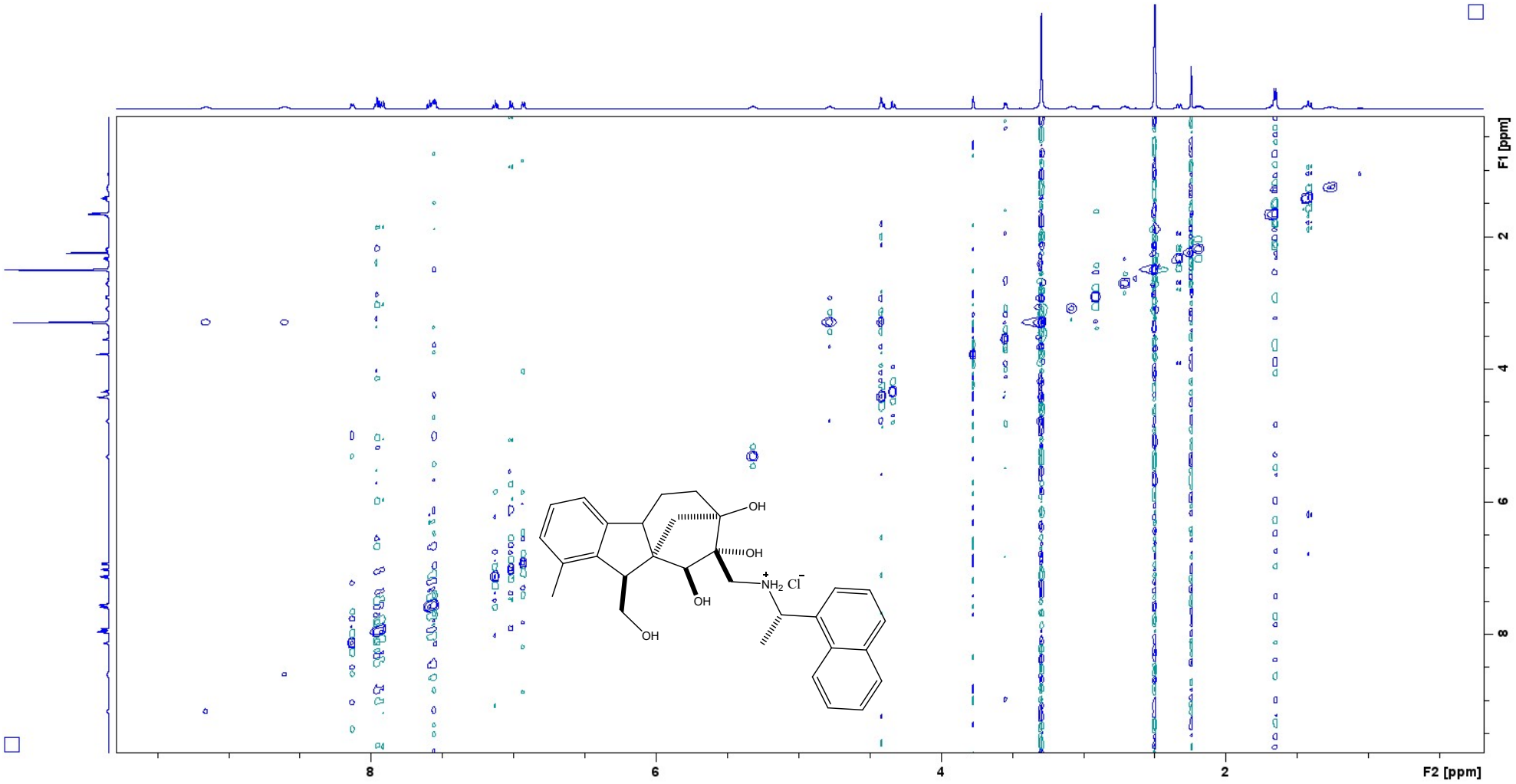
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of (1*S*)-1-(Naphthalen-1-yl)-*N*-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)ethan-1-aminium chloride **25**



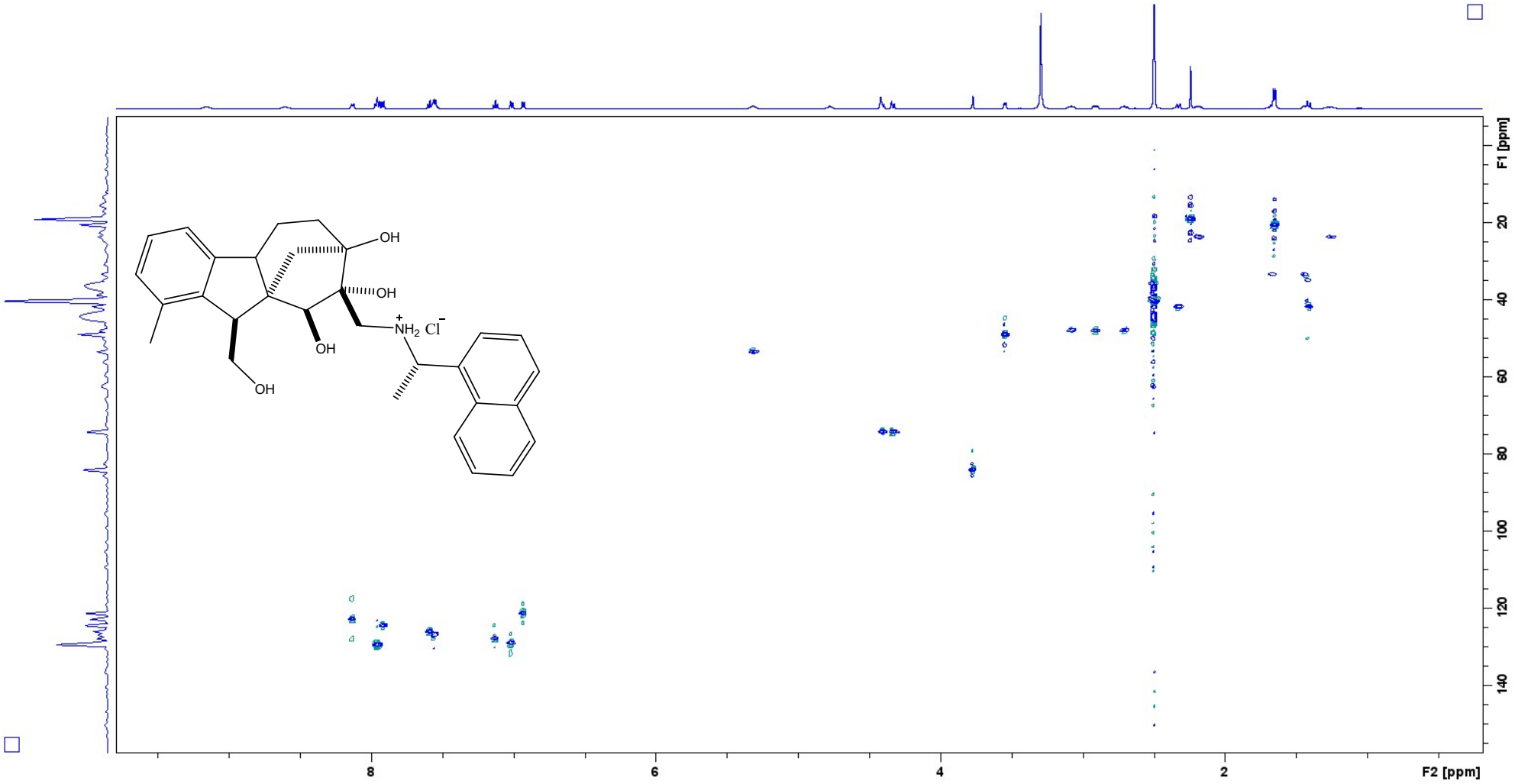
COSY of (1*S*)-1-(Naphthalen-1-yl)-*N*-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)ethan-1-aminium chloride **25**



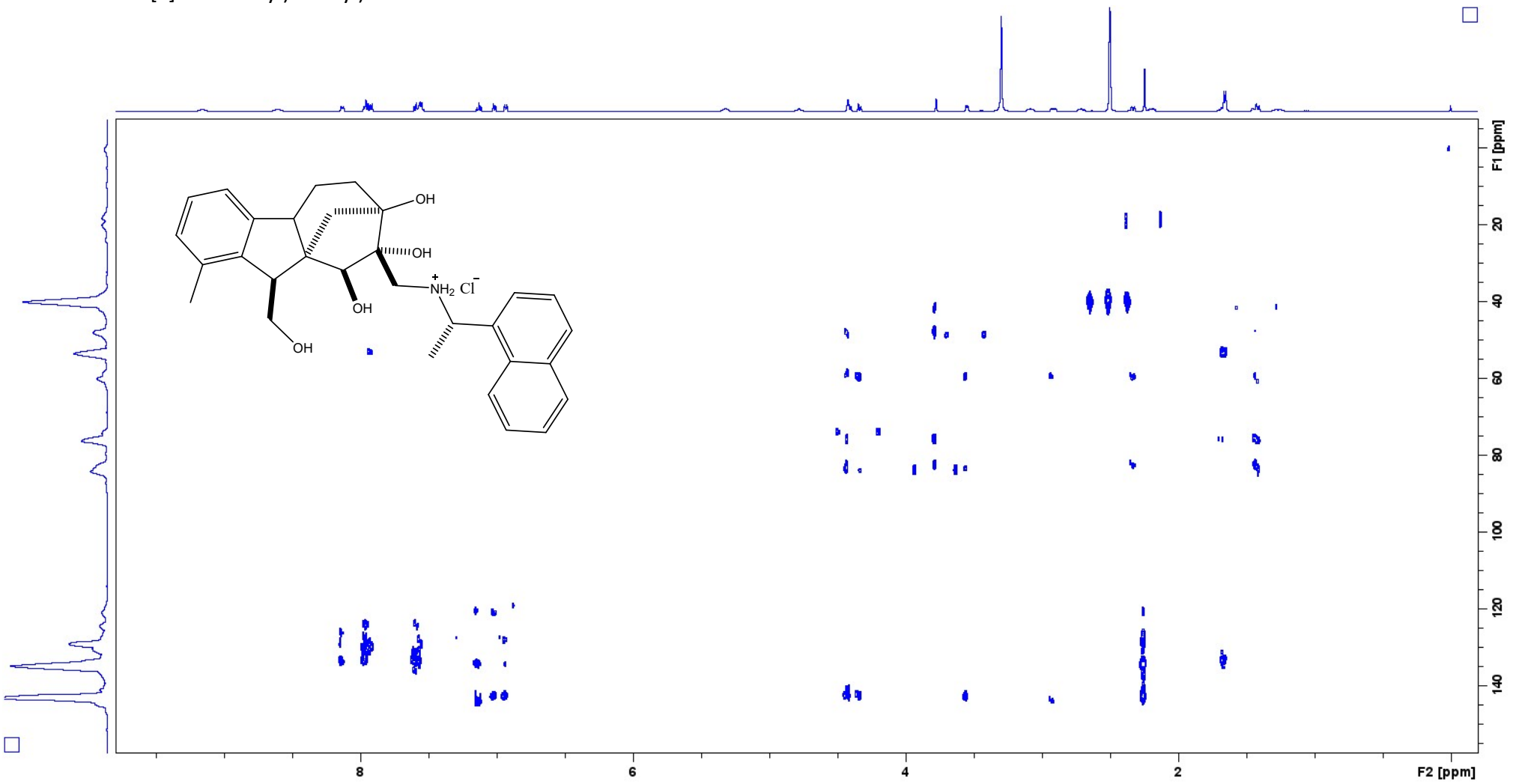
NOESY of (1*S*)-1-(Naphthalen-1-yl)-*N*-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)ethan-1-aminium chloride **25**



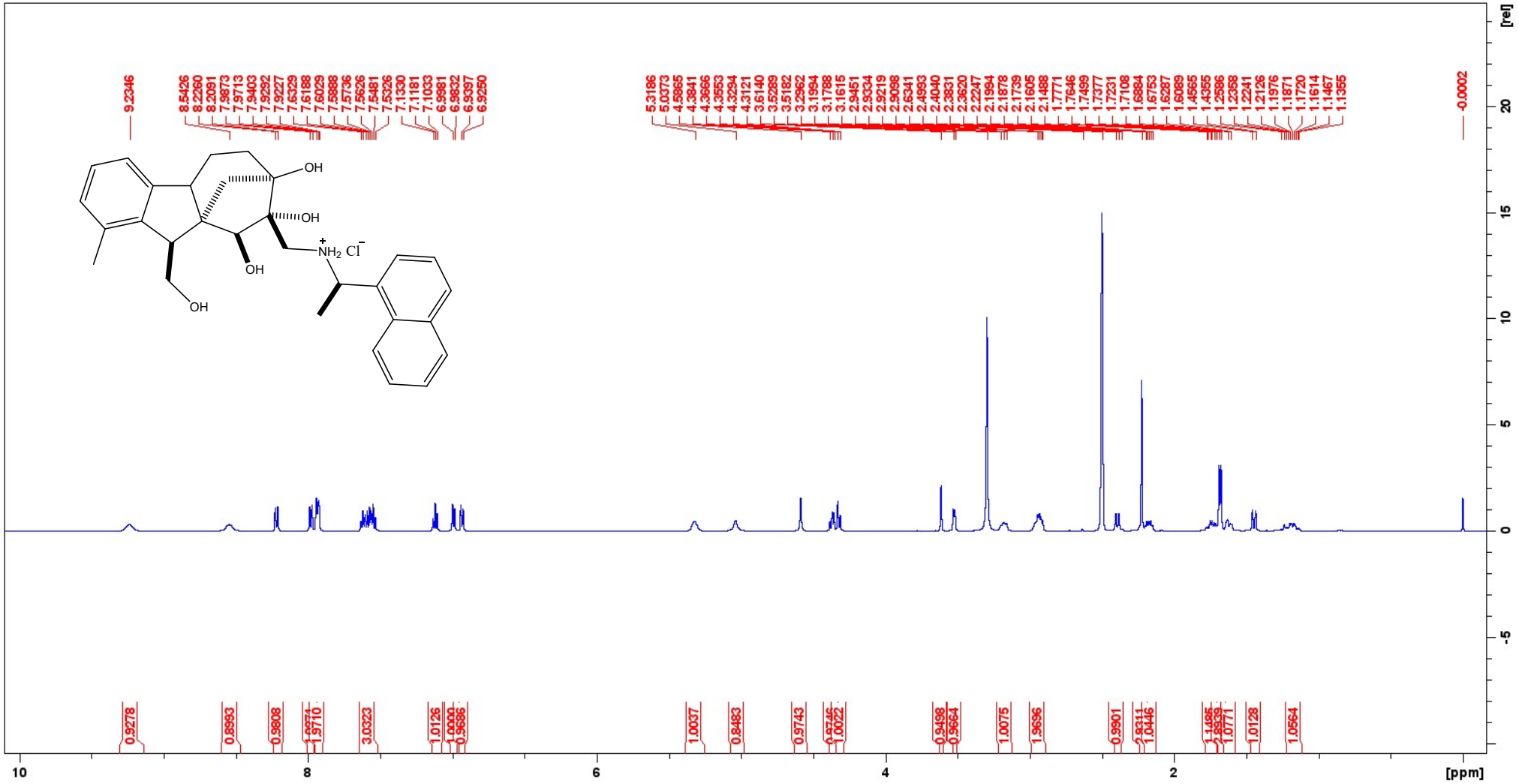
HSQC of (1*S*)-1-(Naphthalen-1-yl)-*N*-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)ethan-1-aminium chloride **25**



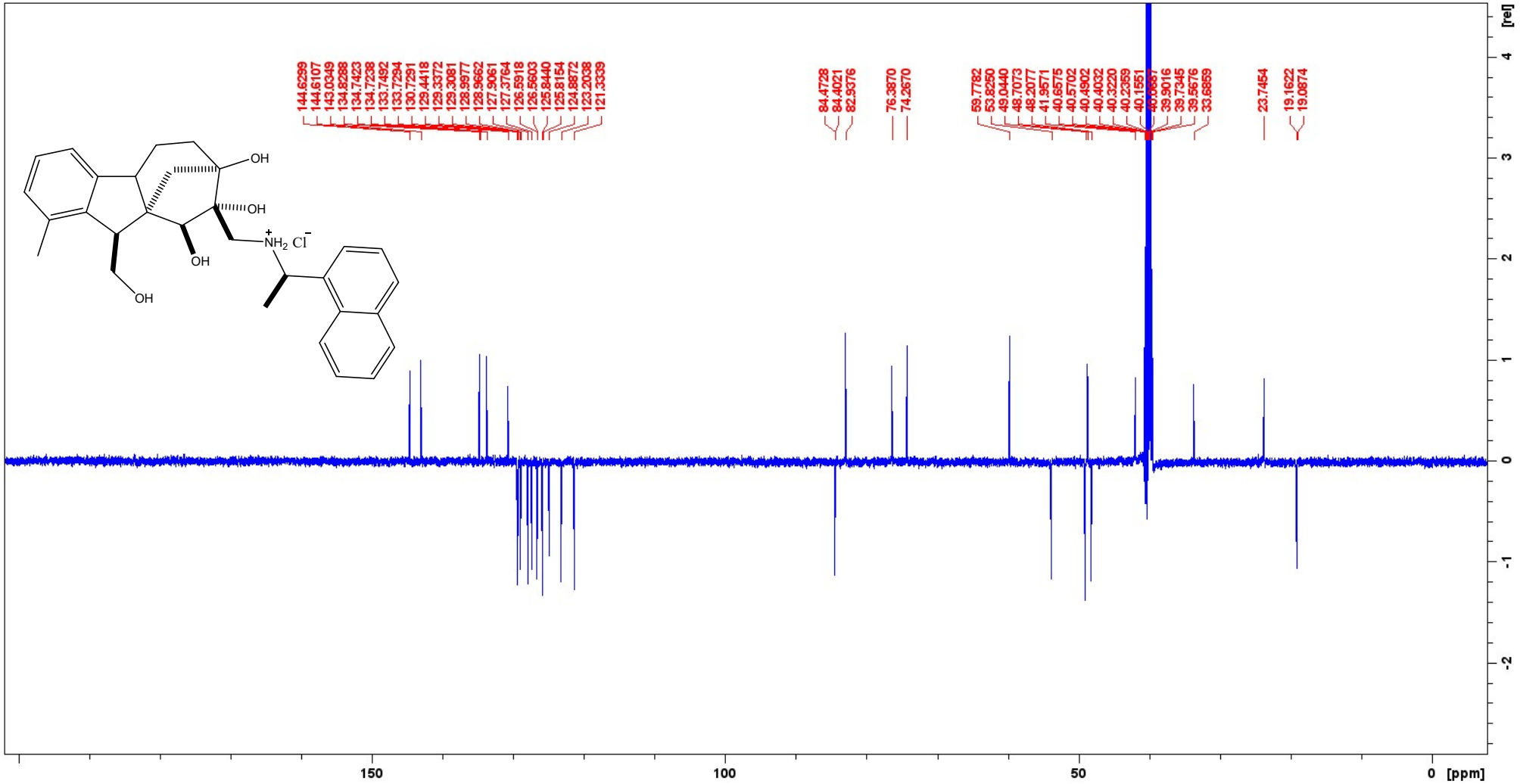
HMBC of (1*S*)-1-(Naphthalen-1-yl)-*N*-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)ethan-1-aminium chloride **25**



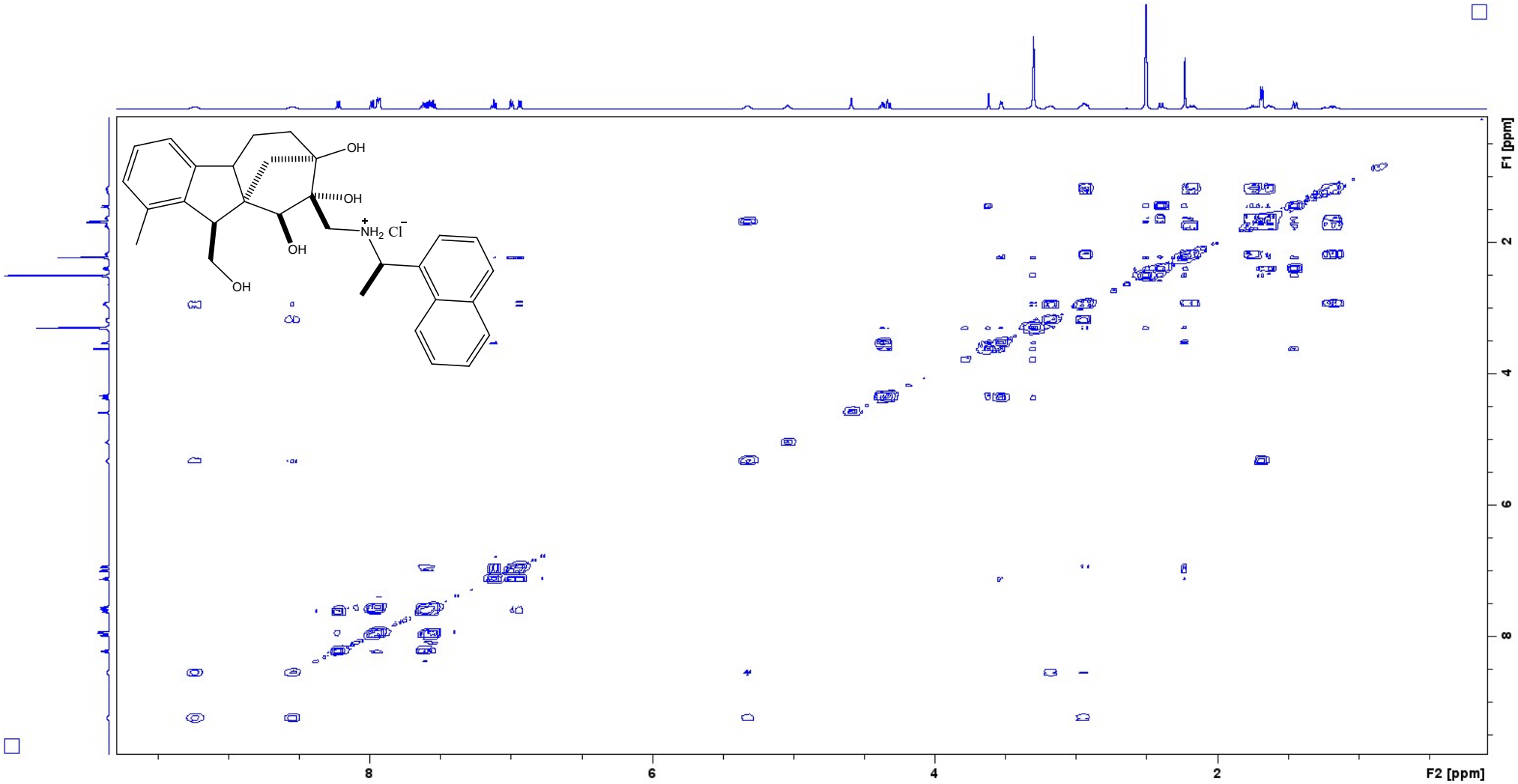
^{1}H-NMR (500 MHz) of (1*R*)-1-(Naphthalen-1-yl)-*N*-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)ethan-1-aminium chloride **26**



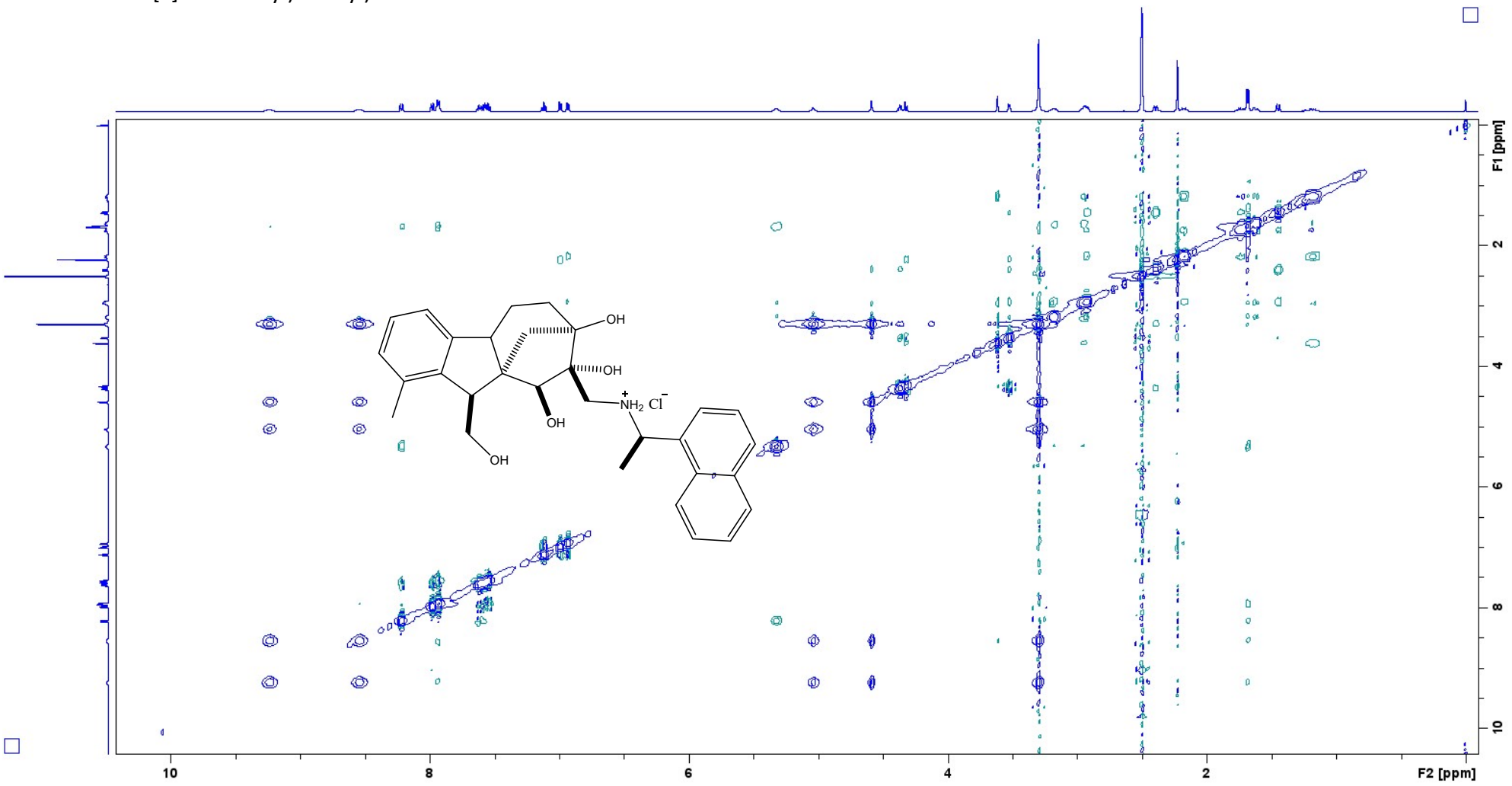
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of (1*R*)-1-(Naphthalen-1-yl)-*N*-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)ethan-1-aminium chloride **26**



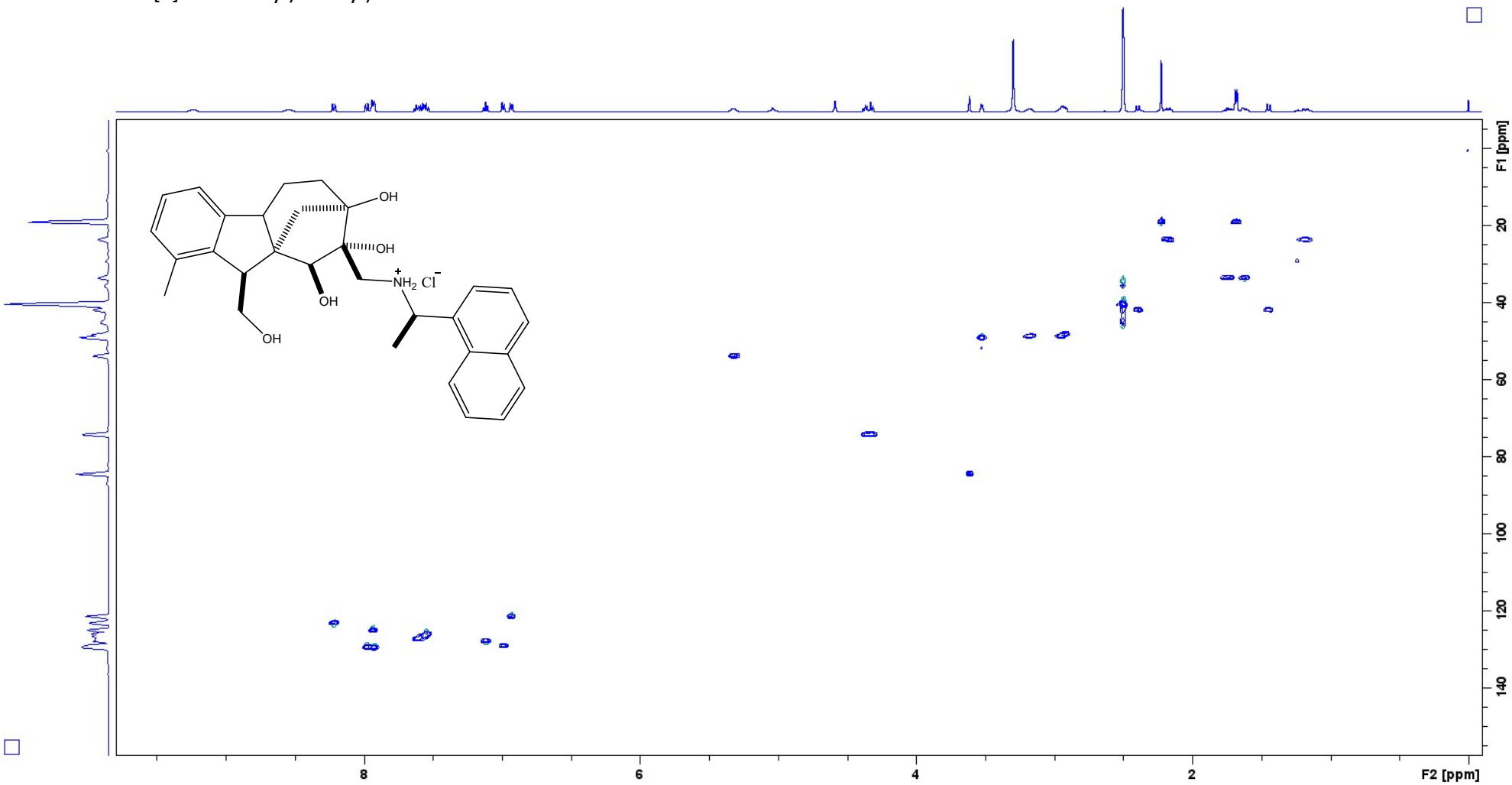
COSY of (1*R*)-1-(Naphthalen-1-yl)-*N*-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)ethan-1-aminium chloride **26**



