

Supporting information

Isolation, structural elucidation, and cytotoxic activity investigation of novel styryl-lactone derivatives from *Goniothalamus elegans*: *in vitro* and *in silico* studies

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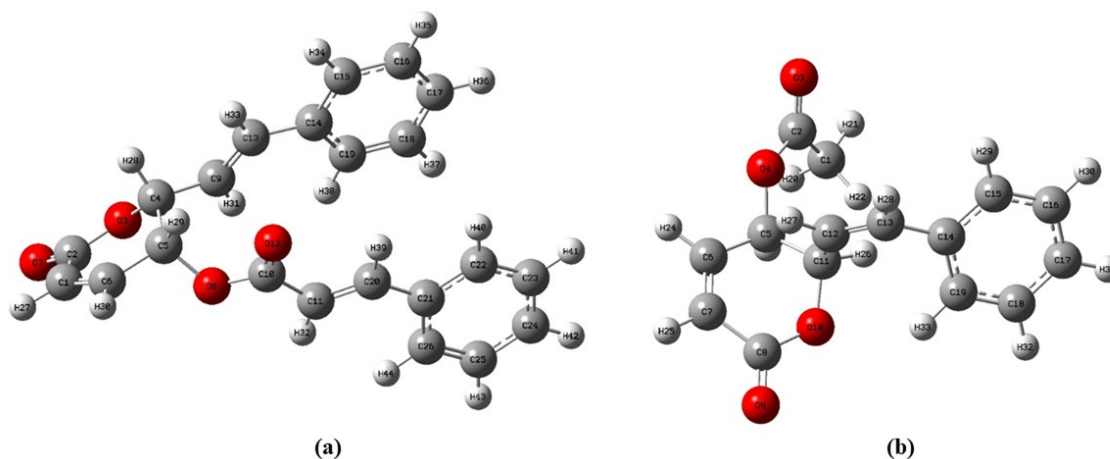
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A. DFT Studies



S1. Optimized geometry of molecular (a) compound (1), (b) compound (2) calculated by DFT/M052X level of calculations through 6-311++G(d,p) basis set

S2. Ground state electronic energy. thermodynamic parameters. dipole moment of investigated compounds in the gas phase using M052X/6-311++G(d,p) method.

Parameter	Compounds	
	1	2
Ground state electronic energy. E (Hartree)	-1150.23	-881.03
Sum of electronic and thermal Enthalpies. H (Hartree/Particle)	-1149.85	-880.75
Sum of electronic and thermal Free Energies. G (Hartree/Particle)	-1149.93	-880.81
Dipole moment (Debye)	5.04	2.47
Polarizability α (a.u)	266.65	178.83

S3. Quantum descriptors of investigated compounds calculated by NBO at M052X/def2TZVPP level

Compound properties	Quantum description	Unit	Compounds	
			1	2
E_{HOMO}	Energy of HOMO	eV	-7.856	-8.227
E_{LUMO}	Energy of LUMO	eV	-1.277	-0.865
Energy gap (E_g)	$E_g = E_{\text{LUMO}} - E_{\text{HOMO}}$	eV	6.579	7.361
Ionization potential (IP)	$IP = -E_{\text{HOMO}}$	eV	7.856	8.227
Electron affinity (EA)	$EA = -E_{\text{LUMO}}$	eV	1.277	0.865
Electronegativity (χ)	$\chi = -(E_{\text{LUMO}} + E_{\text{HOMO}})/2$	eV	4.566	4.546
Chemical hardness (η)	$\eta = (E_{\text{LUMO}} - E_{\text{HOMO}})/2$	eV	3.290	3.681

Chemical potential (μ)	$\mu = -\chi = (E_{\text{LUMO}} + E_{\text{HOMO}})/2$	eV	-4.566	-4.546
Chemical softness (S)	$S = 1/2\eta$	eV	0.152	0.136
Electrophilicity index (ω)	$\omega = \mu^2/2\eta$	eV	3.169	2.807

S4. Calculated geometric parameters of compound 1

Parameters	Bond lengths (Å)	Parameters	Bond angles (°)	Parameters	Dihedral angle
					(°)
R(1,2)	1.4825	A(2,1,6)	122.0616	D(6,1,2,3)	-7.8013
R(1,6)	1.3277	A(2,1,27)	114.6508	D(6,1,2,7)	168.4746
R(1,27)	1.0801	A(6,1,27)	123.0325	D(27,1,2,3)	177.838
R(2,3)	1.35	A(1,2,3)	117.3456	D(27,1,2,7)	-5.8861
R(2,7)	1.1978	A(1,2,7)	122.3783	D(2,1,6,5)	6.4241
R(3,4)	1.4367	A(3,2,7)	120.1711	D(2,1,6,30)	-172.9151
R(4,5)	1.5312	A(2,3,4)	120.0304	D(27,1,6,5)	-179.6911
R(4,9)	1.4983	A(3,4,5)	112.9375	D(27,1,6,30)	0.9697
R(4,28)	1.0926	A(3,4,9)	106.3784	D(1,2,3,4)	-18.6226
R(5,6)	1.494	A(3,4,28)	108.0319	D(7,2,3,4)	165.0152
R(5,8)	1.4351	A(5,4,9)	110.6028	D(2,3,4,5)	43.2819
R(5,29)	1.0888	A(5,4,28)	107.4607	D(2,3,4,9)	164.7913
R(6,30)	1.0824	A(9,4,28)	111.4574	D(2,3,4,28)	-75.43
R(8,10)	1.3648	A(4,5,6)	111.7588	D(3,4,5,6)	-41.2766
R(9,13)	1.3302	A(4,5,8)	109.8011	D(3,4,5,8)	79.6706
R(9,31)	1.0823	A(4,5,29)	107.7409	D(3,4,5,29)	-162.8195
R(10,11)	1.47	A(6,5,8)	108.8925	D(9,4,5,6)	-160.3677
R(10,12)	1.2023	A(6,5,29)	110.4752	D(9,4,5,8)	-39.4206
R(11,20)	1.3368	A(8,5,29)	108.1015	D(9,4,5,29)	78.0894
R(11,32)	1.0802	A(1,6,5)	120.65	D(28,4,5,6)	77.7667
R(13,14)	1.4702	A(1,6,30)	121.4763	D(28,4,5,8)	-161.2862
R(13,33)	1.0866	A(5,6,30)	117.8705	D(28,4,5,29)	-43.7762
R(14,15)	1.3961	A(5,8,10)	115.8586	D(3,4,9,13)	156.5709
R(14,19)	1.3992	A(4,9,13)	123.0228	D(3,4,9,31)	-29.6277
R(15,16)	1.3891	A(4,9,31)	114.293	D(5,4,9,13)	-80.4417

R(15,34)	1.0826	A(13,9,31)	122.3806	D(5,4,9,31)	93.3596
R(16,17)	1.3885	A(8,10,11)	110.3784	D(28,4,9,13)	39.0426
R(16,35)	1.0814	A(8,10,12)	123.2459	D(28,4,9,31)	-147.156
R(17,18)	1.3923	A(11,10,12)	126.3433	D(4,5,6,1)	18.1832
R(17,36)	1.0815	A(10,11,20)	118.3698	D(4,5,6,30)	-162.4543
R(18,19)	1.3856	A(10,11,32)	117.0889	D(8,5,6,1)	-103.2905
R(18,37)	1.0816	A(20,11,32)	124.1932	D(8,5,6,30)	76.072
R(19,38)	1.0809	A(9,13,14)	126.2482	D(29,5,6,1)	138.1335
R(20,21)	1.4628	A(9,13,33)	118.6325	D(29,5,6,30)	-42.504
R(20,39)	1.0851	A(14,13,33)	115.0428	D(4,5,8,10)	97.4764
R(21,22)	1.3969	A(13,14,15)	118.7149	D(6,5,8,10)	-139.8641
R(21,26)	1.3987	A(13,14,19)	122.8163	D(29,5,8,10)	-19.8086
R(22,23)	1.3881	A(15,14,19)	118.4381	D(5,8,10,11)	-157.42
R(22,40)	1.0824	A(14,15,16)	120.9822	D(5,8,10,12)	20.6287
R(23,24)	1.3888	A(14,15,34)	119.1795	D(4,9,13,14)	170.227
R(23,41)	1.0813	A(16,15,34)	119.8381	D(4,9,13,33)	-6.4231
R(24,25)	1.3927	A(15,16,17)	119.9933	D(31,9,13,14)	-3.0809
R(24,42)	1.0813	A(15,16,35)	119.8057	D(31,9,13,33)	-179.7309
R(25,26)	1.3851	A(17,16,35)	120.2009	D(8,10,11,20)	163.1153
R(25,43)	1.0813	A(16,17,18)	119.6049	D(8,10,11,32)	-10.3981
R(26,44)	1.0812	A(16,17,36)	120.2507	D(12,10,11,20)	-14.8586
		A(18,17,36)	120.144	D(12,10,11,32)	171.628
		A(17,18,19)	120.324	D(10,11,20,21)	-174.0705
		A(17,18,37)	120.0832	D(10,11,20,39)	3.1154
		A(19,18,37)	119.5857	D(32,11,20,21)	-1.0547
		A(14,19,18)	120.6552	D(32,11,20,39)	176.1312
		A(14,19,38)	120.2091	D(9,13,14,15)	176.4519
		A(18,19,38)	119.1261	D(9,13,14,19)	-5.5959
		A(11,20,21)	126.9302	D(33,13,14,15)	-6.7934
		A(11,20,39)	116.7972	D(33,13,14,19)	171.1589
		A(21,20,39)	116.2176	D(13,14,15,16)	178.5979
		A(20,21,22)	118.2326	D(13,14,15,34)	-1.2526
		A(20,21,26)	122.9045	D(19,14,15,16)	0.5549

