Peptides *N*-Connected to Hydroxycoumarin and cinnamic acid derivatives: Synthesis and Fluorescence Spectroscopic, Antioxidant and Antimicrobial Properties.

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Contents

Characterization data:

Starting materials:

2-Oxo-2H-chromene-3-carboxylic acid (3a).[1] White crystal (177 mg, 93%), M.P.: 191-192°C [190-192 °C], IR (KBr): 3063, 1744, 1660, 1608, 1564, 1418, 1211 cm^{-1}.

6-Nitro-2-oxo-2H-chromene-3-carboxylic acid (3b).[2] White crystal (221 mg, 94%), M.P.: 233-234°C [234-236 °C], IR (KBr): 3243, 1720, 1616, 1526, 1350, 1233, 1204 cm^{-1}.

7-Hydroxy-2-oxo-2H-chromene-3-carboxylic acid (3c).[1] Light yellow crystal (187 mg, 91%), M.P.: 264-265°C [263.4 - 265.3 °C], IR (KBr): 3158, 2759, 1736, 1672, 1607, 1435, 1293, 1225 cm^{-1}.

6-Bromo-2-oxo-2H-chromene-3-carboxylic acid (3d).[3] White crystal (260mg, 97 %), M.P.: 200°C [195-196 °C], IR (KBr): 2807, 1771, 1369, 1197, 1024 cm^{-1}.

3-Oxo-3H-benzo[*f*]chromene-2-carboxylic acid (3e).[2] Brown crystal (216mg, 90%), M.P.: 233-234°C (decomposed) [236-237 °C (decomposed)], IR (KBr): 3417, 3064, 1746, 1684, 1565, 1388, 1210, 1038, 791, 711 cm^{-1}.

6-Methyl-2-oxo-2H-chromene-3-carboxylic acid (3f).[4] White crystal (200mg, 98%), M.P.: 165-166°C [165 - 166 °C], IR (KBr): 3419, 3042, 1745, 1674, 1615, 1570, 1372, 1222, 1083, 804 cm^{-1}.

8-Ethoxy-2-oxo-2H-chromene-3-carboxylic acid (3g).[5] Light yellow crystal (229mg, 98 %), M.P.: 197- 198°C [197 - 198 °C], IR (KBr): 3047, 2983, 1750, 1677, 1605, 1467, 1423, 1380, 1284, 1211 cm^{-1}.

7, 8-Dihydroxy-2-oxo-2H-chromene-3-carboxylic acid (3h). Yellow crystal (211 mg, 95%), M.P.: 270-271°C, IR (KBr): 3421, 3261, 3040, 1735, 1688, 1494, 1401, 1295 cm^{-1}, ^{1}H NMR (300 MHz, DMSO-d_6): δ(ppm) = 6.85 (*d*, *J* = 8.4 Hz, 1H, H-Ar), 7.24 (*d*, *J* = 8.5 Hz, 1H, H-Ar), 8.62 (*s*, 1H, =CH), 9.76 (*s*, 1H, OH), 10.69 (br*s*, 1H, OH), 11.5 (brs.1H, -CO2H), ^{13}C NMR (75 MHz, DMSO-d_6): δ (ppm) = 111.6, 112.3, 113.5, 121.8, 132.0, 144.9, 150.3, 152.6, 158.0, 164.5.

8-Methoxy-2-oxo-2H-chromene-3-carboxylic acid (3i).[6] Light yellow crystal (218mg, 99 %), M.P.: 215- 218°C [218 - 219 °C], IR (KBr): 3472, 2843, 1769, 1676, 1606, 1473, 1264, 1094, 964, 799, 739 cm^{-1}.

7-(Diethylamino)-2-oxo-2H-chromene-3-carboxylic acid (3j).[7] Orange crystal (253mg, 97 %), M.P.: 222-223°C [222 °C], IR (KBr): 3421, 2936, 1738, 1610, 1581, 1511, 1406, 1196 cm^{-1}.

8-Hydroxy-2-oxo-2H-chromene-3-carboxylic acid (3k).[8]Green crystal (187mg, 91), M.P.: 292-293°C (decomposed) [291 - 292 °C (decomposed)], IR (KBr): 2018, 2053, 1774, 1031 cm^{-1}.

2-(5-Methoxy-2-oxo-2H-chromen-3-yl) acetic acid (4).[9] Yellow solid (166 mg, 71%), ^{1}H NMR (300 MHz, DMSO-*d*$_6$): δ(ppm) = 3.49 (*s*, 2H, -CH_2), 3.91 (*s*, 3H, -CH_3), 7.06 – 7.51 (*m*, 3H, H-Ar), 7.95 (*s*, 1H, =CH), 12.49 (*brs*, 1H, OH), ^{13}C NMR (75 MHz, DMSO-*d*$_6$): δ(ppm) = 35.9, 56.1, 101.6, 111.5, 113.8, 119.6, 123.3, 136.7, 141.9, 146.4, 161.4, 169.6.

Methyl 7, 8-dihydroxy-2-oxo-2H-chromene-3-carboxylate. ^{1}H NMR (300 MHz, DMSO-*d*$_6$): δ(ppm) = 3.79 (*s*, 3H, -OMe), 6.86 (*dd*, *J* = 8.5, 1.1 Hz, 1H, H-Ar), 7.27 (*d*, *J* = 8.5 Hz, 1H, H-Ar), 8.65 (*d*, *J* = 1.1 Hz, 1H, =CH), 9.57 (*brs*, 1H, OH), 10.64 (*brs*, 1H, OH).

Methyl 7, 8-dimethoxy-2-oxo-2H-chromene-3-carboxylate. ^{1}H NMR (300 MHz, DMSO-*d*$_6$): δ (ppm) = 3.81 (*s*, 3H, -OMe), 3.83 (*s*, 3H, -OMe), 3.95 (*s*, 3H, -OMe), 7.20 (*d*, *J* = 8.9 Hz, 1H, H-Ar), 7.68 (*d*, *J* = 8.8 Hz, 1H, H-Ar), 8.74 (*s*, 1H, =CH).

7, 8-Dimethoxy-2-oxo-2H-chromene-3-carboxylic acid (5). Yellow crystal (218 mg, 87 %), M.P.: 186-188°C, IR (KBr): 3418, 3194, 1738, 1613, 1468, 1204, 1078, 802, 610 cm^{-1}, ^{1}H NMR (300 MHz, DMSO-*d*$_6$): δ (ppm) = 3.79 (*s*, 3H, -OCH3), 3.80 (*s*, 3H, -OCH3) 6.86 (*dd*, *J* = 8.4, 1.0 Hz, 1H, H-Ar), 7.27 (*d*, *J* = 8.5 Hz, 1H, H-Ar), 8.66 (*d*, *J* = 1.0, 1H, =CH), 9.69 (*s*, 1H, -COOH), ^{13}C NMR (75 MHz, DMSO-*d*$_6$): δ (ppm) = 52.1, 56.5, 111.2, 111.6, 113.3, 121.8, 131.8, 144.9, 150.4, 152.6, 156.4, 163.6.

6-(Benzyloxy)-2-oxo-2H-chromene-3-carboxylic acid (6).[10] White crystal. (243 mg, 82 %), ^{1}H NMR (300 MHz, DMSO-*d*$_6$): δ(ppm) = 5.24 (*s*, 2H, -CH_2), 6.94 – 7.19 (*m*, 2H, H-Ar), 7.24 – 7.56 (*m*, 5H, H-Ar), 7.83 (*d*, *J* = 8.4 Hz, 1H, H-Ar), 8.69 (*s*, 1H, =CH), 12.87 (*s*, 1H,

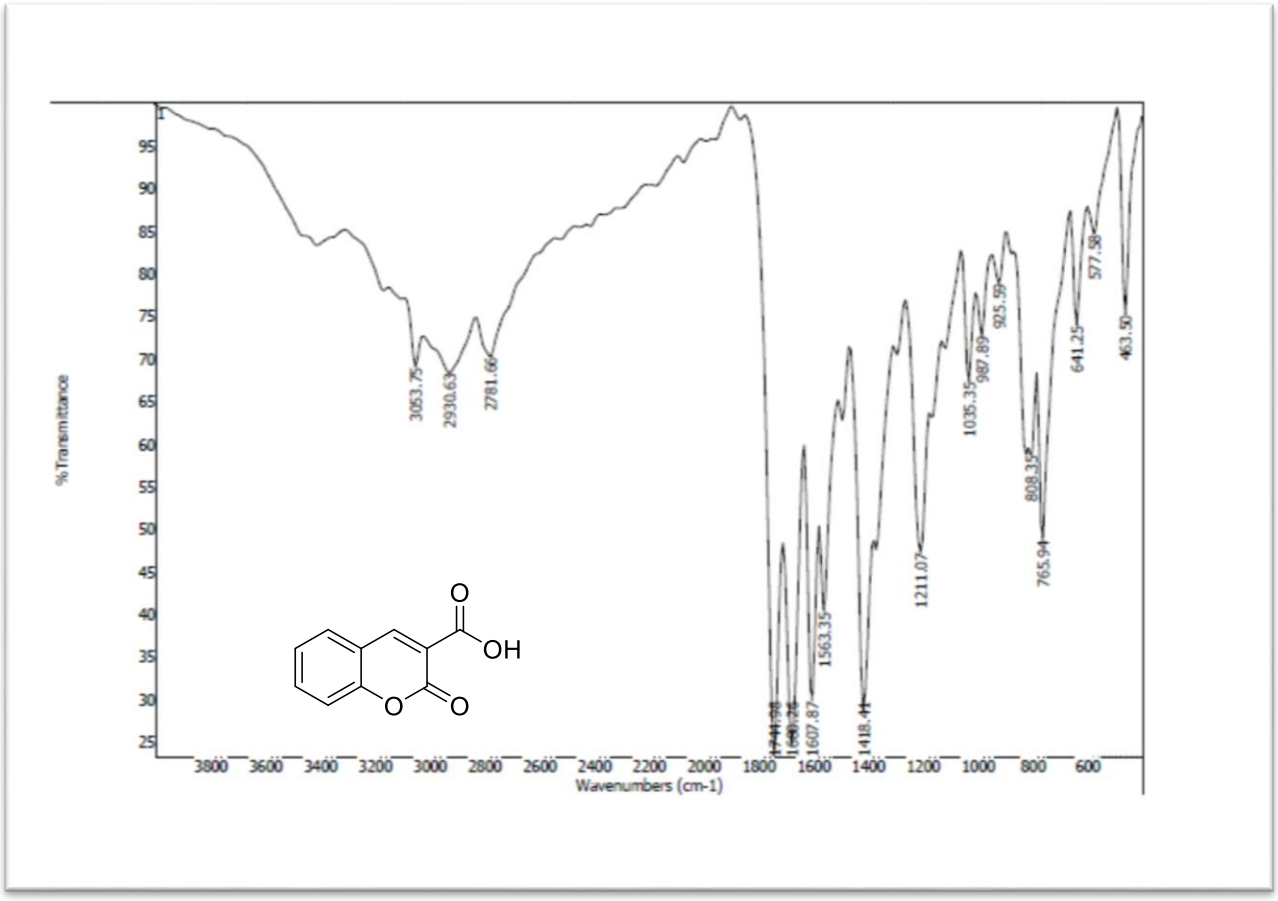
OH), ^{13}C NMR (75 MHz, DMSO-d_6): δ(ppm) = 70.2, 101.2, 111.8, 113.8, 114.0, 128.0, 128.3, 128.6, 131.7, 136.0, 149.0, 156.8, 157.2, 163.6, 164.2.

7-Methoxy-2-oxo-2H-chromene-3-carboxylic acid (7).[4] White crystal (212 mg, 96 %), M.P.: 193-194°C [193-195 °C], IR (KBr): 3453, 3042, 1736, 1691, 1610, 1502, 1421, 1380, 1257, 1212, 1111, 1010, 799 cm^{-1}.