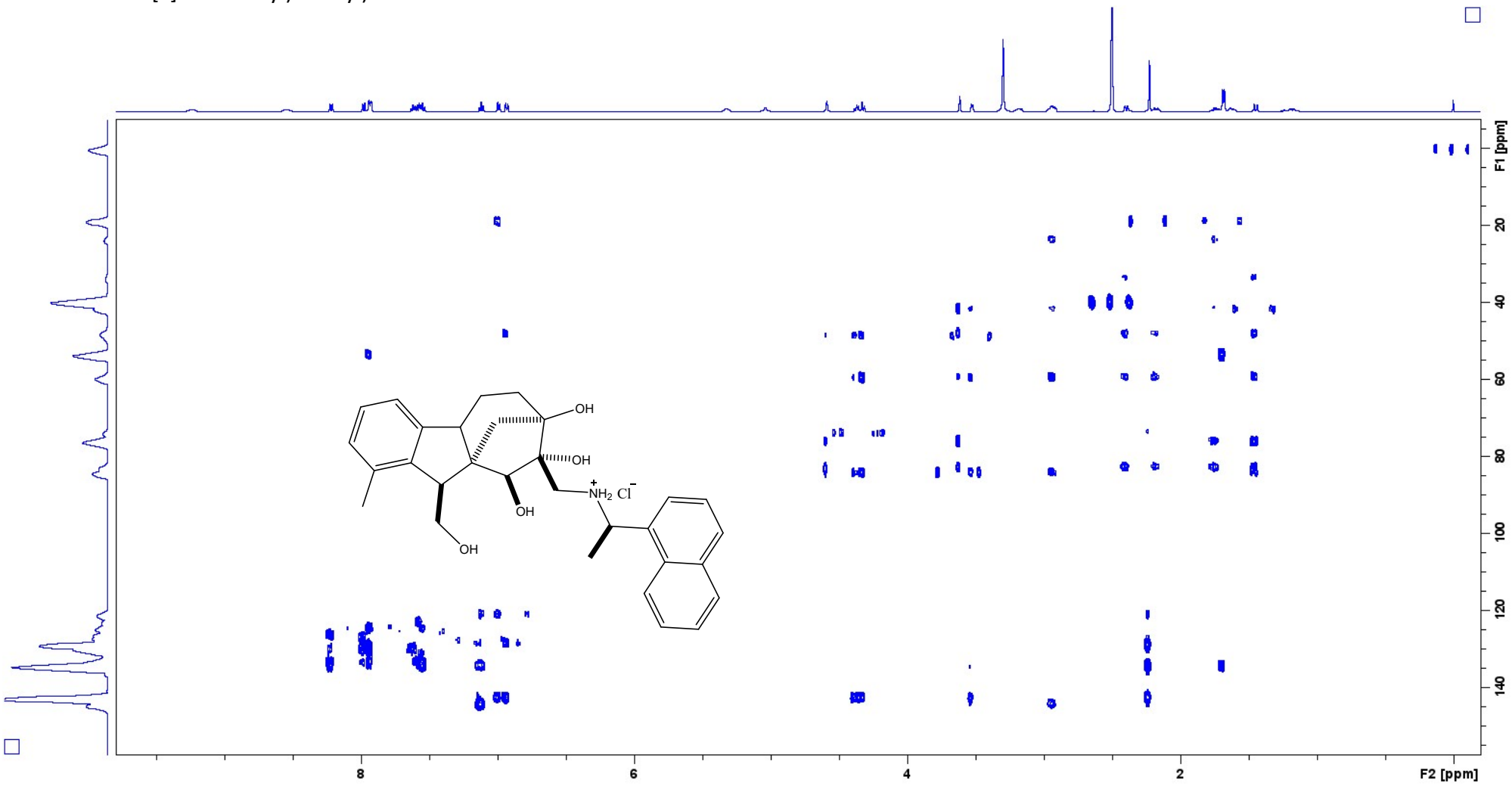
NOESY of (1*R*)-1-(Naphthalen-1-yl)-*N*-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)ethan-1-aminium chloride **26**



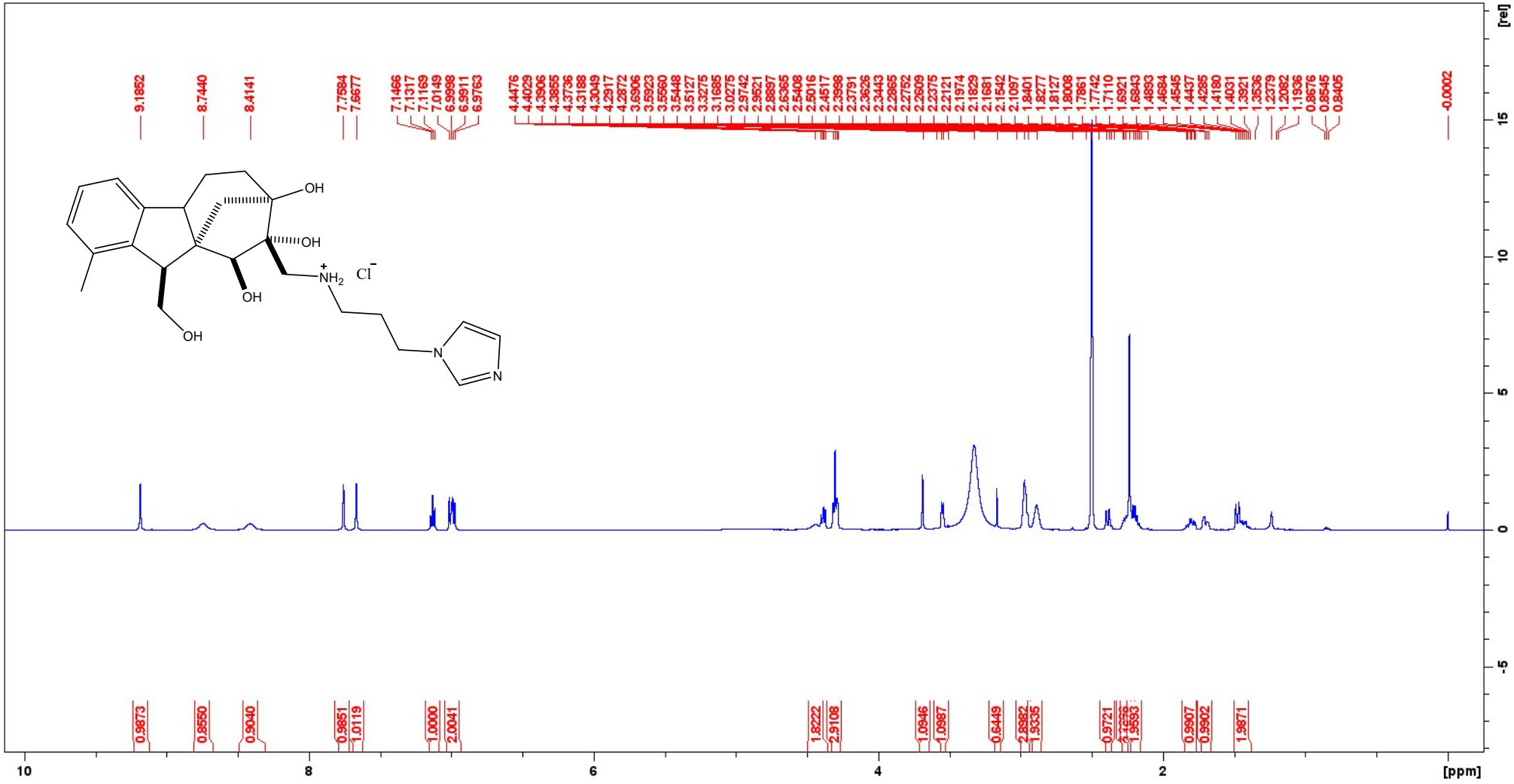
HSQC of (1*R*)-1-(Naphthalen-1-yl)-*N*-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)ethan-1-aminium chloride **26**



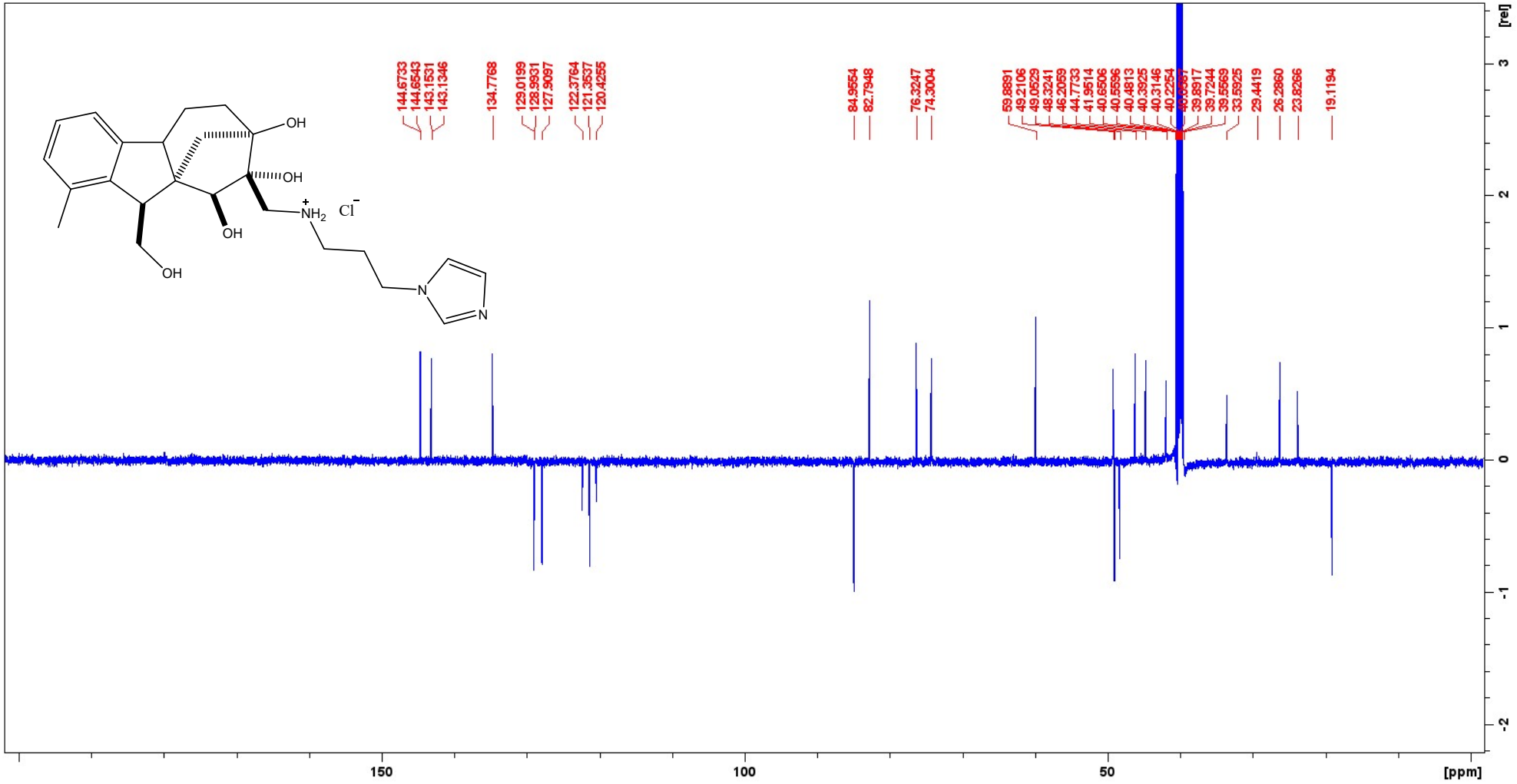
HMBC of (1*R*)-1-(Naphthalen-1-yl)-*N*-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)ethan-1-aminium chloride **26**



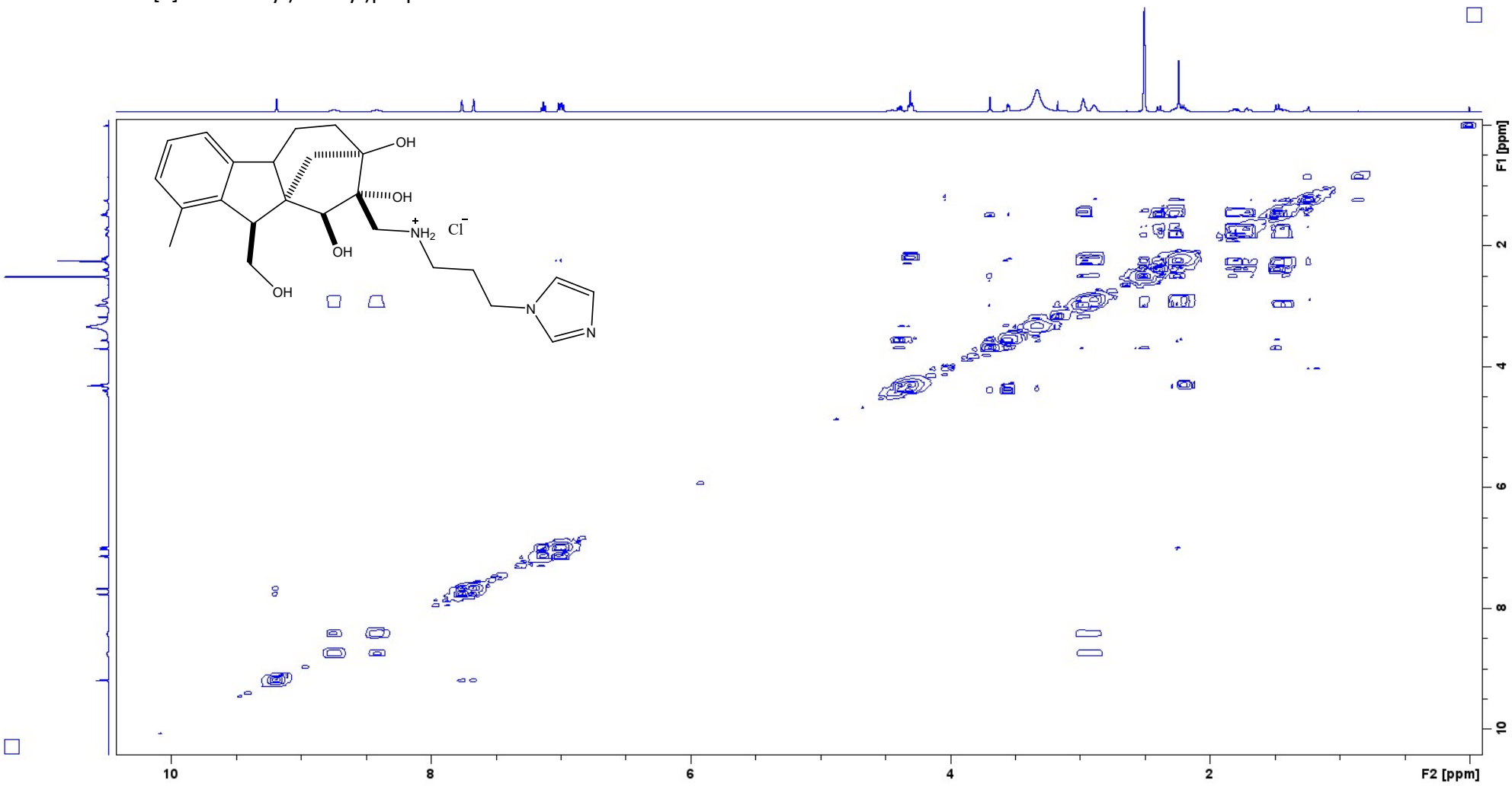
^{1}H-NMR (500 MHz) of 3-(1*H*-Imidazol-1-yl)-*N*-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)propan-1-aminium chloride **27**



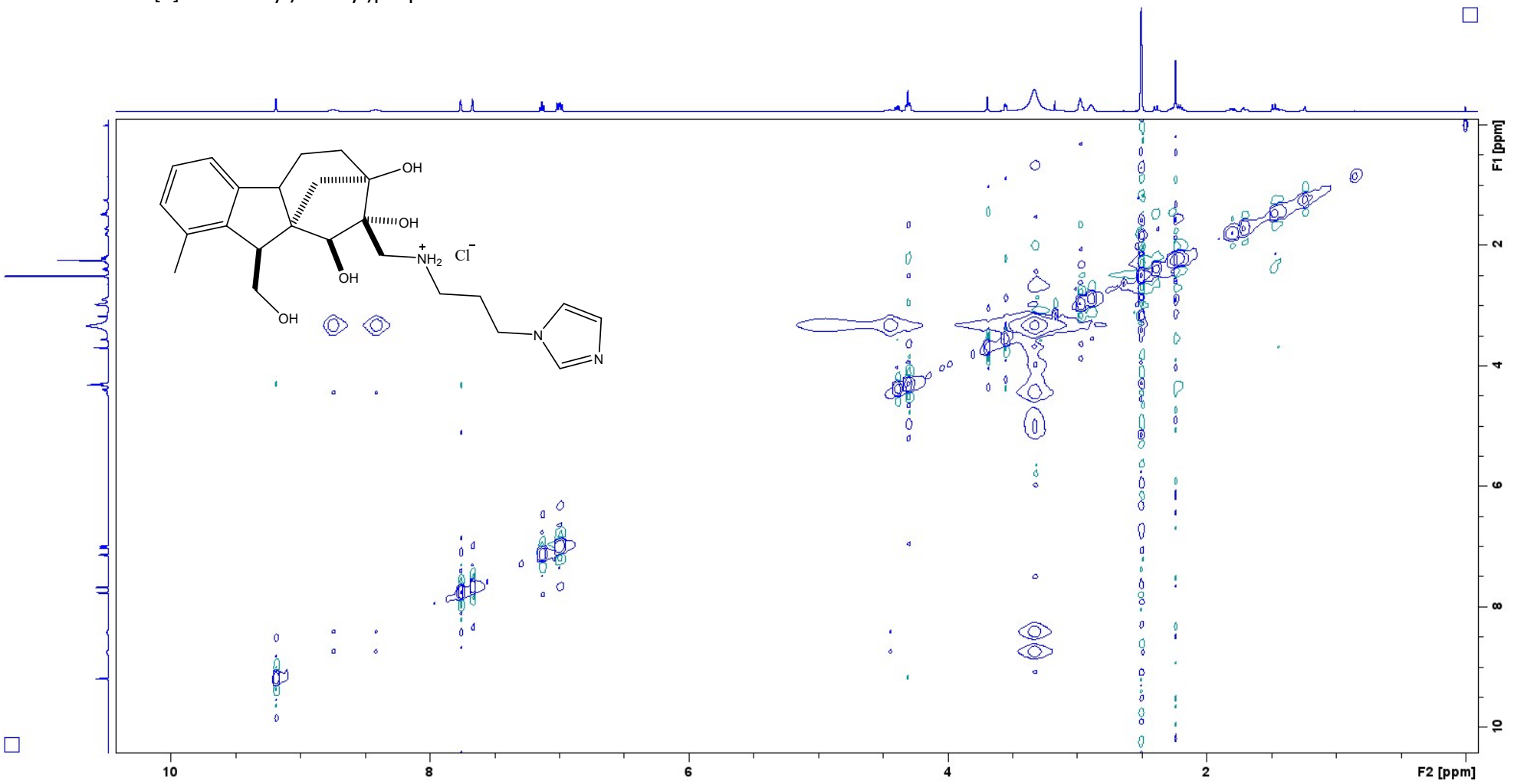
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of 3-(1*H*-Imidazol-1-yl)-*N*-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)propan-1-aminium chloride **27**



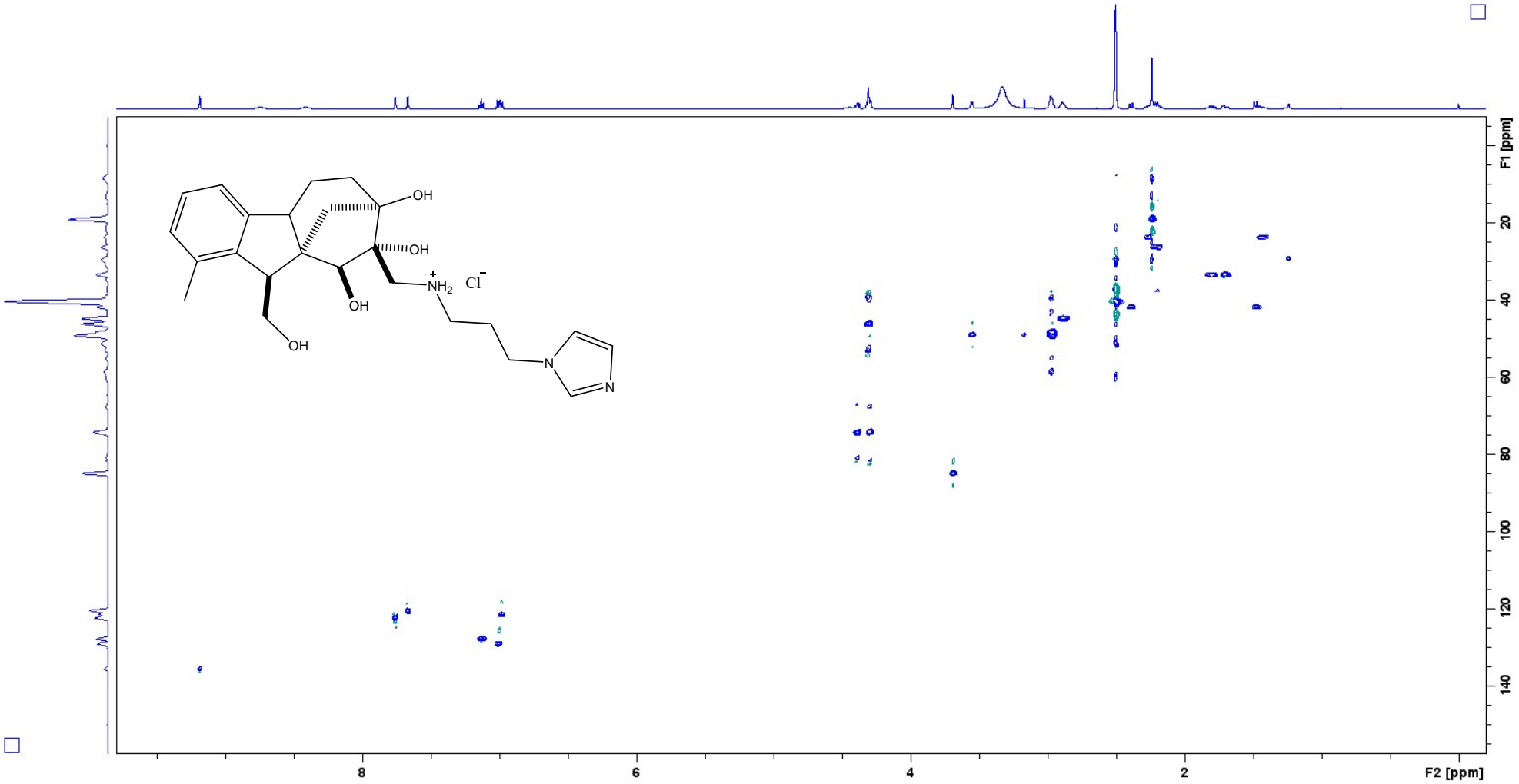
COSY of 3-(1*H*-Imidazol-1-yl)-*N*-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)propan-1-aminium chloride **27**



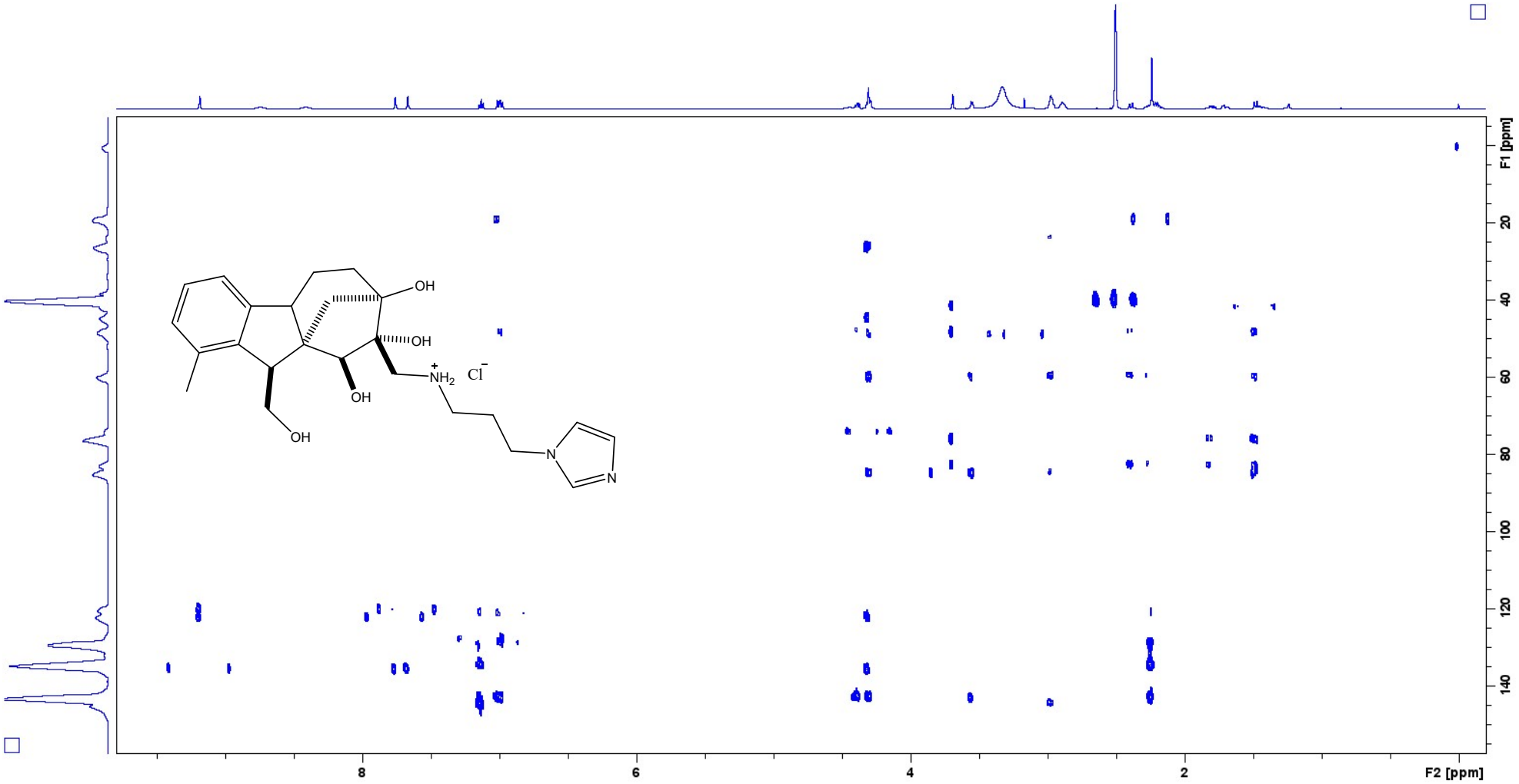
NOESY of 3-(1*H*-Imidazol-1-yl)-*N*-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)propan-1-aminium chloride **27**



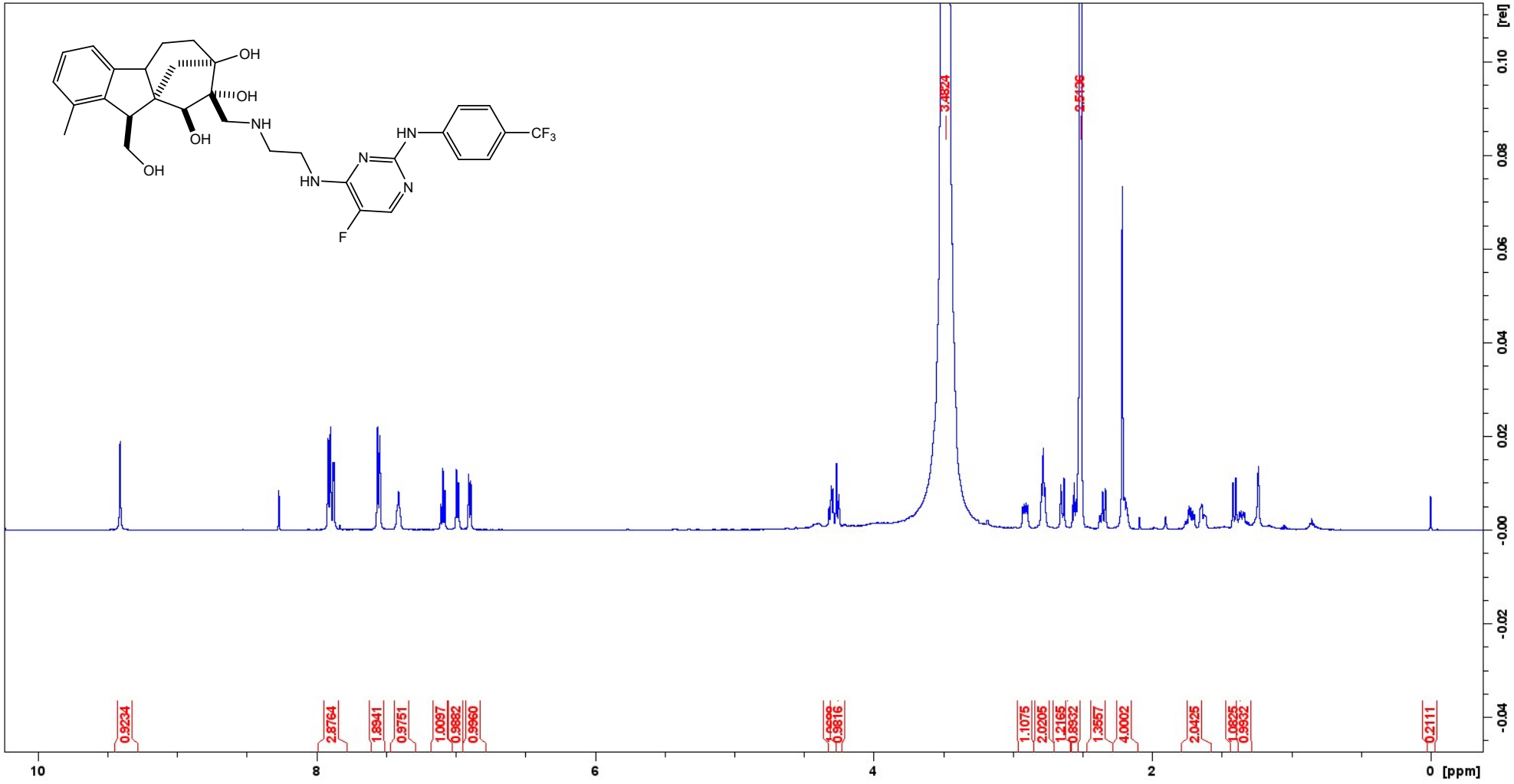
HSQC of 3-(1*H*-Imidazol-1-yl)-*N*-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)propan-1-aminium chloride **27**