		A(22,21,26)	118.8563	D(19,14,15,34)	-179.2955
		A(21,22,23)	120.7367	D(13,14,19,18)	-178.4777
		A(21,22,40)	119.097	D(13,14,19,38)	0.3823
		A(23,22,40)	120.1598	D(15,14,19,18)	-0.5201
		A(22,23,24)	119.8942	D(15,14,19,38)	178.34
		A(22,23,41)	119.9211	D(14,15,16,17)	-0.2601
		A(24,23,41)	120.1846	D(14,15,16,35)	179.84
		A(23,24,25)	119.8722	D(34,15,16,17)	179.5894
		A(23,24,42)	120.1395	D(34,15,16,35)	-0.3105
		A(25,24,42)	119.9873	D(15,16,17,18)	-0.0804
		A(24,25,26)	120.2248	D(15,16,17,36)	-179.8478
		A(24,25,43)	119.9857	D(35,16,17,18)	179.8191
		A(26,25,43)	119.7889	D(35,16,17,36)	0.0517
		A(21,26,25)	120.4132	D(16,17,18,19)	0.1135
		A(21,26,44)	120.0397	D(16,17,18,37)	-178.908
		A(25,26,44)	119.5434	D(36,17,18,19)	179.8812
				D(36,17,18,37)	0.8597
				D(17,18,19,14)	0.1925
				D(17,18,19,38)	-178.6798
				D(37,18,19,14)	179.2188
				D(37,18,19,38)	0.3465
				D(11,20,21,22)	168.1925
				D(11,20,21,26)	-10.8591
				D(39,20,21,22)	-9.0076
				D(39,20,21,26)	171.9409
				D(20,21,22,23)	-178.5076
				D(20,21,22,40)	0.5651
				D(26,21,22,23)	0.5832
				D(26,21,22,40)	179.6559
				D(20,21,26,25)	178.5686
				D(20,21,26,44)	-2.1407
				D(22,21,26,25)	-0.4773
				D(22,21,26,44)	178.8134

				D(21,22,23,24)	-0.2792
				D(21,22,23,41)	179.8243
				D(40,22,23,24)	-179.3421
				D(40,22,23,41)	0.7615
				D(22,23,24,25)	-0.1379
				D(22,23,24,42)	-179.7901
				D(41,23,24,25)	179.7582
				D(41,23,24,42)	0.1061
				D(23,24,25,26)	0.2422
				D(23,24,25,43)	-179.4653
				D(42,24,25,26)	179.8948
				D(42,24,25,43)	0.1874
				D(24,25,26,21)	0.0697
				D(24,25,26,44)	-179.2244
				D(43,25,26,21)	179.7778
				D(43,25,26,44)	0.4836

S5. Calculated geometric parameters of compound 2

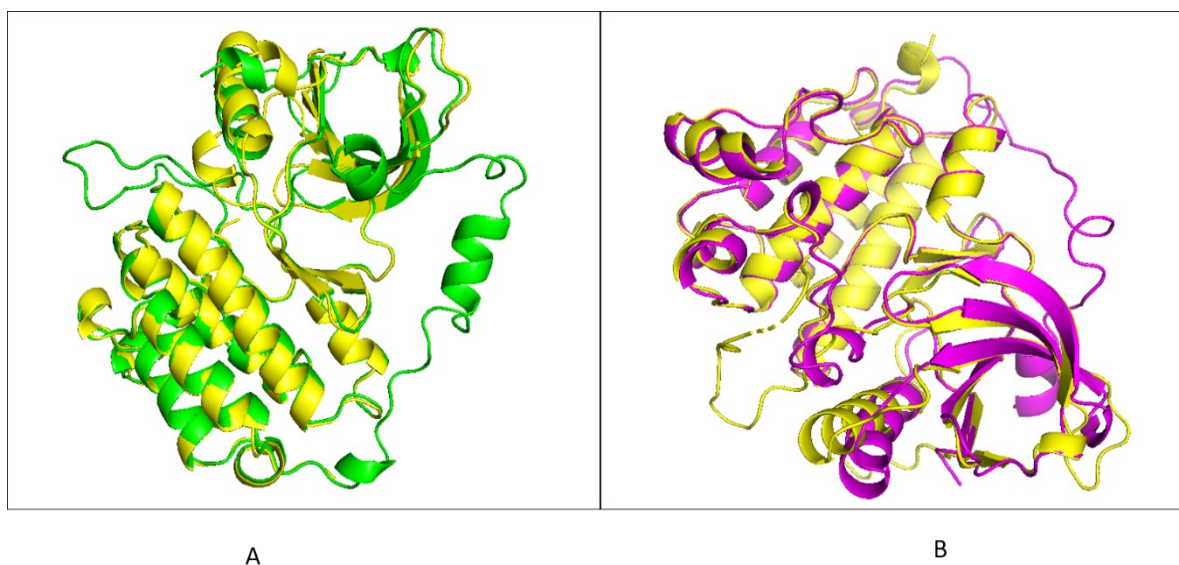
Parameters	Bond lengths	Parameters	Bond angles	Parameters	Dihedral angle
	(Å)		(°)		(°)
R(1,2)	1.5082	A(2,1,20)	110.2621	D(20,1,2,3)	-113.9383
R(1,20)	1.0904	A(2,1,21)	107.1878	D(20,1,2,4)	63.7991
R(1,21)	1.0844	A(2,1,22)	112.1796	D(21,1,2,3)	4.8347
R(1,22)	1.0883	A(20,1,21)	109.2112	D(21,1,2,4)	-177.4278
R(2,3)	1.1927	A(20,1,22)	108.4659	D(22,1,2,3)	125.0569
R(2,4)	1.3641	A(21,1,22)	109.4957	D(22,1,2,4)	-57.2057
R(4,5)	1.4254	A(1,2,3)	123.6197	D(1,2,4,5)	9.173
R(5,6)	1.4988	A(1,2,4)	118.1046	D(3,2,4,5)	-172.9656
R(5,11)	1.5297	A(3,2,4)	118.2384	D(2,4,5,6)	-155.4448
R(5,23)	1.0919	A(2,4,5)	122.4239	D(2,4,5,11)	85.2297
R(6,7)	1.3275	A(4,5,6)	106.9915	D(2,4,5,23)	-36.5241
R(6,24)	1.0823	A(4,5,11)	110.7263	D(4,5,6,7)	-149.2566
R(7,8)	1.4826	A(4,5,23)	110.8562	D(4,5,6,24)	31.1817
R(7,25)	1.0796	A(6,5,11)	109.5516	D(11,5,6,7)	-29.176
R(8,9)	1.1961	A(6,5,23)	109.1562	D(11,5,6,24)	151.2624
R(8,10)	1.3577	A(11,5,23)	109.5095	D(23,5,6,7)	90.7273
R(10,11)	1.45	A(5,6,7)	120.3286	D(23,5,6,24)	-88.8344
R(11,12)	1.4993	A(5,6,24)	117.1301	D(4,5,11,10)	171.2582
R(11,26)	1.0864	A(7,6,24)	122.5398	D(4,5,11,12)	46.2146
R(12,13)	1.334	A(6,7,8)	120.9537	D(4,5,11,26)	-76.1279
R(12,27)	1.0824	A(6,7,25)	123.3986	D(6,5,11,10)	53.4866
R(13,14)	1.4744	A(8,7,25)	115.5404	D(6,5,11,12)	-71.557
R(13,28)	1.0848	A(7,8,9)	123.1897	D(6,5,11,26)	166.1004
R(14,15)	1.398	A(7,8,10)	116.7413	D(23,5,11,10)	-66.2002
R(14,19)	1.3978	A(9,8,10)	119.9775	D(23,5,11,12)	168.7562
R(15,16)	1.3867	A(8,10,11)	119.3915	D(23,5,11,26)	46.4137
R(15,29)	1.0826	A(5,11,10)	108.2311	D(5,6,7,8)	-2.9112
R(16,17)	1.391	A(5,11,12)	112.2991	D(5,6,7,25)	-178.9752
R(16,30)	1.0813	A(5,11,26)	110.4813	D(24,6,7,8)	176.6261
R(17,18)	1.3891	A(10,11,12)	112.6985	D(24,6,7,25)	0.5621
R(17,31)	1.0813	A(10,11,26)	103.4539	D(6,7,8,9)	-166.9707
R(18,19)	1.3898	A(12,11,26)	109.3244	D(6,7,8,10)	9.5426
R(18,32)	1.0814	A(11,12,13)	123.9727	D(25,7,8,9)	9.3879
R(19,33)	1.0817	A(11,12,27)	117.0535	D(25,7,8,10)	-174.0988
		A(13,12,27)	118.8887	D(7,8,10,11)	20.0595
		A(12,13,14)	127.0425	D(9,8,10,11)	-163.3089
		A(12,13,28)	117.5288	D(8,10,11,5)	-51.6235
		A(14,13,28)	115.4055	D(8,10,11,12)	73.1832

	A(13,14,15)	118.8199	D(8,10,11,26)	-168.855
	A(13,14,19)	122.2391	D(5,11,12,13)	-143.9002
	A(15,14,19)	118.9261	D(5,11,12,27)	32.6978
	A(14,15,16)	120.6636	D(10,11,12,13)	93.5476
	A(14,15,29)	119.2963	D(10,11,12,27)	-89.8544
	A(16,15,29)	120.0355	D(26,11,12,13)	-20.9044
	A(15,16,17)	120.0182	D(26,11,12,27)	155.6936
	A(15,16,30)	119.8632	D(11,12,13,14)	-3.1779
	A(17,16,30)	120.1176	D(11,12,13,28)	174.9768
	A(16,17,18)	119.7767	D(27,12,13,14)	-179.7175
	A(16,17,31)	120.0916	D(27,12,13,28)	-1.5627
	A(18,17,31)	120.1261	D(12,13,14,15)	139.3809
	A(17,18,19)	120.3302	D(12,13,14,19)	-42.0393
	A(17,18,32)	120.1077	D(28,13,14,15)	-38.8076
	A(19,18,32)	119.5569	D(28,13,14,19)	139.7722
	A(14,19,18)	120.256	D(13,14,15,16)	-179.3475
	A(14,19,33)	119.6815	D(13,14,15,29)	-0.1281
	A(18,19,33)	120.035	D(19,14,15,16)	2.025
			D(19,14,15,29)	-178.7556
			D(13,14,19,18)	179.771
			D(13,14,19,33)	-2.1382
			D(15,14,19,18)	-1.6507
			D(15,14,19,33)	176.4401
			D(14,15,16,17)	-1.0512
			D(14,15,16,30)	179.3142
			D(29,15,16,17)	179.7351
			D(29,15,16,30)	0.1005
			D(15,16,17,18)	-0.3192
			D(15,16,17,31)	-179.4575
			D(30,16,17,18)	179.3145
			D(30,16,17,31)	0.1761
			D(16,17,18,19)	0.6867
			D(16,17,18,32)	-178.4769
			D(31,17,18,19)	179.8248
			D(31,17,18,32)	0.6611
			D(17,18,19,14)	0.3117
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			D(32,18,19,14)	179.48
			D(32,18,19,33)	1.396