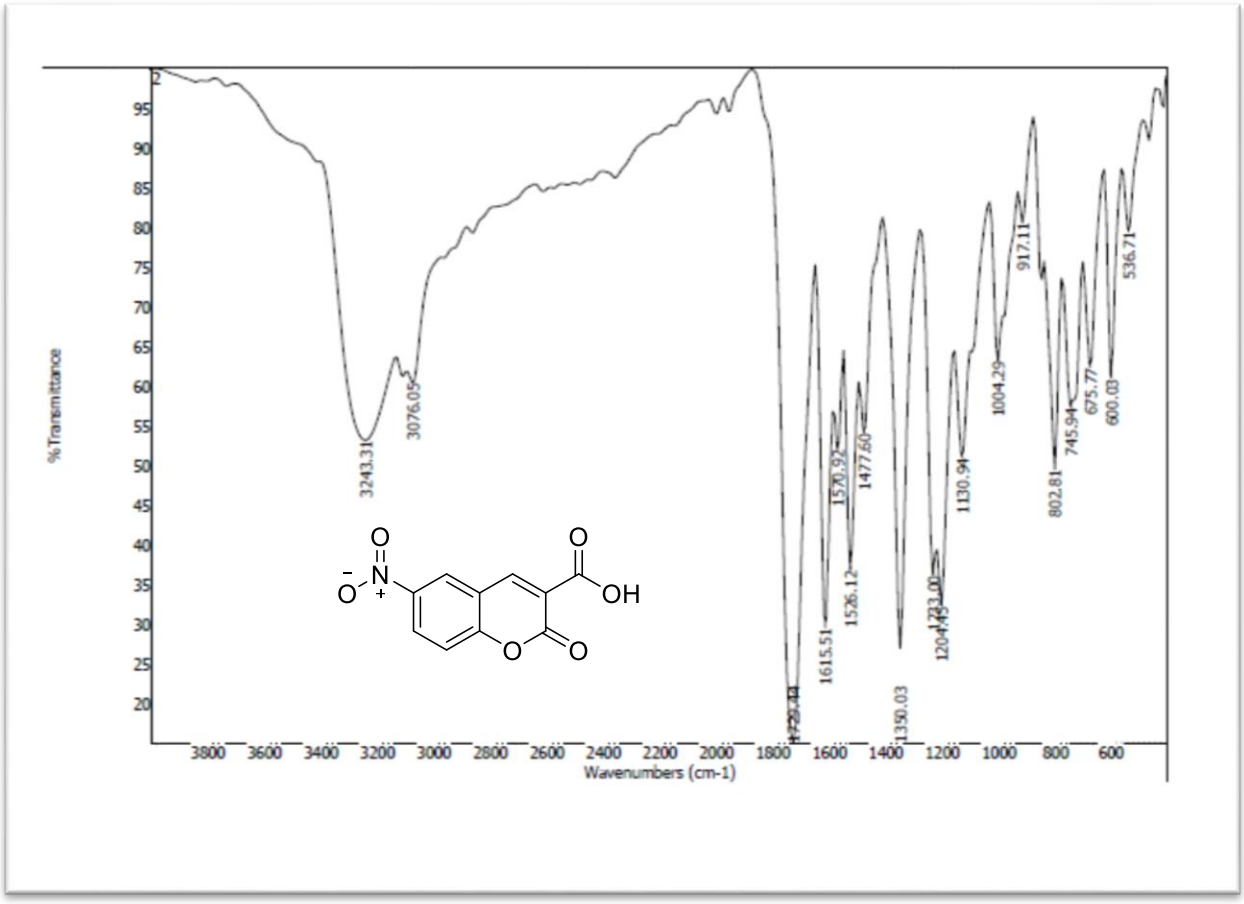
(E)-3-(4-methoxyphenyl) acrylic acid (9a).[3] Light yellow crystal (166 mg, 93 %), M.P.: 170-171°C [170-171°C],

(**E)-3-(2, 2-Dimethylbenzo[d][1,3] dioxol-5-yl)acrylic acid (10a).**[11] Light green crystal (194 mg, 88 %), ^{1}H NMR (300 MHz, DMSO-d_6): δ(ppm) = 1.65 (*s*, 6H, 2-CH_3), 6.37 (*d*, *J* = 15.8 Hz, 1H, =CH), 6.85 (*d*, *J* = 7.9 Hz, 1H, H-Ar), 7.10 (*dd*, *J* = 8.0, 1.7 Hz, 1H, H-Ar), 7.27 (*d*, *J* = 1.8 Hz, 1H, H-Ar), 7.47 (*d*, *J* = 15.9 Hz, 1H, =CH), ^{13}C NMR (75 MHz, DMSO-d_6): δ(ppm) = 25.6, 106.5, 108.4, 116.8, 118.9, 124.3, 128.3, 144.1, 147.7, 148.8, 168.0.

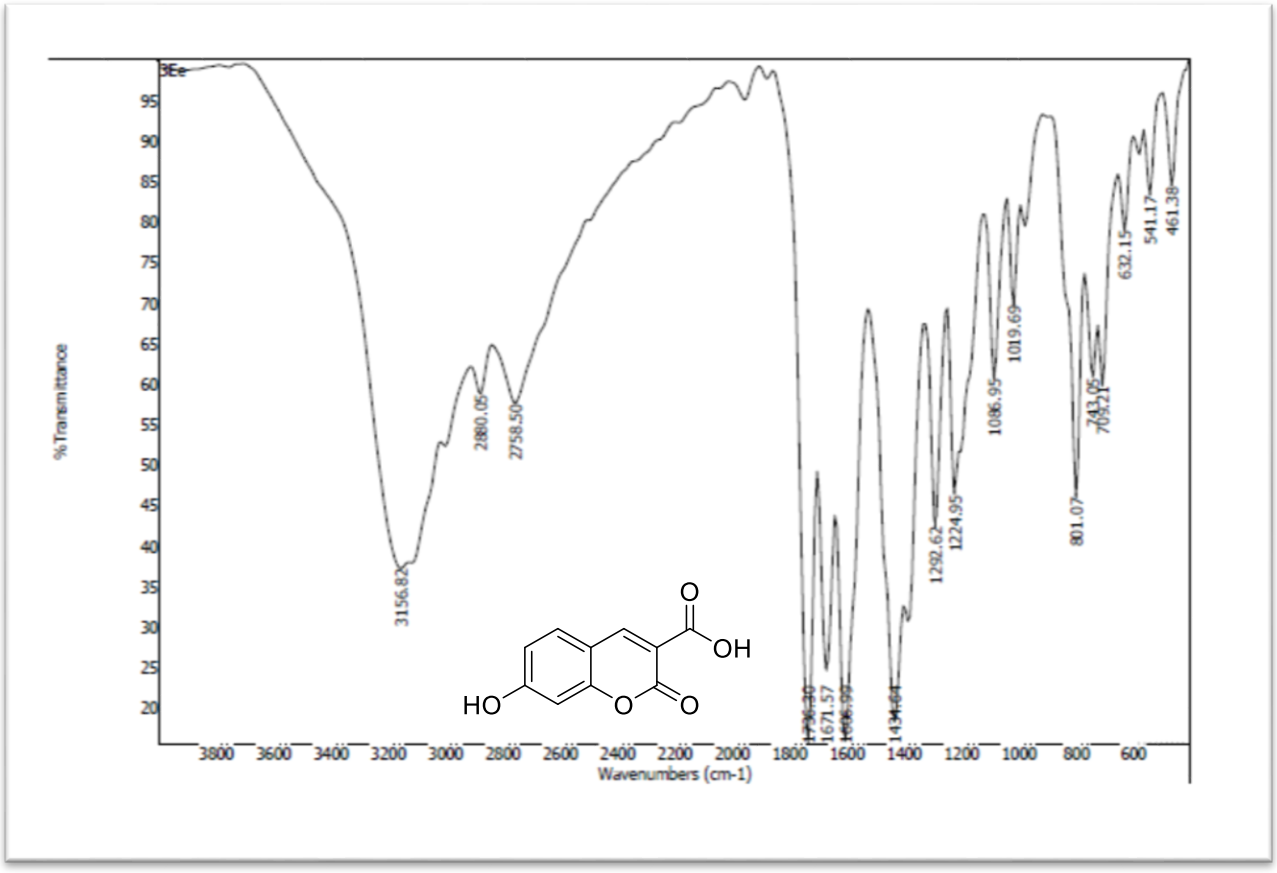
IR Spectra



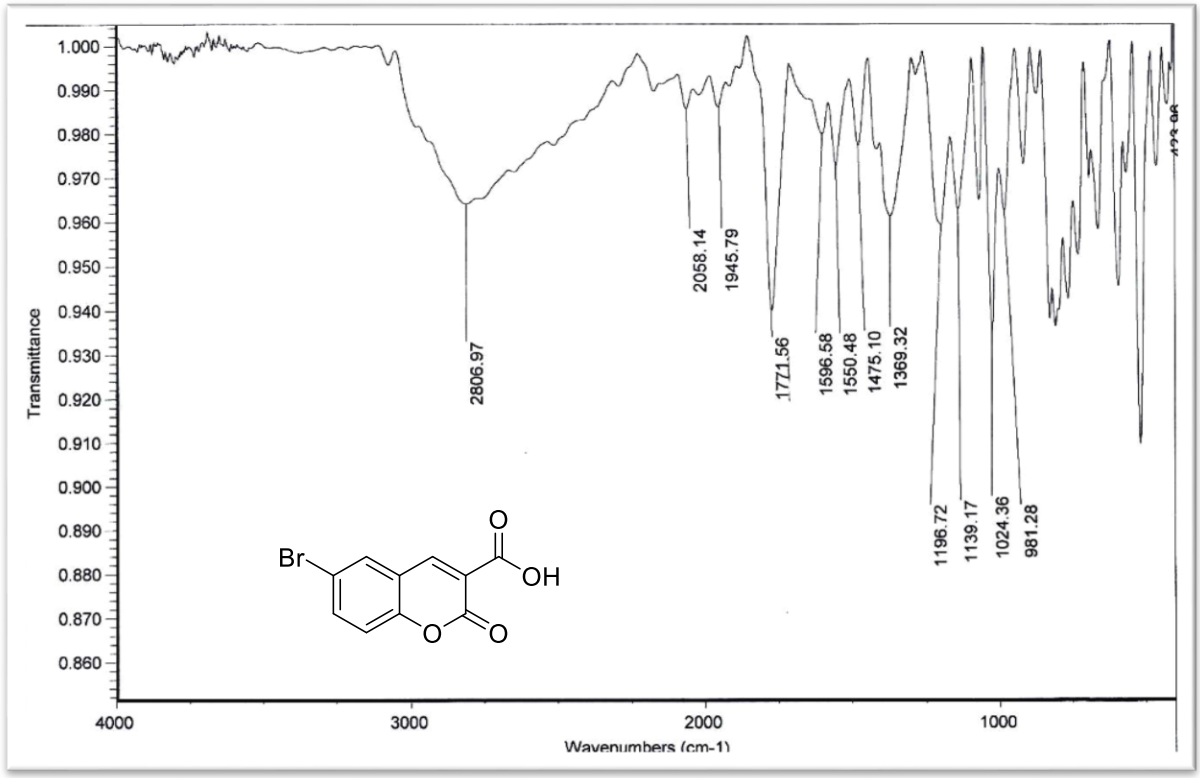
IR (KBr, cm^{-1}) spectra of 2-oxo-2H-chromene-3-carboxylic acid (**3a**)



IR (KBr, cm^{-1}) spectra of 6-nitro-2-oxo-2H-chromene-3-carboxylic acid (**3b**)



IR (KBr, cm^{-1}) spectra of 7-hydroxy-2-oxo-2H-chromene-3-carboxylic acid (**3c**)



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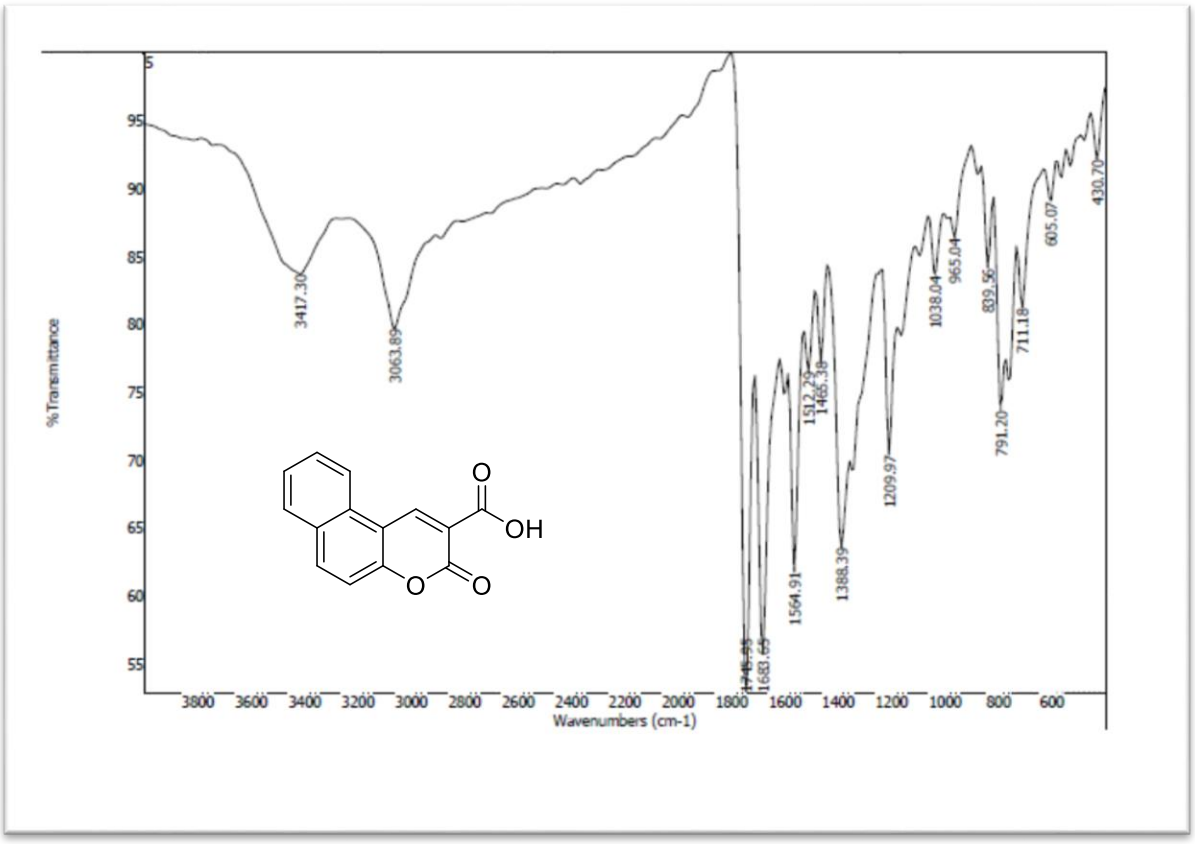