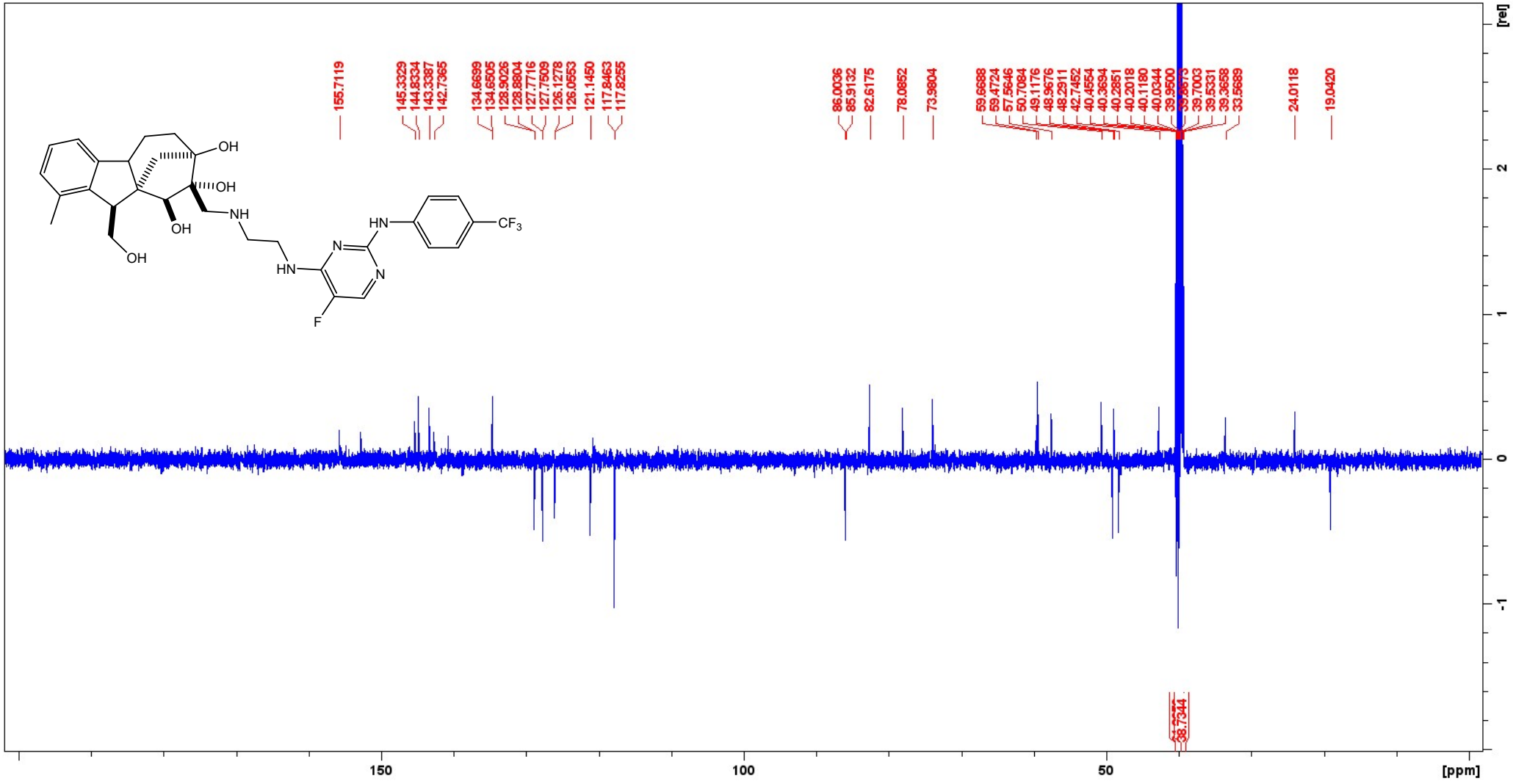
HMBC of 3-(1*H*-Imidazol-1-yl)-*N*-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)propan-1-aminium chloride **27**



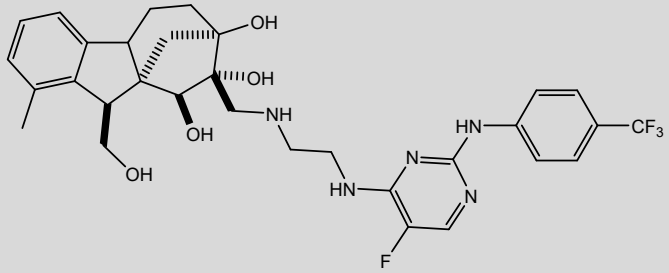
^{1}H-NMR (500 MHz) of (7*S*,8*R*,9*S*,9a*R*,10*S*)-8-(((2-((5-Fluoro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)ethyl)amino)methyl)-10-(hydroxymethyl)-1-methyl-4b,5,6,8,9,10-hexahydro-7*H*-7,9a-methanobenzo[a]azulene-7,8,9-triol **28**



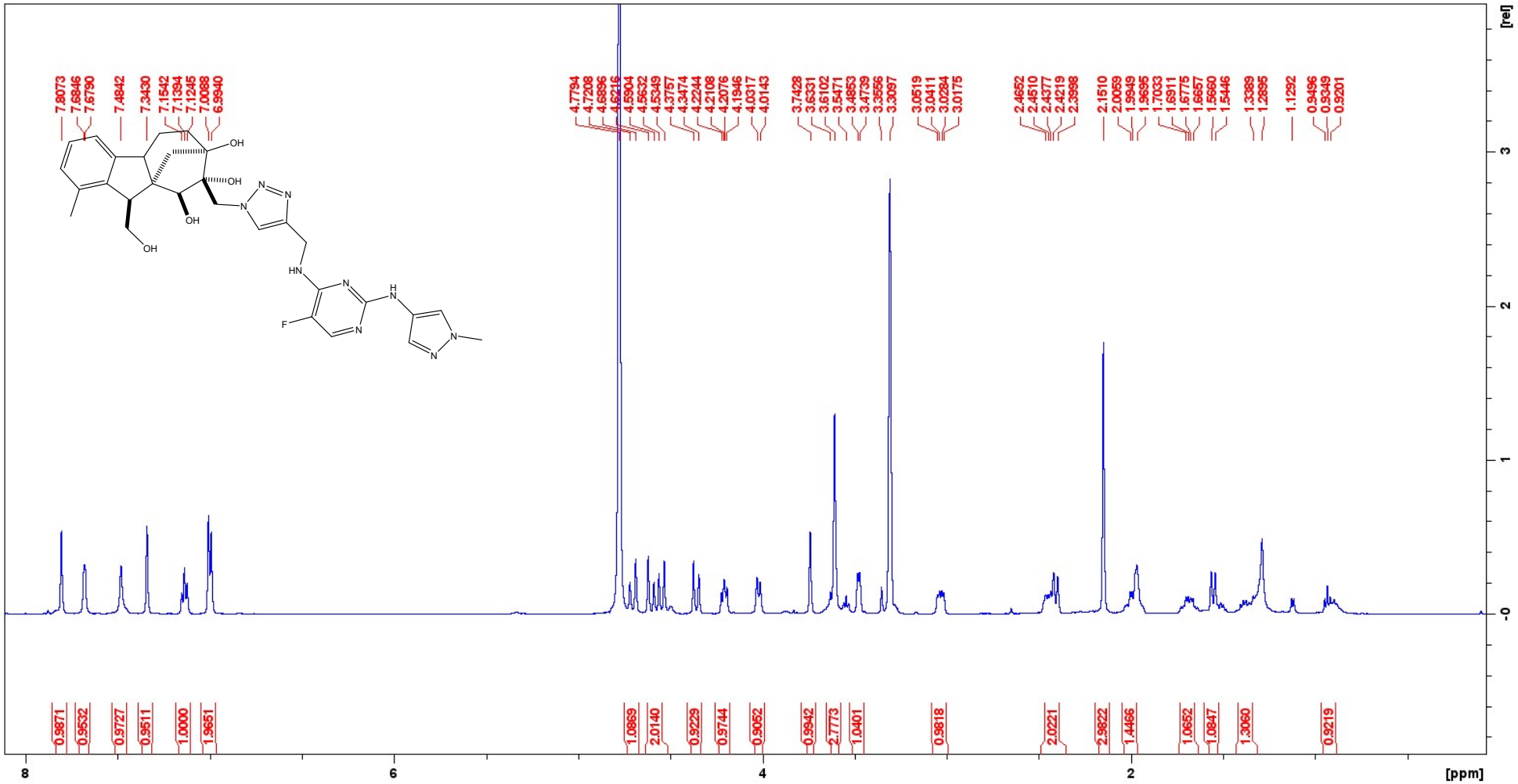
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of (7*S*,8*R*,9*S*,9a*R*,10*S*)-8-(((2-((5-Fluoro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)ethyl)amino)methyl)-10-(hydroxymethyl)-1-methyl-4b,5,6,8,9,10-hexahydro-7*H*-7,9a-methanobenzo[a]azulene-7,8,9-triol **28**



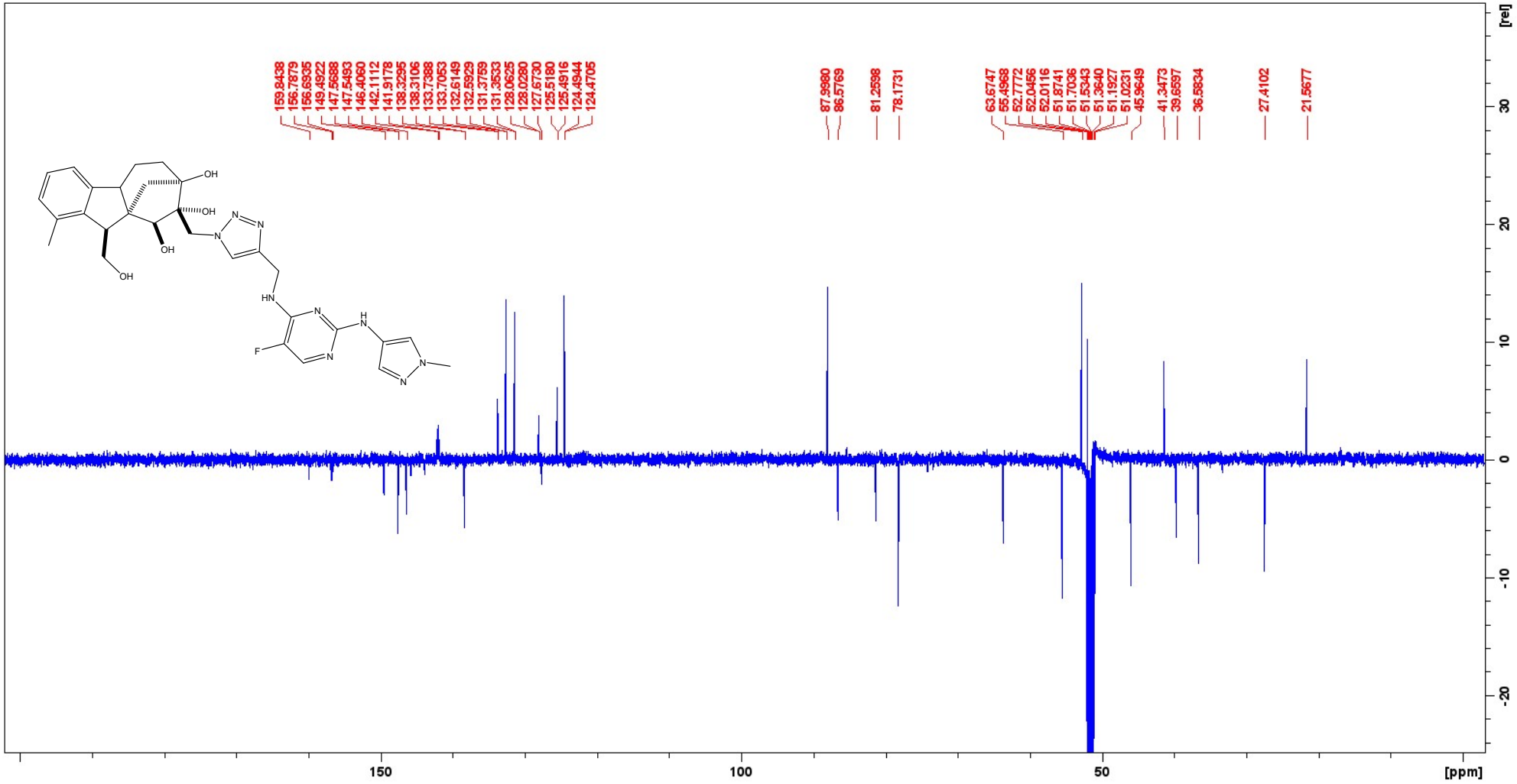
^{19}FNMR (470 MHz) of (7*S*,8*R*,9*S*,9a*R*,10*S*)-8-(((2-((5-Fluoro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)ethyl)amino)methyl)-10-(hydroxymethyl)-1-methyl-4b,5,6,8,9,10-hexahydro-7*H*-7,9a-methanobenzo[a]azulene-7,8,9-triol **28**



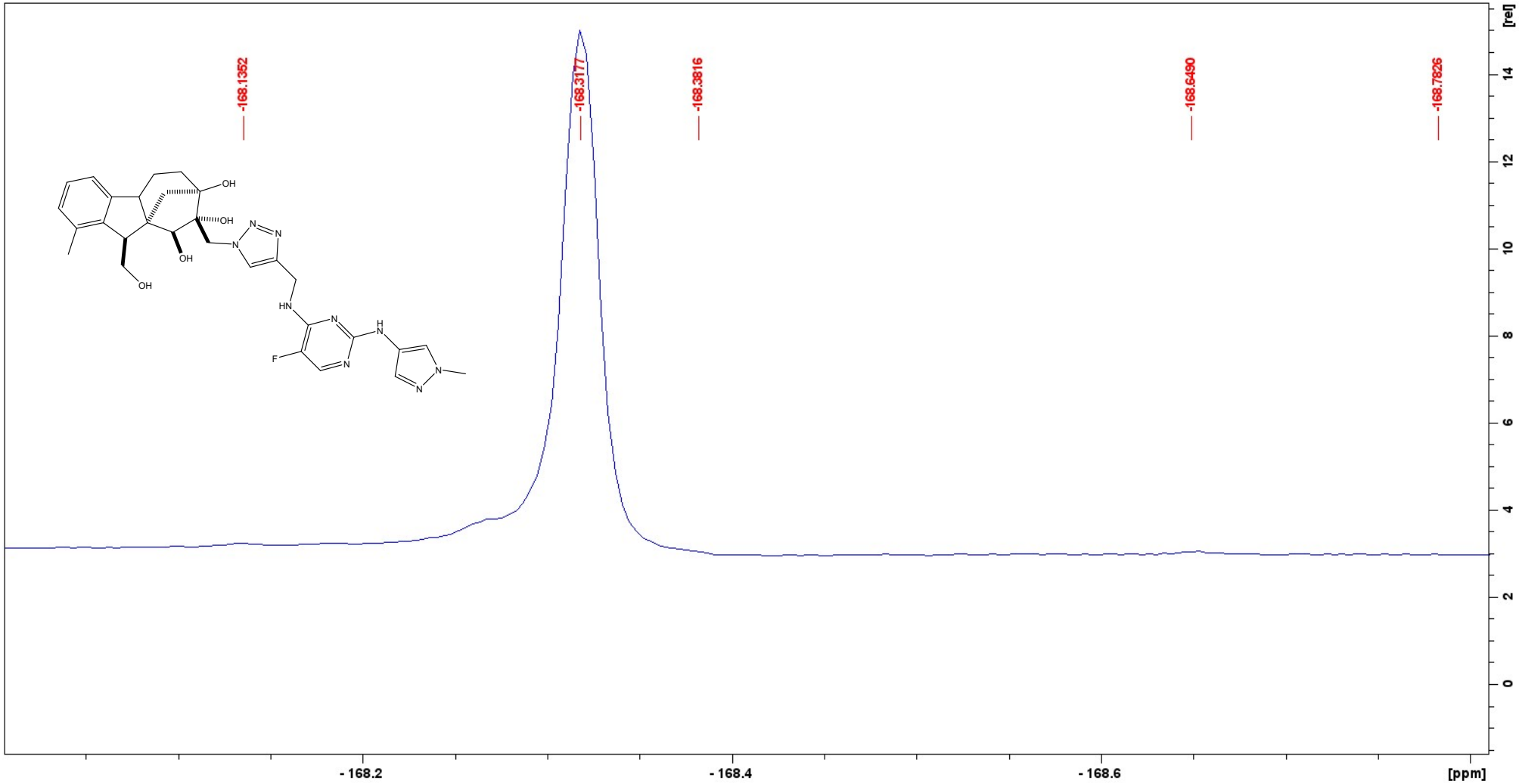
^{1}H-NMR (500 MHz) of (7*S*,8*R*,9*S*,9a*R*,10*S*)-8-((4-(((5-Fluoro-2-((1-methyl-1H-pyrazol-4-yl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-10-(hydroxymethyl)-1-methyl-4b,5,6,8,9,10-hexahydro-7*H*-7,9a-methanobenzo[a]azulene-7,8,9-triol **36**



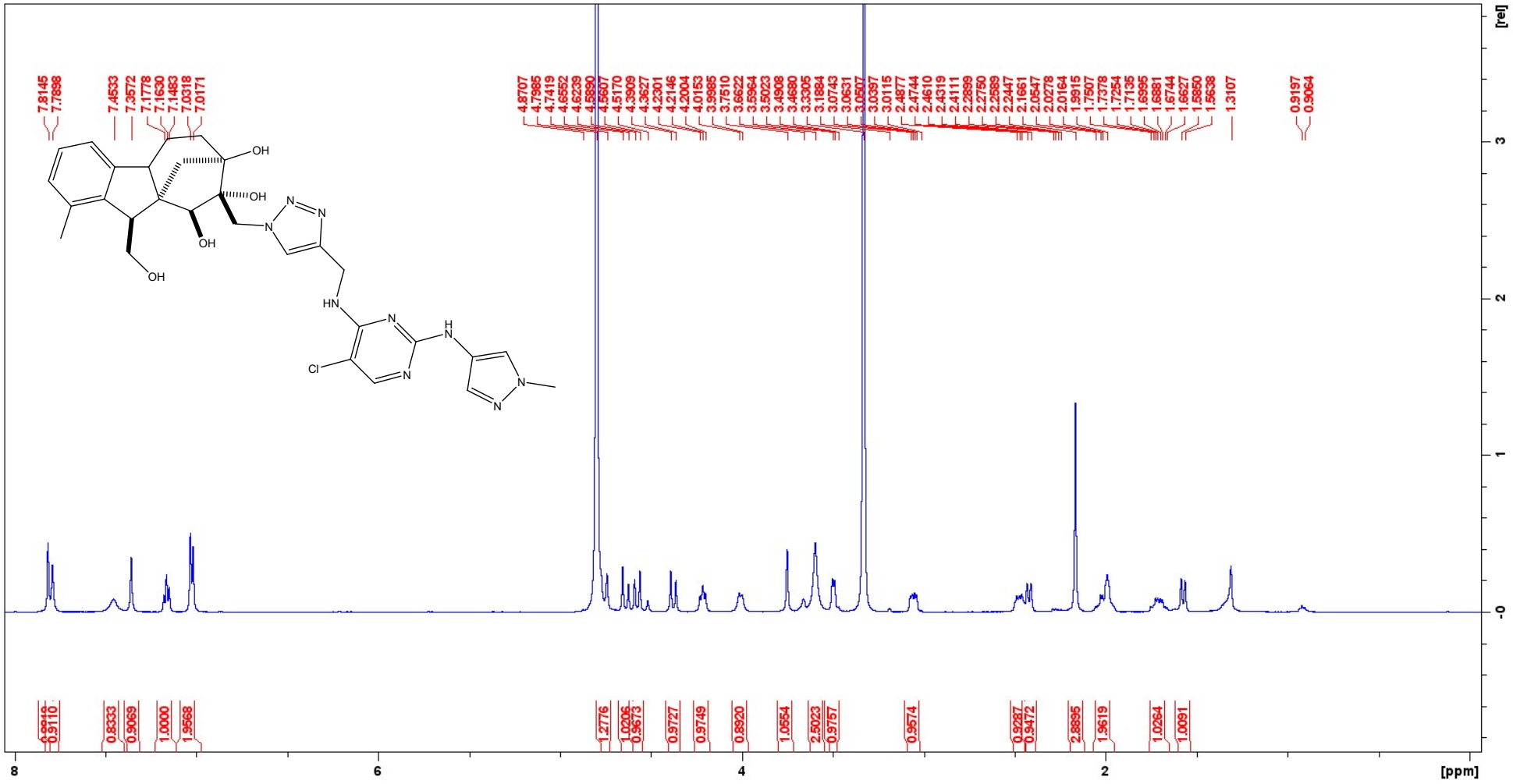
$^{13}C\{1H\}$ NMR (125 MHz) of (7*S*,8*R*,9*S*,9a*R*,10*S*)-8-((4-(((5-Fluoro-2-((1-methyl-1H-pyrazol-4-yl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-10-(hydroxymethyl)-1-methyl-4b,5,6,8,9,10-hexahydro-7*H*-7,9a-methanobenzo[a]azulene-7,8,9-triol **36**



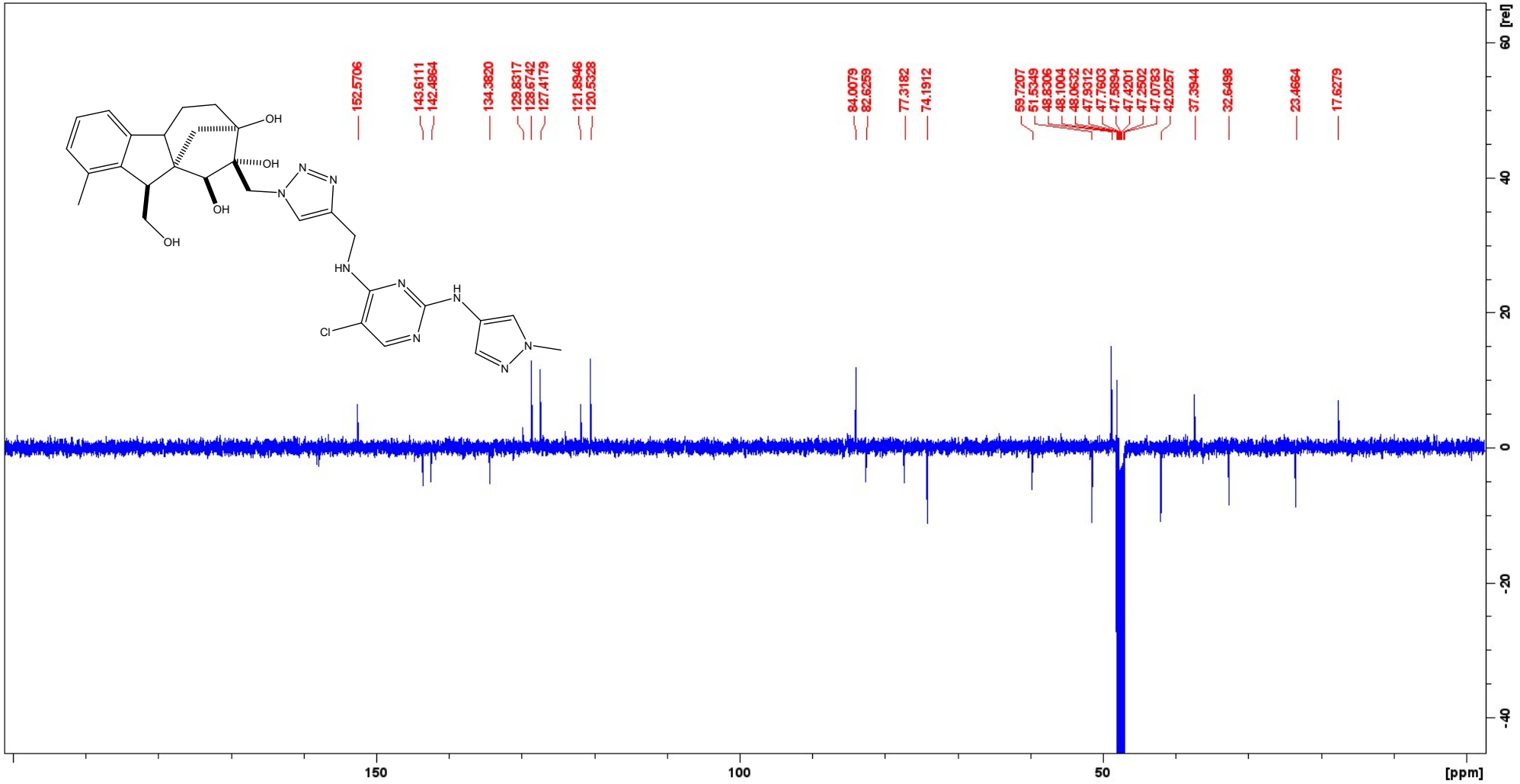
^{19}F *J*-MOD NMR (470 MHz) of (7*S*,8*R*,9*S*,9a*R*,10*S*)-8-((4-(((5-Fluoro-2-((1-methyl-1H-pyrazol-4-yl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-10-(hydroxymethyl)-1-methyl-4b,5,6,8,9,10-hexahydro-7*H*-7,9a-methanobenzo[a]azulene-7,8,9-triol **36**



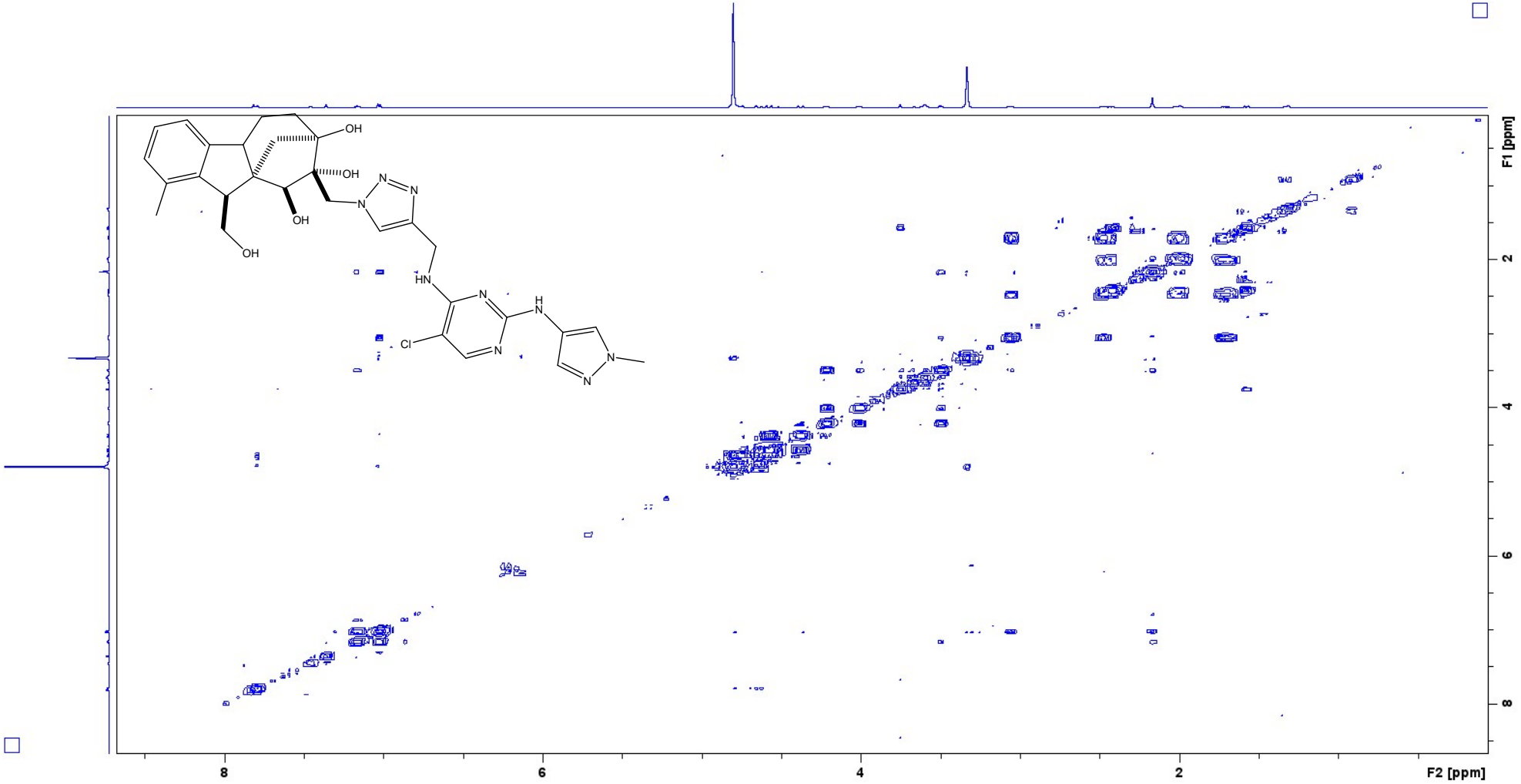
^{1}H-NMR (500 MHz) of (7*S*,8*R*,9*S*,9a*R*,10*S*)-8-((4-(((5-Chloro-2-((1-methyl-1*H*-pyrazol-4-yl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-10-(hydroxymethyl)-1-methyl-4b,5,6,8,9,10-hexahydro-7*H*-7,9a-methanobenzo[a]azulene-7,8,9-triol **37**