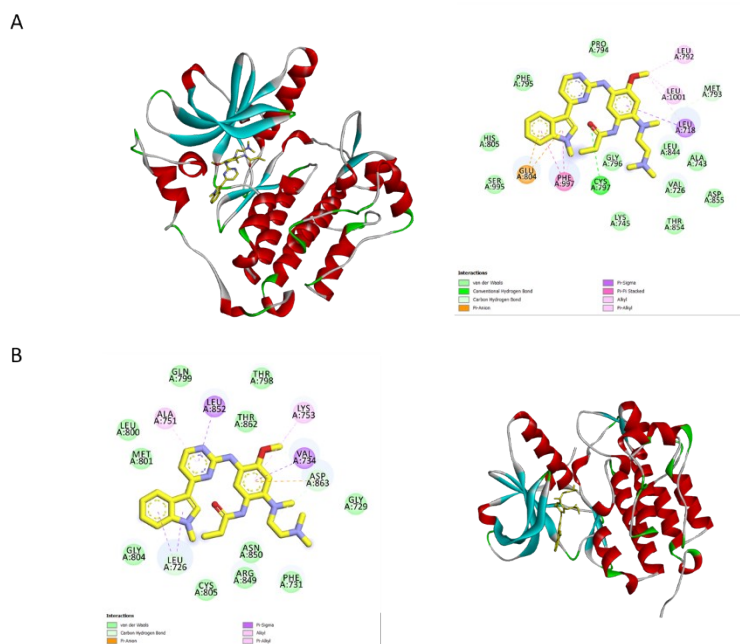
B. Molecular docking analysis

S6. Binding energy of compounds towards EGFR and HER2

Compound	EGFR (kcal/mol)	HER2 (kcal/mol)
1	-8.6	-8.7
2	-6.4	-6.9
Osimertinib ^{a)}	-8.1	-7.9

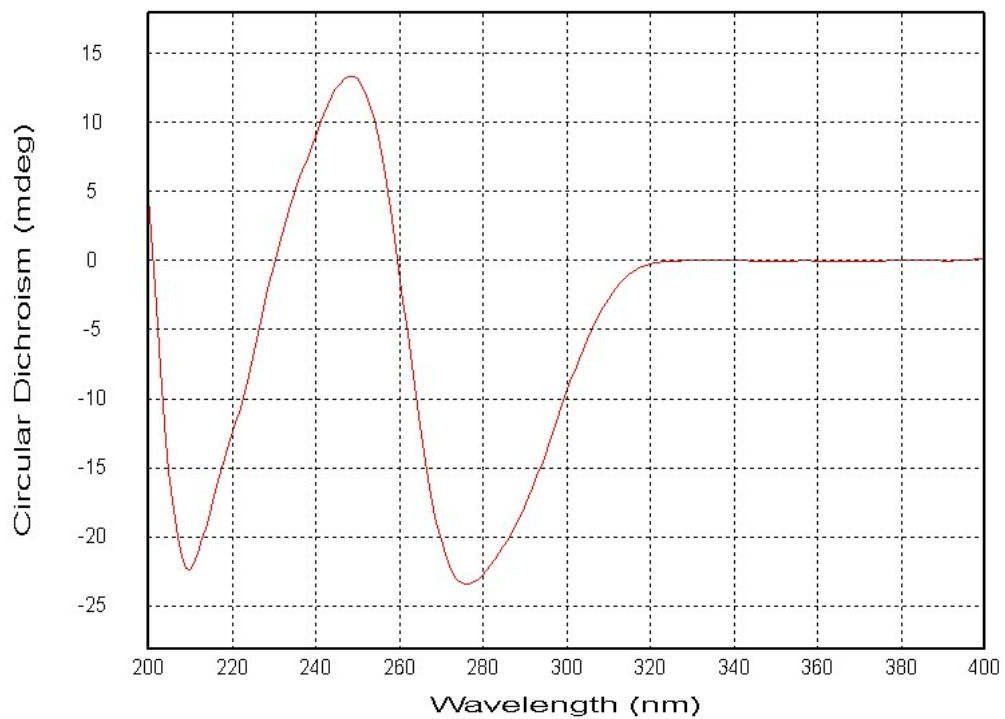


S6. Validation structure between PDB database (yellow) and AlphaFold predicted (green and purple) (A) EGFR (B) HER-2

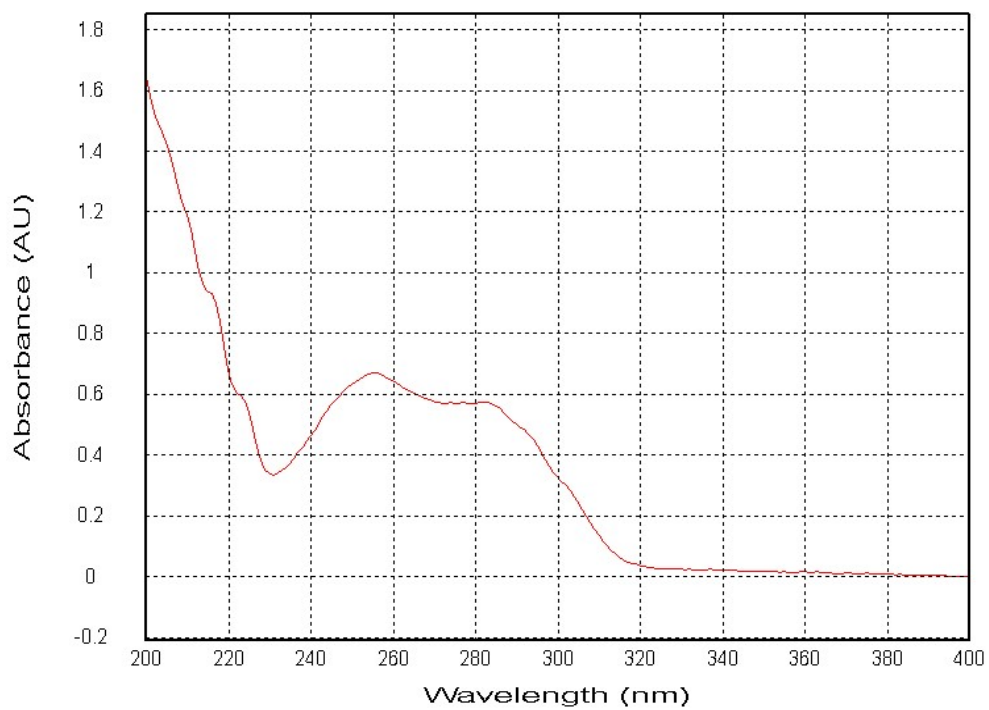


S7. 3D and 2D interaction between Osimertinib and protein (A) EGFR (B) HER-2

C. Characterization data for compound 1



S8. CD spectrum of compound 1

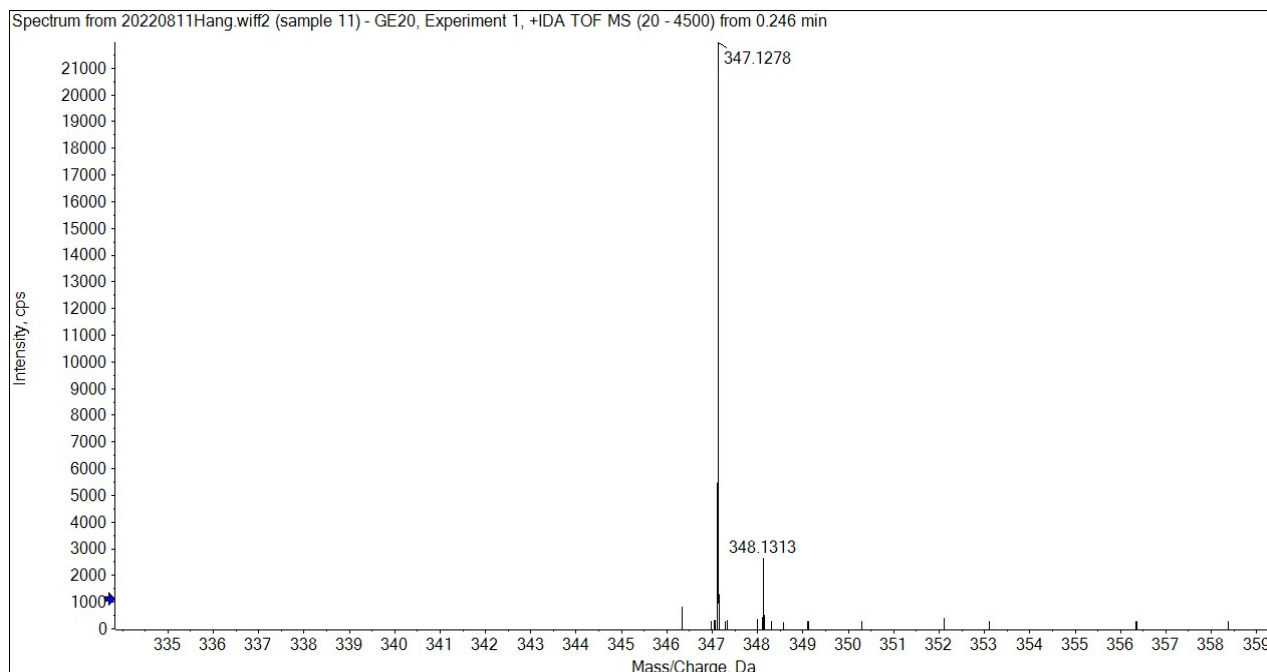
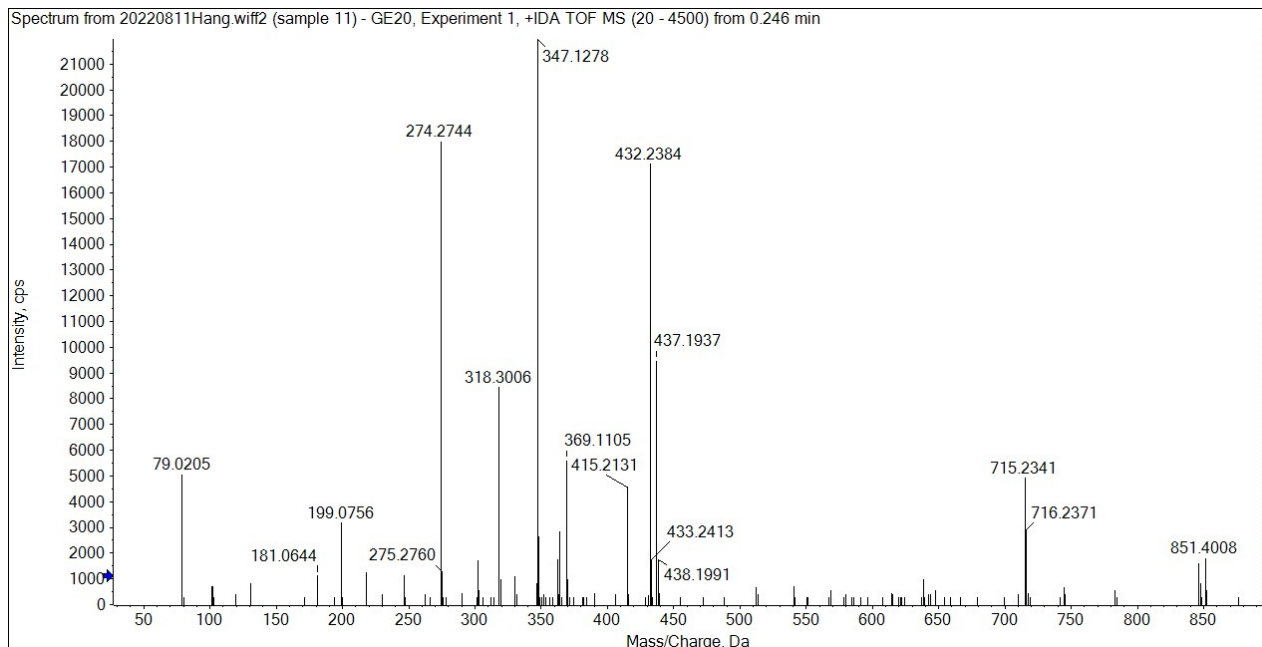