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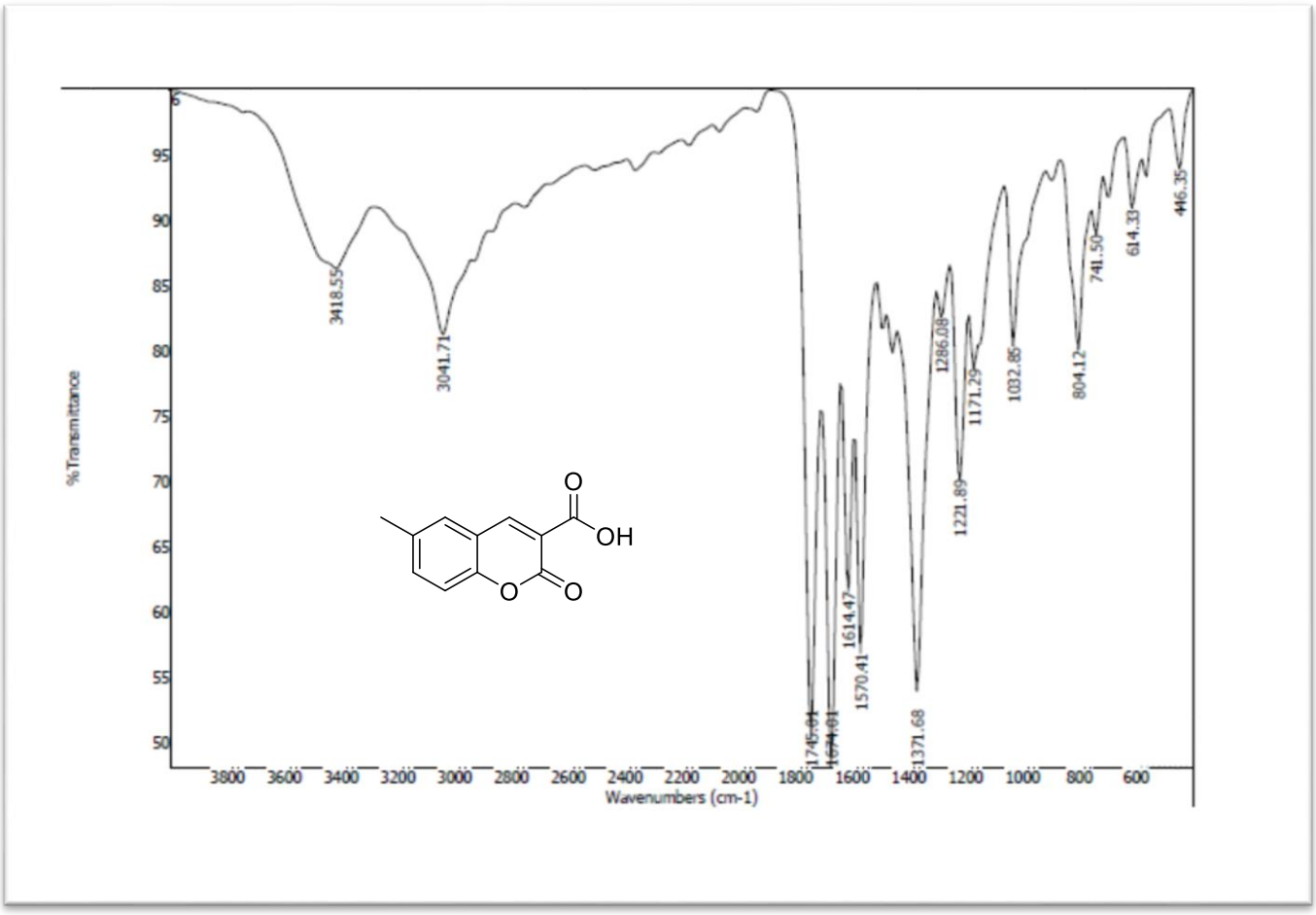

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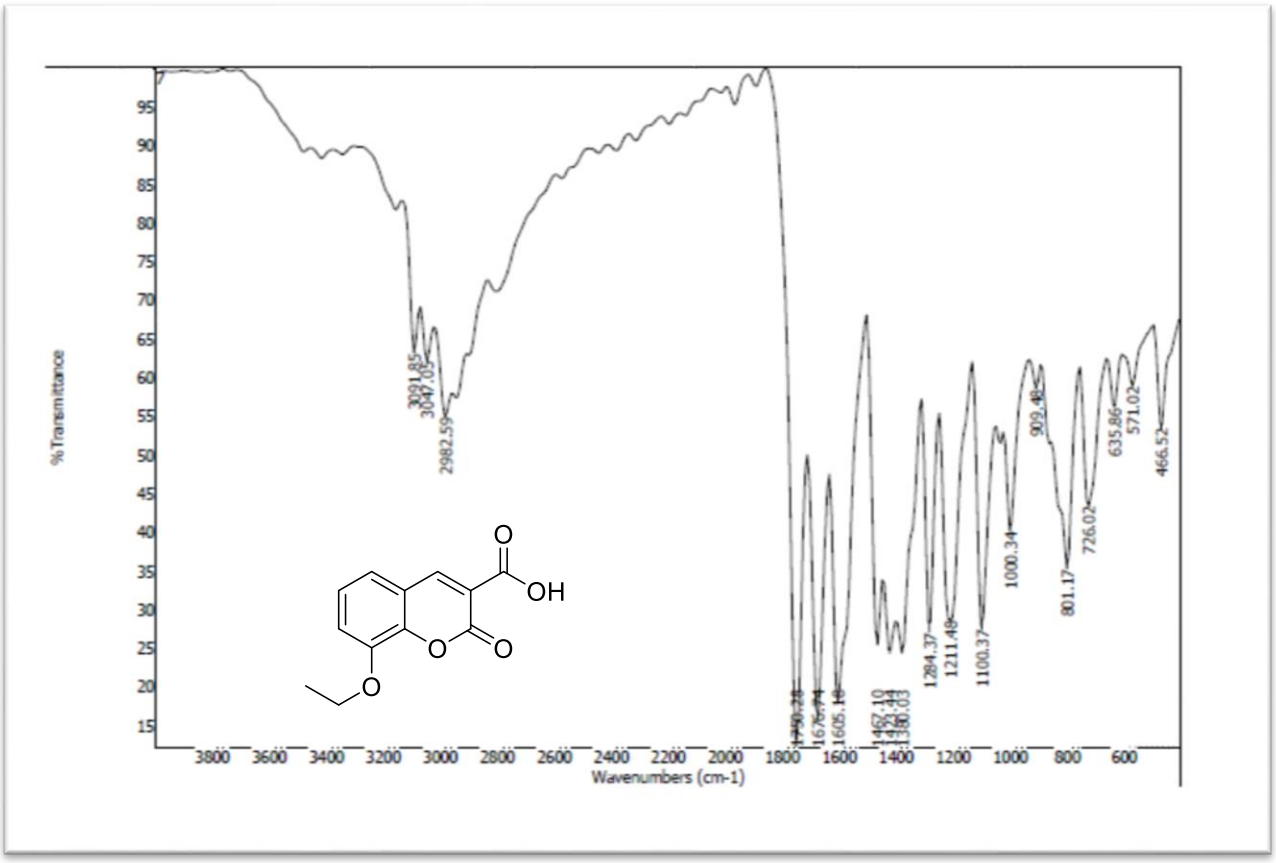
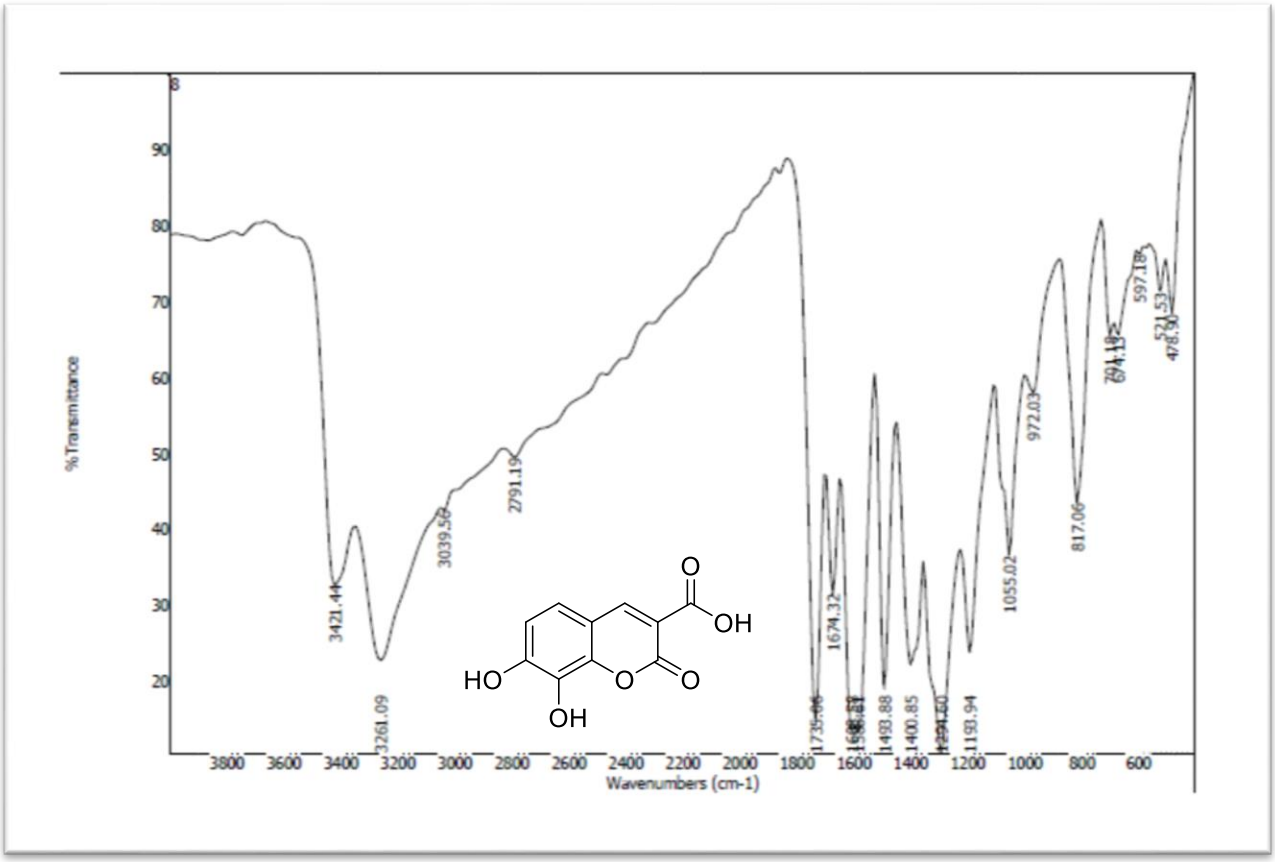
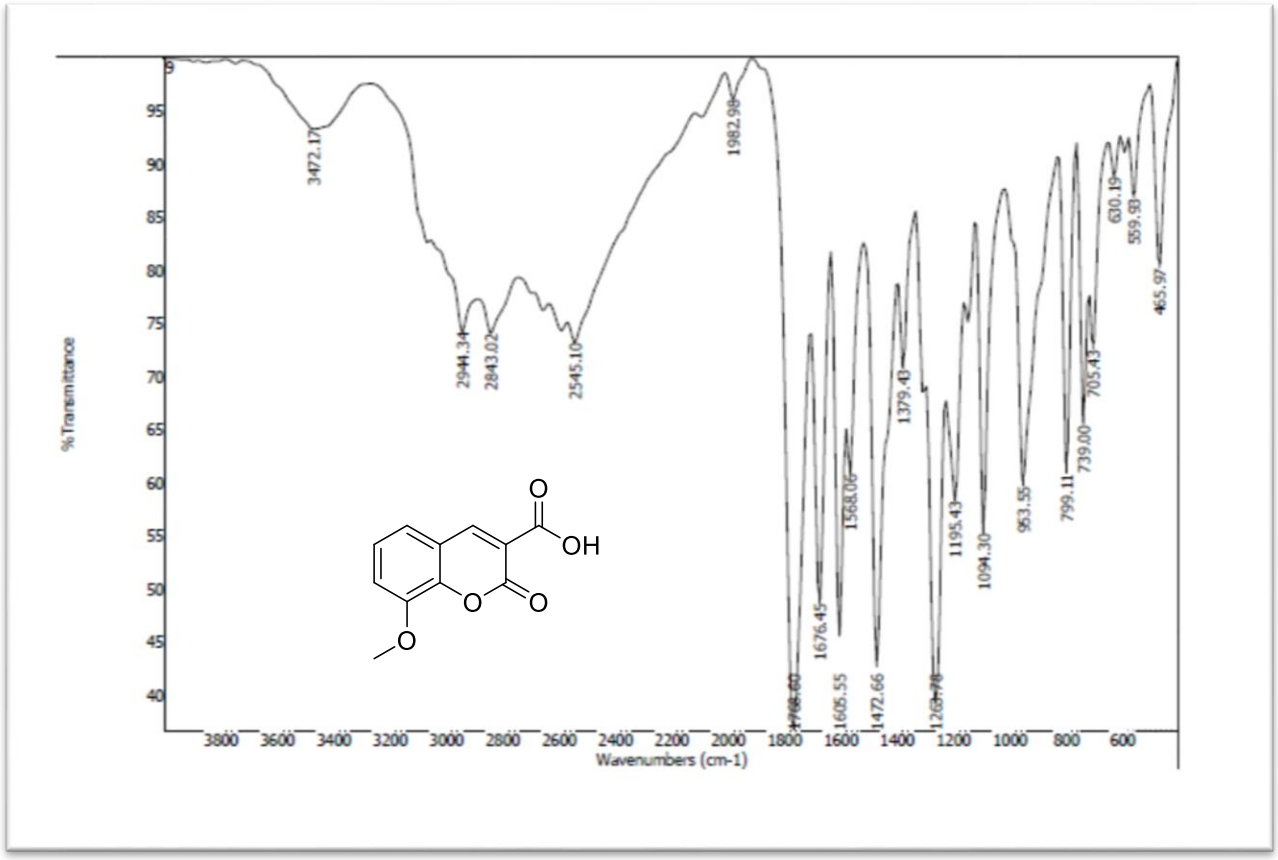