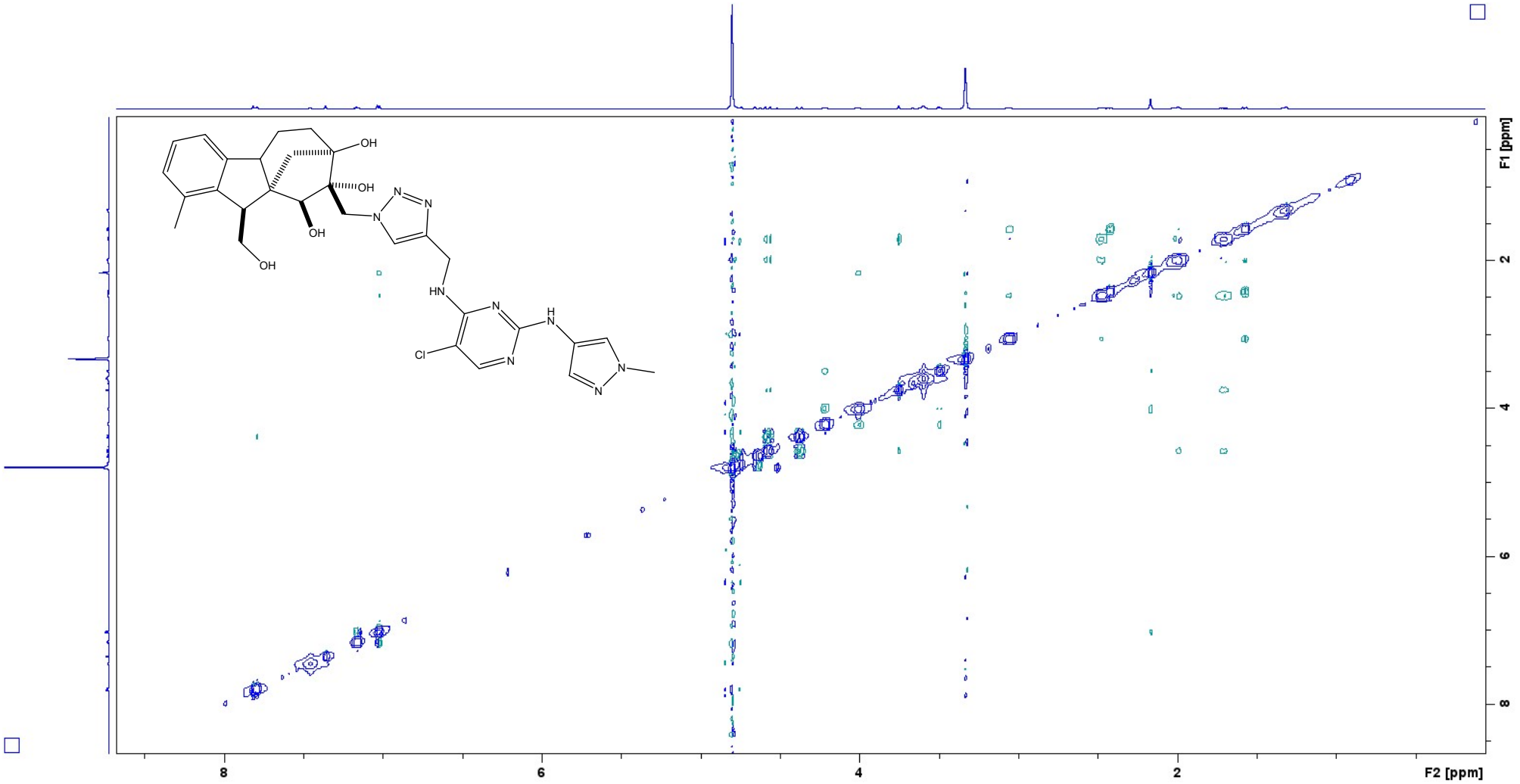
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of (7*S*,8*R*,9*S*,9a*R*,10*S*)-8-((4-(((5-Chloro-2-((1-methyl-1*H*-pyrazol-4-yl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-10-(hydroxymethyl)-1-methyl-4b,5,6,8,9,10-hexahydro-7*H*-7,9a-methanobenzo[a]azulene-7,8,9-triol **37**



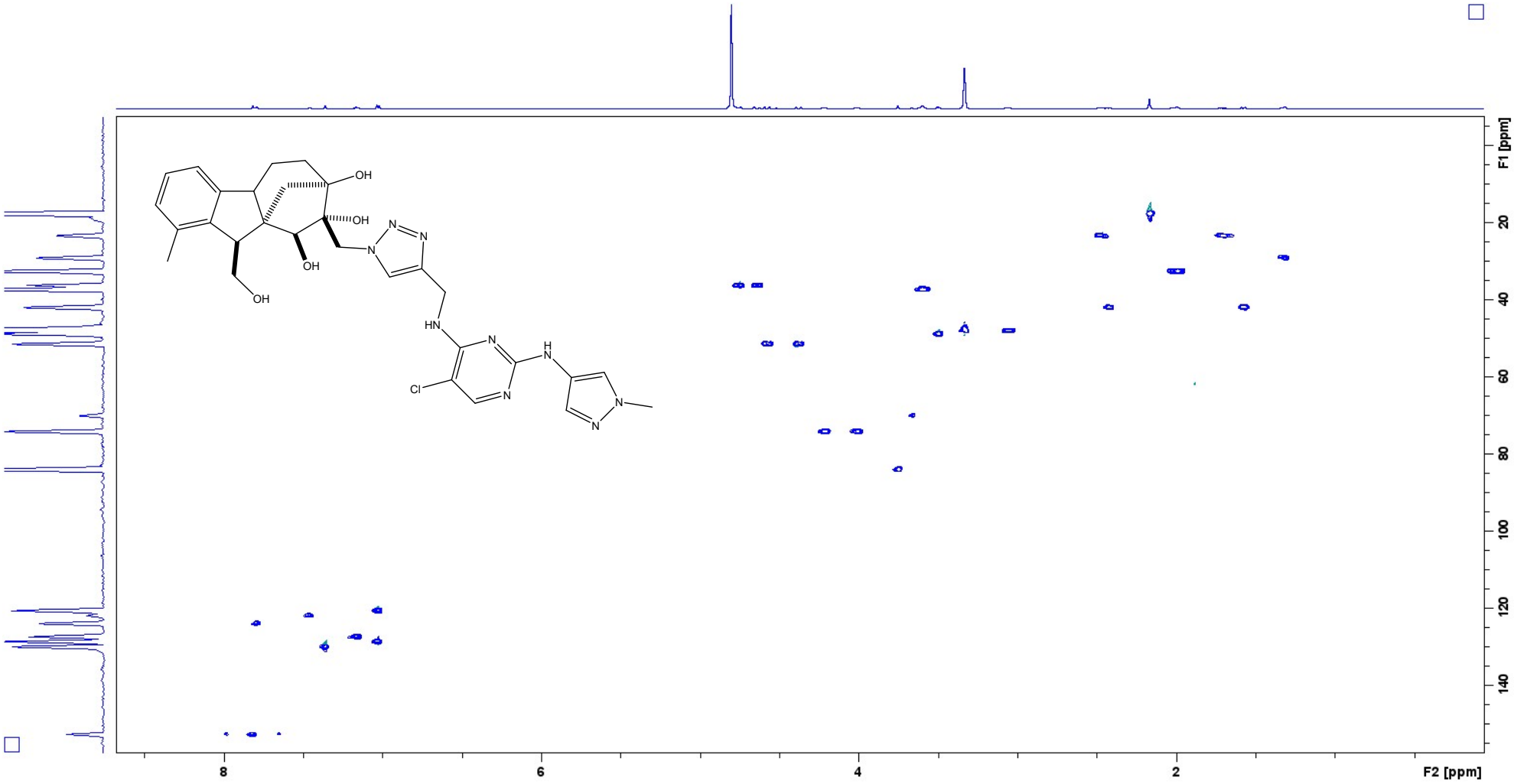
COSY of (7*S*,8*R*,9*S*,9a*R*,10*S*)-8-((4-(((5-Chloro-2-((1-methyl-1*H*-pyrazol-4-yl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-10-(hydroxymethyl)-1-methyl-4b,5,6,8,9,10-hexahydro-7*H*-7,9a-methanobenzo[a]azulene-7,8,9-triol **37**



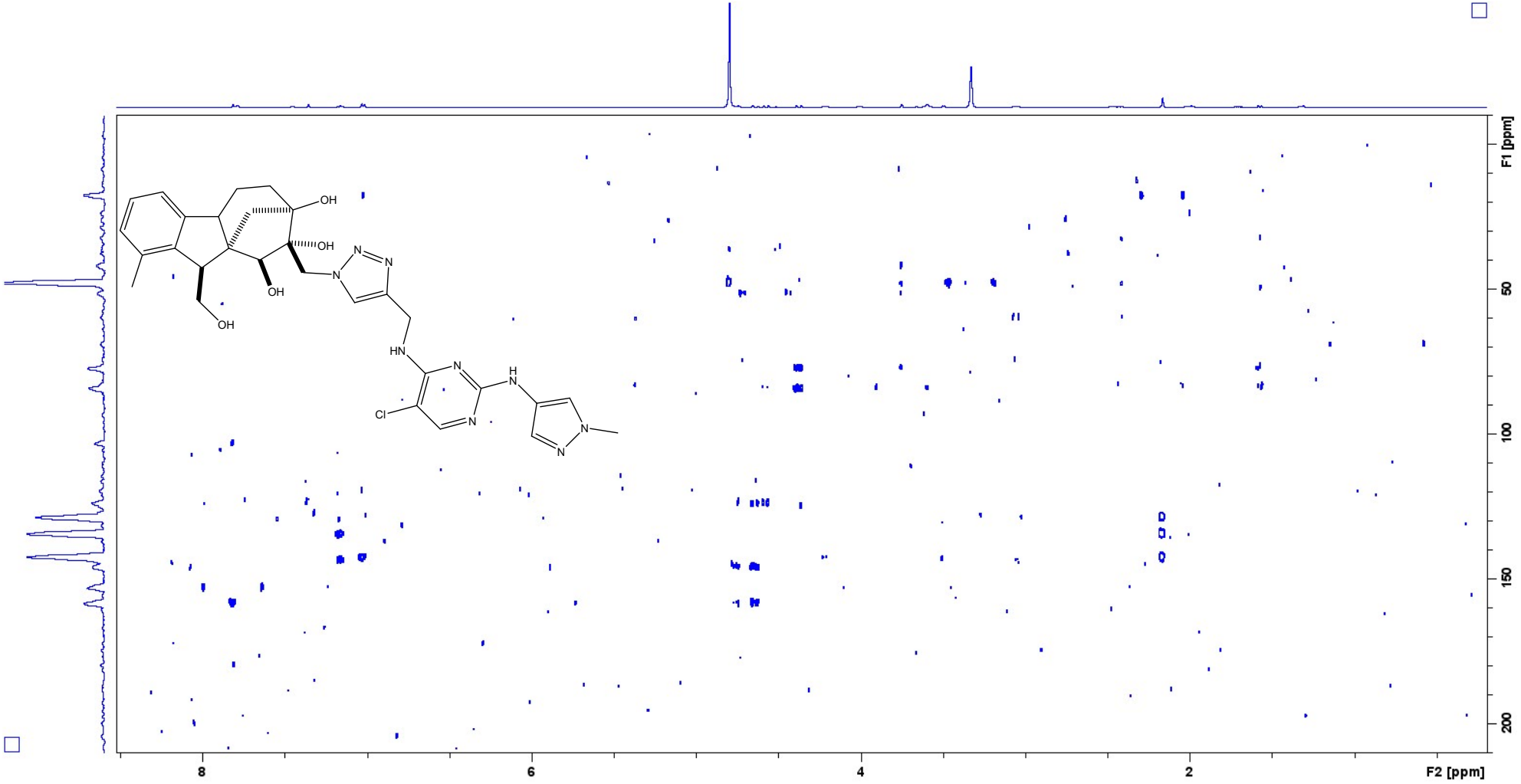
NOESY of (7*S*,8*R*,9*S*,9a*R*,10*S*)-8-((4-(((5-Chloro-2-((1-methyl-1*H*-pyrazol-4-yl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-10-(hydroxymethyl)-1-methyl-4b,5,6,8,9,10-hexahydro-7*H*-7,9a-methanobenzo[a]azulene-7,8,9-triol **37**



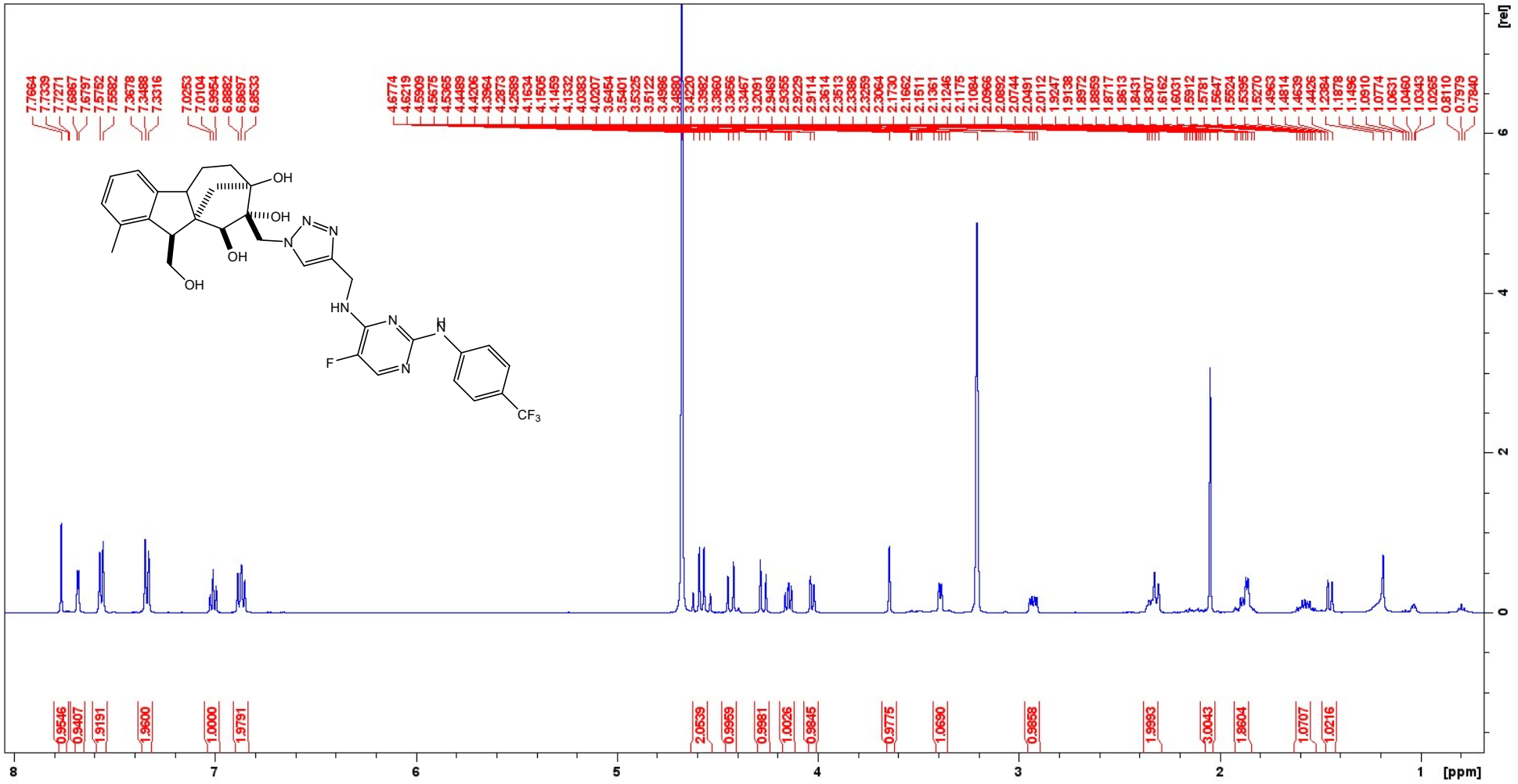
HSQC of (7*S*,8*R*,9*S*,9a*R*,10*S*)-8-((4-(((5-Chloro-2-((1-methyl-1*H*-pyrazol-4-yl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-10-(hydroxymethyl)-1-methyl-4b,5,6,8,9,10-hexahydro-7*H*-7,9a-methanobenzo[a]azulene-7,8,9-triol **37**



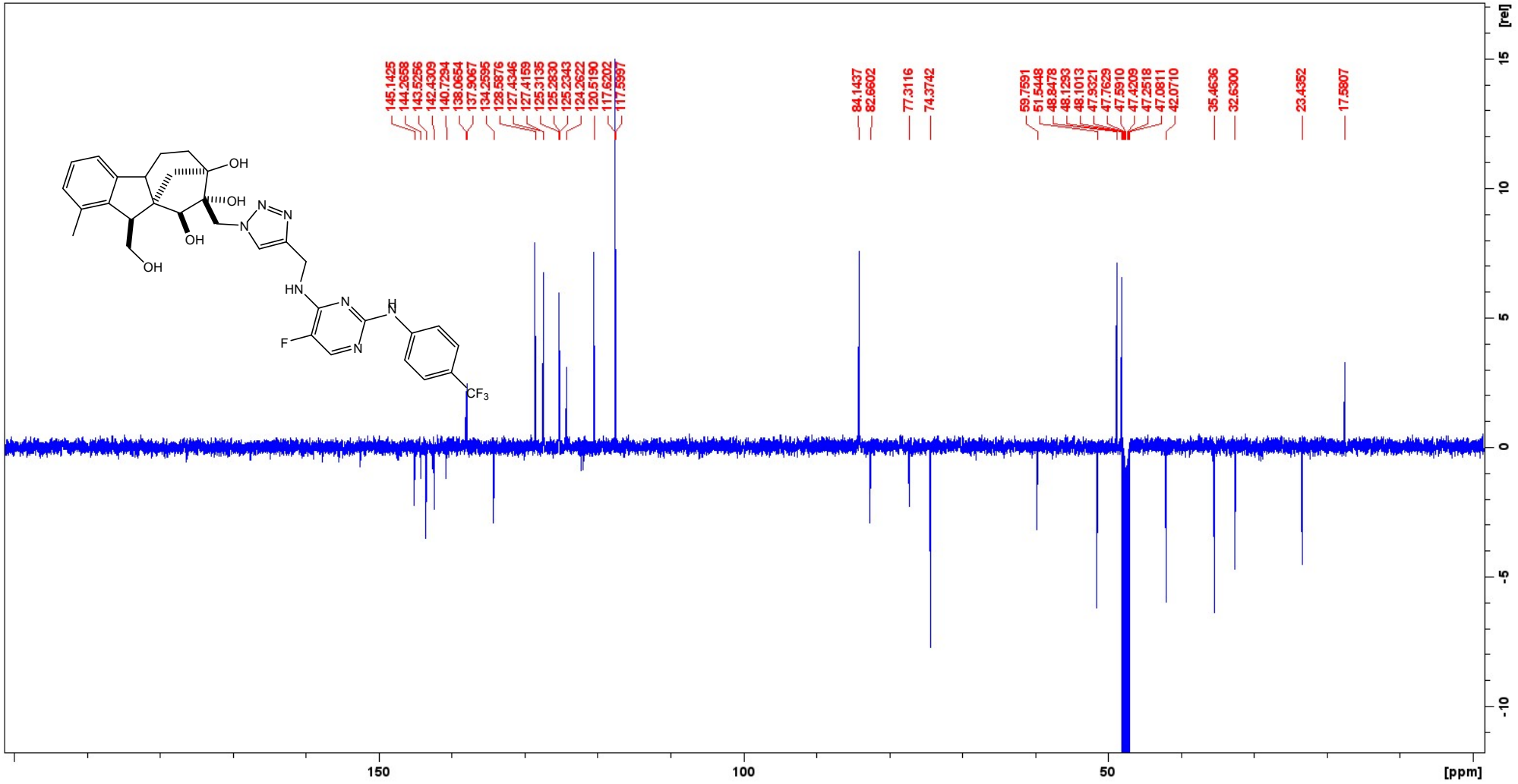
HMBC of (7*S*,8*R*,9*S*,9a*R*,10*S*)-8-((4-(((5-Chloro-2-((1-methyl-1*H*-pyrazol-4-yl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-10-(hydroxymethyl)-1-methyl-4b,5,6,8,9,10-hexahydro-7*H*-7,9a-methanobenzo[a]azulene-7,8,9-triol **37**



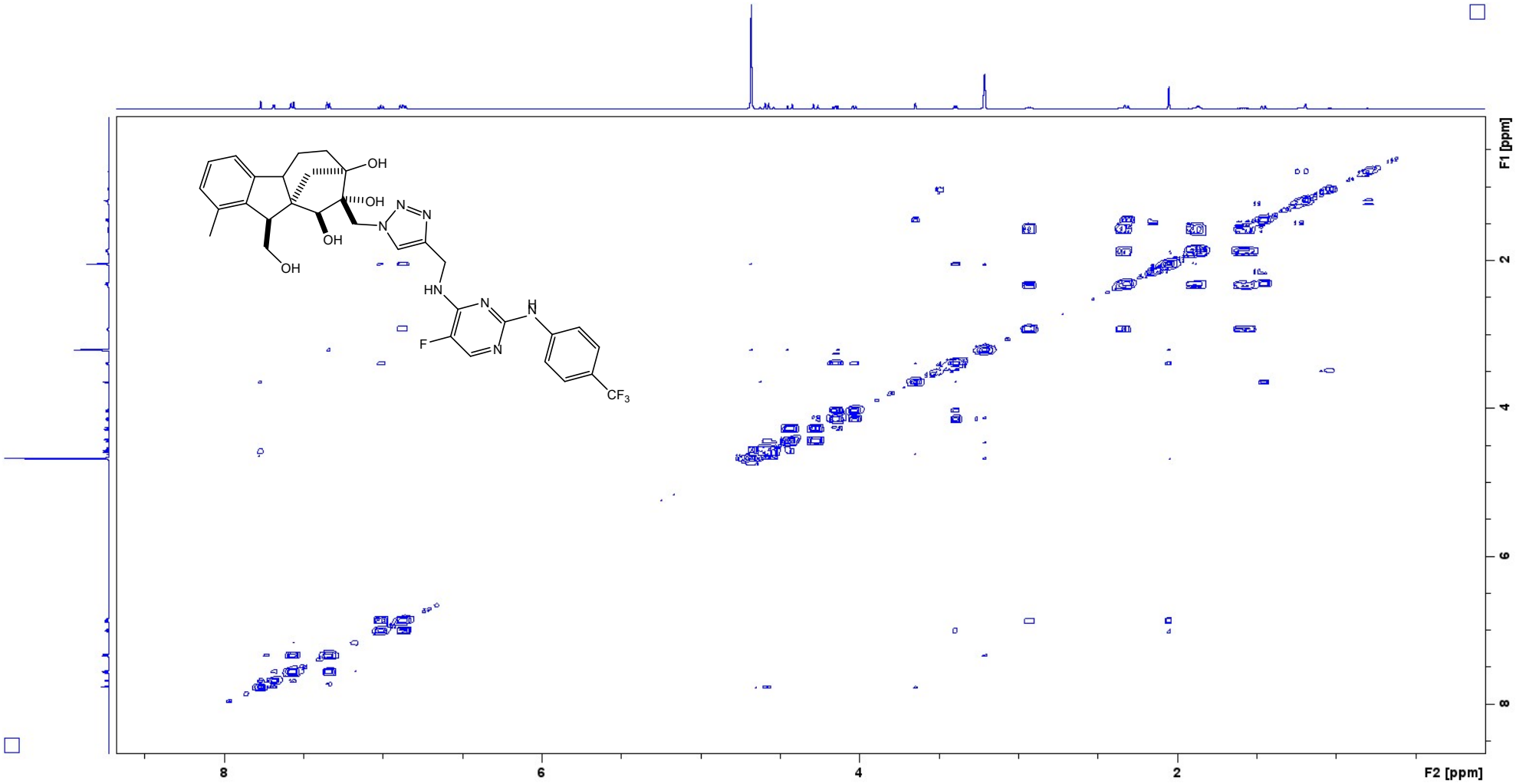
^{1}H-NMR (500 MHz) of (7*S*,8*R*,9*S*,9a*R*,10*S*)-8-((4-(((5-Fluoro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-10-(hydroxymethyl)-1-methyl-4b,5,6,8,9,10-hexahydro-7*H*-7,9a-methanobenzo[*a*]azulene-7,8,9-triol **38**



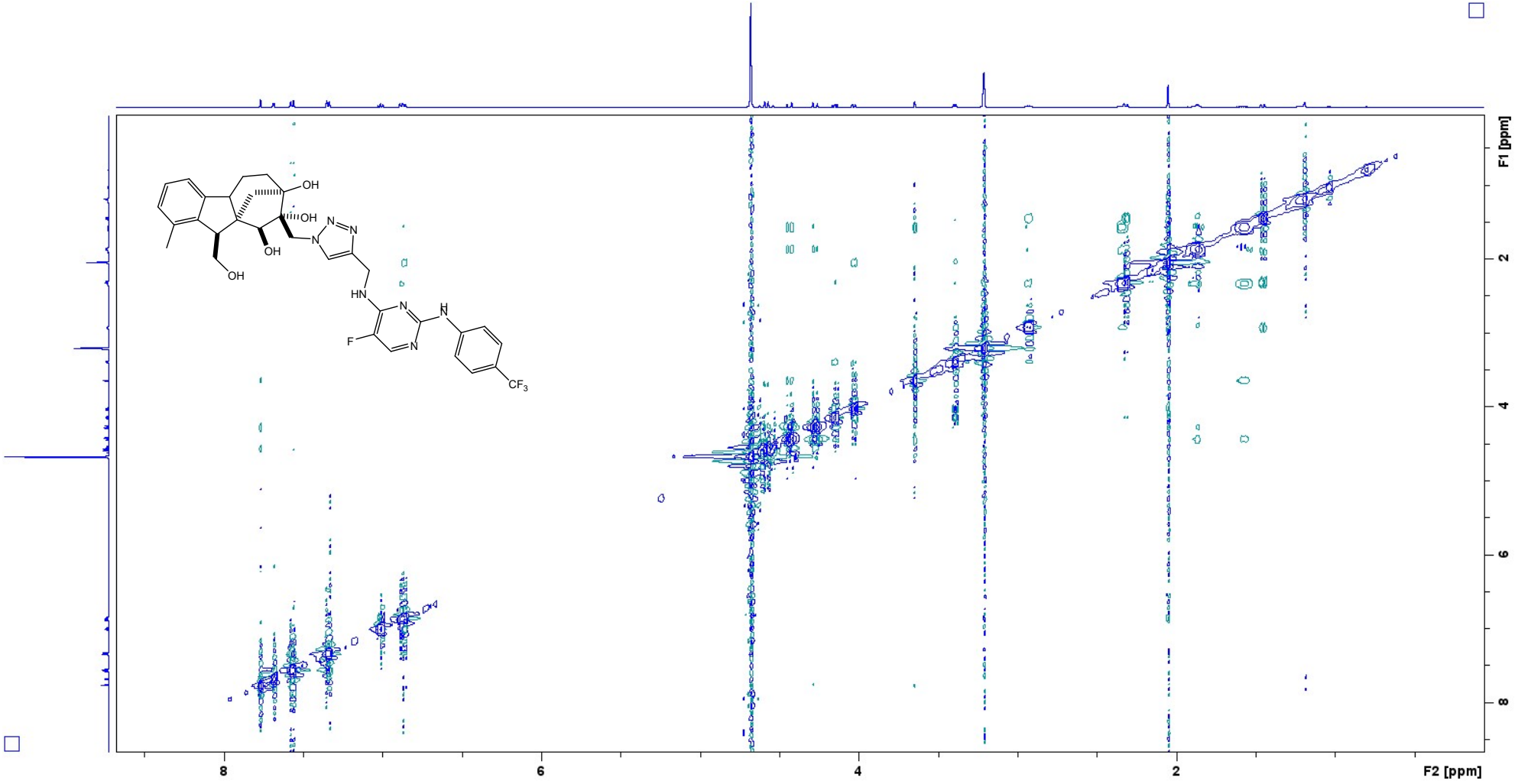
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of (7*S*,8*R*,9*S*,9a*R*,10*S*)-8-((4-(((5-Fluoro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-10-(hydroxymethyl)-1-methyl-4b,5,6,8,9,10-hexahydro-7*H*-7,9a-methanobenzo[*a*]azulene-7,8,9-triol **38**



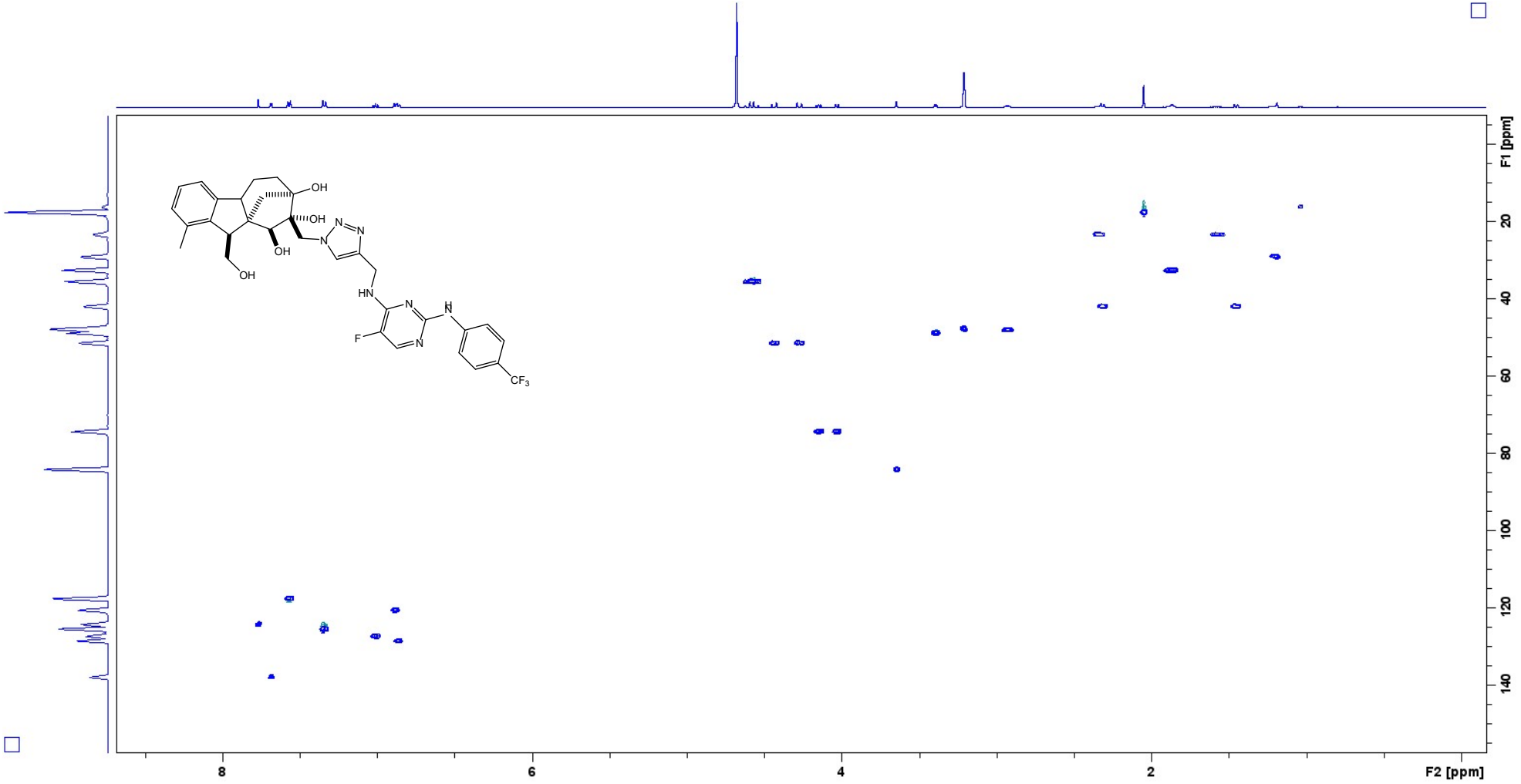
COSY of (7*S*,8*R*,9*S*,9a*R*,10*S*)-8-((4-(((5-Fluoro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-10-(hydroxymethyl)-1-methyl-4b,5,6,8,9,10-hexahydro-7*H*-7,9a-methanobenzo[*a*]azulene-7,8,9-triol **38**