S9. UV Spectrum of compound 1

MS spectra

Method: +IDA TOF MS/MS

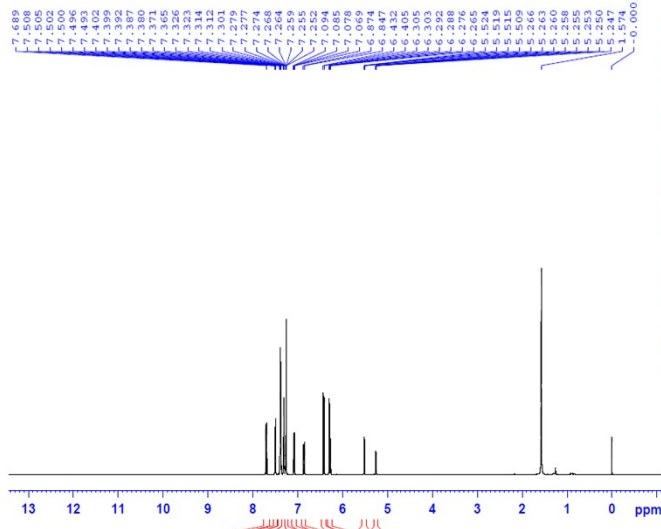
Date: 2022.08.11



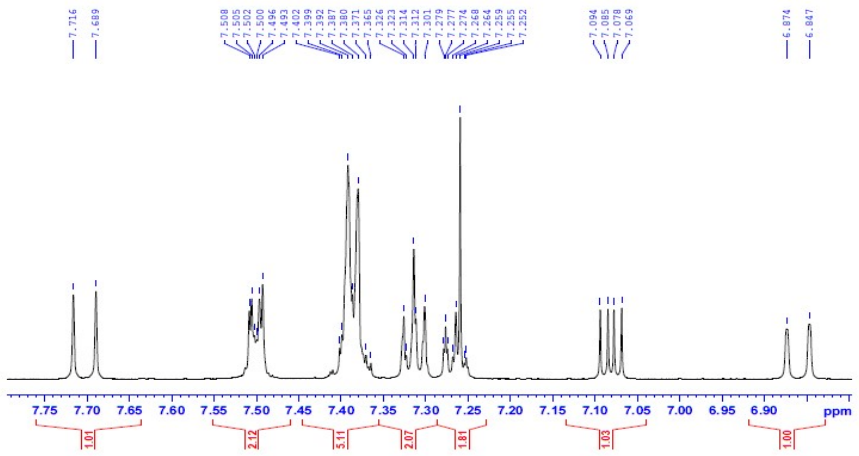
Hit	Formula	m/z	RDB	ppm	MS Rank	MSMS ppm	MSMS Rank	Found
1	C22H18O4	347.12779	14.0	0.2	1			NA/NA

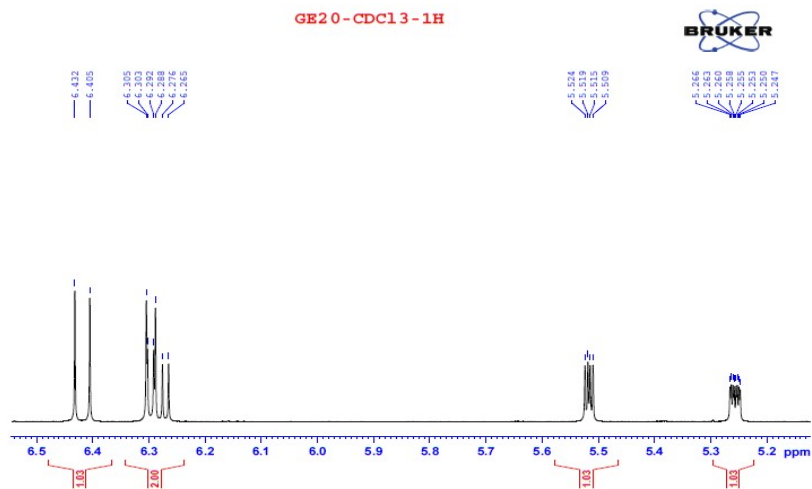
S10. MS spectrum of compound 1

GE20-CDCl3-1H

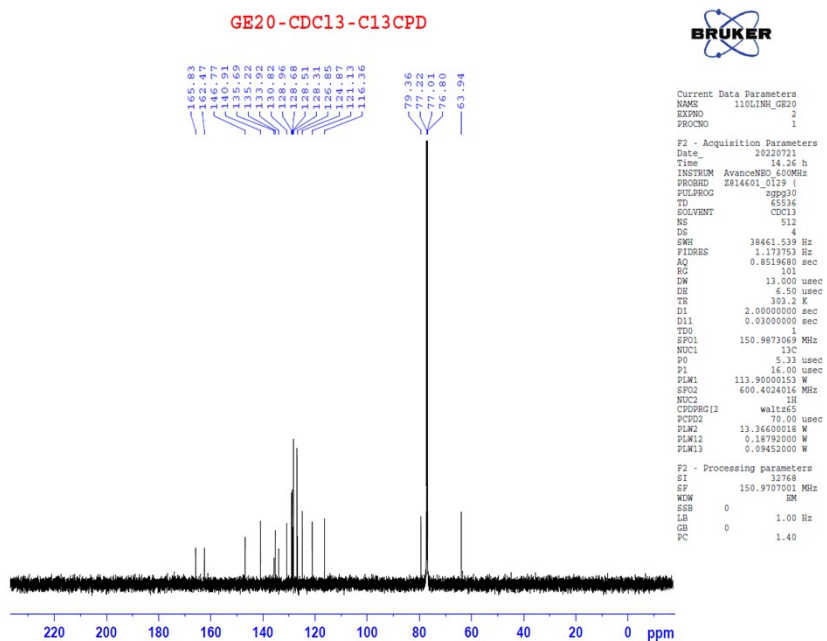


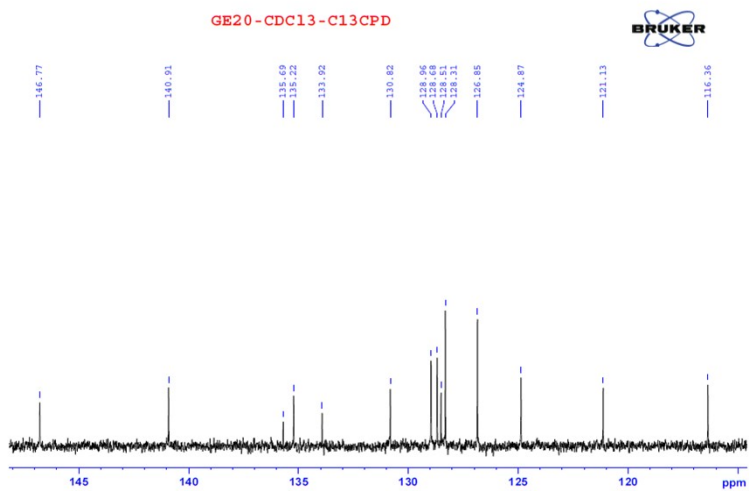
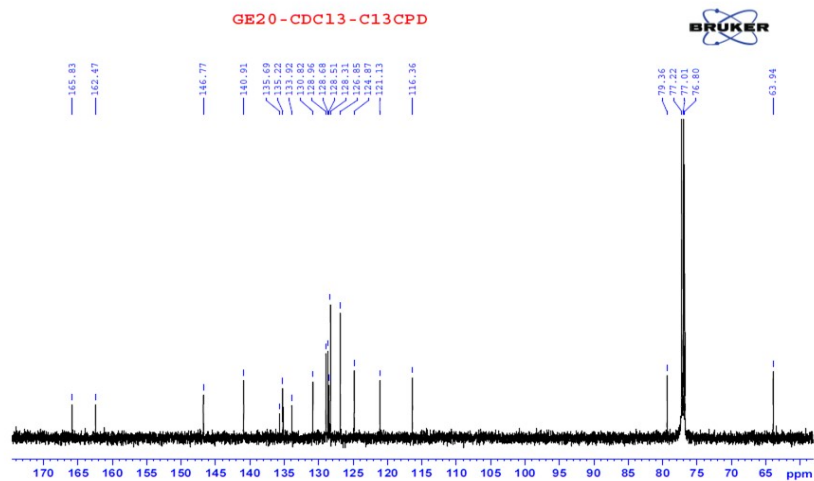
GE20-CDCl3-1H