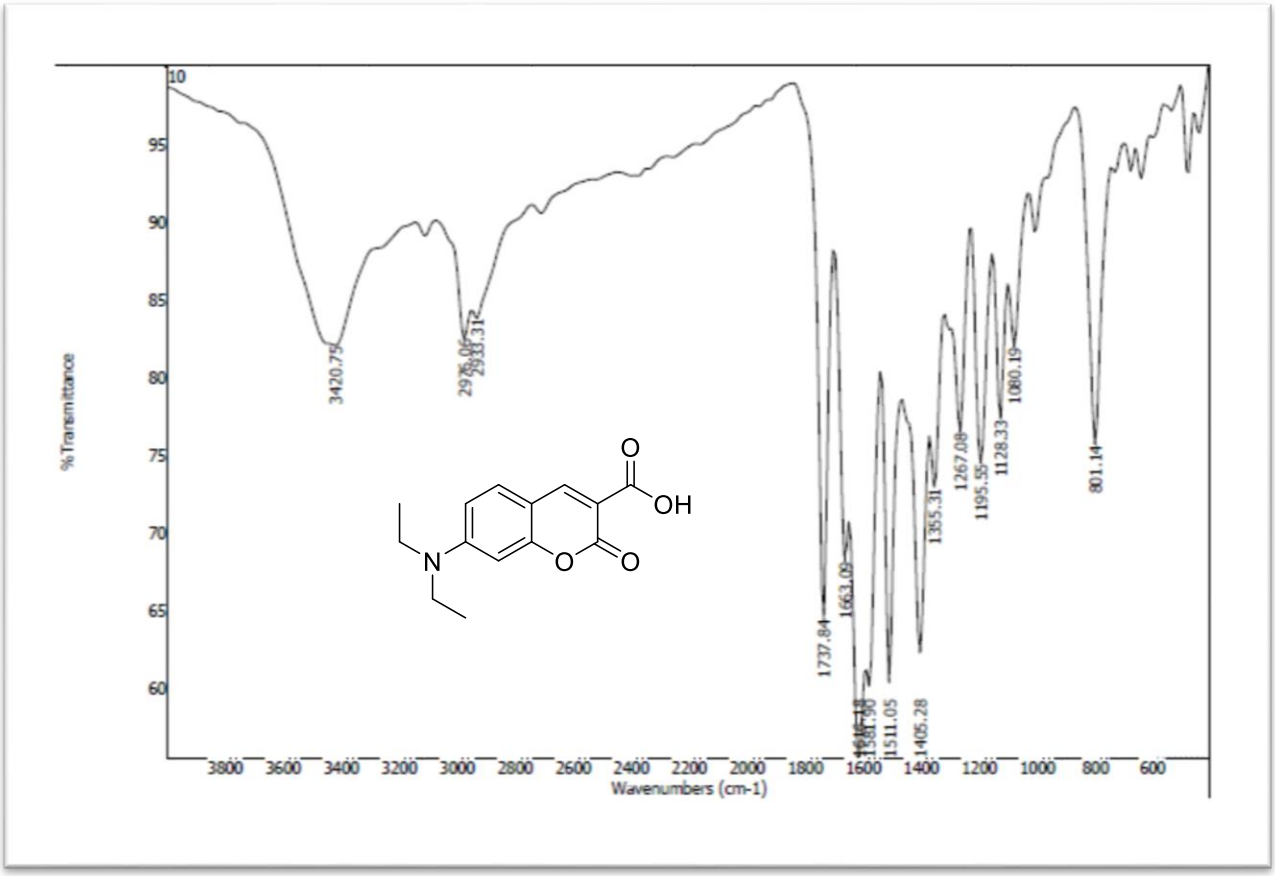
IR (KBr, cm^{-1}) spectra of 8-ethoxy-2-oxo-2H-chromene-3-carboxylic acid (**3g**)



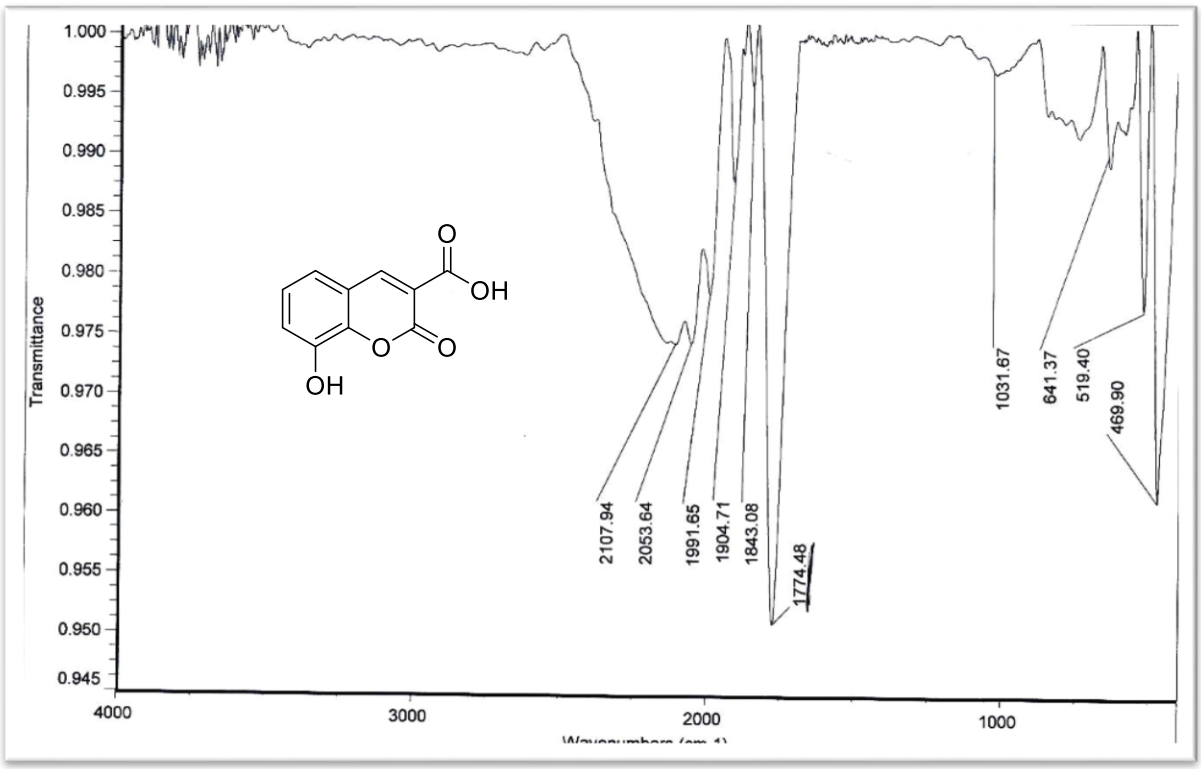
IR (KBr, cm^{-1}) spectra of 7, 8-dihydroxy-2-oxo-2H-chromene-3-carboxylic acid (**3h**)



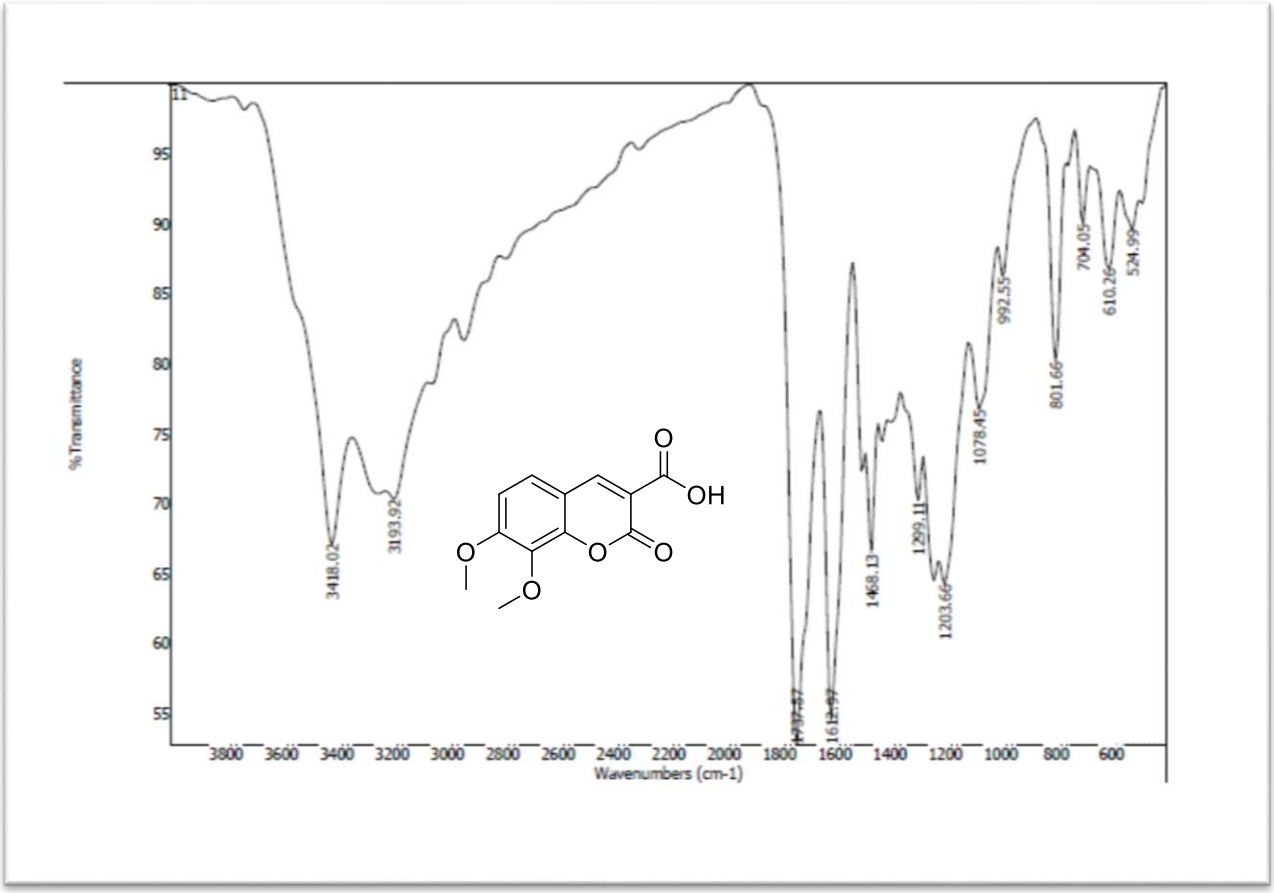
IR (KBr, cm^{-1}) spectra of 8-methoxy-2-oxo-2H-chromene-3-carboxylic acid (**3i**)



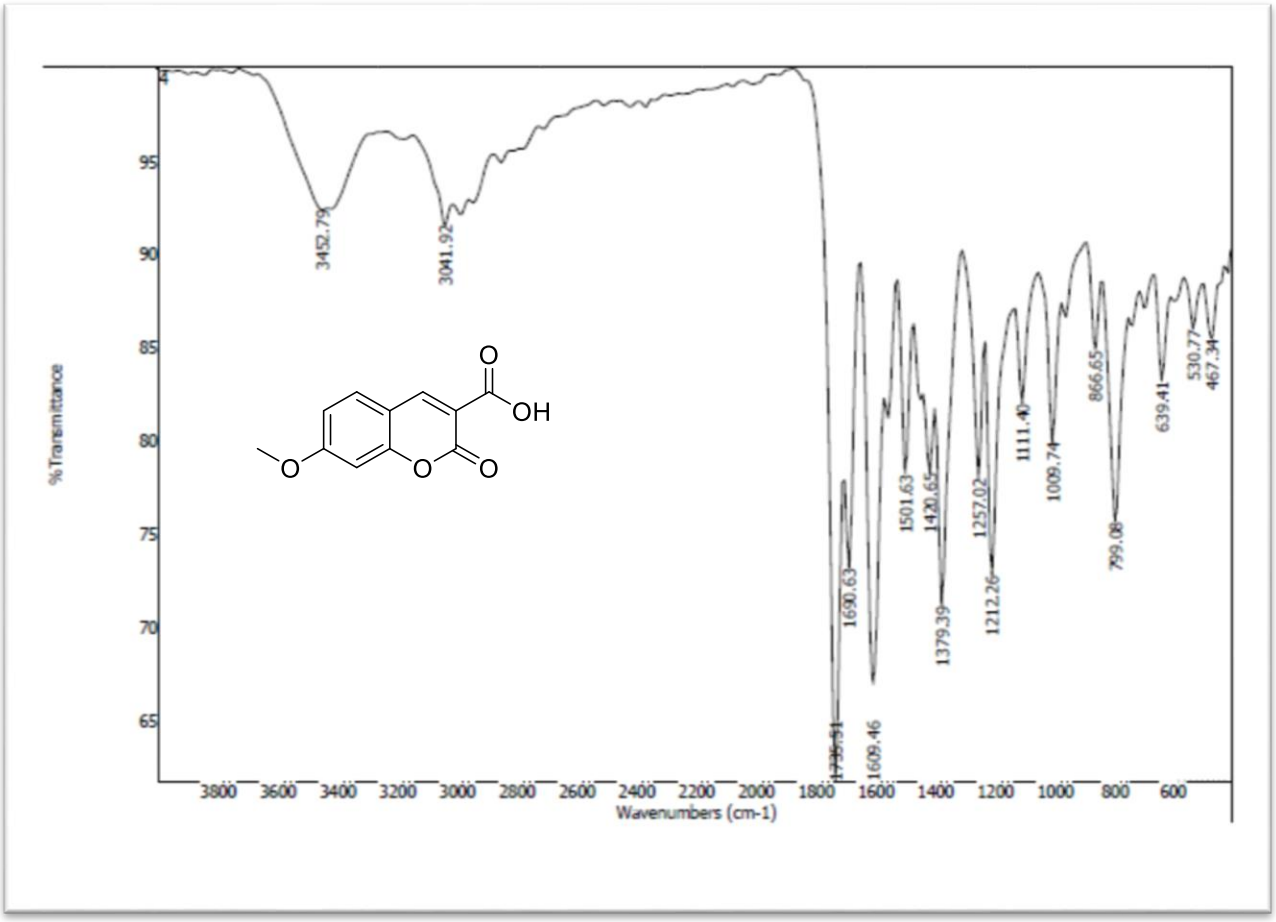
IR (KBr, cm^{-1}) spectra of 7-(diethylamino)-2-oxo-2H-chromene-3-carboxylic acid (**3j**)