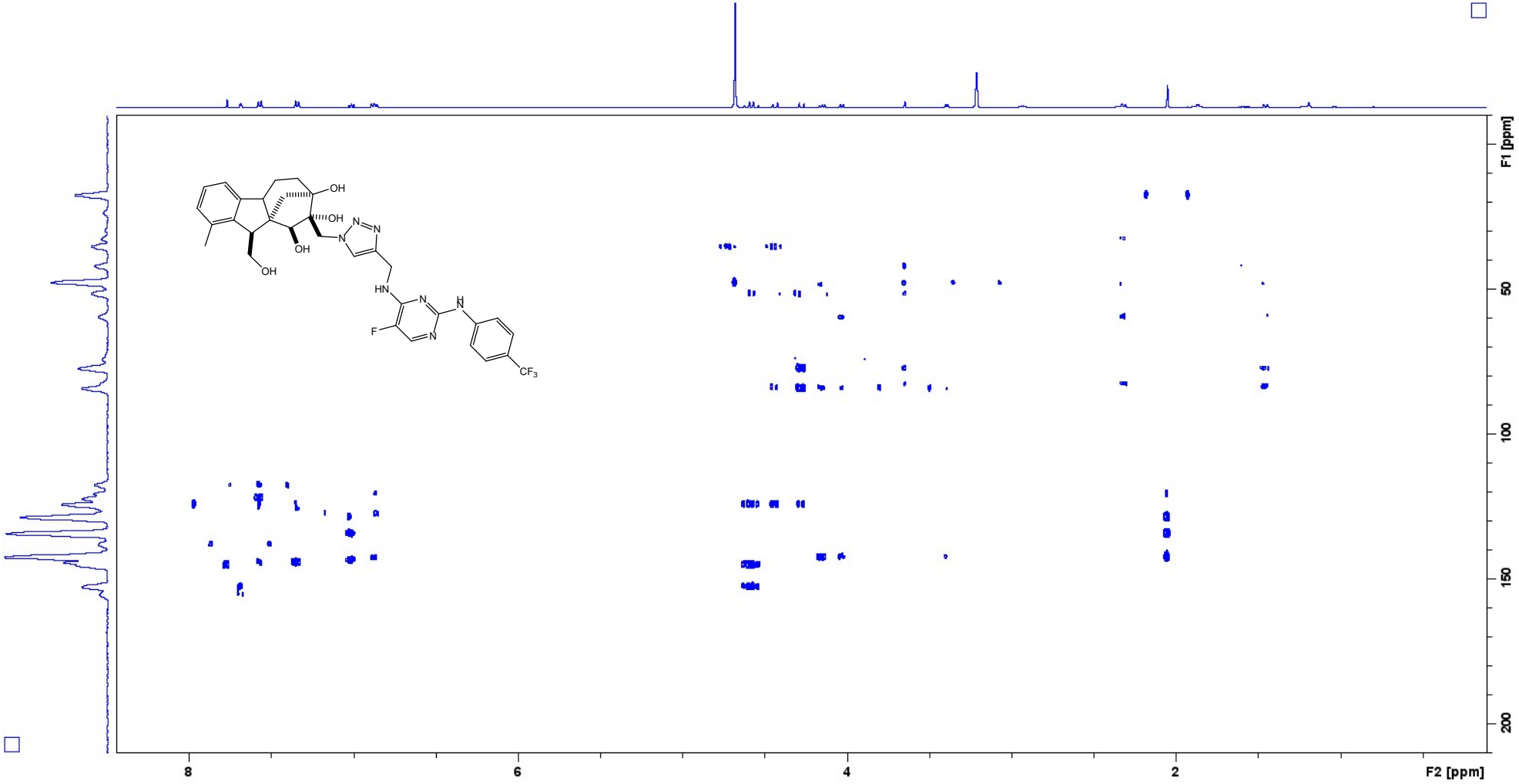
NOESY of (7*S*,8*R*,9*S*,9a*R*,10*S*)-8-((4-(((5-Fluoro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-10-(hydroxymethyl)-1-methyl-4b,5,6,8,9,10-hexahydro-7*H*-7,9a-methanobenzo[*a*]azulene-7,8,9-triol **38**



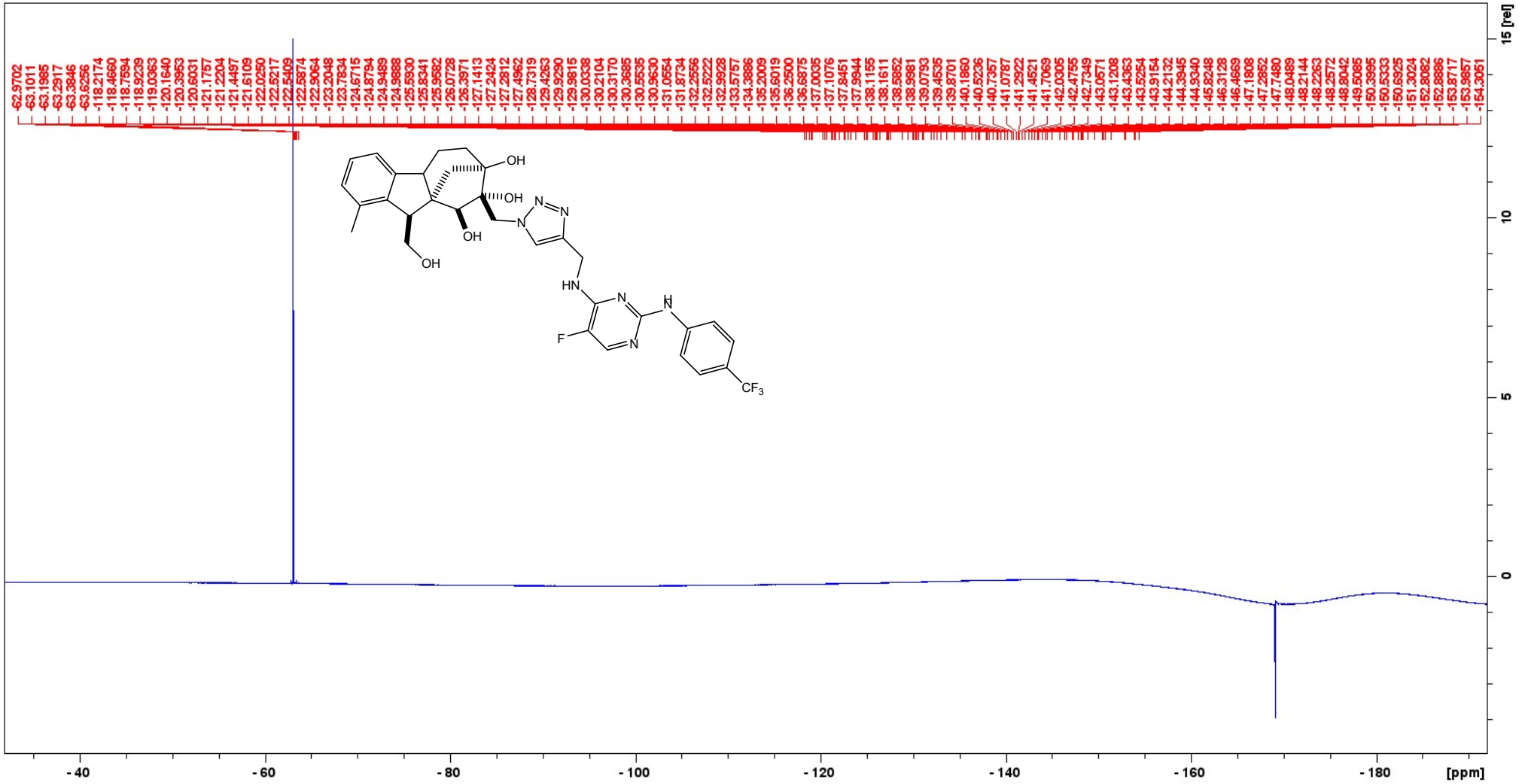
HSQC of (7*S*,8*R*,9*S*,9a*R*,10*S*)-8-((4-(((5-Fluoro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-10-(hydroxymethyl)-1-methyl-4b,5,6,8,9,10-hexahydro-7*H*-7,9a-methanobenzo[*a*]azulene-7,8,9-triol **38**



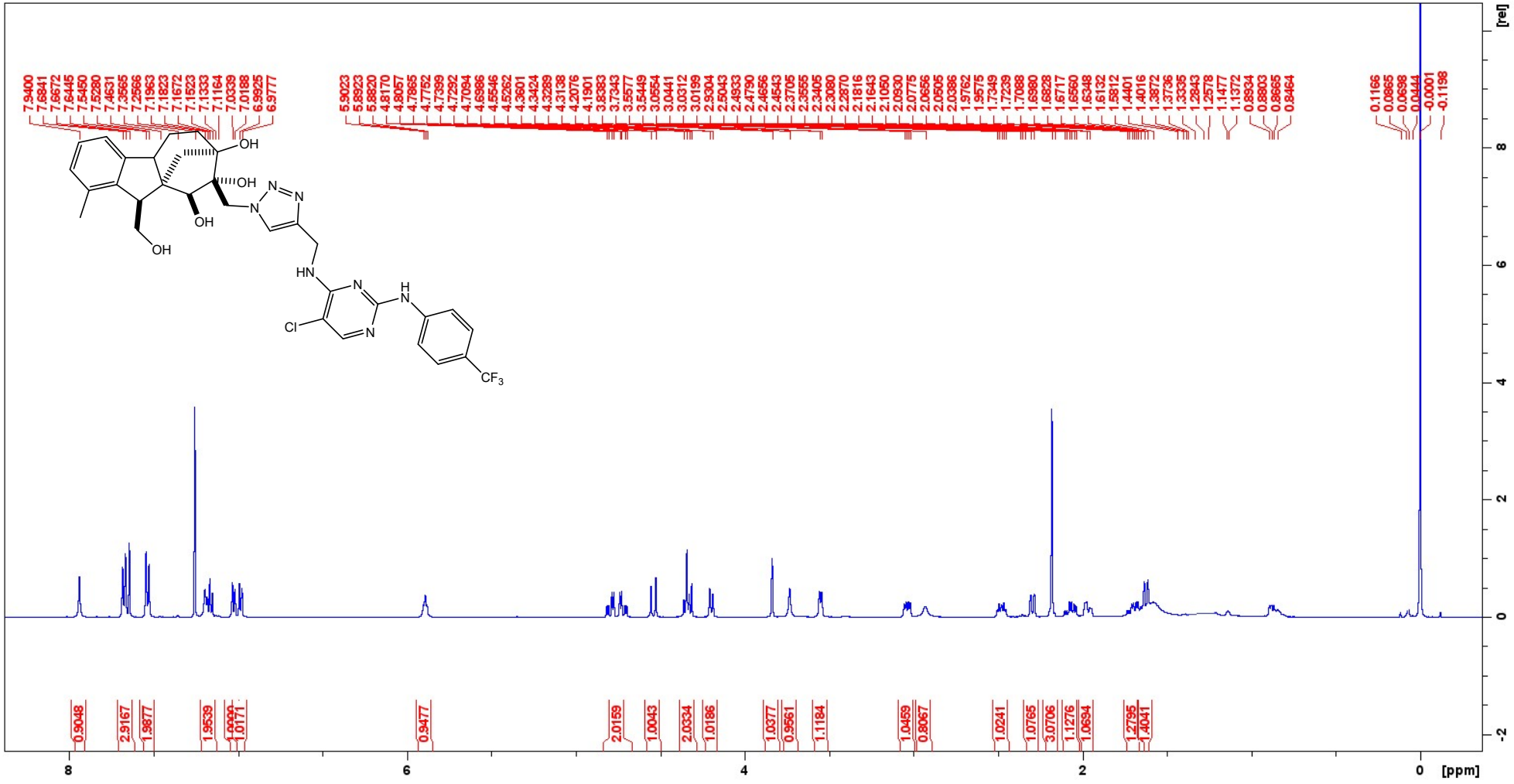
HMBC of (7*S*,8*R*,9*S*,9a*R*,10*S*)-8-((4-(((5-Fluoro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-10-(hydroxymethyl)-1-methyl-4b,5,6,8,9,10-hexahydro-7*H*-7,9a-methanobenzo[*a*]azulene-7,8,9-triol **38**



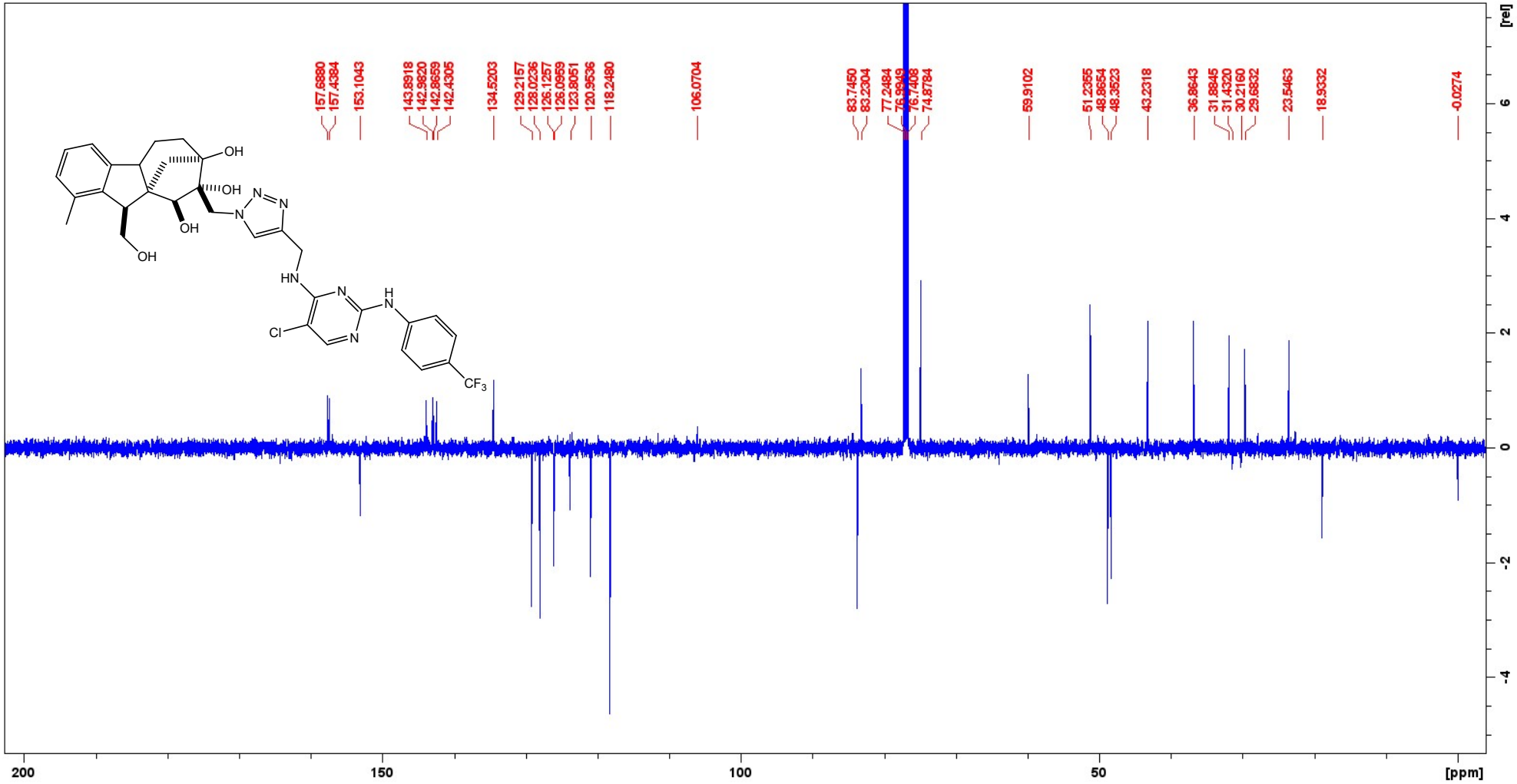
^{19}F *J*-MOD NMR (470 MHz) of (7*S*,8*R*,9*S*,9a*R*,10*S*)-8-((4-(((5-Fluoro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-10-(hydroxymethyl)-1-methyl-4b,5,6,8,9,10-hexahydro-7*H*-7,9a-methanobenzo[*a*]azulene-7,8,9-triol **38**



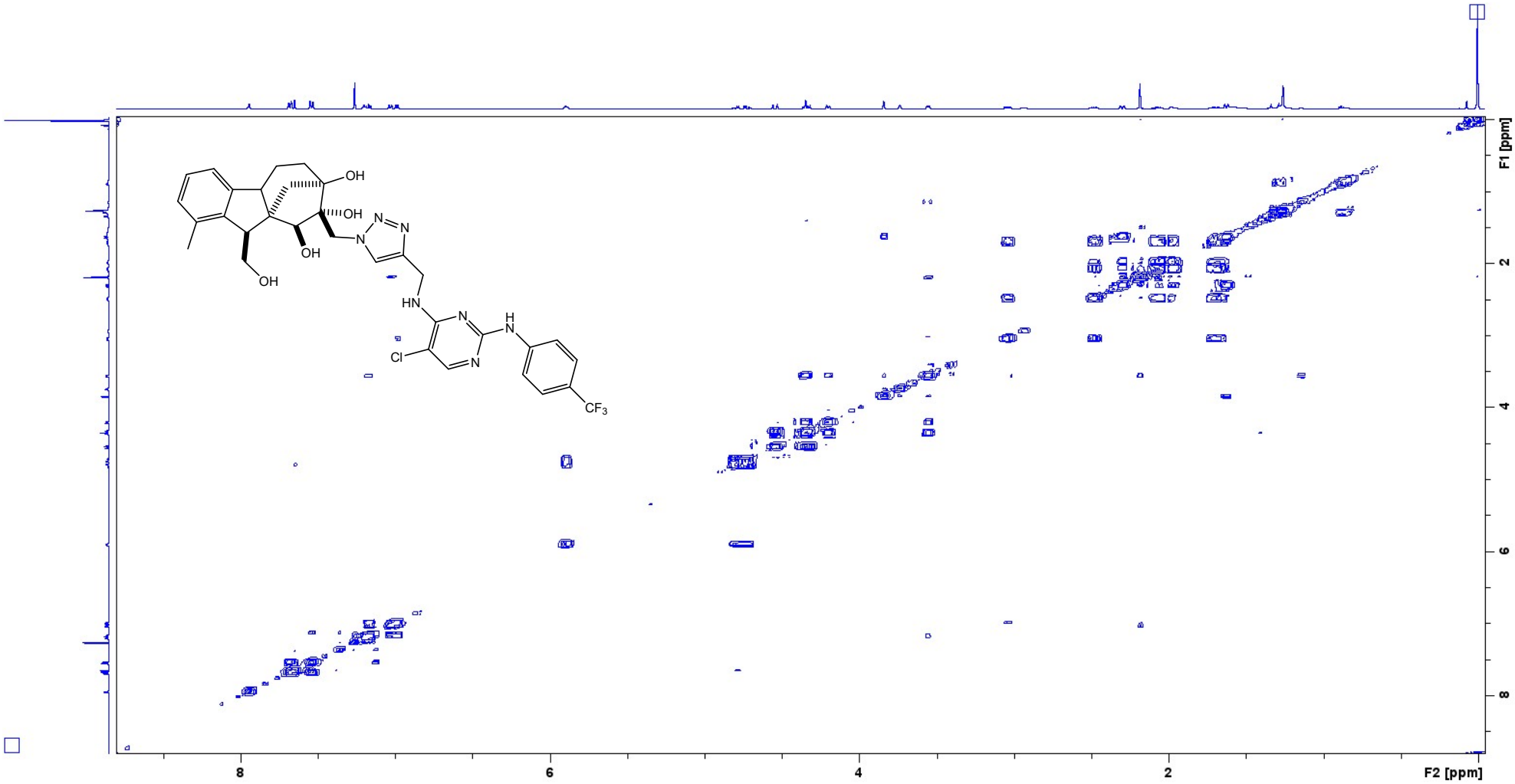
^{1}H-NMR (500 MHz) of (7*S*,8*R*,9*S*,9a*R*,10*S*)-8-((4-(((5-chloro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-10-(hydroxymethyl)-1-methyl-4b,5,6,8,9,10-hexahydro-7*H*-7,9a-methanobenzo[a]azulene-7,8,9-triol **39**



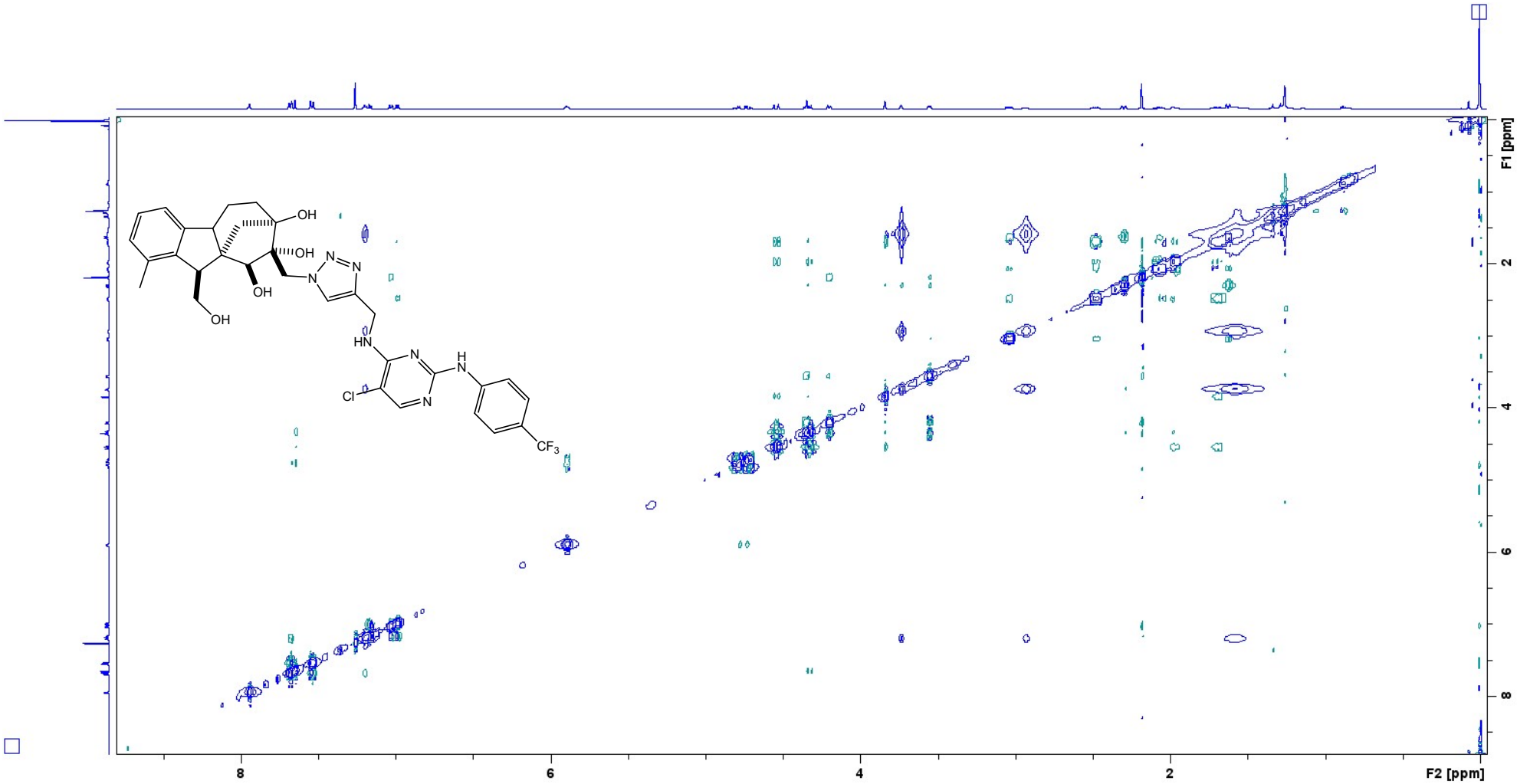
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of (7*S*,8*R*,9*S*,9a*R*,10*S*)-8-((4-(((5-chloro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-10-(hydroxymethyl)-1-methyl-4b,5,6,8,9,10-hexahydro-7*H*-7,9a-methanobenzo[a]azulene-7,8,9-triol **39**



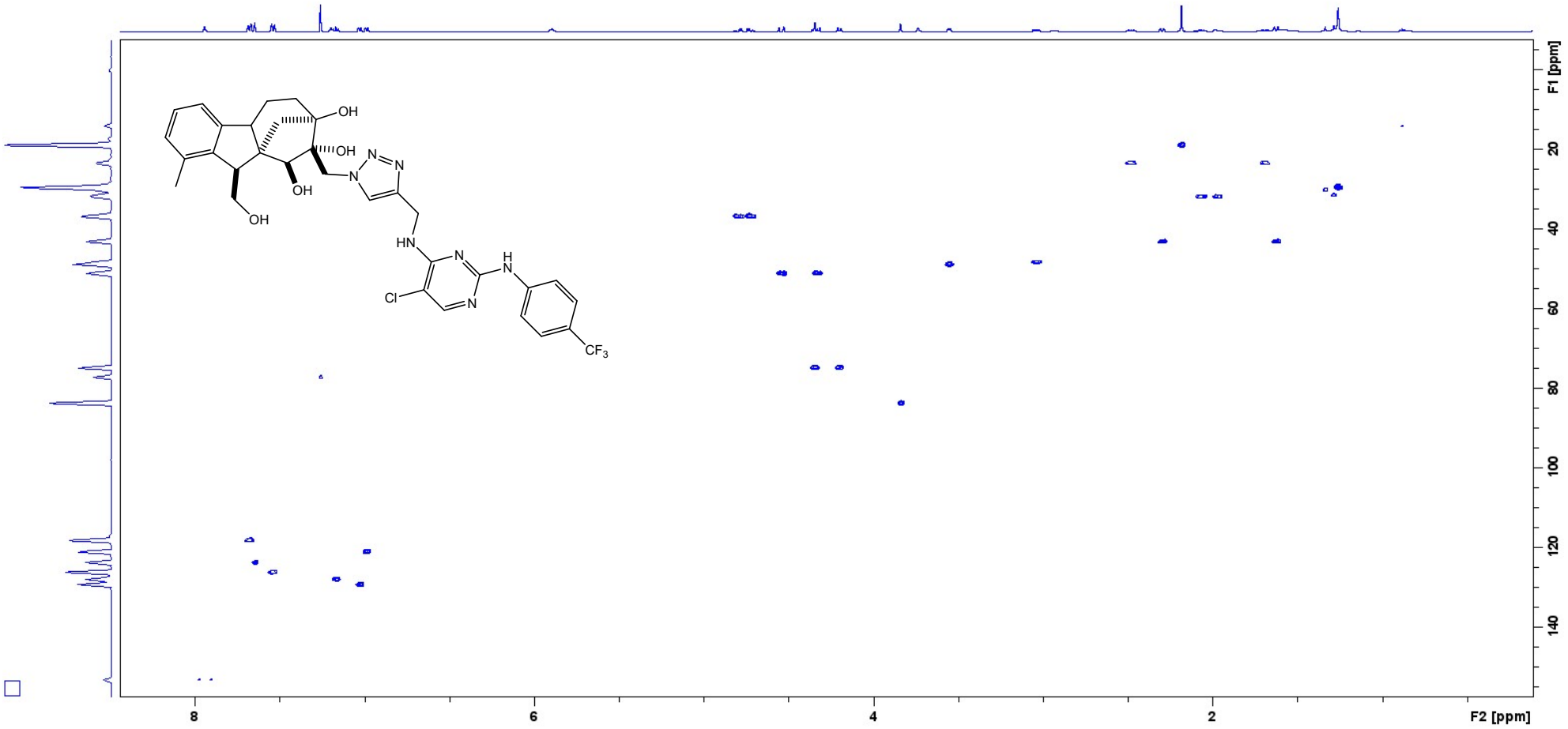
COSY of (7*S*,8*R*,9*S*,9a*R*,10*S*)-8-((4-(((5-chloro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-10-(hydroxymethyl)-1-methyl-4b,5,6,8,9,10-hexahydro-7*H*-7,9a-methanobenzo[a]azulene-7,8,9-triol **39**