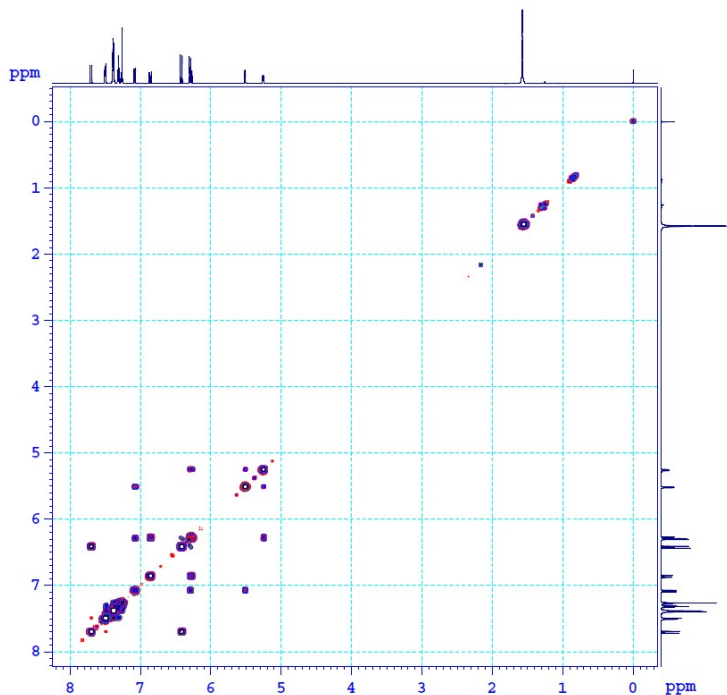
S11. ^1H - NMR spectrum of compound 1





S12. ^{13}C - NMR spectrum of compound 1

GE20 - CDC13 - COSYGP



```

Current Data Parameters
NAME      110LINH_GE20
EXPNO    7
PROCNO   1

F2 - Acquisition Parameters
Date_    20220726
Time     11:16 h
INSTRUM  AvanceBO 600MHz
PROBHD   Z114607_0862 (
PULPROG  cosygpqpgf
TD       2048
SOLVENT  CDC13
NS       4
DS       8
SWH      9090.909 Hz
FIDRES   8.977641 Hz
AQ       0.1126400 sec
RG       101
AQ       55.000 usec
DE       6.50 usec
TE       303.2 K
D0       0.00000300 sec
D1       0.77881569 sec
D11      0.00000000 sec
D12      0.00002000 sec
D13      0.00004000 sec
D14      0.00020000 sec
IN0      0.00011000 sec
SPARSELI 0
TDav     1
SFO1     600.4042028 MHz
NUC1     1H
P0       10.50 usec
P1       10.50 usec
P17      2500.00 usec
PLW1     27.03700666 W
PLW10    4.76929998 W
CPDPRM(1) SWSQ10 100
CPZ1     10.00 %
P16     1000.00 usec

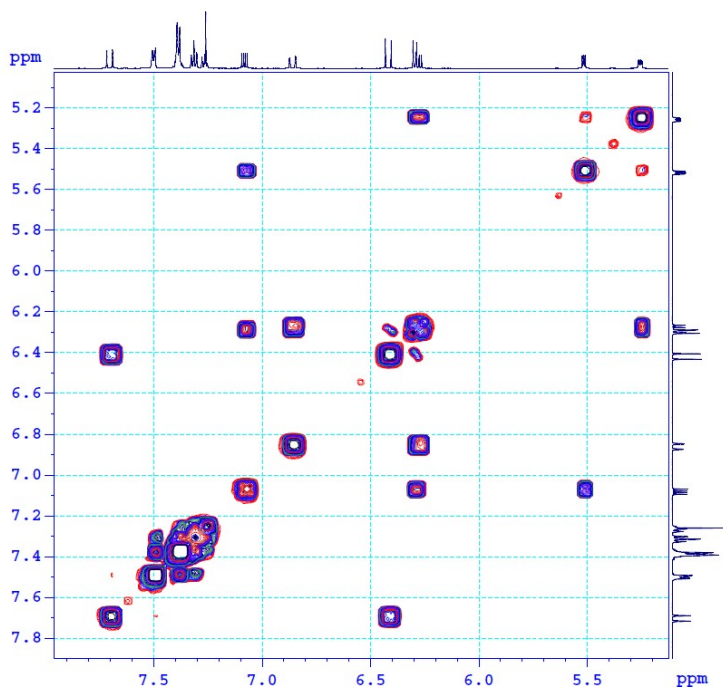
***** F1 INDIRECT DIMENSION *****
td1      160
sw_F1    15.141288

F1 - Acquisition parameters
TD       80
SFO1     600.4042 MHz
FIDRES   227.272720 Hz
SW       15.141 ppm
PnMODE   QF

F2 - Processing parameters
SI       1024
SF       600.4002462 MHz
WDW      QSLINE
SSB      0
LB       0 Hz
GB       0
PC       1.40

F1 - Processing parameters
SI       1024
MC2      QF
SF       600.4002462 MHz
WDW      QSLINE
SSB      0
LB       0 Hz
GB       0
    
```

GE20 - CDC13 - COSYGP



```

Current Data Parameters
NAME      110LINH_GE20
EXPNO    7
PROCNO   1

F2 - Acquisition Parameters
Date_    20220726
Time     11:16 h
INSTRUM  AvanceBO 600MHz
PROBHD   Z114607_0862 (
PULPROG  cosygpqpgf
TD       2048
SOLVENT  CDC13
NS       4
DS       8
SWH      9090.909 Hz
FIDRES   8.977641 Hz
AQ       0.1126400 sec
RG       101
AQ       55.000 usec
DE       6.50 usec
TE       303.2 K
D0       0.00000300 sec
D1       0.77881569 sec
D11      0.00000000 sec
D12      0.00002000 sec
D13      0.00004000 sec
D14      0.00020000 sec
IN0      0.00011000 sec
SPARSELI 0
TDav     1
SFO1     600.4042028 MHz
NUC1     1H
P0       10.50 usec
P1       10.50 usec
P17      2500.00 usec
PLW1     27.03700666 W
PLW10    4.76929998 W
CPDPRM(1) SWSQ10 100
CPZ1     10.00 %
P16     1000.00 usec

***** F1 INDIRECT DIMENSION *****
td1      160
sw_F1    15.141288

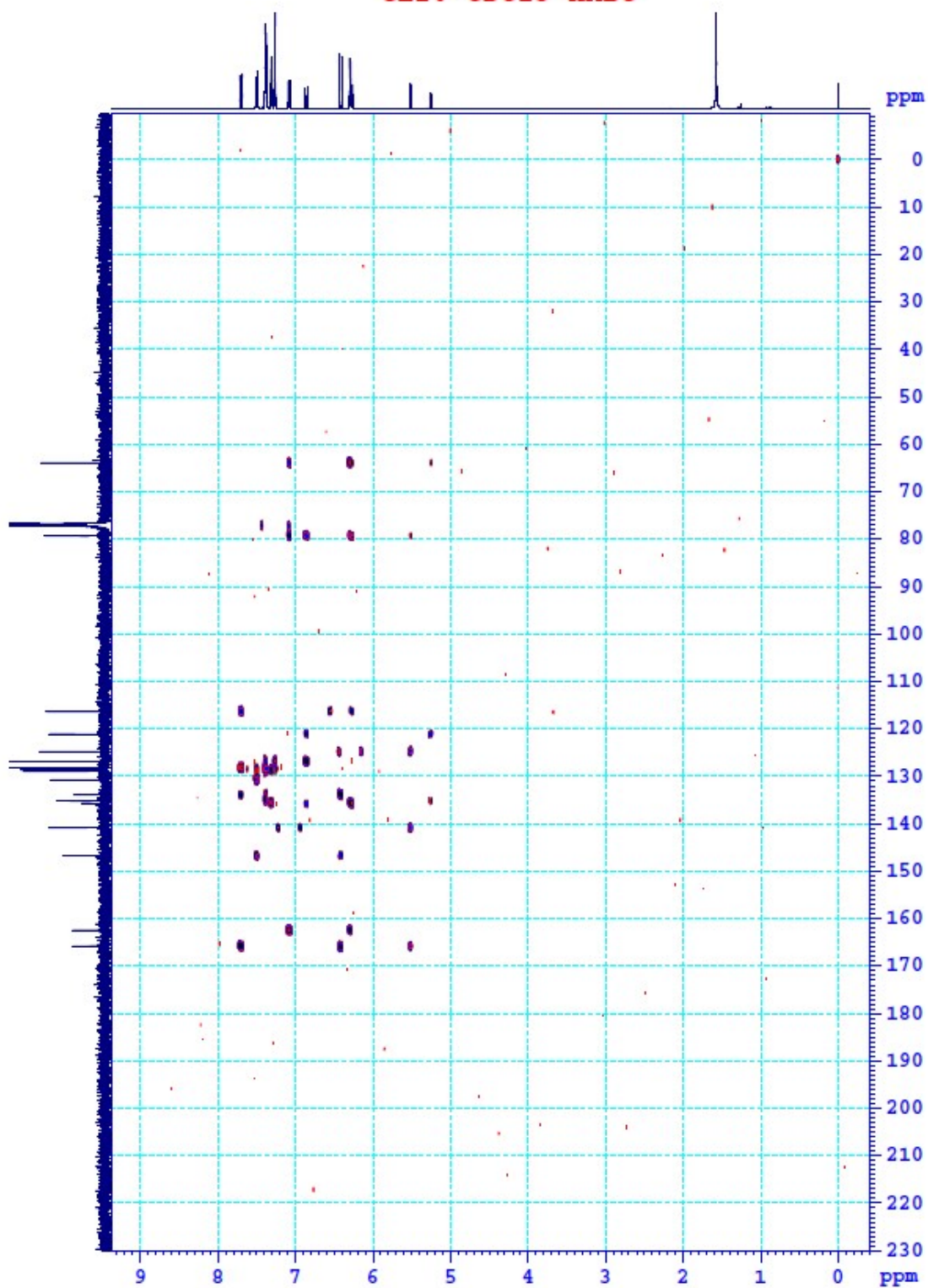
F1 - Acquisition parameters
TD       80
SFO1     600.4042 MHz
FIDRES   227.272720 Hz
SW       15.141 ppm
PnMODE   QF

F2 - Processing parameters
SI       1024
SF       600.4002462 MHz
WDW      QSLINE
SSB      0
LB       0 Hz
GB       0
PC       1.40

F1 - Processing parameters
SI       1024
MC2      QF
SF       600.4002462 MHz
WDW      QSLINE
SSB      0
LB       0 Hz
GB       0
    
```