IR (KBr, cm^{-1}) spectra of 8-hydroxy-2-oxo-2H-chromene-3-carboxylic acid (**3K**)

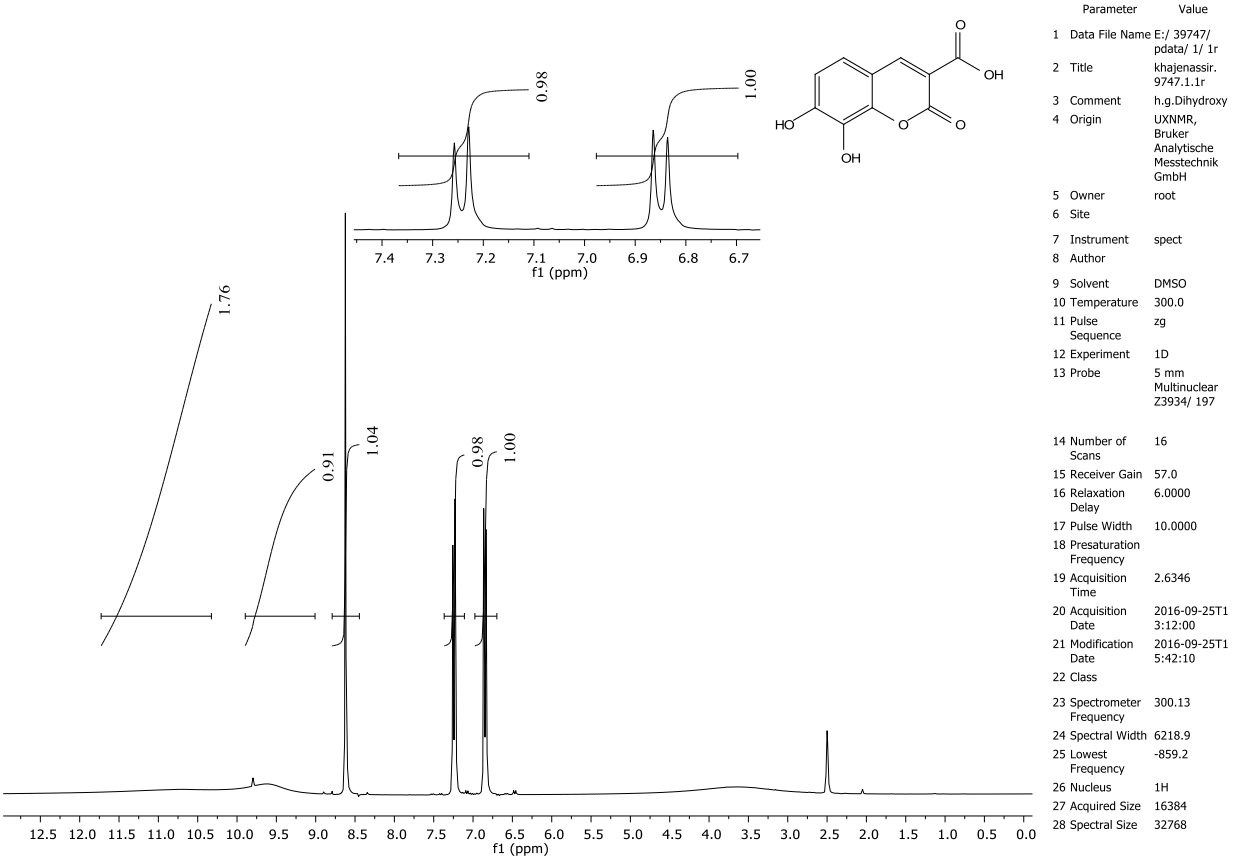


IR (KBr, cm^{-1}) spectra of 7, 8-dimethoxy-2-oxo-2H-chromene-3-carboxylic acid (**5**)



IR (KBr, cm^{-1}) spectra of 7-methoxy-2-oxo-2H-chromene-3-carboxylic acid (**7**)

NMR spectra



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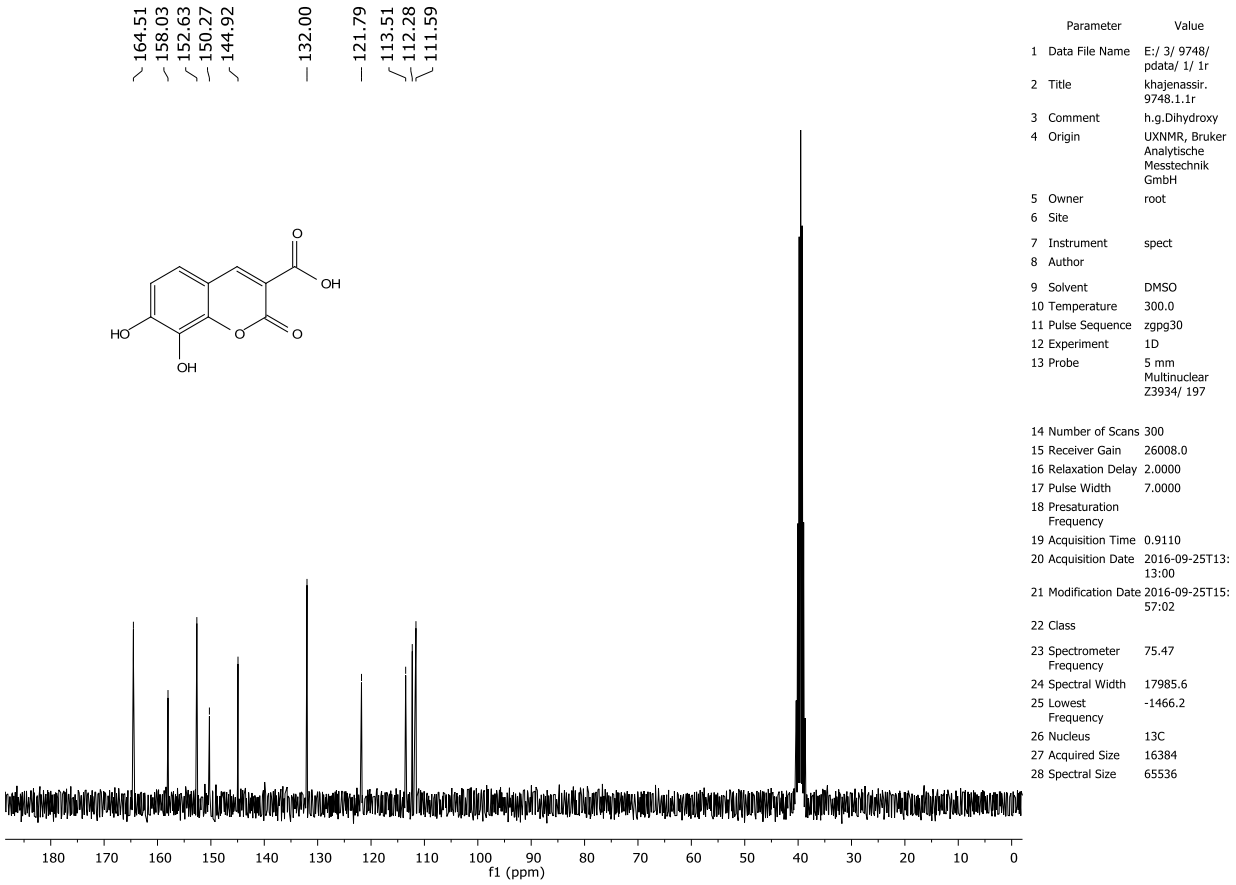
^{1}H NMR (300 MHz, DMSO-d_6) spectra of 7, 8-dihydroxy-2-oxo-2H-chromene-3-carboxylic acid (**3h**)



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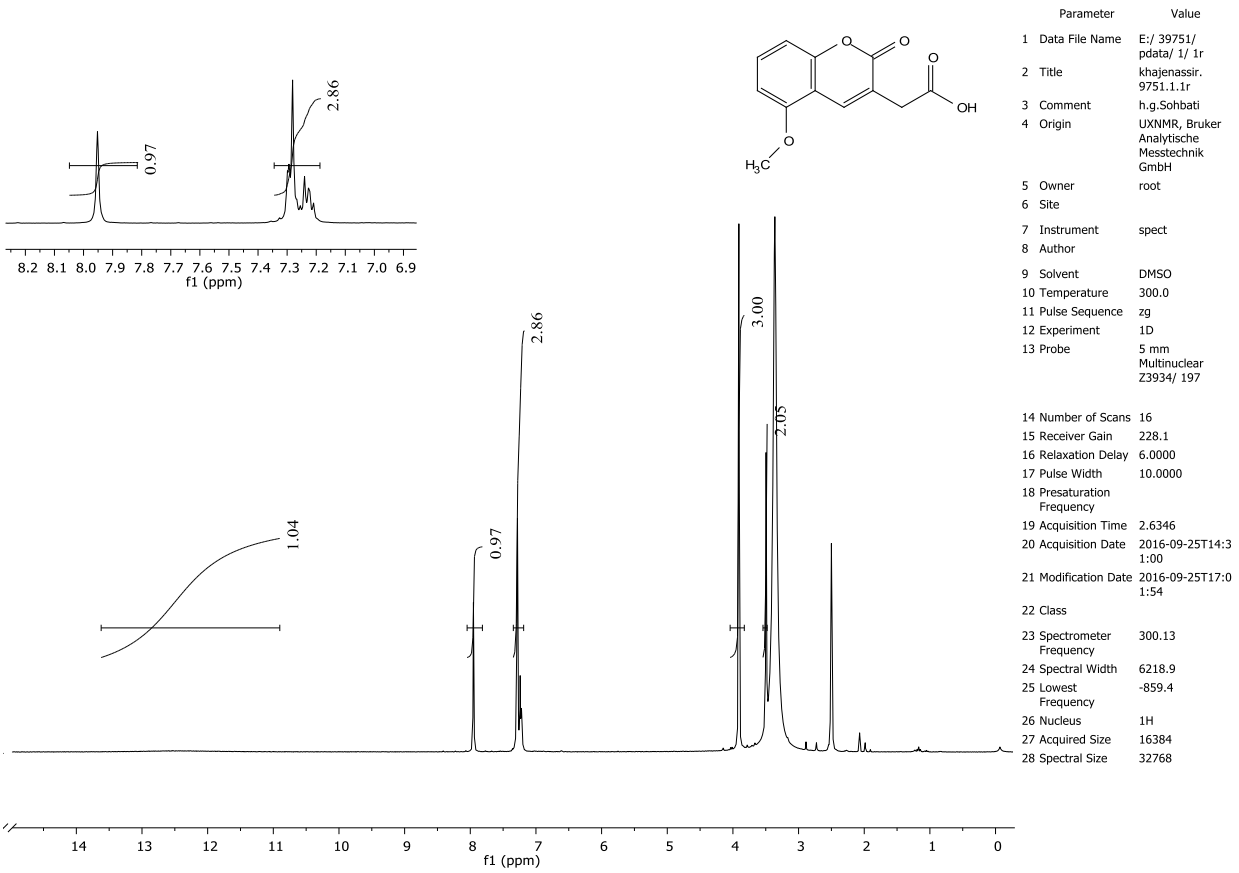
^{13}C NMR (75 MHz, DMSO-d_6) spectra 7, 8-dihydroxy-2-oxo-2H-chromene-3-carboxylic acid (**3h**)