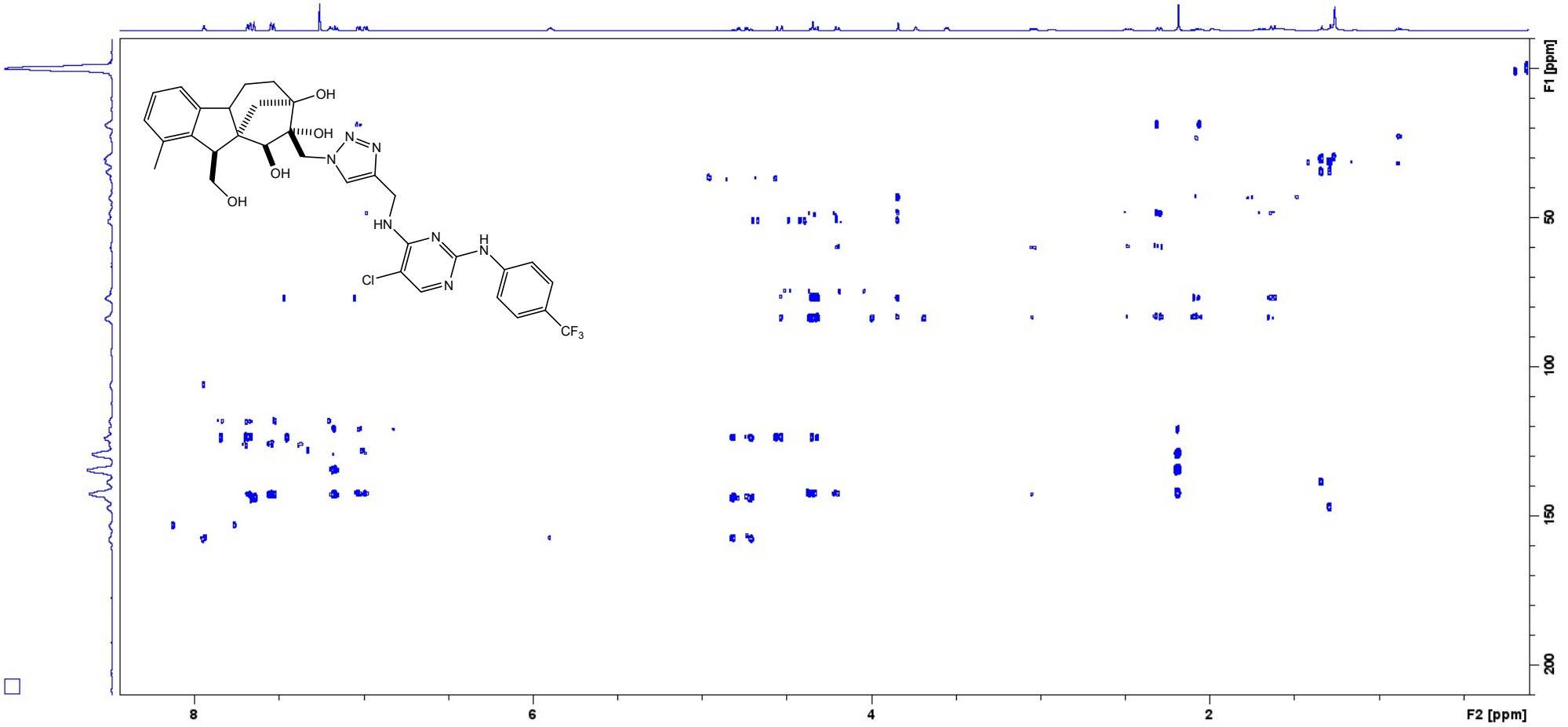
NOESY of (7*S*,8*R*,9*S*,9a*R*,10*S*)-8-((4-(((5-chloro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-10-(hydroxymethyl)-1-methyl-4b,5,6,8,9,10-hexahydro-7*H*-7,9a-methanobenzo[a]azulene-7,8,9-triol **39**



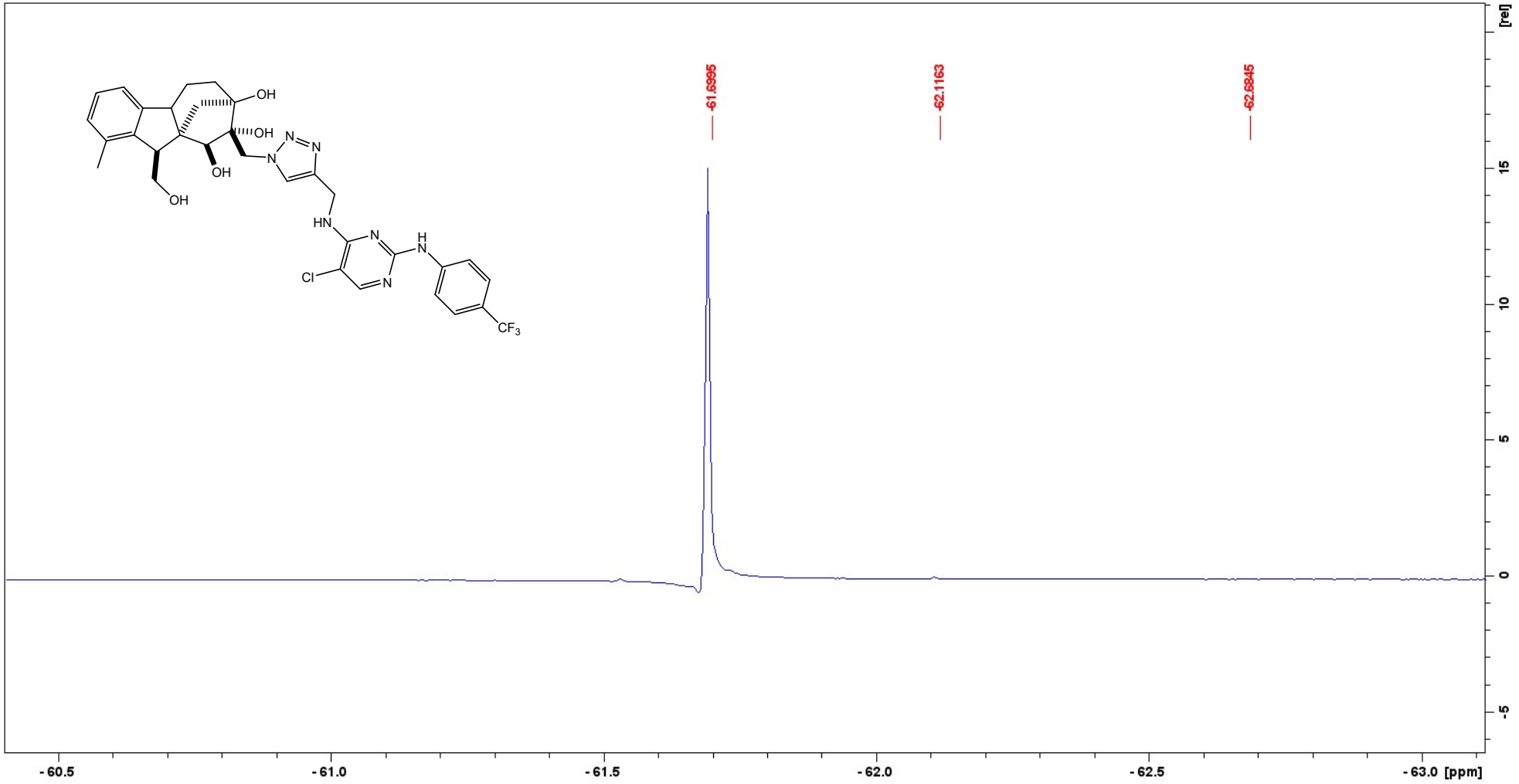
HSQC of (7*S*,8*R*,9*S*,9a*R*,10*S*)-8-((4-(((5-chloro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-10-(hydroxymethyl)-1-methyl-4b,5,6,8,9,10-hexahydro-7*H*-7,9a-methanobenzo[a]azulene-7,8,9-triol **39**



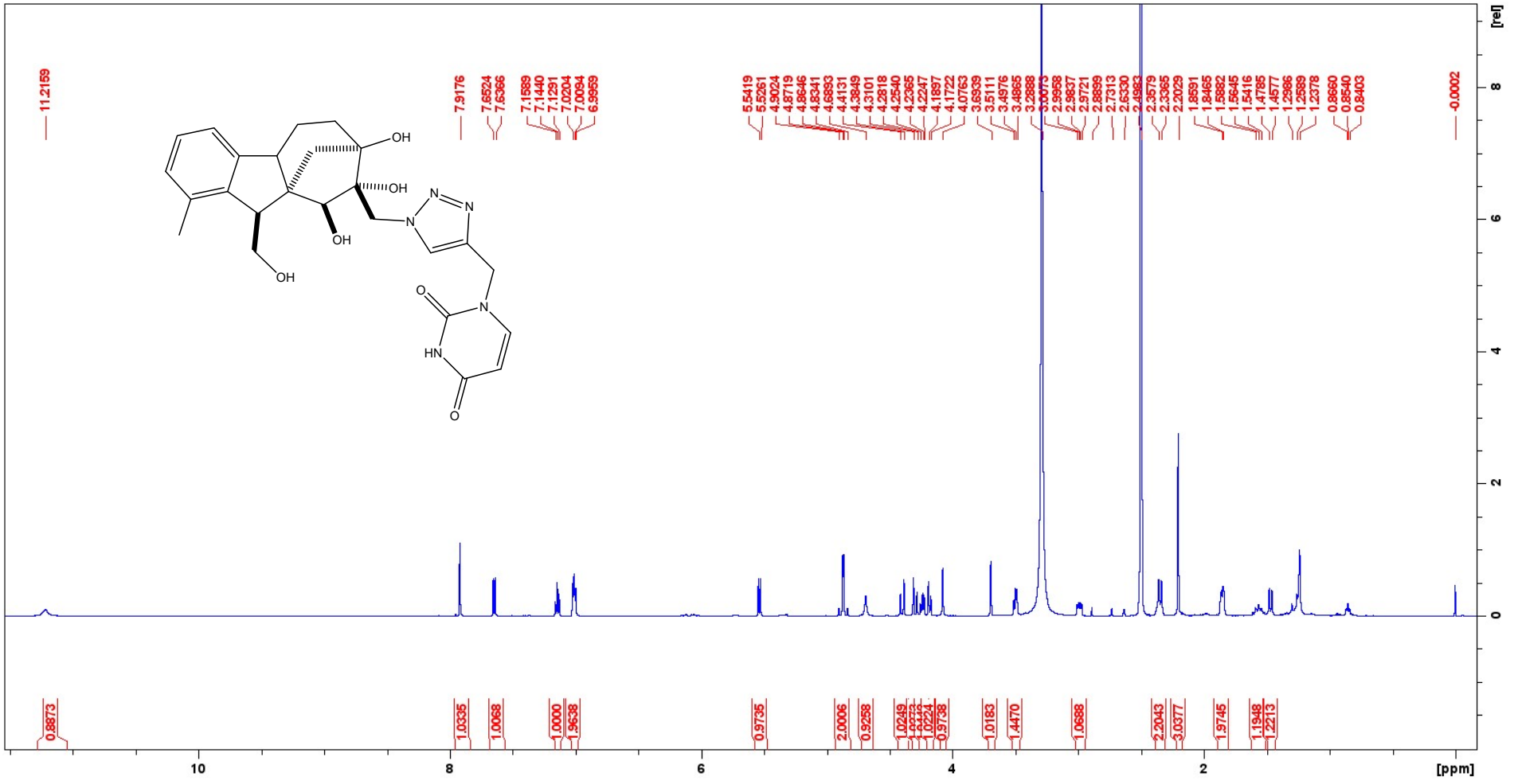
HMBC of (7*S*,8*R*,9*S*,9a*R*,10*S*)-8-((4-(((5-chloro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-10-(hydroxymethyl)-1-methyl-4b,5,6,8,9,10-hexahydro-7*H*-7,9a-methanobenzo[a]azulene-7,8,9-triol **39**



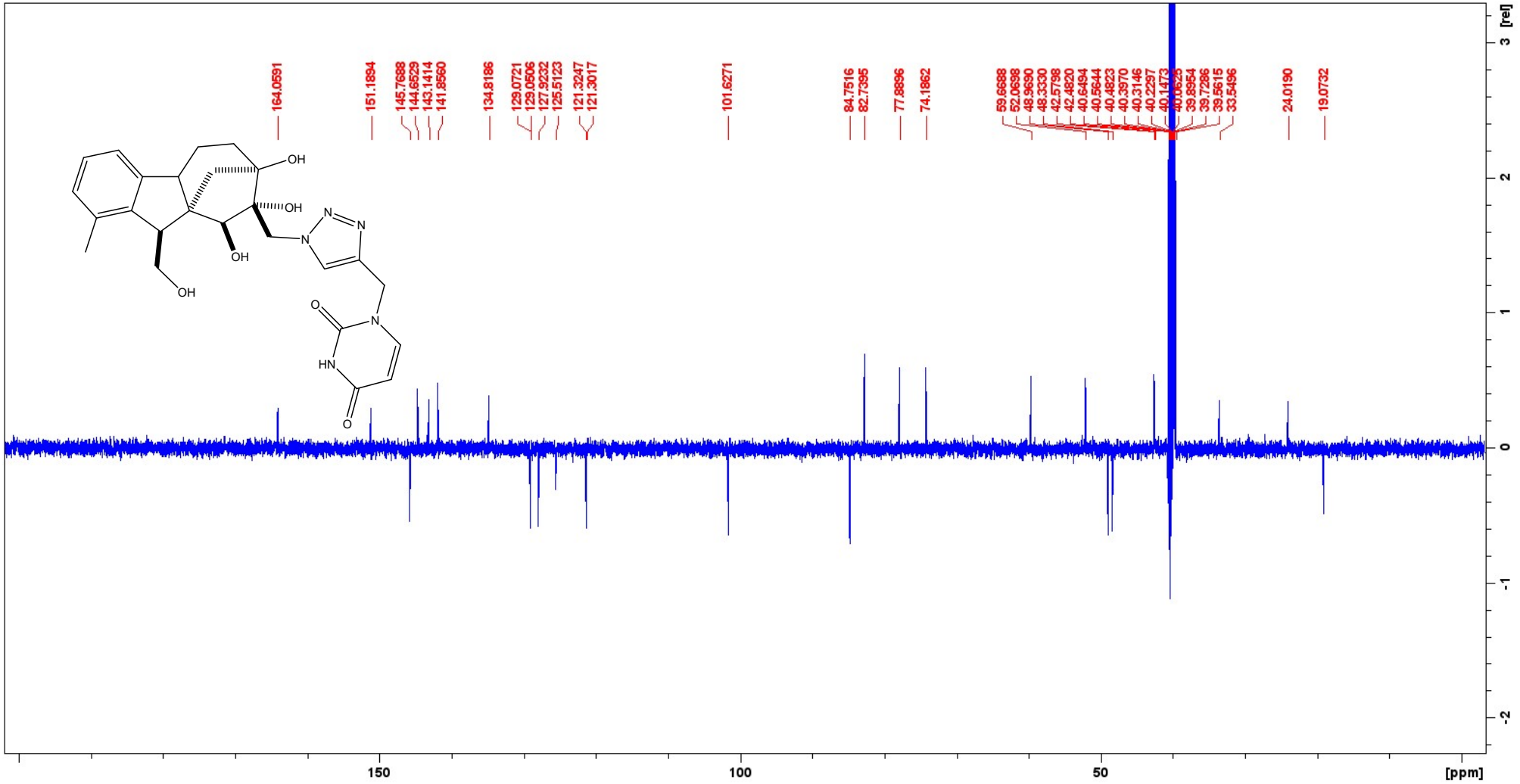
^{19}F *J*-MOD NMR (470 MHz) of (7*S*,8*R*,9*S*,9a*R*,10*S*)-8-((4-(((5-chloro-2-((4-(trifluoromethyl)phenyl)amino)pyrimidin-4-yl)amino)methyl)-1*H*-1,2,3-triazol-1-yl)methyl)-10-(hydroxymethyl)-1-methyl-4b,5,6,8,9,10-hexahydro-7*H*-7,9a-methanobenzo[a]azulene-7,8,9-triol **39**



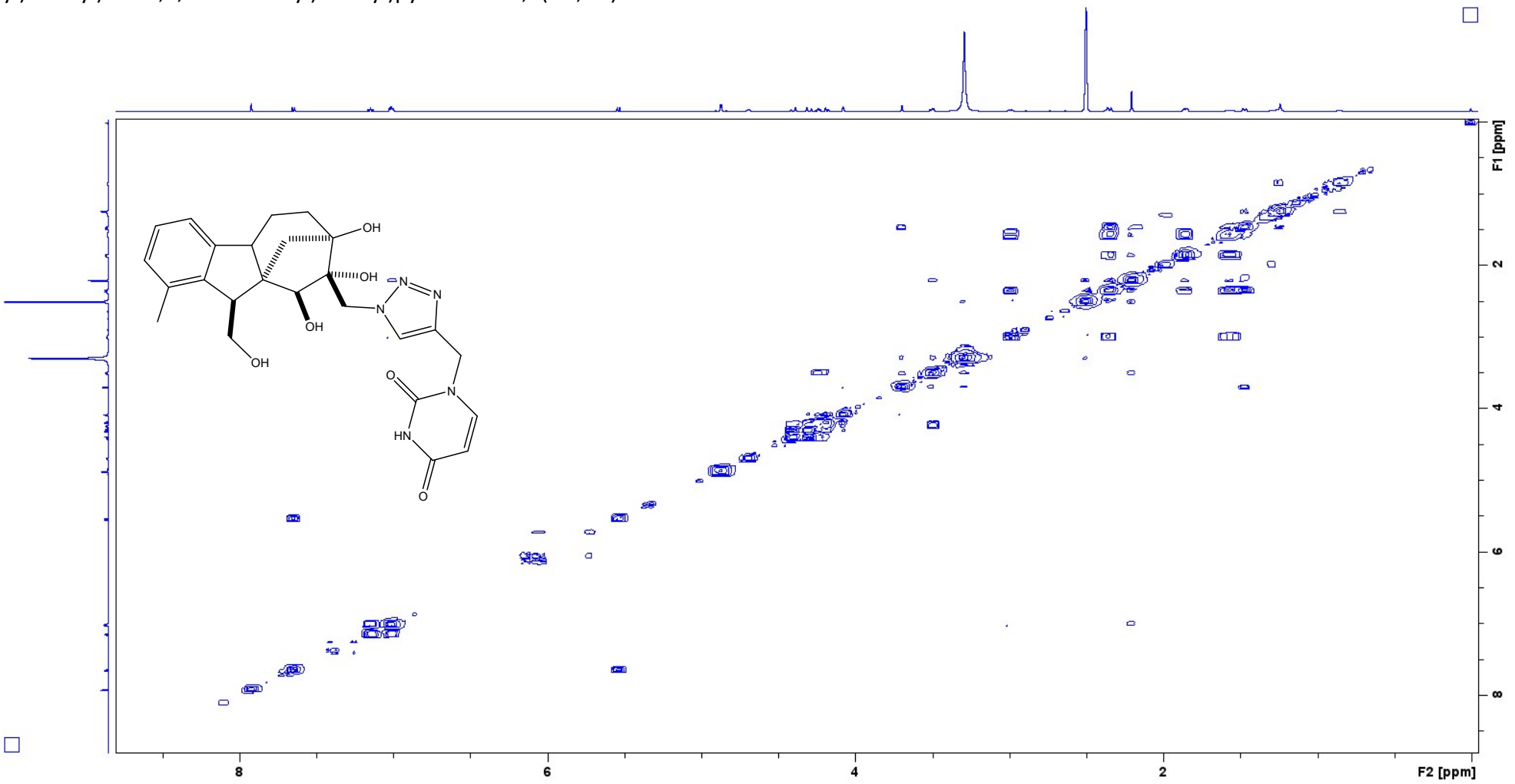
^{1}H-NMR (500 MHz) of 1-((1-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-Trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)-1*H*-1,2,3-triazol-4-yl)methyl)pyrimidine-2,4(1*H*,3*H*)-dione **40**



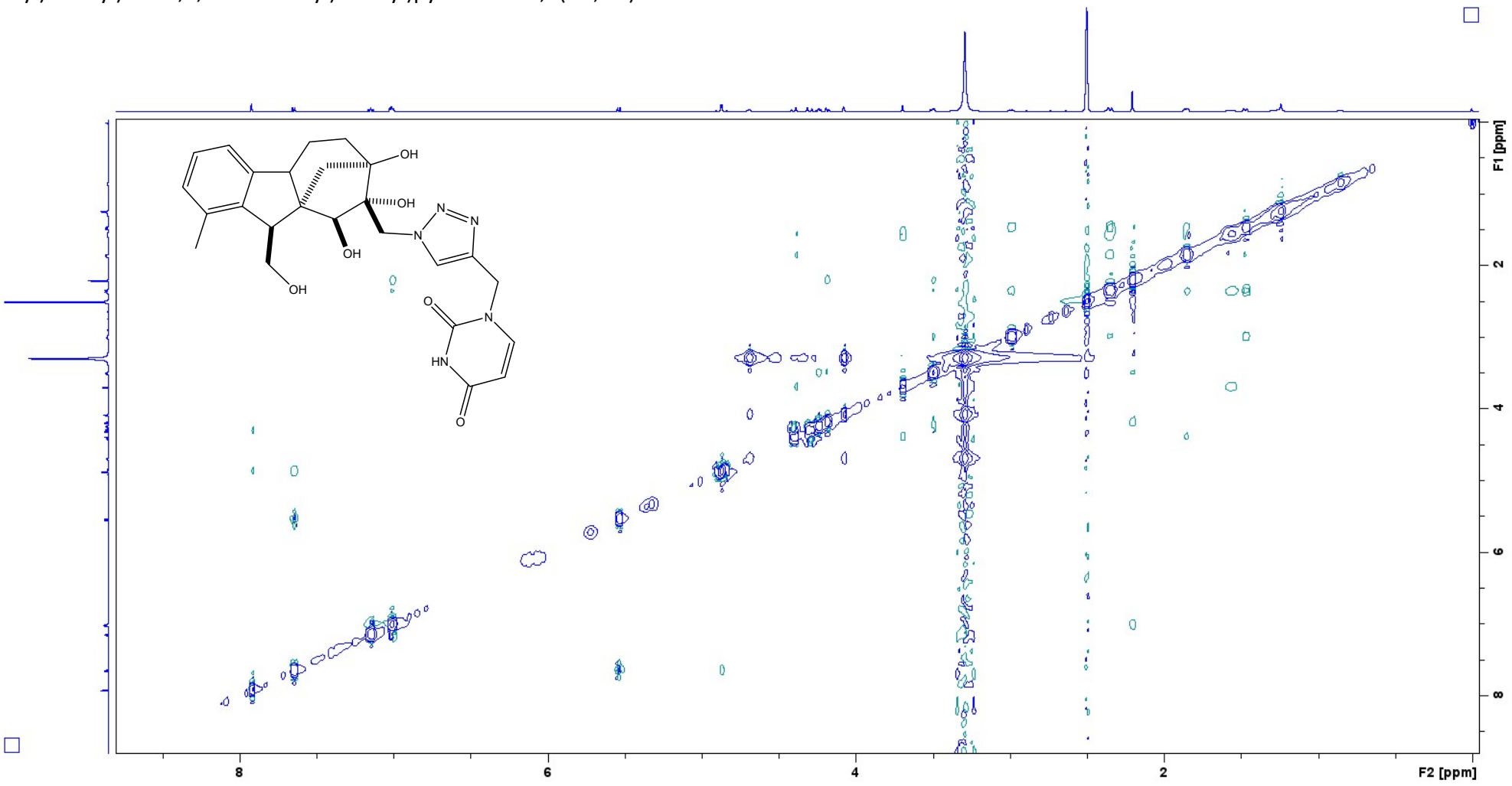
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of 1-((1-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-Trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)-1*H*-1,2,3-triazol-4-yl)methyl)pyrimidine-2,4(1*H*,3*H*)-dione **40**



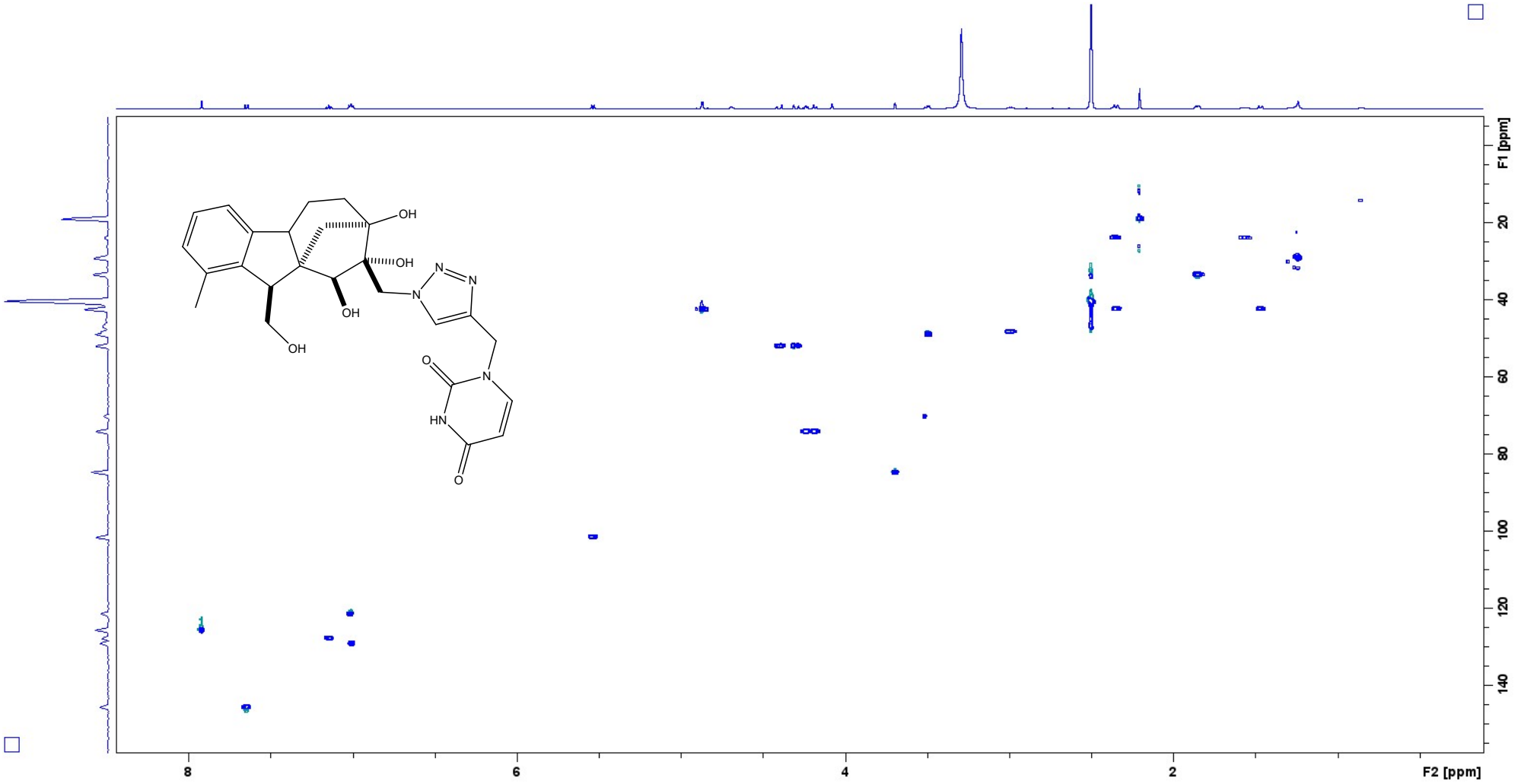
COSY of 1-((1-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-Trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)-1*H*-1,2,3-triazol-4-yl)methyl)pyrimidine-2,4(1*H*,3*H*)-dione **40**



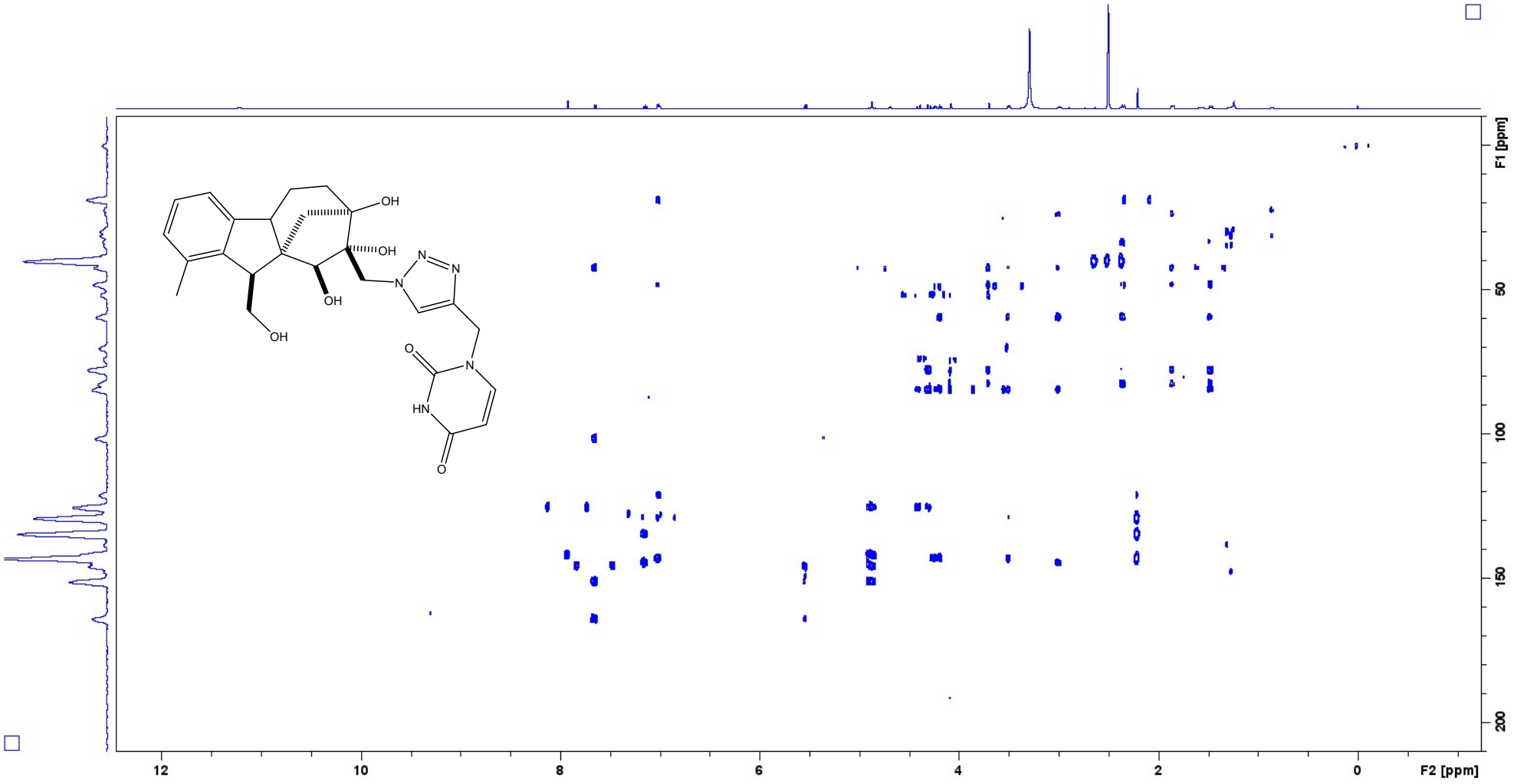
NOESY of 1-((1-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-Trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)-1*H*-1,2,3-triazol-4-yl)methyl)pyrimidine-2,4(1*H*,3*H*)-dione **40**