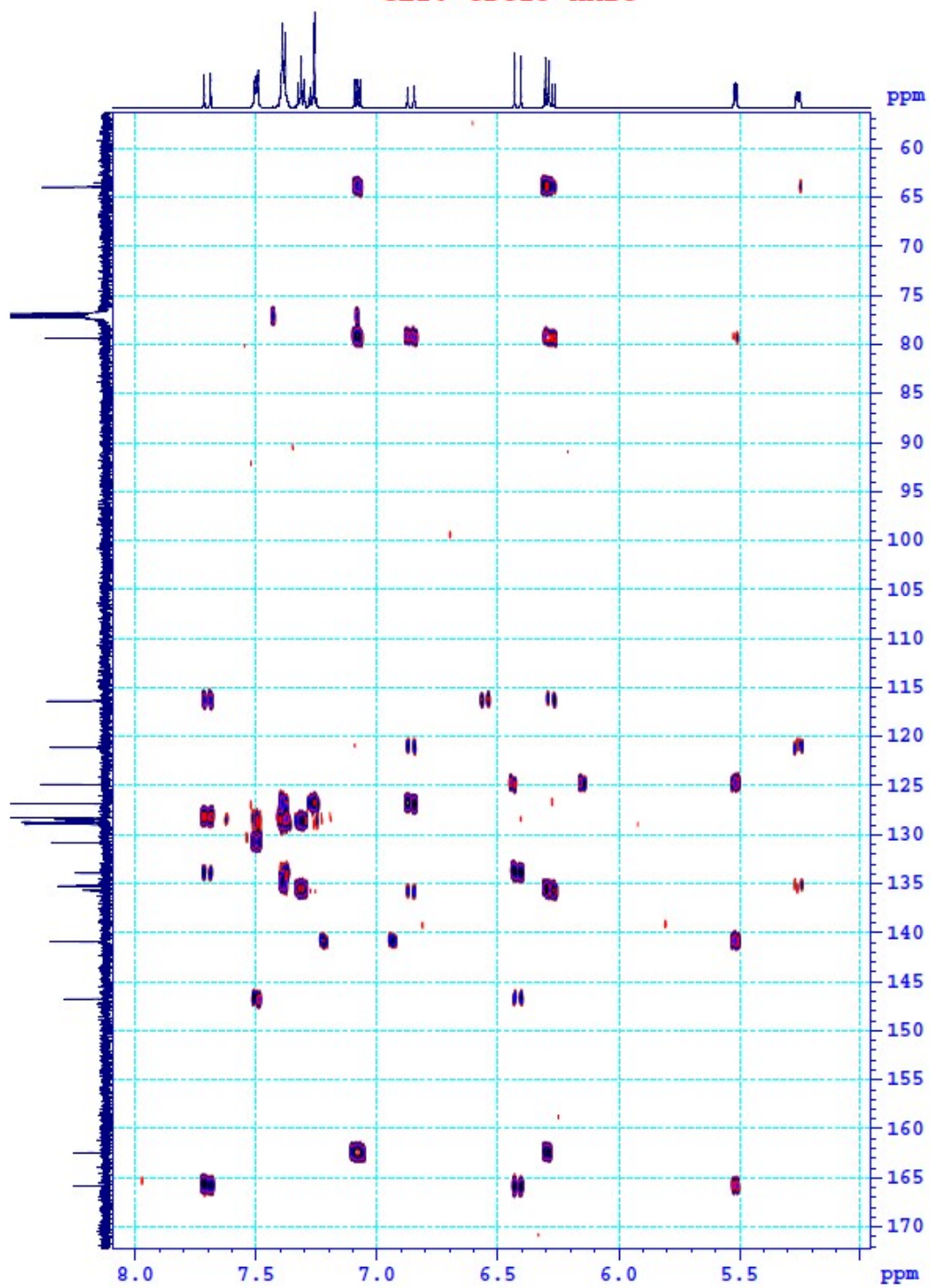
S13. COSY- NMR spectrum of compound 1

GE20-CDC13-HMBC



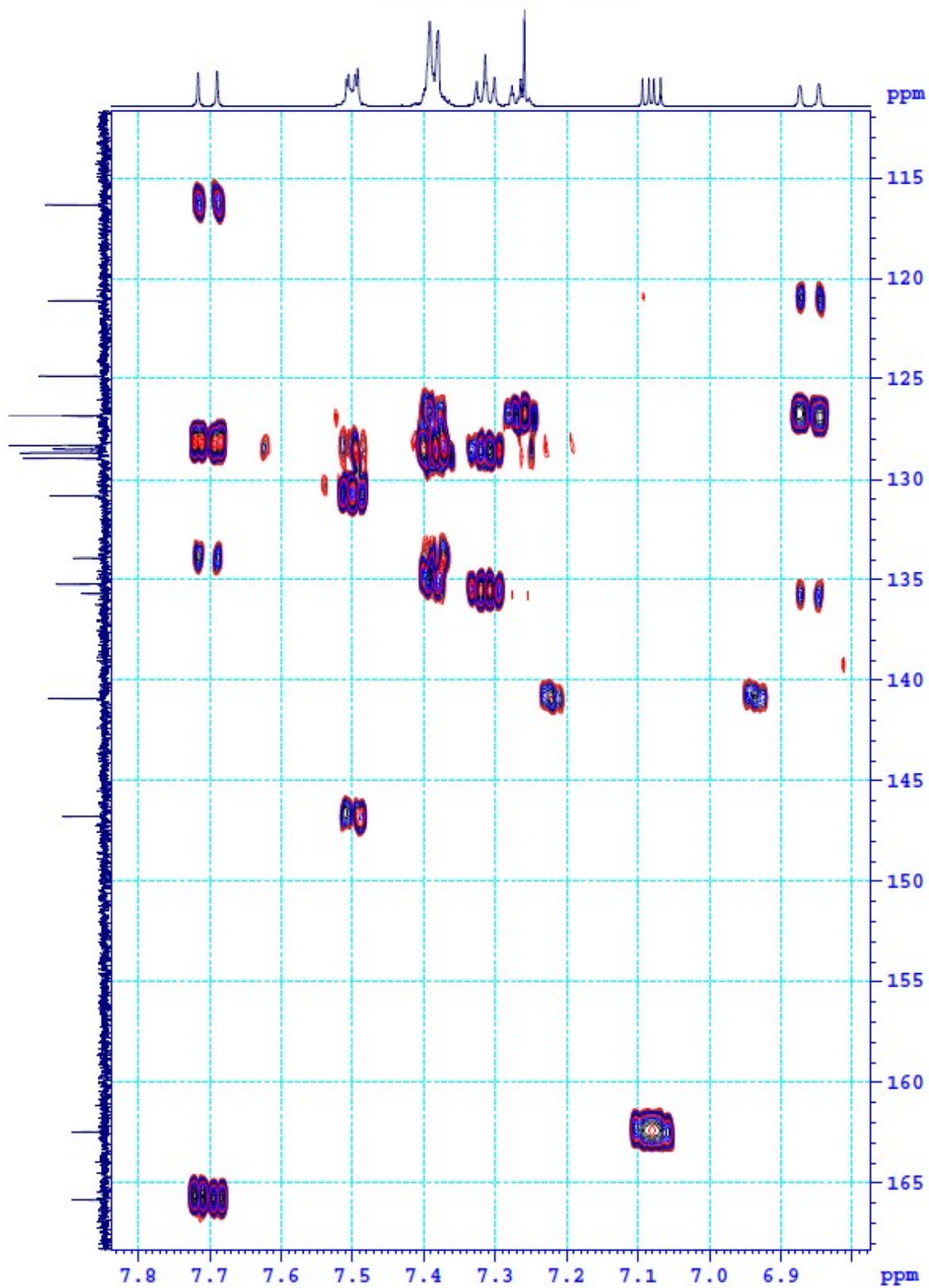
S14. HMBC - NMR spectrum of compound 1

GE20 - CDC13 - HMBC



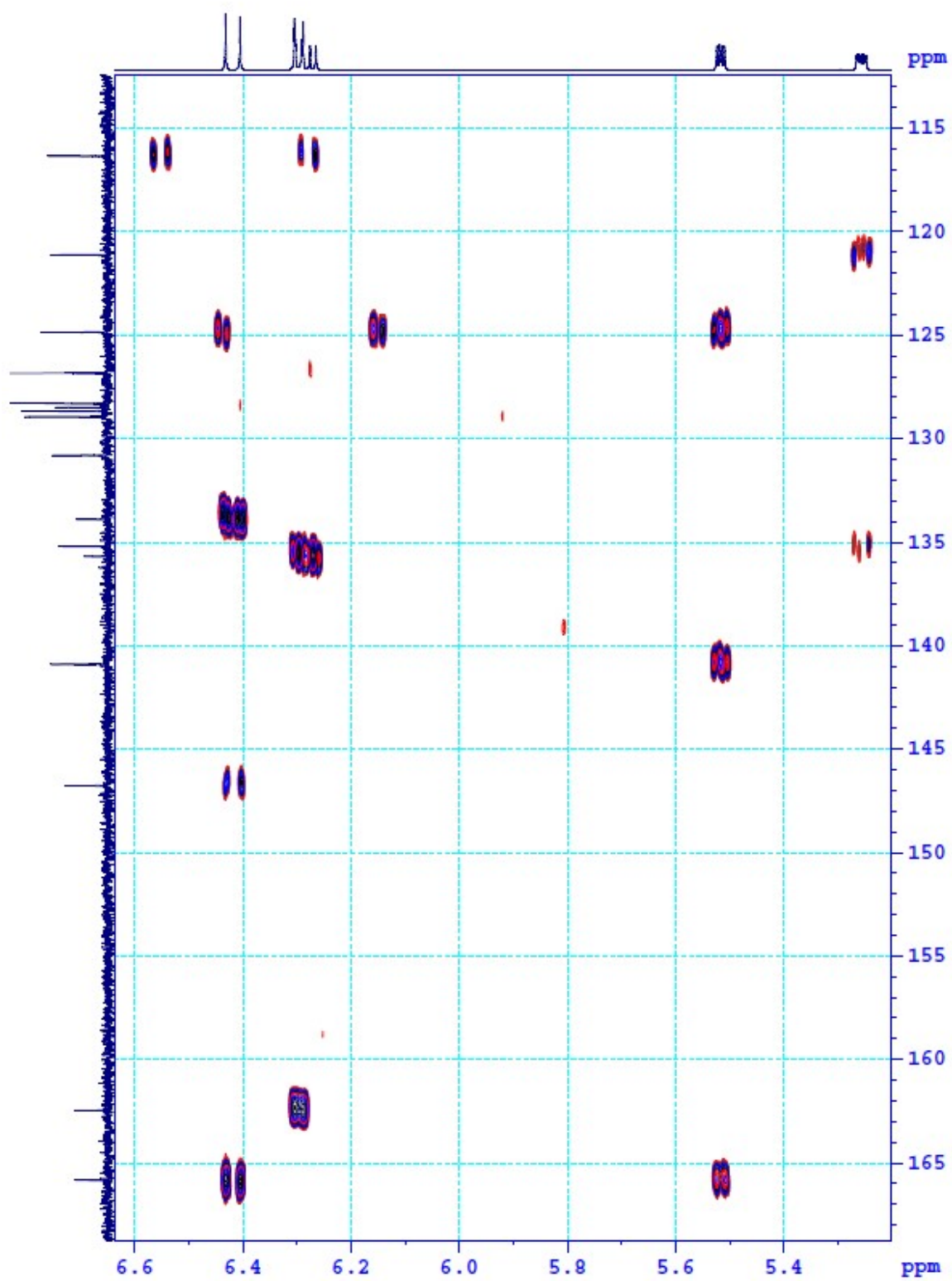
S15. HMBC - NMR spectrum of compound 1

GE20-CDC13-HMBC

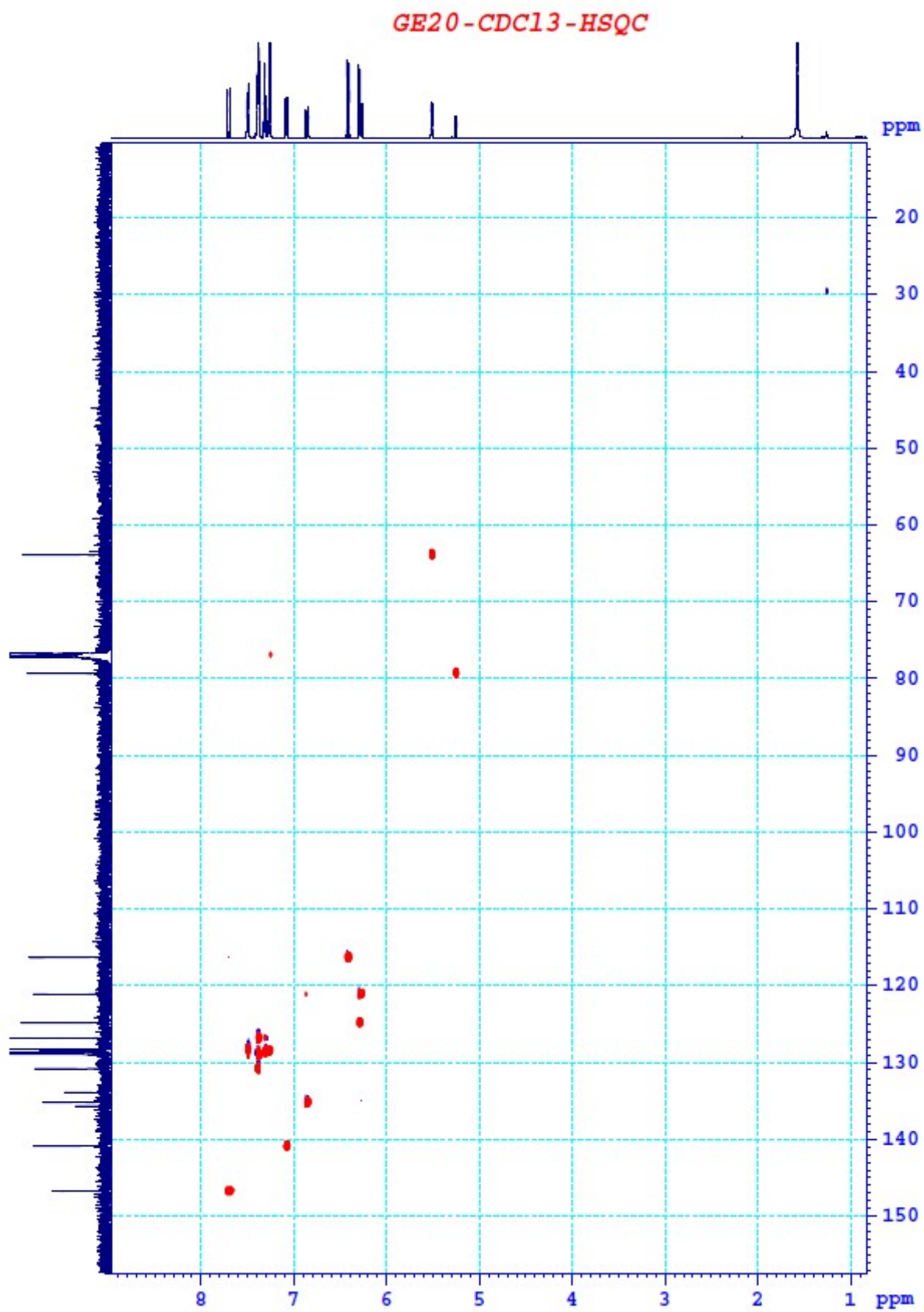


S16. HMBC - NMR spectrum of compound 1

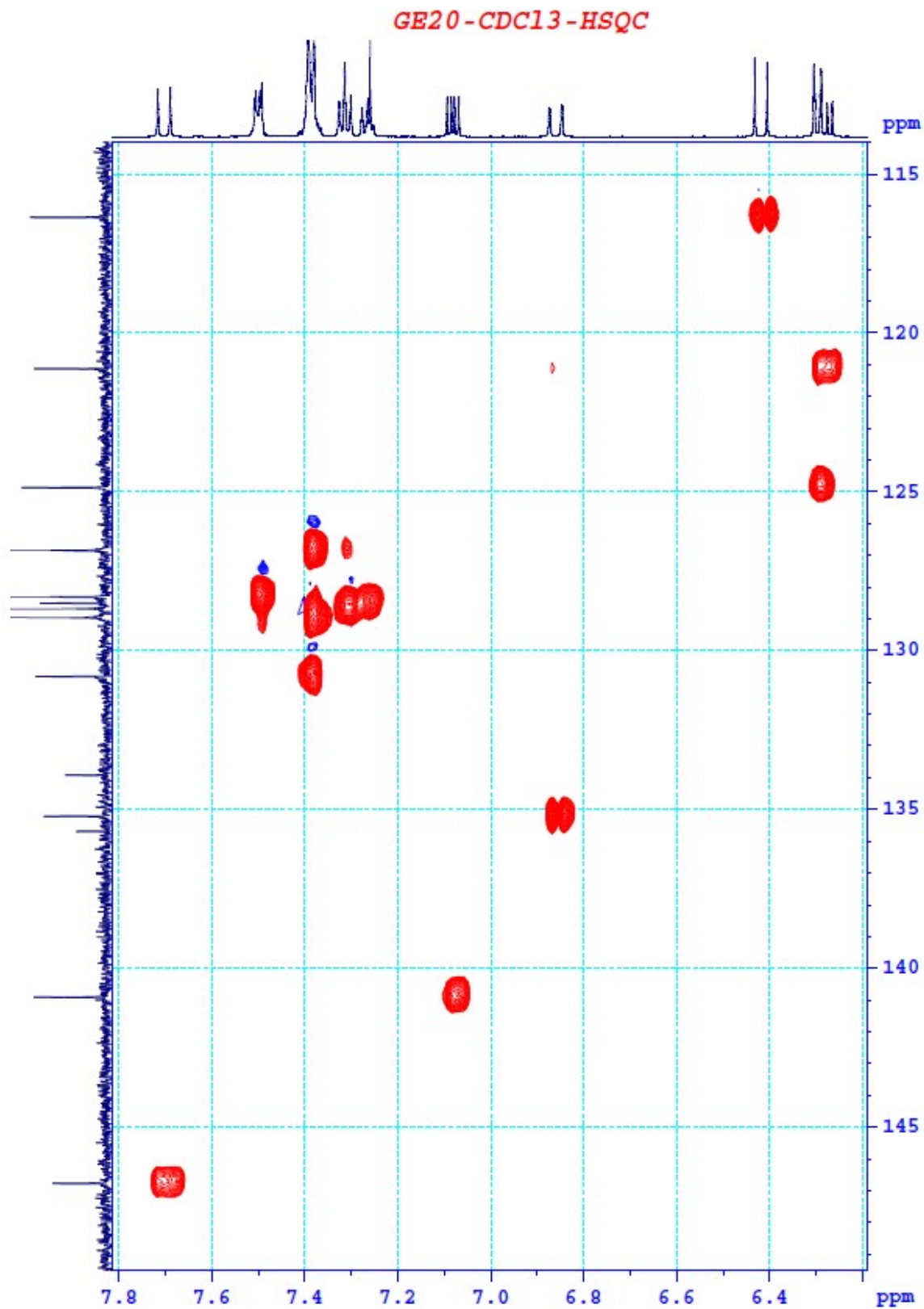
GE20 - CDC13 - HMBC



S17. HMBC - NMR spectrum of compound 1

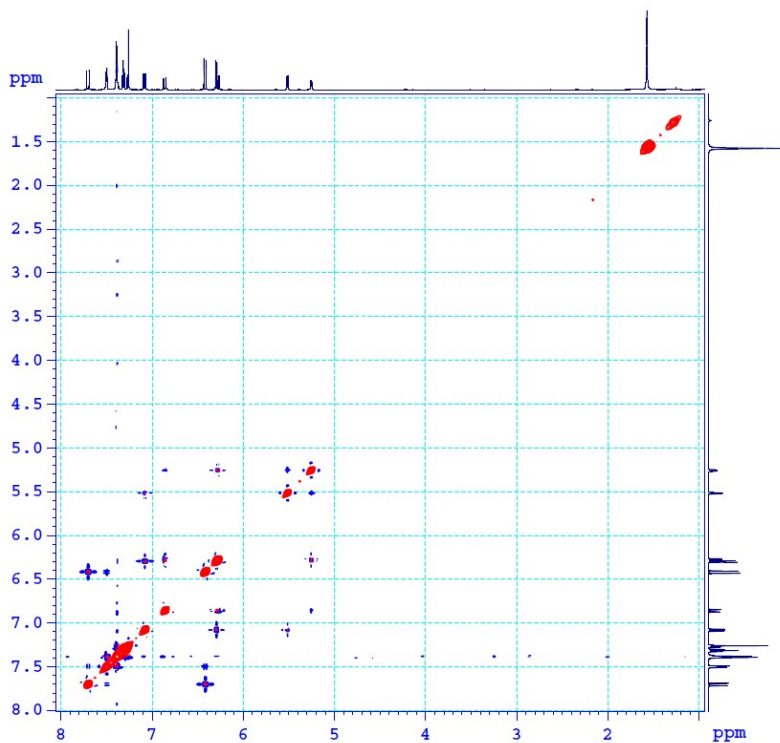


S18. HSQC - NMR spectrum of compound 1



S19. HSQC - NMR spectrum of compound 1

GE20 - CDCl3 - NOESY



```

Current Data Parameters
NAME      110LINH_GE20
EXPNO    8
PROCNO   1