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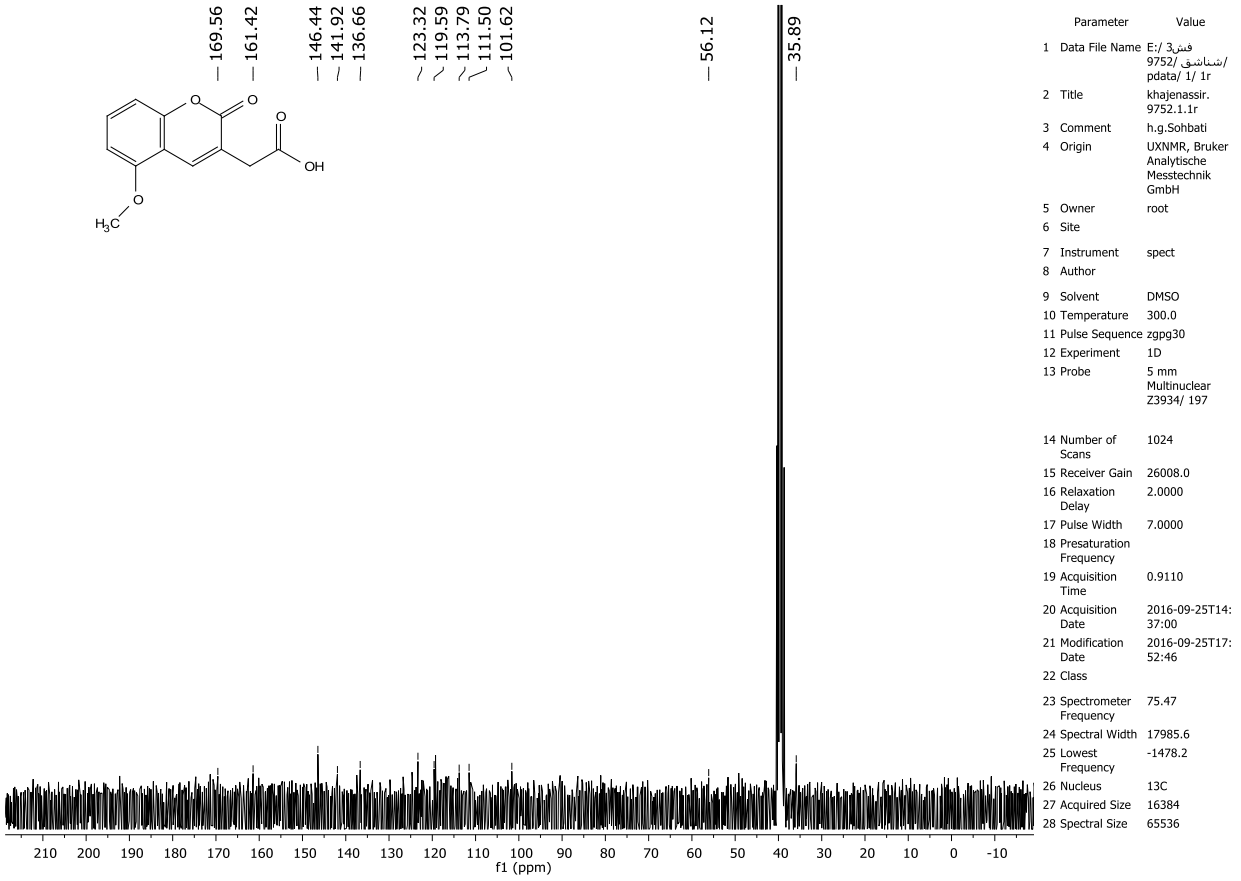
^{1}H NMR (300 MHz, DMSO-d_6) spectra of 2-(5-methoxy-2-oxo-2H-chromen-3-yl) acetic acid (**4**)



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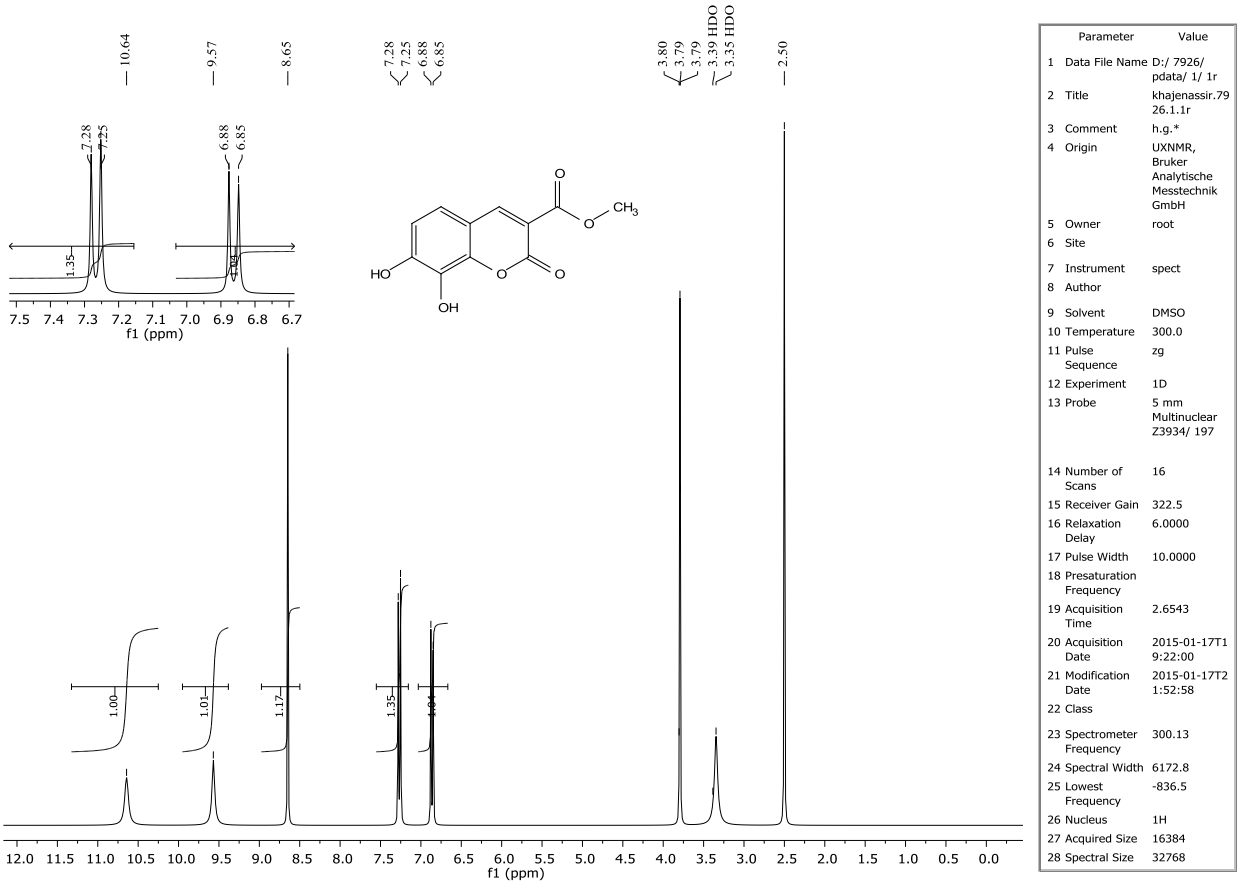
^{13}C NMR (75 MHz, DMSO-d_6) spectra of 2-(5-methoxy-2-oxo-2H-chromen-3-yl) acetic acid (**4**)



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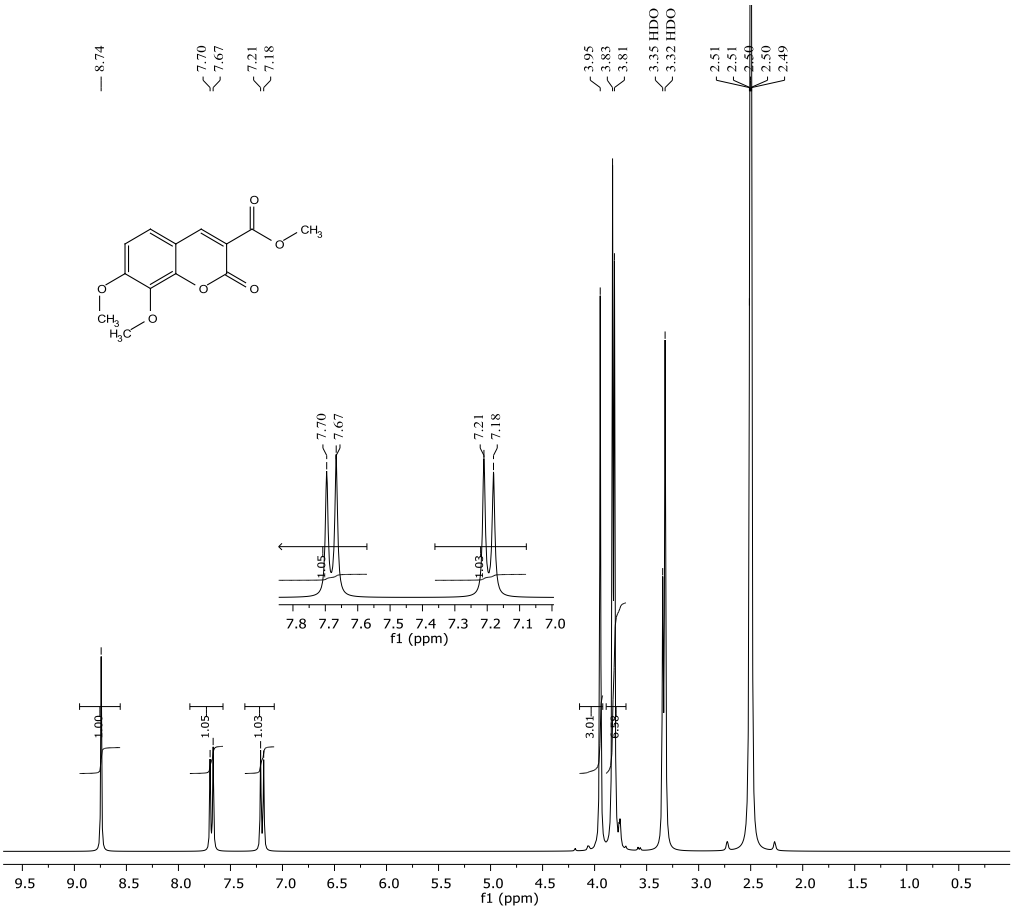
^{1}H NMR (300 MHz, DMSO-d_6) spectra of Methyl 7, 8-dihydroxy-2-oxo-2H-chromene-3-carboxylate