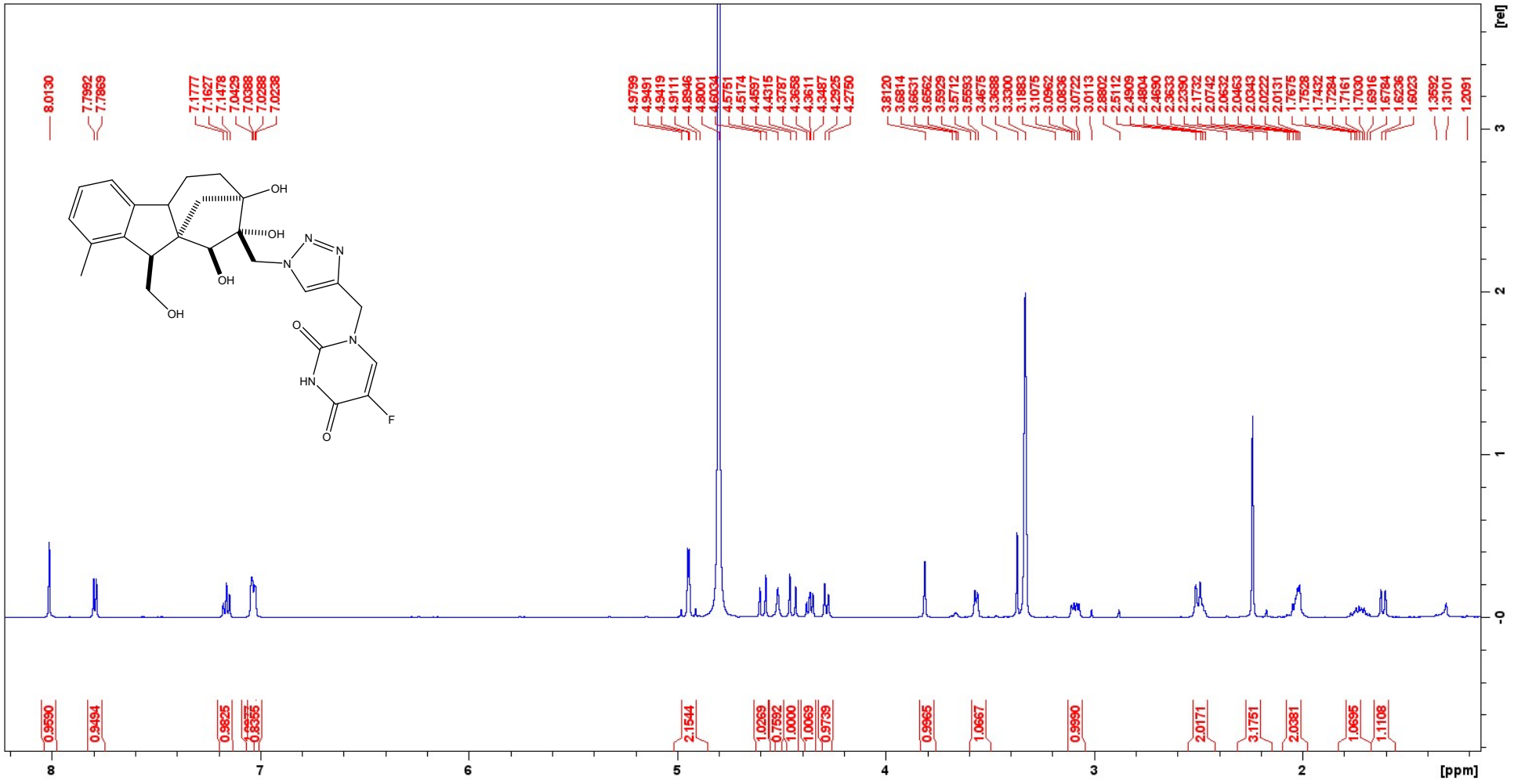
HSQC of 1-((1-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-Trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)-1*H*-1,2,3-triazol-4-yl)methyl)pyrimidine-2,4(1*H*,3*H*)-dione **40**



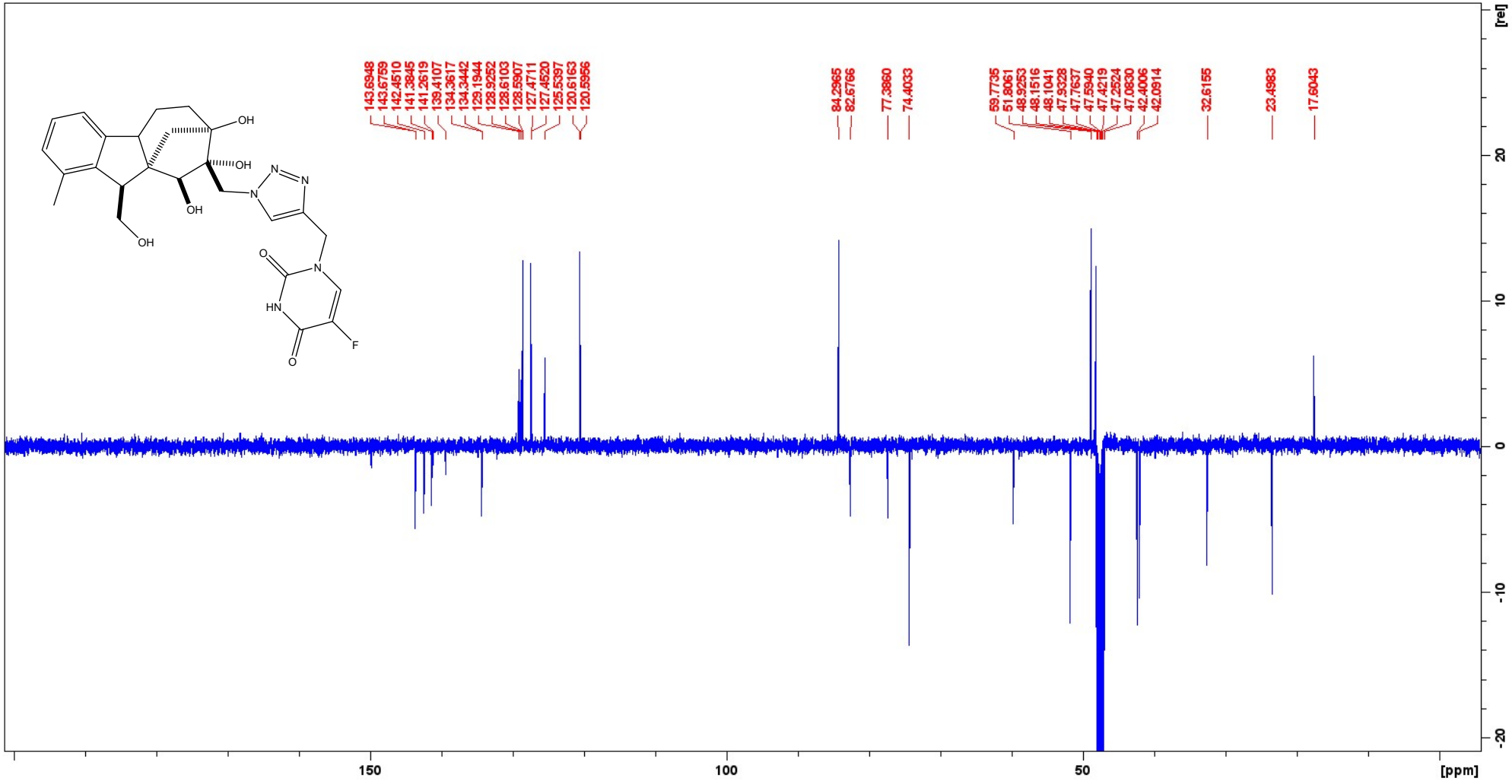
HMBC of 1-((1-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-Trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)-1*H*-1,2,3-triazol-4-yl)methyl)pyrimidine-2,4(1*H*,3*H*)-dione **40**



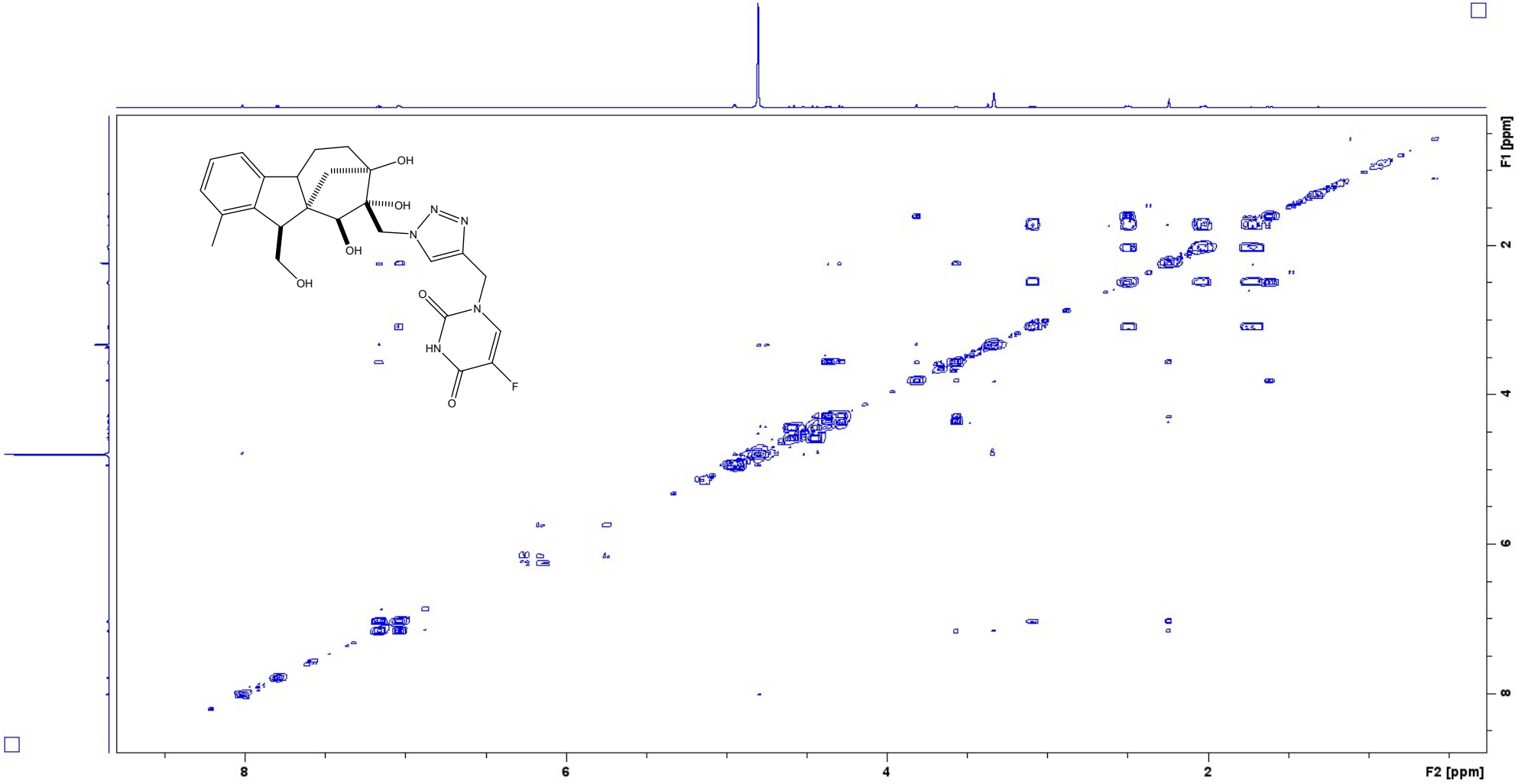
^{1}H-NMR (500 MHz) of 5-Fluoro-1-((1-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)-1*H*-1,2,3-triazol-4-yl)methyl)pyrimidine-2,4(1*H*,3*H*)-dione **41**



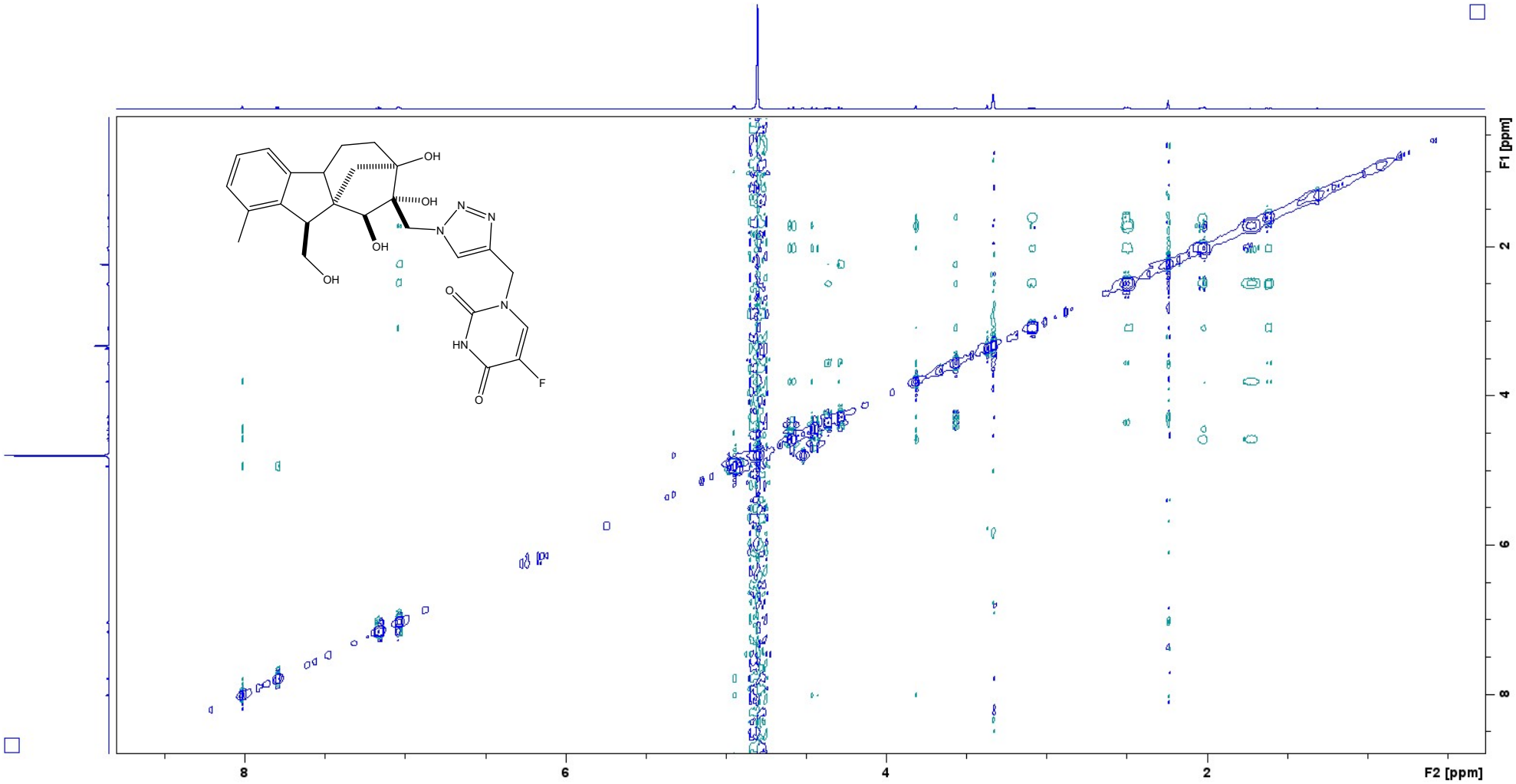
$^{13}C\{1H\}$ *J*-MOD NMR (125 MHz) of 5-Fluoro-1-((1-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)-1*H*-1,2,3-triazol-4-yl)methyl)pyrimidine-2,4(1*H*,3*H*)-dione **41**



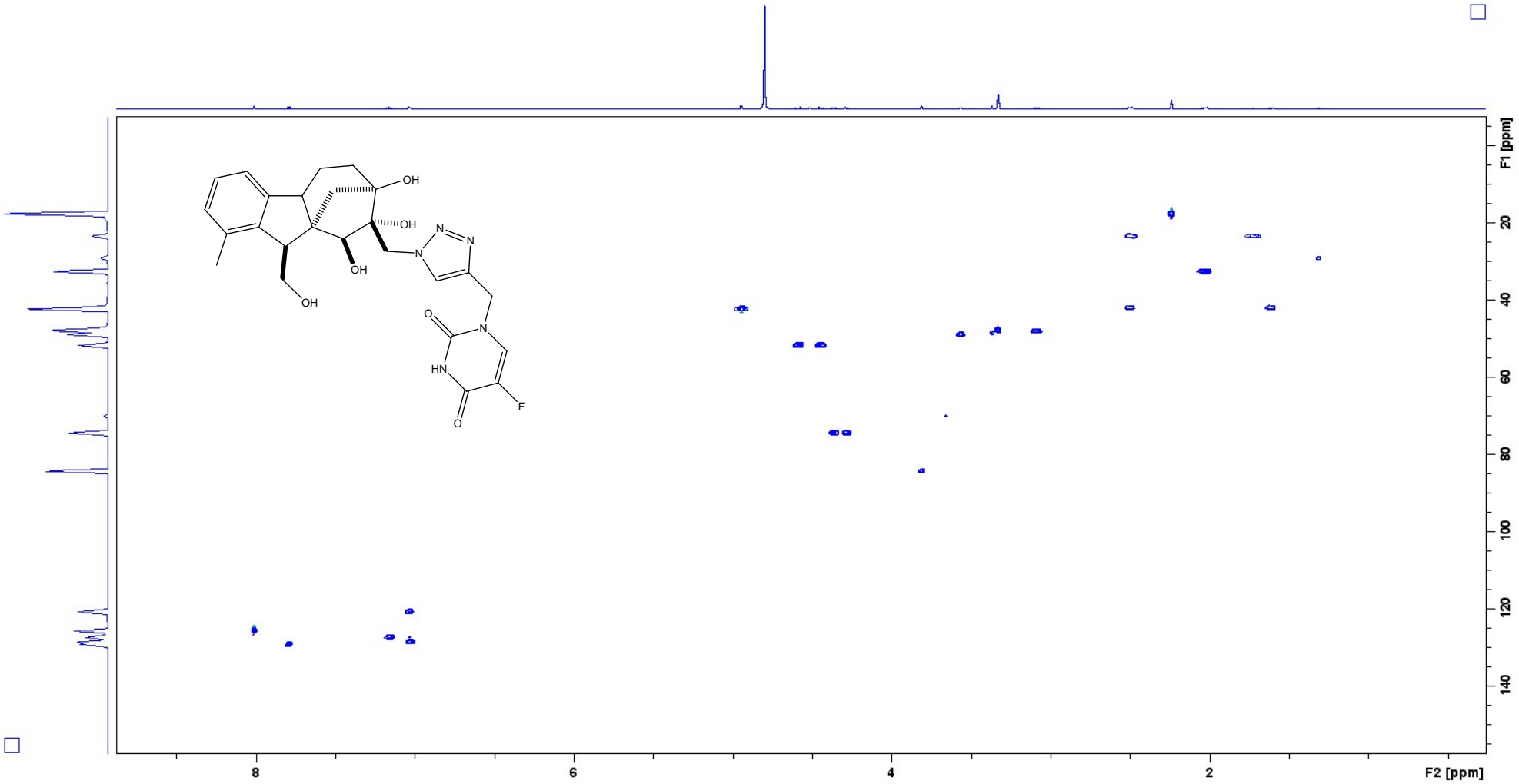
COSY of 5-Fluoro-1-((1-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)-1*H*-1,2,3-triazol-4-yl)methyl)pyrimidine-2,4(1*H*,3*H*)-dione **41**



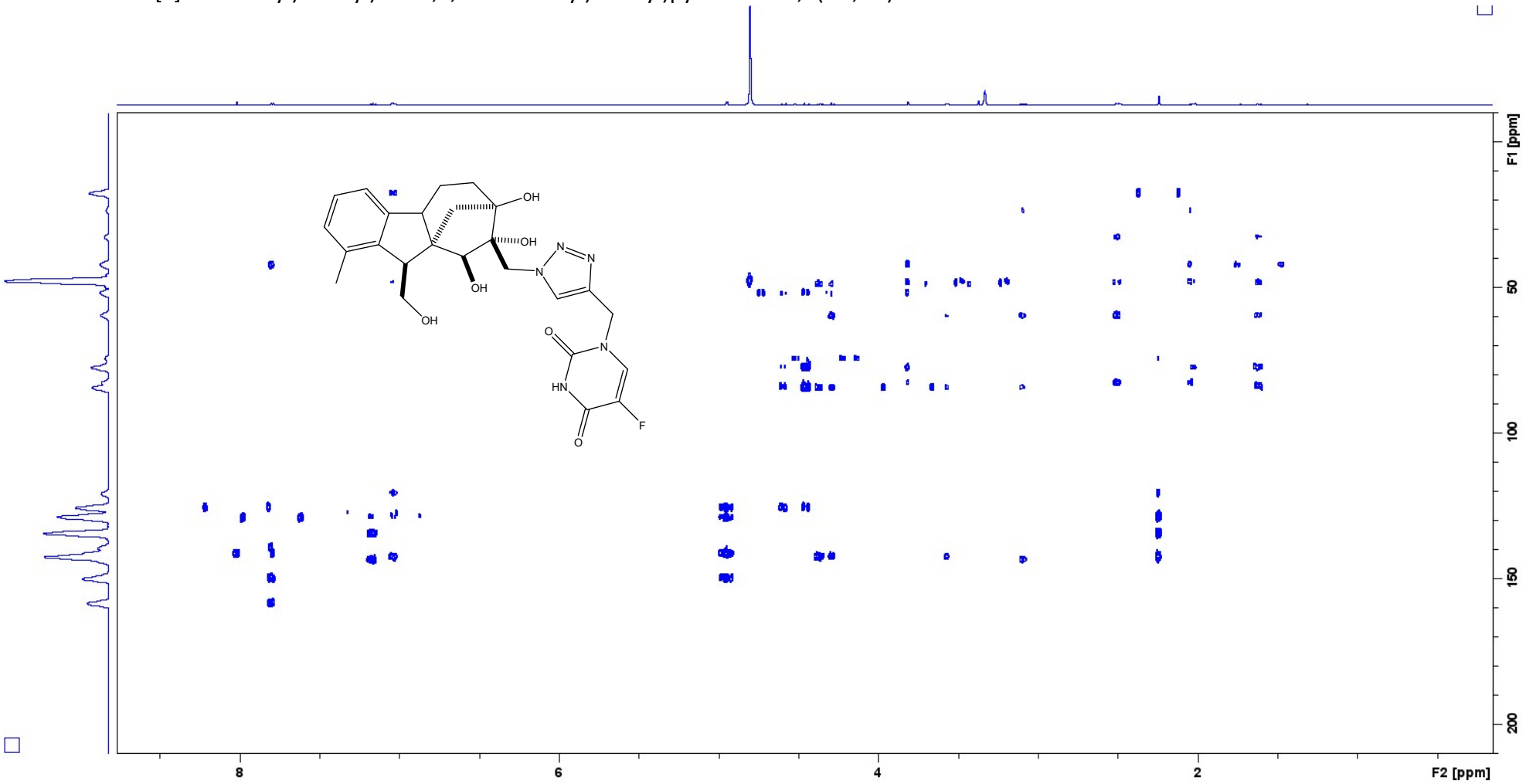
NOESY of 5-Fluoro-1-((1-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)-1*H*-1,2,3-triazol-4-yl)methyl)pyrimidine-2,4(1*H*,3*H*)-dione **41**



HSQC of 5-Fluoro-1-((1-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)-1*H*-1,2,3-triazol-4-yl)methyl)pyrimidine-2,4(1*H*,3*H*)-dione **41**



HMBC of 5-Fluoro-1-((1-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)-1*H*-1,2,3-triazol-4-yl)methyl)pyrimidine-2,4(1*H*,3*H*)-dione **41**



^{19}F *J*-MOD NMR (470 MHz) of 5-Fluoro-1-((1-(((7*S*,8*R*,9*S*,9a*R*,10*S*)-7,8,9-trihydroxy-10-(hydroxymethyl)-1-methyl-4b,6,7,8,9,10-hexahydro-5*H*-7,9a-methanobenzo[a]azulen-8-yl)methyl)-1*H*-1,2,3-triazol-4-yl)methyl)pyrimidine-2,4(1*H*,3*H*)-dione **41**