F2 - Acquisition Parameters
Date_    20220726
Time     12.22 h
INSTRUM  AvanceNeo 600MHz
PROBHD   E114607_0862 (
PULPROG  noesyzgpgpp
TD        2048
SOLVENT  CDCl3
NS        4
DS        32
SWH       5263.158 Hz
FIDRES    5.139802 Hz
AQ        0.1945600 sec
RG        181
DW        95.000 usec
DE        17.07 usec
TE        303.2 K
D0        0.0008163 sec
D1        1.97542405 sec
D8        0.30000001 sec
D11       0.03000000 sec
D12       0.00002000 sec
D16       0.00020000 sec
IN0       0.00019000 sec
TDav      1
SFO1      600.4025921 MHz
NUC1      1H
P1        10.50 usec
P2        21.00 usec
P17       2500.00 usec
PLW1      27.03700066 W
PLW10     4.75323998 W
GPNAM[1]  SMO10_100
GPZ1      40.00 %
P16       1000.00 usec

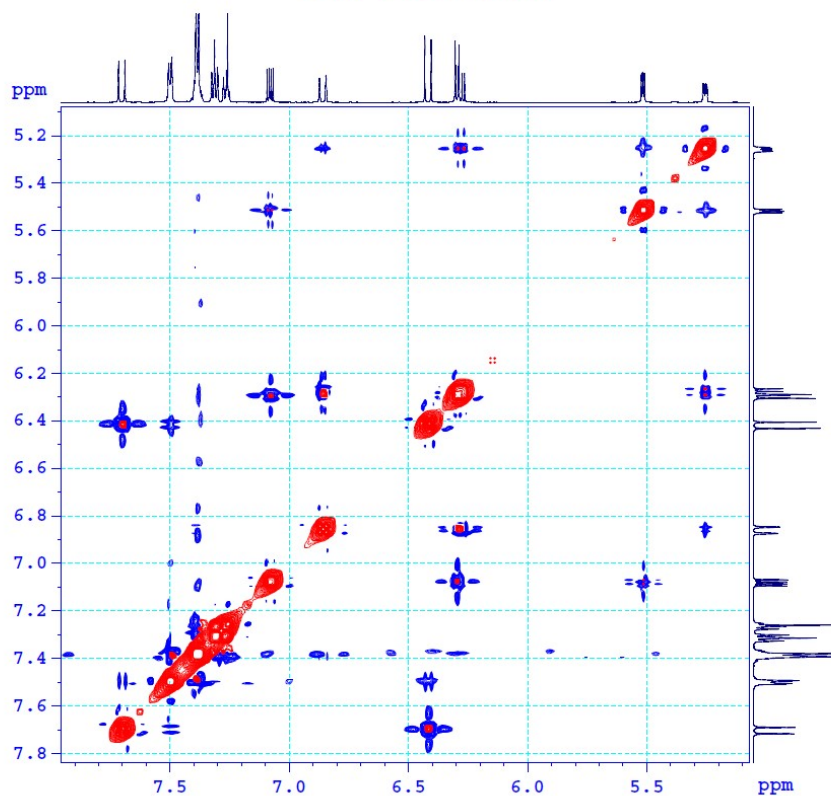
***** F1 INDIRECT DIMENSION *****
cd1       256
sw_F1     8.766048

F1 - Acquisition parameters
TD        256
SFO1      600.4026 MHz
FIDRES    41.118420 Hz
SW        8.766 ppm
F0MODE    States-TPPI

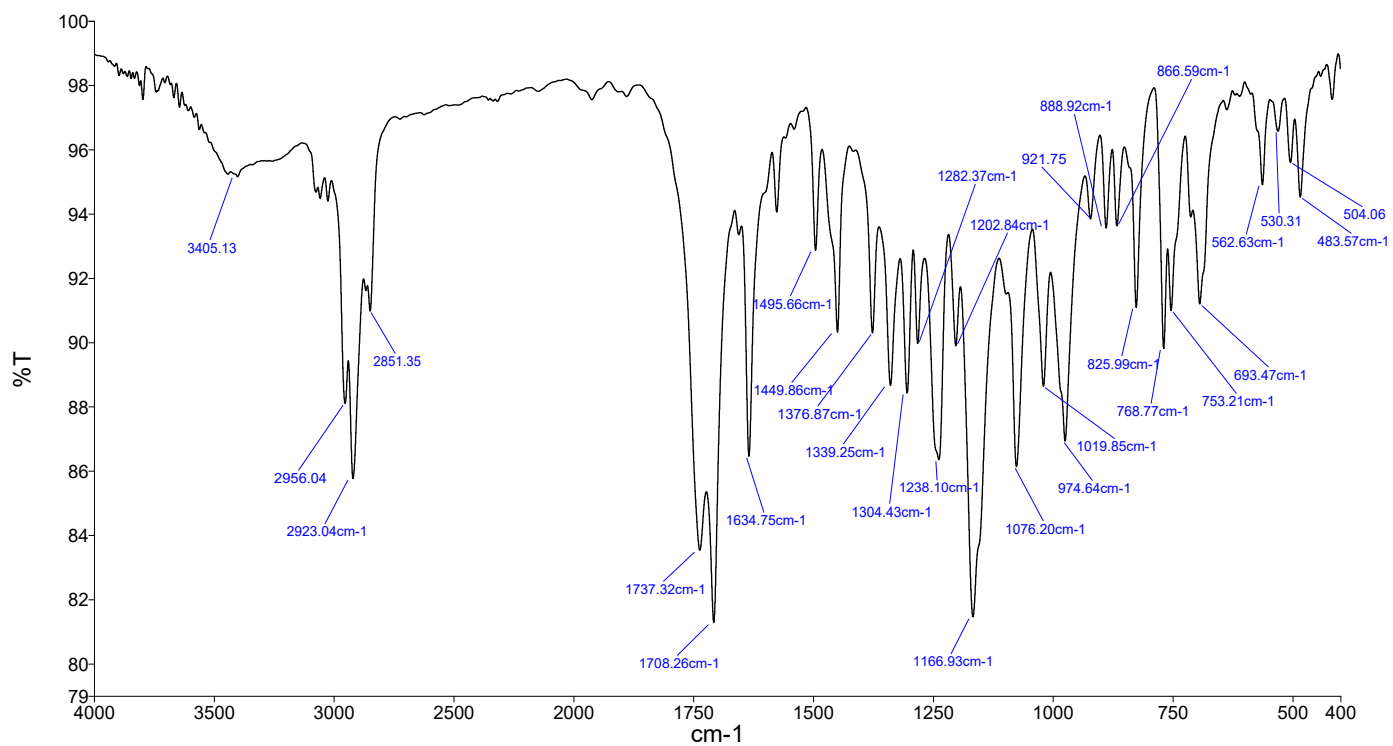
F2 - Processing parameters
SI         1024
SF         600.4000152 MHz
WDW        QSINE
SSB        2
LB         0 Hz
GB         0
PC         1.00

F1 - Processing parameters
SI         1024
MC2       States-TPPI
SF         600.4000152 MHz
WDW        QSINE
SSB        2
LB         0 Hz
GB         0
    
```

GE20 - CDCl3 - NOESY



S20. NOESY - NMR spectrum of compound 1



S21. IR spectrum of compound 1