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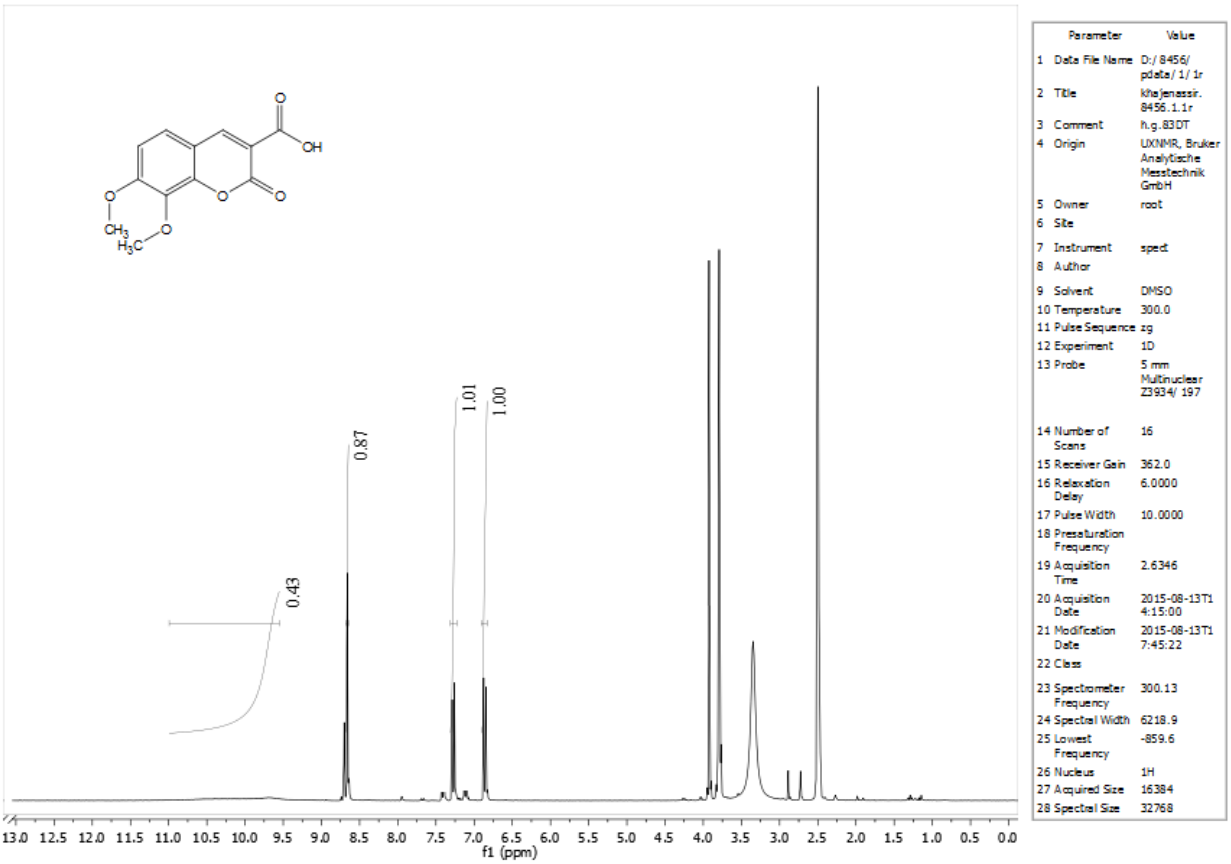
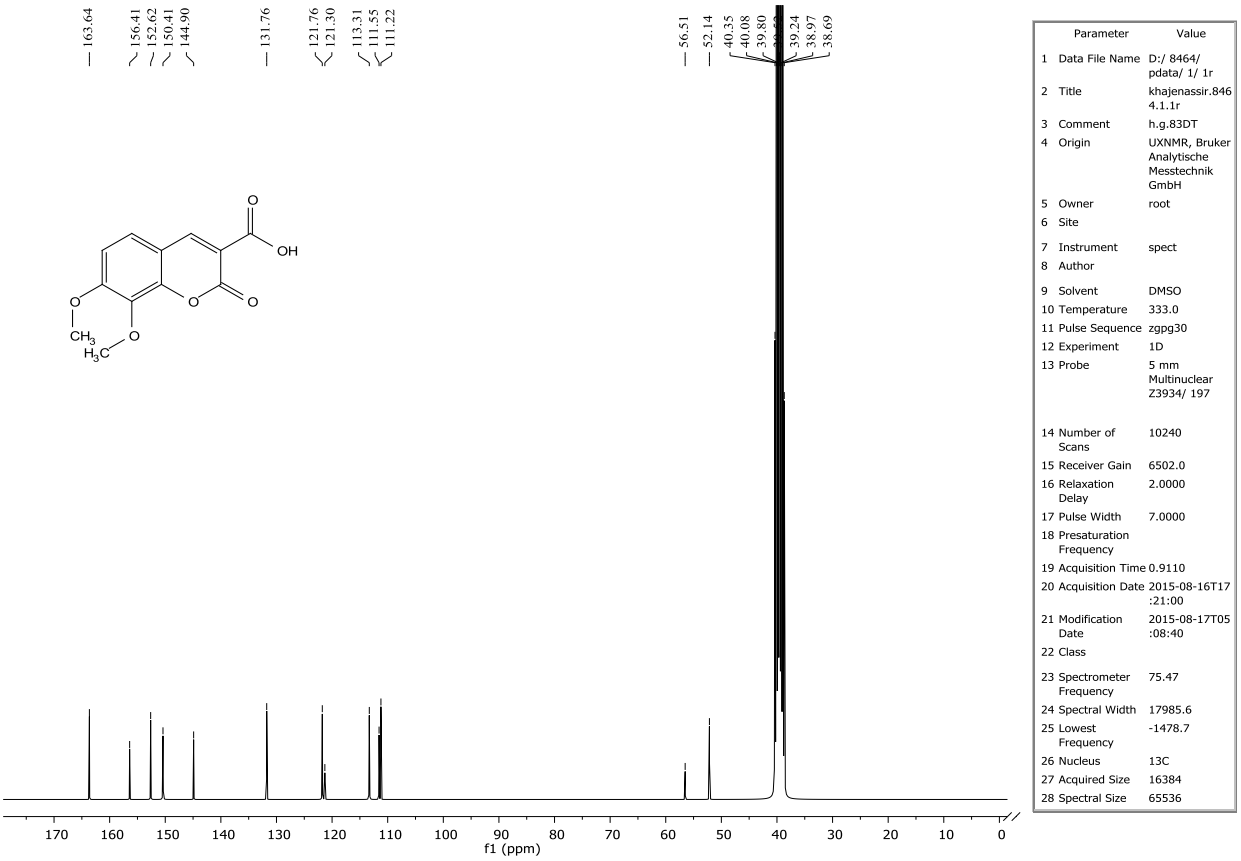
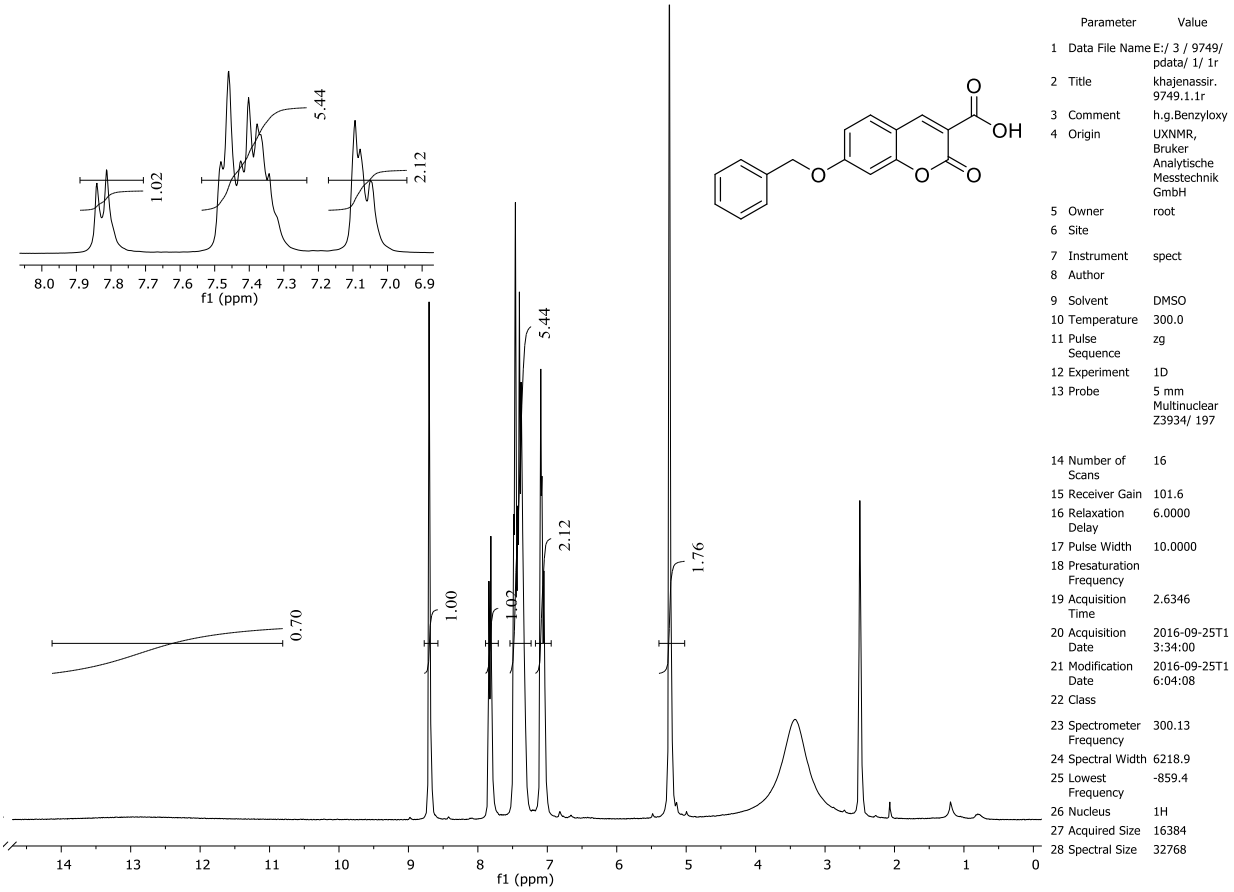
^{1}H NMR (300 MHz, DMSO-d_6) spectra of Methyl 7, 8-dimethoxy-2-oxo-2H-chromene-3-carboxylate



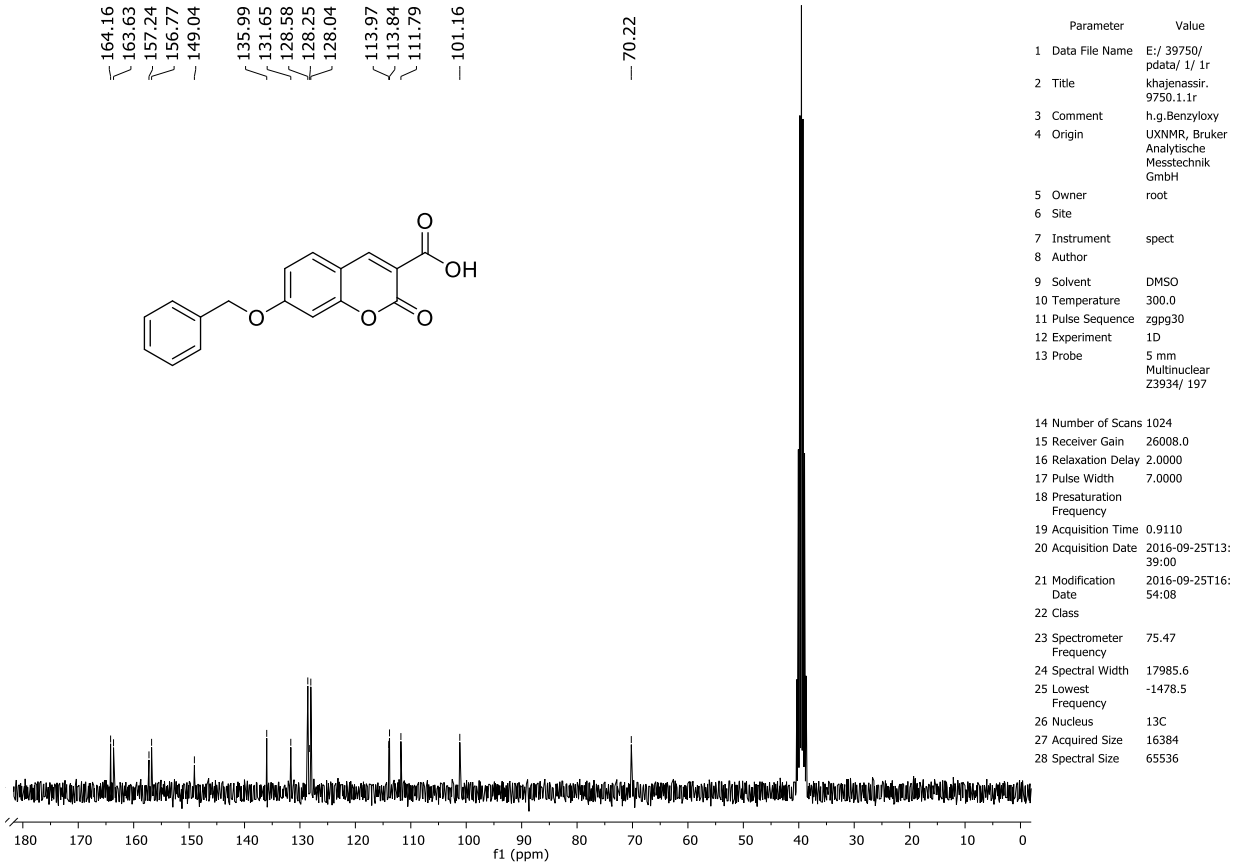
^{1}H NMR (300 MHz, DMSO-d_6) spectra of 7, 8-dimethoxy-2-oxo-2H-chromene-3-carboxylic acid (**5**)



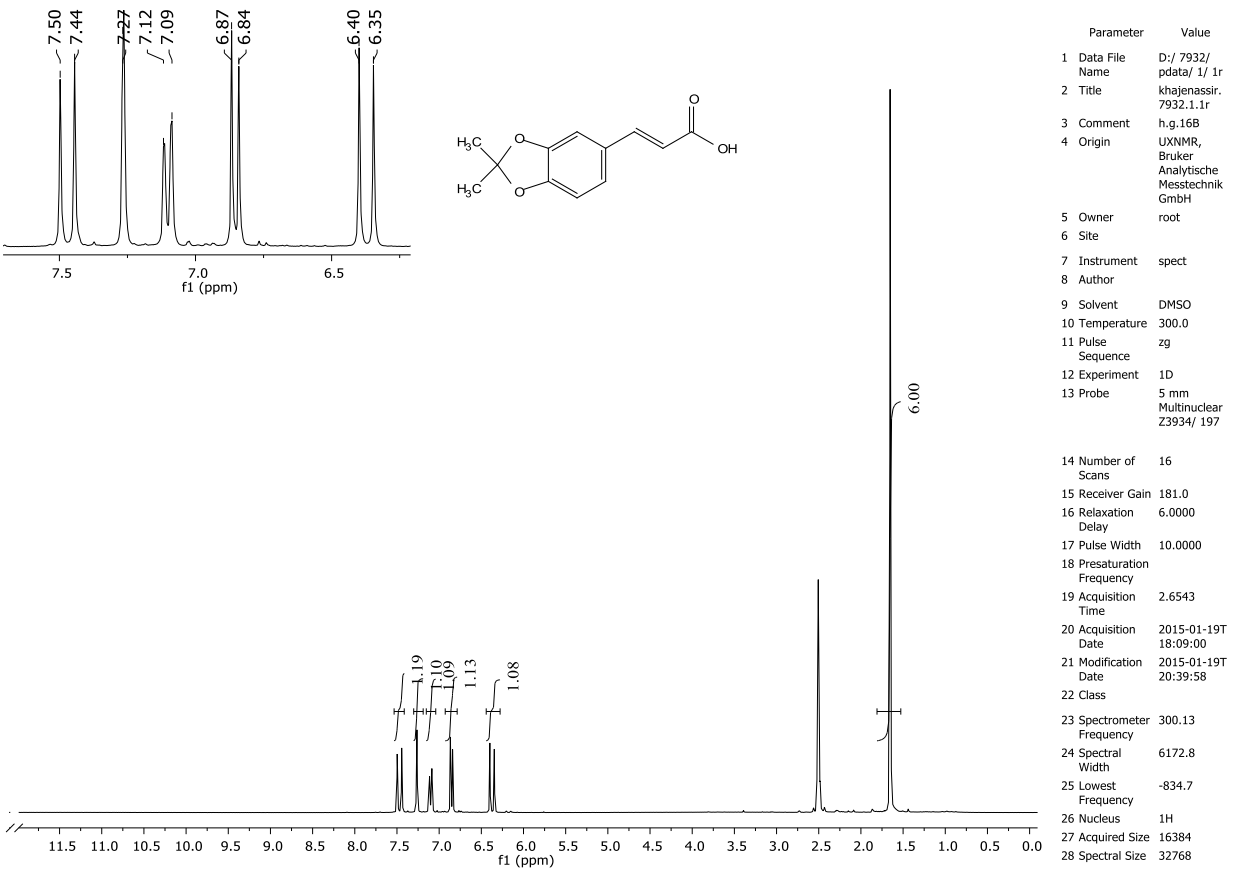
^{13}C NMR (75 MHz, DMSO-d_6) spectra of 7, 8-dimethoxy-2-oxo-2H-chromene-3-carboxylic acid (**5**)