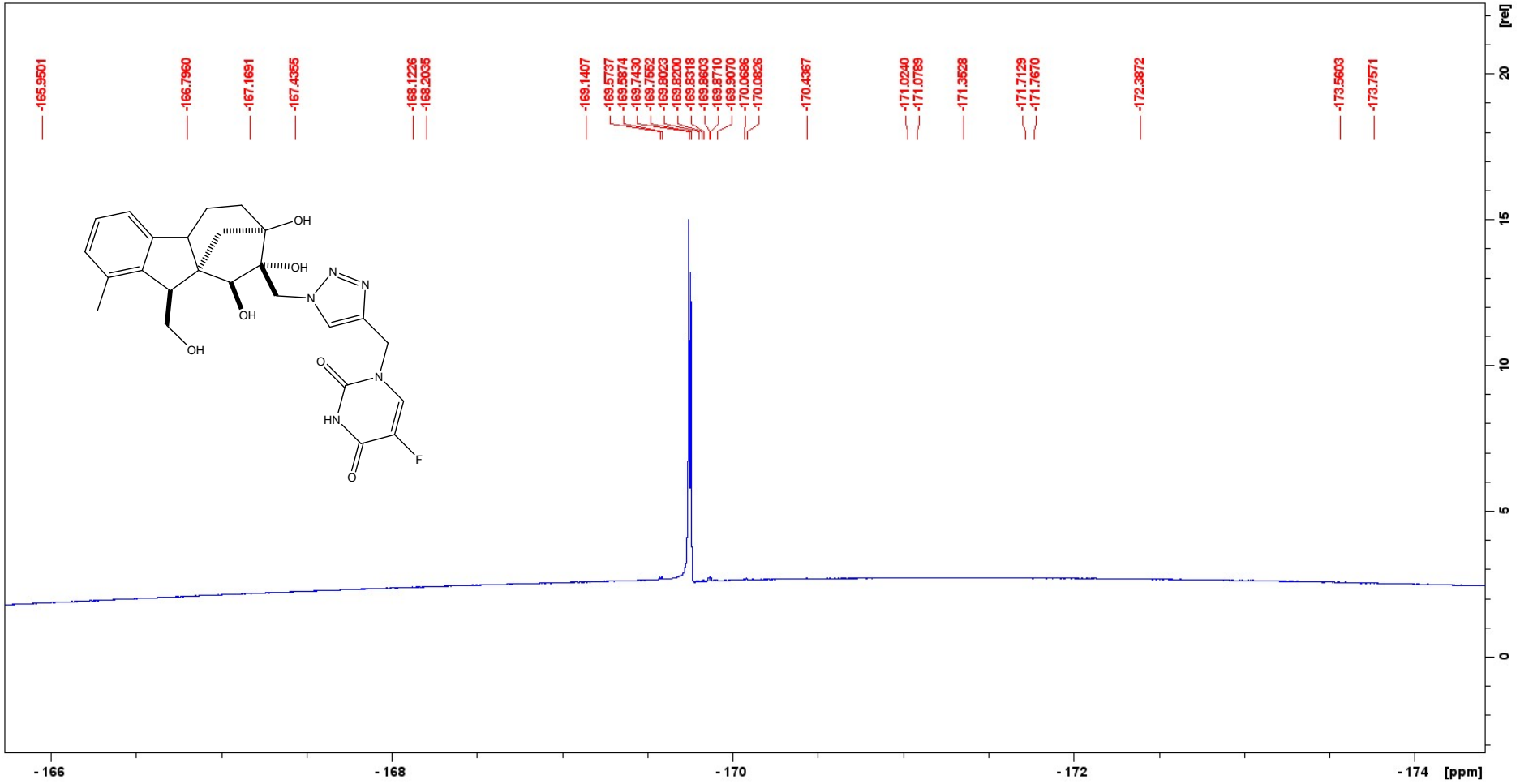
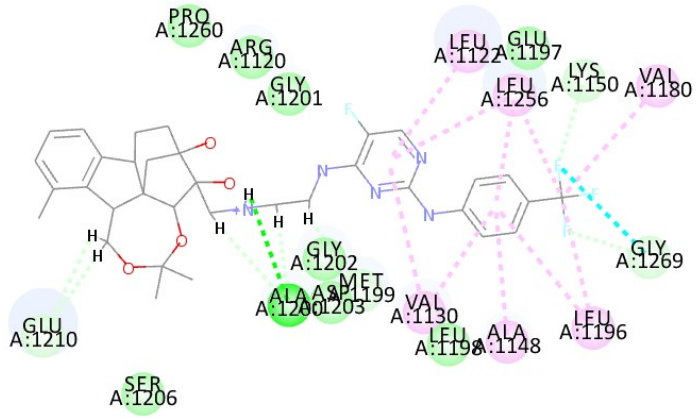
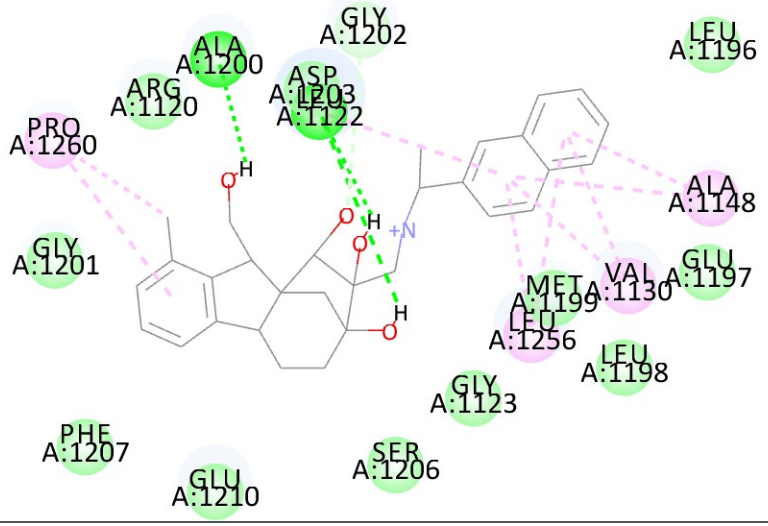
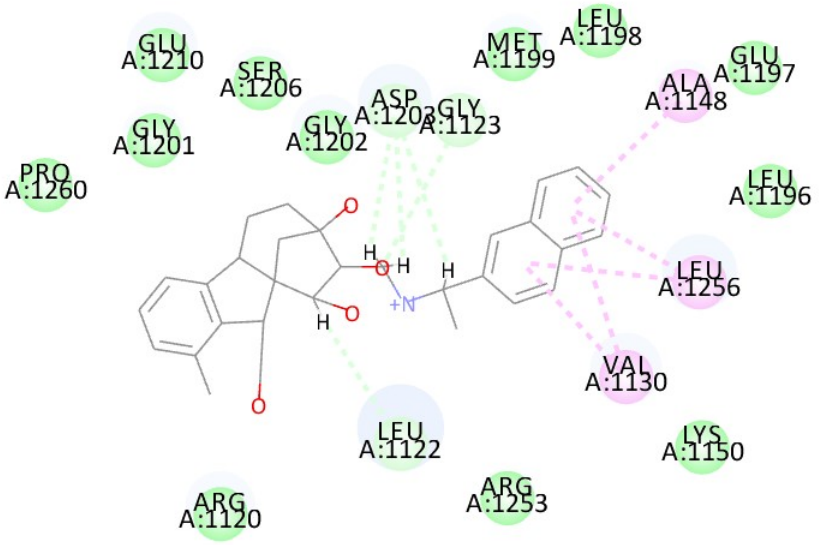
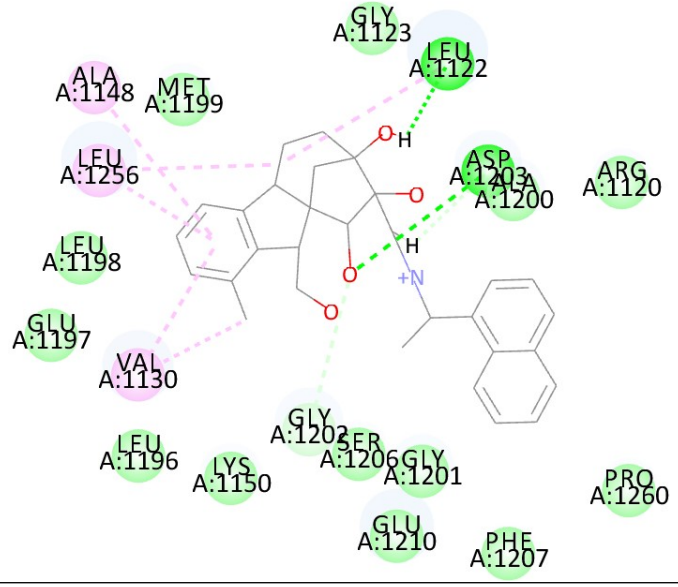
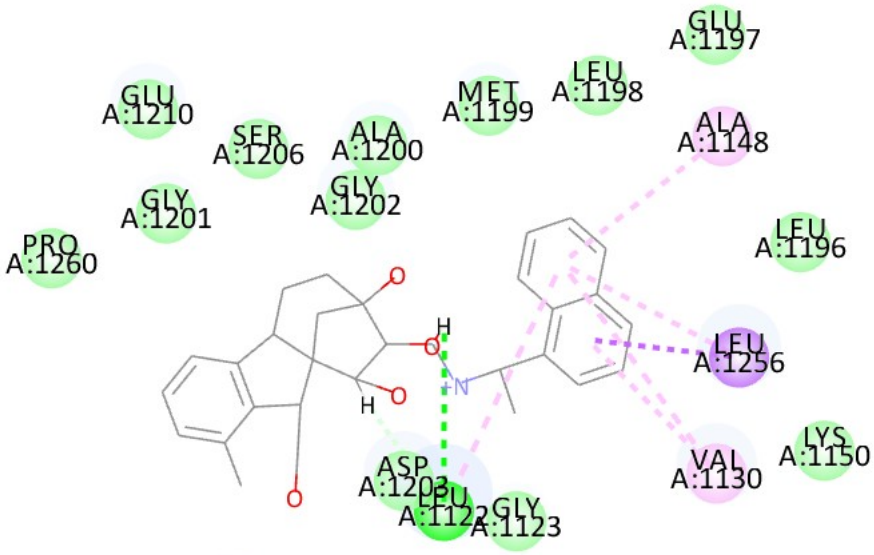
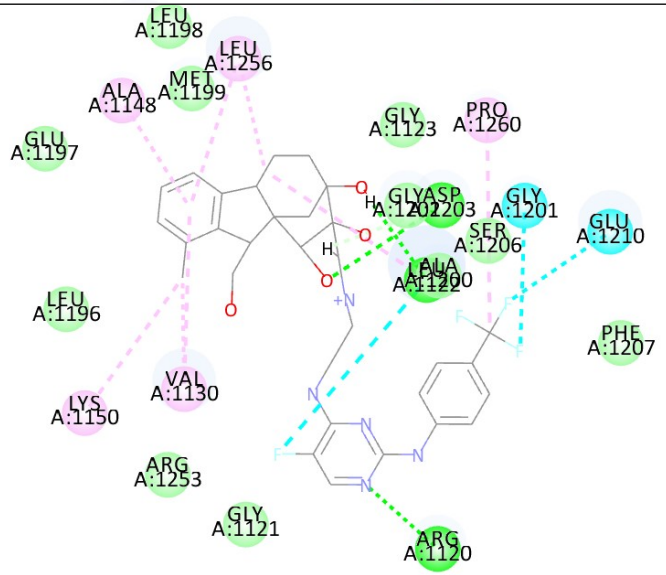
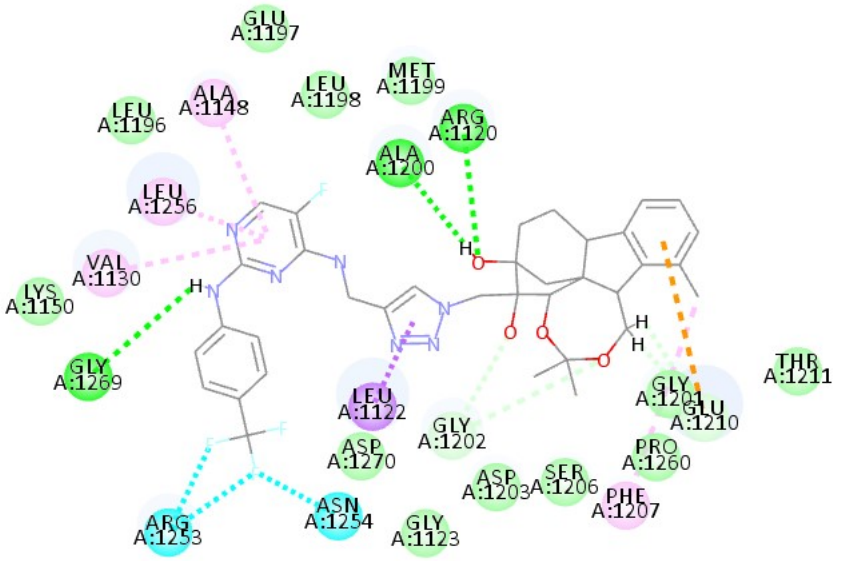
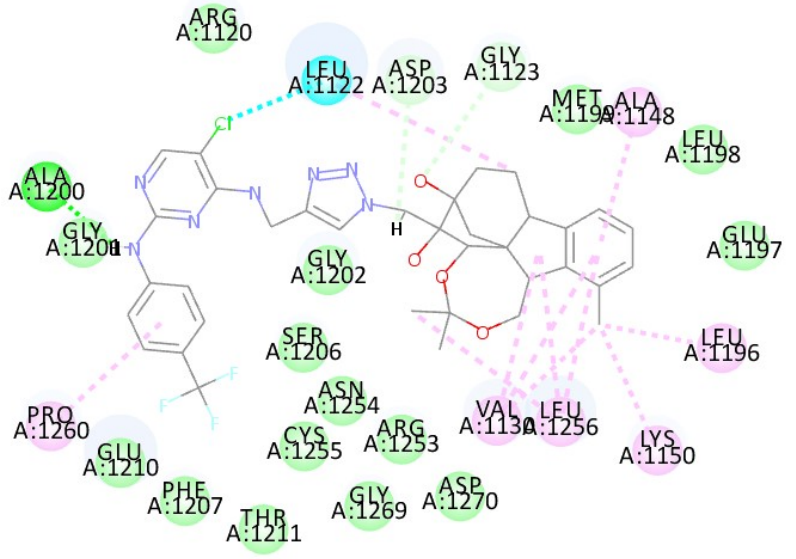


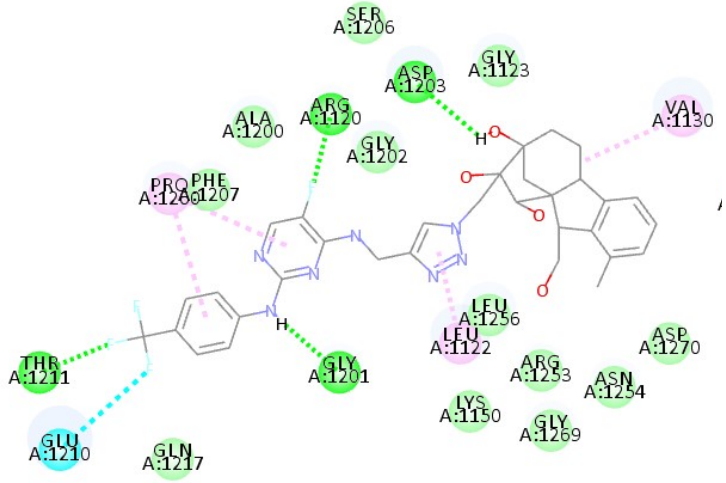
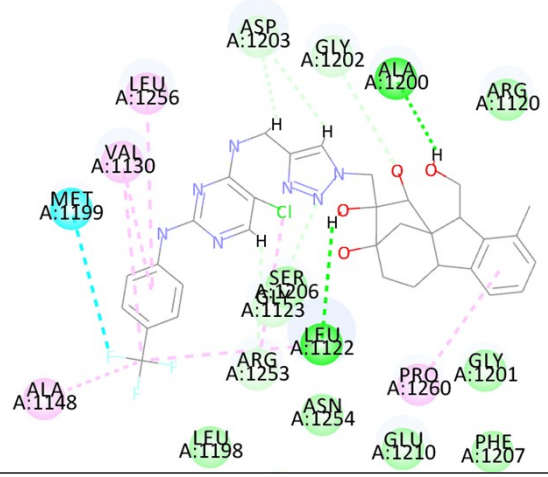
Table S2 Docking Study

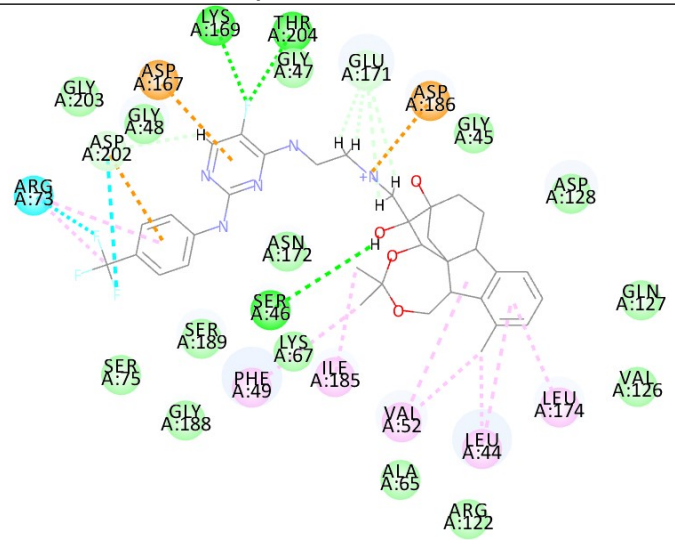
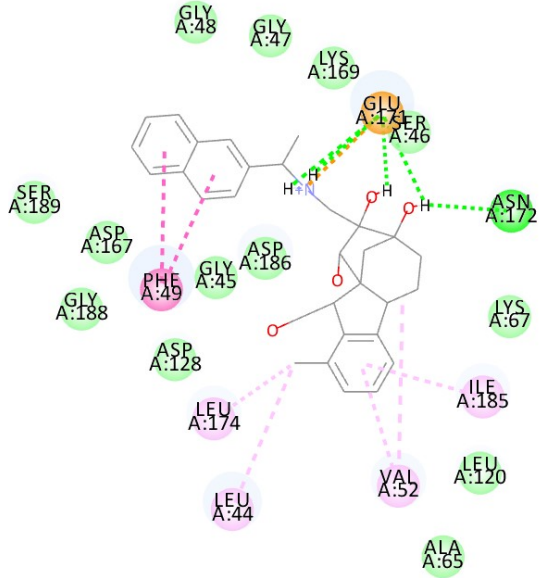
Compound	Interactions with ALK (PDB code: 3AOX, resolution: 1.75 Å)
18	
23	

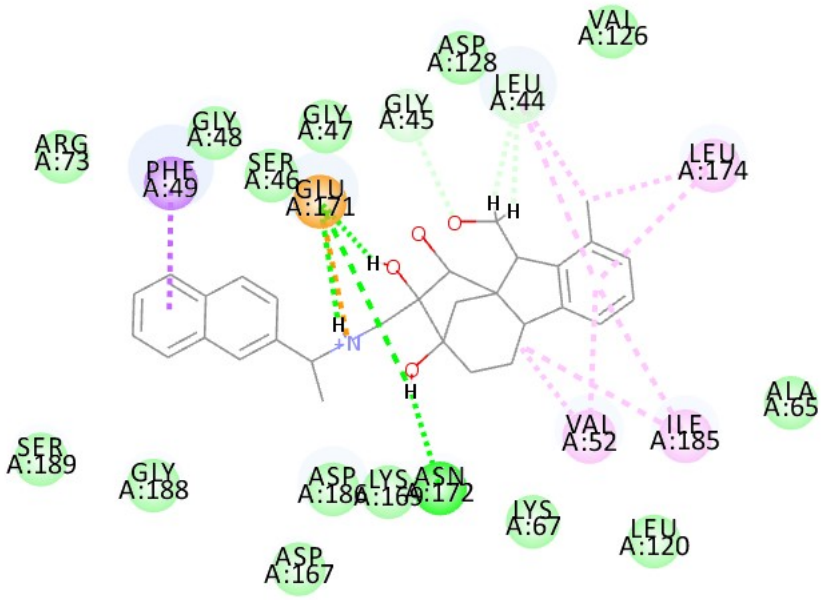
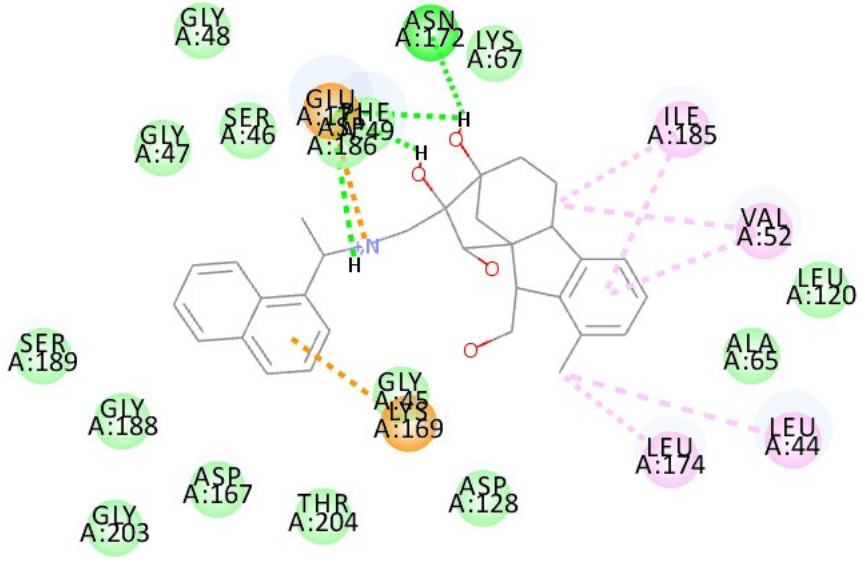
24	 GLU A:1210 SER A:1206 MET A:1199 LEU A:1198 GLU A:1197 ALA A:1148 ASP A:1203 GLY A:1123 GLY A:1201 GLY A:1202 PRO A:1260 LEU A:1196 LEU A:1256 VAL A:1130 LEU A:1122 LYS A:1150 ARG A:1120 ARG A:1253
25	 GLY A:1123 LEU A:1122 ALA A:1148 MET A:1199 LEU A:1256 ASP A:1203 ARG A:1120 GLY A:1200 LEU A:1198 GLU A:1197 VAL A:1130 GLY A:1202 SER A:1206 LEU A:1196 LYS A:1150 GLY A:1201 PRO A:1260 GLU A:1210 PHE A:1207

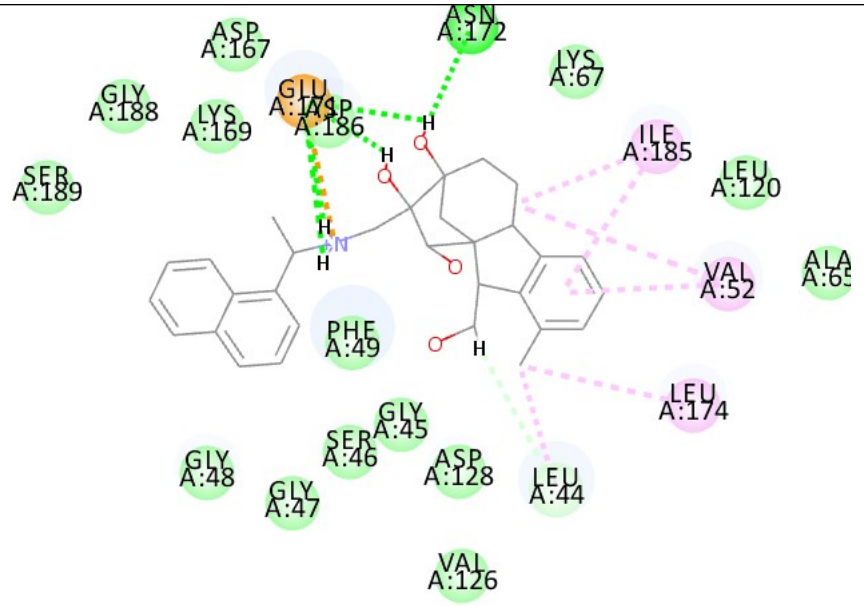
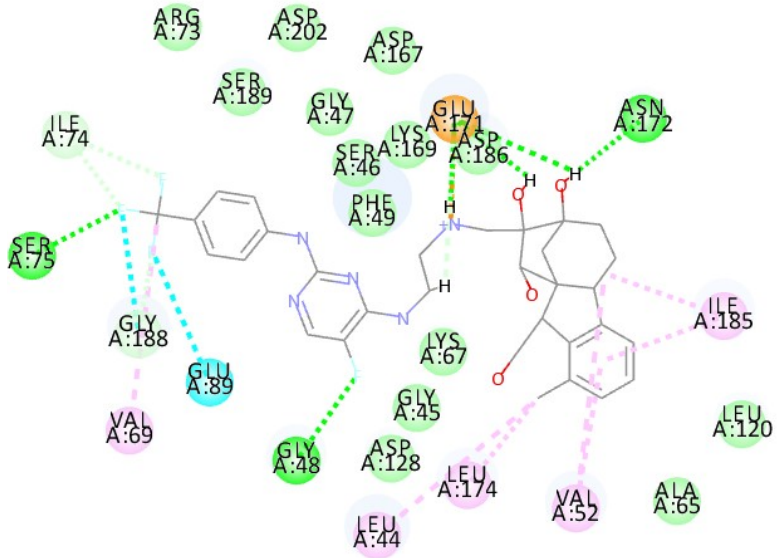
26	 GLU A:1197 LEU A:1198 MET A:1199 GLU A:1210 SER A:1206 ALA A:1200 ALA A:1148 GLY A:1201 GLY A:1202 LEU A:1196 PRO A:1260 LEU A:1256 VAL A:1130 LYS A:1150 ASP A:1203 LEU A:1122 GLY A:1123
28	 LEU A:1198 LEU A:1256 MET A:1199 ALA A:1148 GLY A:1123 PRO A:1260 GLU A:1197 GLY A:1201 SER A:1206 GLU A:1210 LEU A:1196 PHE A:1207 VAL A:1130 LYS A:1150 ARG A:1253 GLY A:1121 ARG A:1120

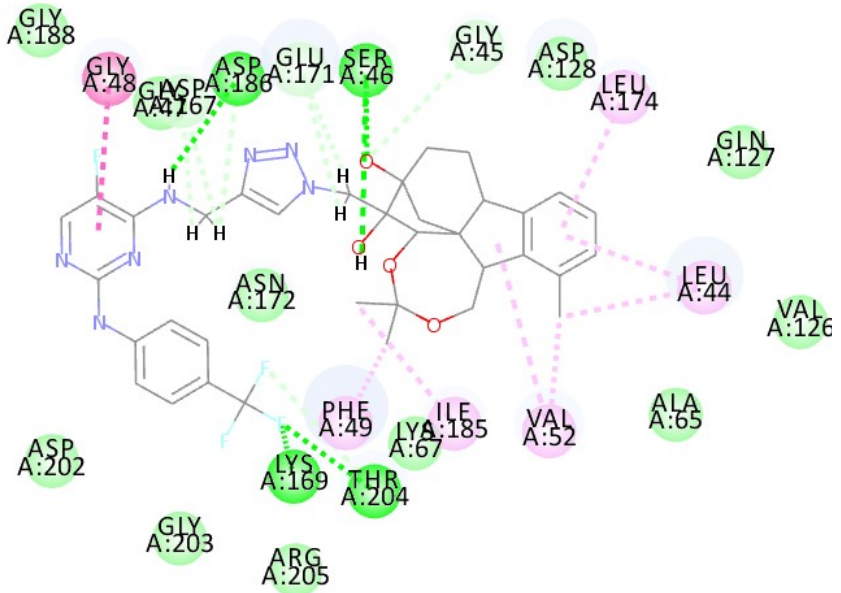
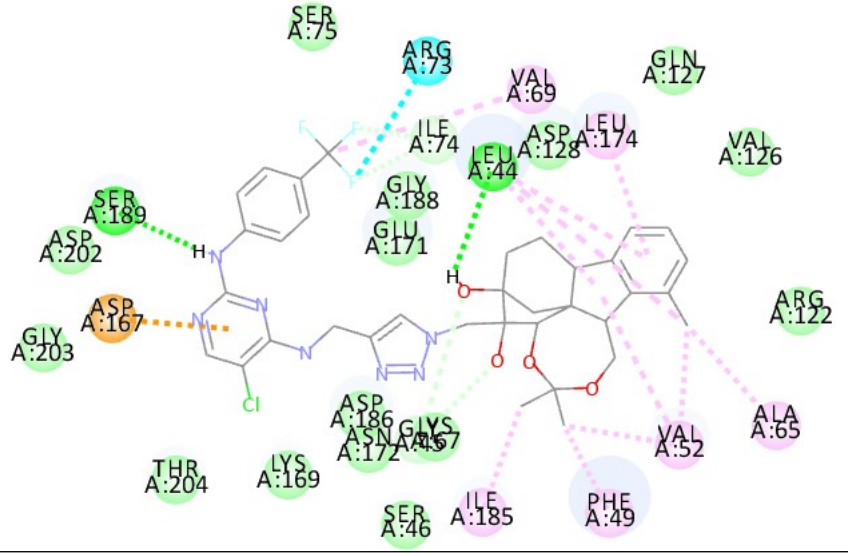
32	 GLU A:1197 MET A:1199 LEU A:1198 ALA A:1148 LEU A:1196 ARG A:1120 ALA A:1200 LEU A:1256 VAL A:1130 LYS A:1150 GLY A:1269 THR A:1211 GLY A:1201 GLU A:1210 LEU A:1122 GLY A:1202 ASP A:1270 PRO A:1260 ASP A:1203 SER A:1206 PHE A:1207 ARG A:1253 ASN A:1254 GLY A:1123
33	 ARG A:1120 LEU A:1122 ASP A:1203 GLY A:1123 MET A:1199 ALA A:1148 LEU A:1198 ALA A:1200 GLY A:1201 GLU A:1197 GLY A:1202 SER A:1206 LEU A:1196 ASN A:1254 PRO A:1260 VAL A:1130 LEU A:1256 CYS A:1255 ARG A:1253 LYS A:1150 GLU A:1210 PHE A:1207 GLY A:1269 ASP A:1270 THR A:1211

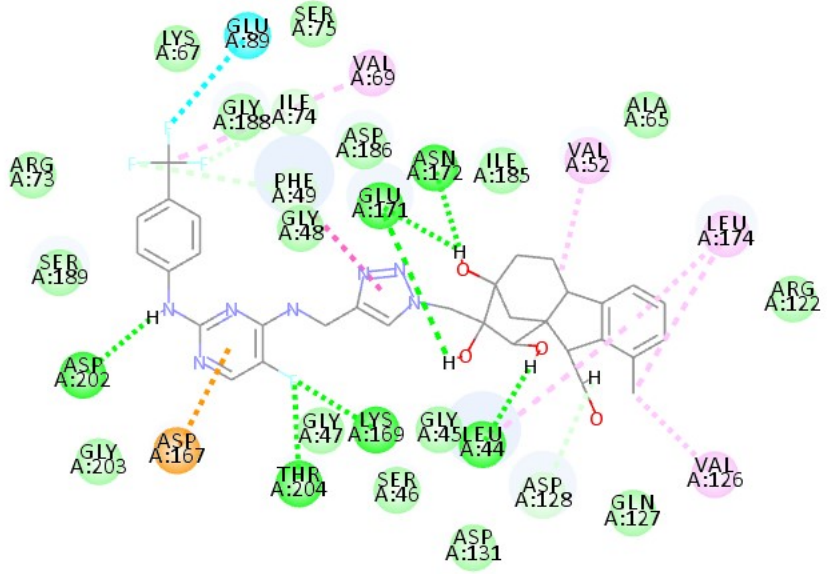
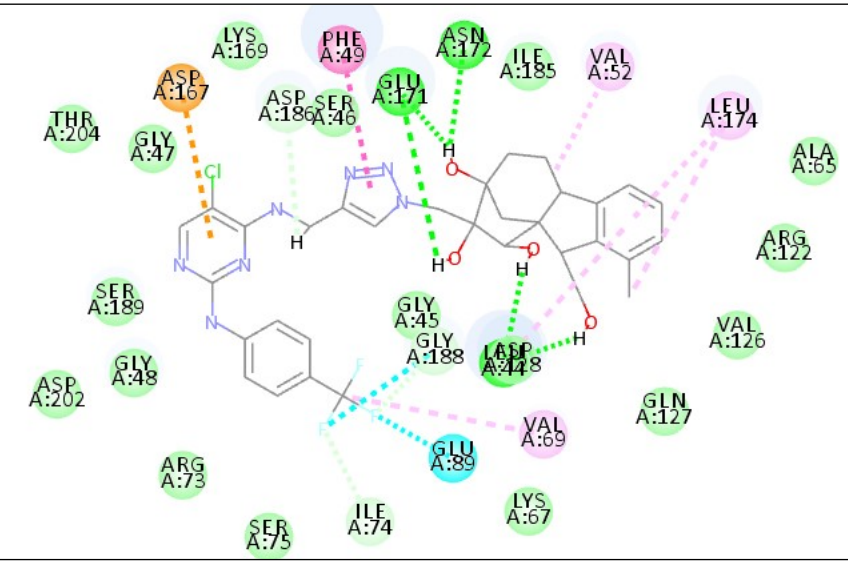
38	 SER A:1206 GLY A:1123 ASP A:1203 ARG A:1120 ALA A:1200 GLY A:1202 VAL A:1130 PRO A:1260 PHE A:1207 LEU A:1256 LEU A:1122 ASP A:1270 THR A:1211 GLY A:1201 ARG A:1253 ASN A:1254 LYS A:1150 GLY A:1269 GLU A:1210 GLN A:1217
39	 ASP A:1203 GLY A:1202 ALA A:1200 ARG A:1120 LEU A:1256 VAL A:1130 MET A:1199 SER A:1206 GLU A:1123 LEU A:1122 ARG A:1253 PRO A:1260 GLY A:1201 ALA A:1148 ASN A:1254 LEU A:1198 GLU A:1210 PHE A:1207

Compound	Interactions with Pim-1 (PDB code: 4ALW, resolution: 1.92 Å)
18	
23	

24	 VAL A:126 ASP A:128 LEU A:44 GLY A:48 GLY A:47 GLY A:45 ARG A:73 PHE A:49 SER A:46 GLU A:171 LEU A:174 ALA A:65 VAL A:52 ILE A:185 SER A:189 GLY A:188 ASP A:186 LYS A:169 ASN A:172 LYS A:67 LEU A:120 ASP A:167
25	 GLY A:48 ASN A:172 LYS A:67 GLU A:171 SER A:46 GLY A:47 ASP A:186 ILE A:185 VAL A:52 LEU A:120 SER A:189 ALA A:65 GLY A:45 LYS A:169 GLY A:188 LEU A:44 LEU A:174 ASP A:167 ASP A:128 THR A:204 GLY A:203

26	 ASP A:167 ASN A:172 LYS A:67 GLY A:188 LYS A:169 GLU A:171 ASP A:186 ILE A:185 SER A:189 LEU A:120 VAL A:52 ALA A:65 PHE A:49 LEU A:174 GLY A:45 SER A:46 GLY A:48 ASP A:128 LEU A:44 GLY A:47 VAL A:126
28	 ARG A:73 ASP A:202 ASP A:167 SER A:189 GLY A:47 GLU A:171 ASN A:172 ILE A:74 LYS A:169 ASP A:186 SER A:46 PHE A:49 SER A:75 ILE A:185 GLY A:188 LYS A:67 GLU A:89 GLY A:45 LEU A:120 VAL A:69 GLY A:48 ASP A:128 LEU A:174 VAL A:52 ALA A:65 LEU A:44

32	 GLY A:188 GLY A:48 ASP A:186 GLU A:171 SER A:46 GLY A:45 ASP A:128 LEU A:174 GLN A:127 ASP A:167 ASN A:172 LEU A:44 VAL A:126 PHE A:49 ILE A:185 VAL A:52 ALA A:65 LYS A:67 ASP A:202 LYS A:169 THR A:204 GLY A:203 ARG A:205
33	 SER A:75 ARG A:73 VAL A:69 GLN A:127 ILE A:74 LEU A:174 ASP A:128 VAL A:126 LEU A:44 GLY A:188 SER A:189 GLU A:171 ASP A:202 ASP A:167 ARG A:122 GLY A:203 ASP A:186 ALA A:65 LYS A:67 VAL A:52 ASN A:172 THR A:204 LYS A:169 SER A:46 ILE A:185 PHE A:49

38	 LYS A:67 GLU A:89 SER A:75 VAL A:69 GLY A:188 ILE A:74 ALA A:65 ASP A:186 ASN A:172 ILE A:185 VAL A:52 ARG A:73 PHE A:49 GLU A:171 GLY A:48 LEU A:174 SER A:189 ARG A:122 ASP A:202 GLY A:47 LYS A:169 GLY A:45 LEU A:44 ASP A:167 GLY A:203 THR A:204 SER A:46 ASP A:128 VAL A:126 GLN A:127 ASP A:131
39	 LYS A:169 PHE A:49 ASN A:172 ILE A:185 VAL A:52 ASP A:167 ASP A:186 SER A:46 GLU A:171 LEU A:174 THR A:204 GLY A:47 ALA A:65 ARG A:122 SER A:189 GLY A:45 VAL A:126 GLY A:188 ASP A:128 GLY A:48 ASP A:202 GLN A:127 VAL A:69 GLU A:89 ARG A:73 LYS A:67 ILE A:74 SER A:75

Key interactions