^{1}H NMR (300 MHz, DMSO-d_6) spectra of 7-(benzyloxy)-2-oxo-2H-chromene-3-carboxylic acid (**6**)



^{13}C NMR (75 MHz, DMSO-d_6) spectra of 7-(benzyloxy)-2-oxo-2H-chromene-3-carboxylic acid (**6**)



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6	Site	
7	Instrument	spect
8	Author	
9	Solvent	DMSO
10	Temperature	300.0
11	Pulse Sequence	zg
12	Experiment	1D
13	Probe	5 mm Multinuclear Z3934/ 197
14	Number of Scans	16
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16	Relaxation Delay	6.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	2.6543
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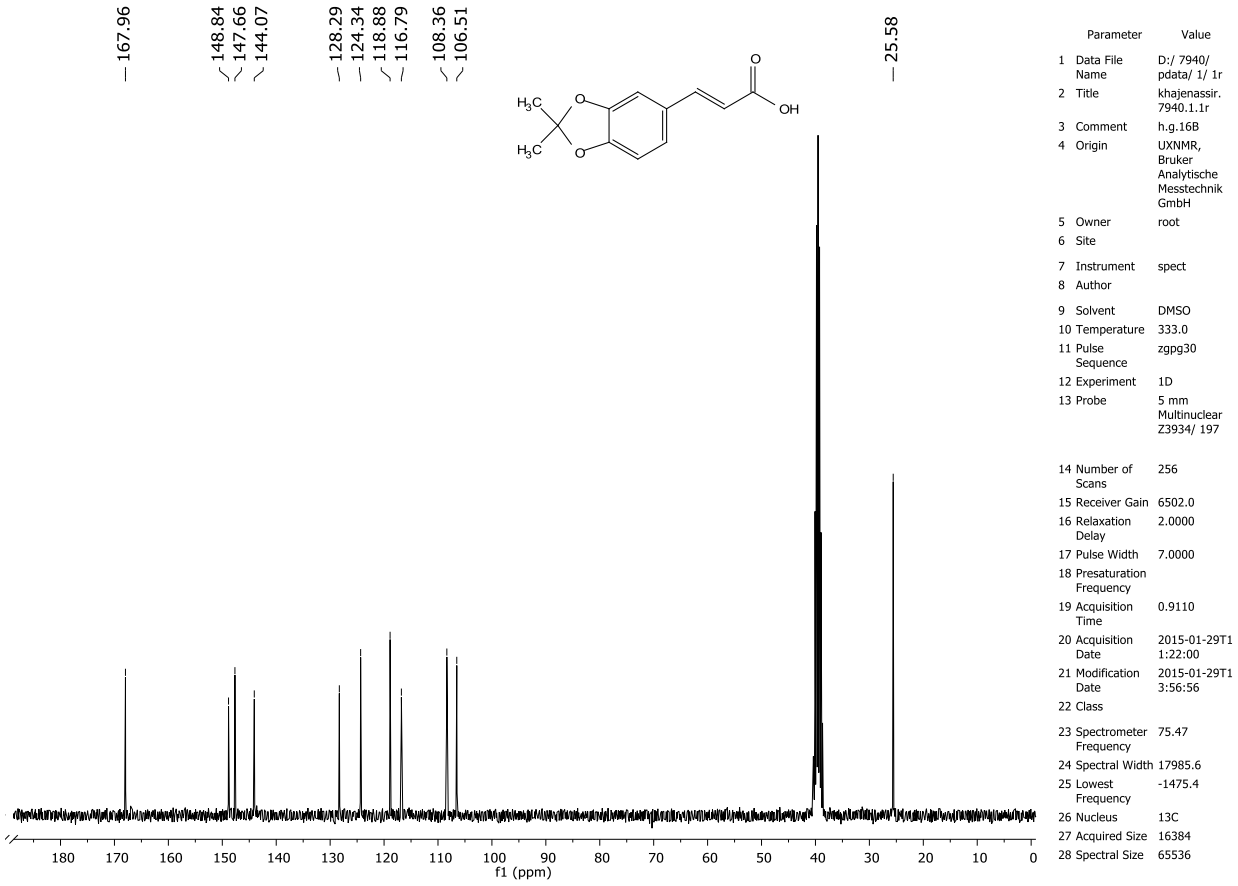
21	Modification Date	2015-01-19T 20:39:58
22	Class	
23	Spectrometer Frequency	300.13
24	Spectral Width	6172.8
25	Lowest Frequency	-834.7
26	Nucleus	1H
27	Acquired Size	16384
28	Spectral Size	32768

^{1}H NMR (300 MHz, DMSO-d_6) spectra of (*E*)-3-(2,2-dimethylbenzo[*d*] [1,3] dioxol-5-yl) acrylic acid (**10a**)



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5	Owner	root
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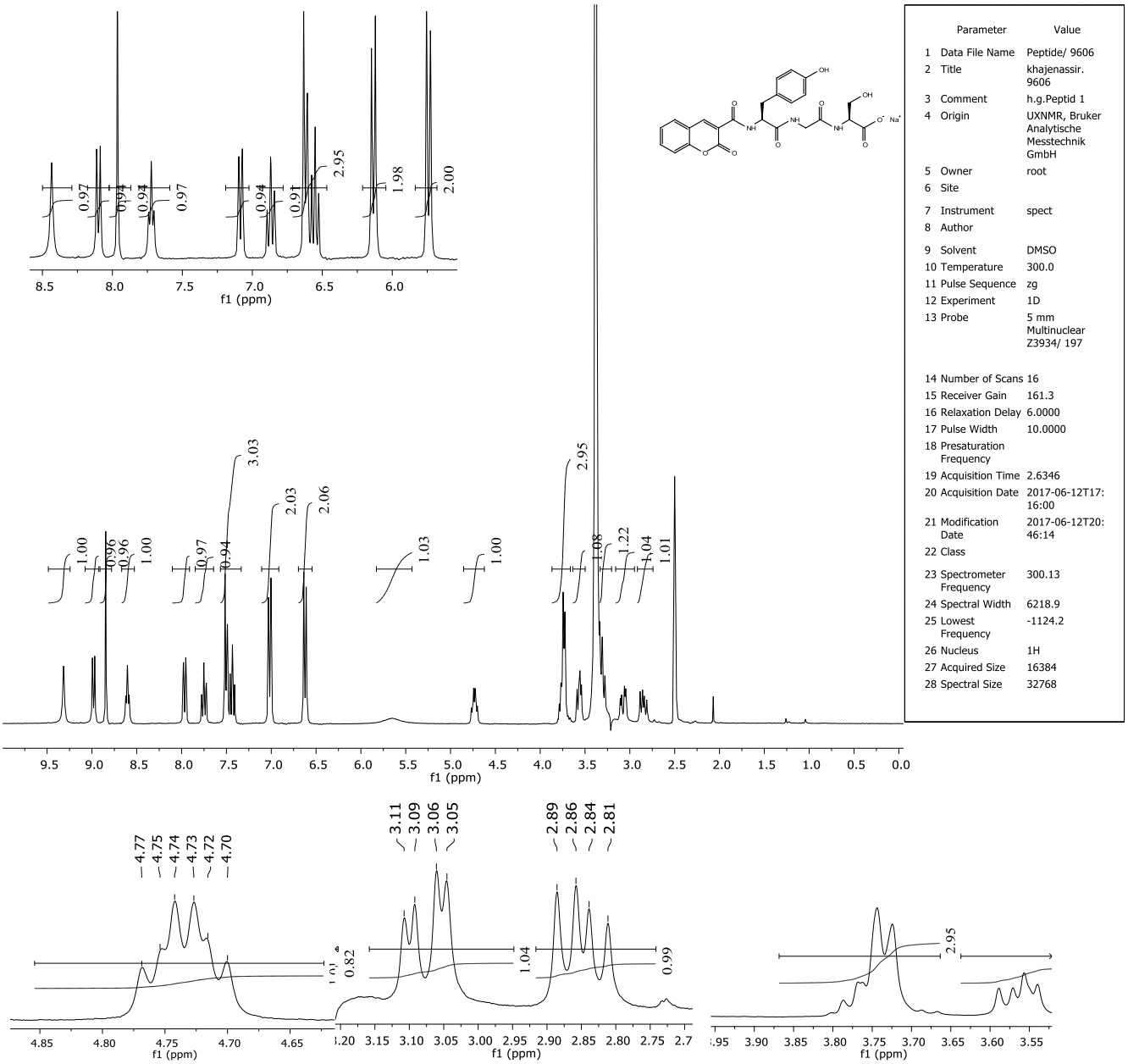
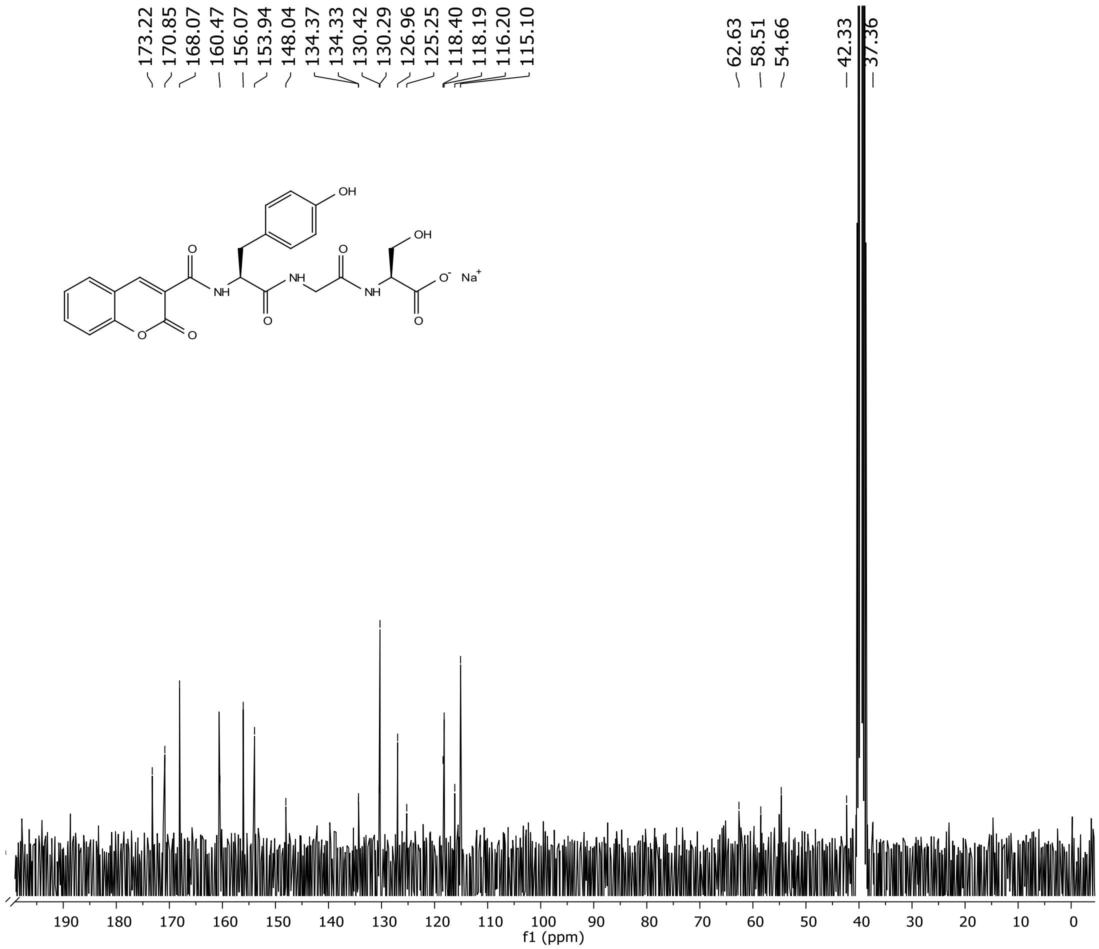
7	Instrument	spect
8	Author	
9	Solvent	DMSO
10	Temperature	333.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm Multinuclear Z3934/ 197
14	Number of Scans	256
15	Receiver Gain	6502.0
16	Relaxation Delay	2.0000
17	Pulse Width	7.0000
18	Presaturation Frequency	
19	Acquisition Time	0.9110
20	Acquisition Date	2015-01-29T11:22:00
21	Modification Date	2015-01-29T13:56:56
22	Class	
23	Spectrometer Frequency	75.47
24	Spectral Width	17985.6
25	Lowest Frequency	-1475.4
26	Nucleus	13C
27	Acquired Size	16384
28	Spectral Size	65536

^{13}C NMR (75 MHz, DMSO-d_6) spectra of (*E*)-3-(2,2-dimethylbenzo[*d*] [1,3] dioxol-5-yl) acrylic acid (**10a**)



^{1}H NMR (300 MHz, DMSO-d_6) spectra of sodium (2-oxo-2H-chromene-3-carbonyl)-*L*-tyrosylglycyl-*L*-serinate (**11**)



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5	Owner	root
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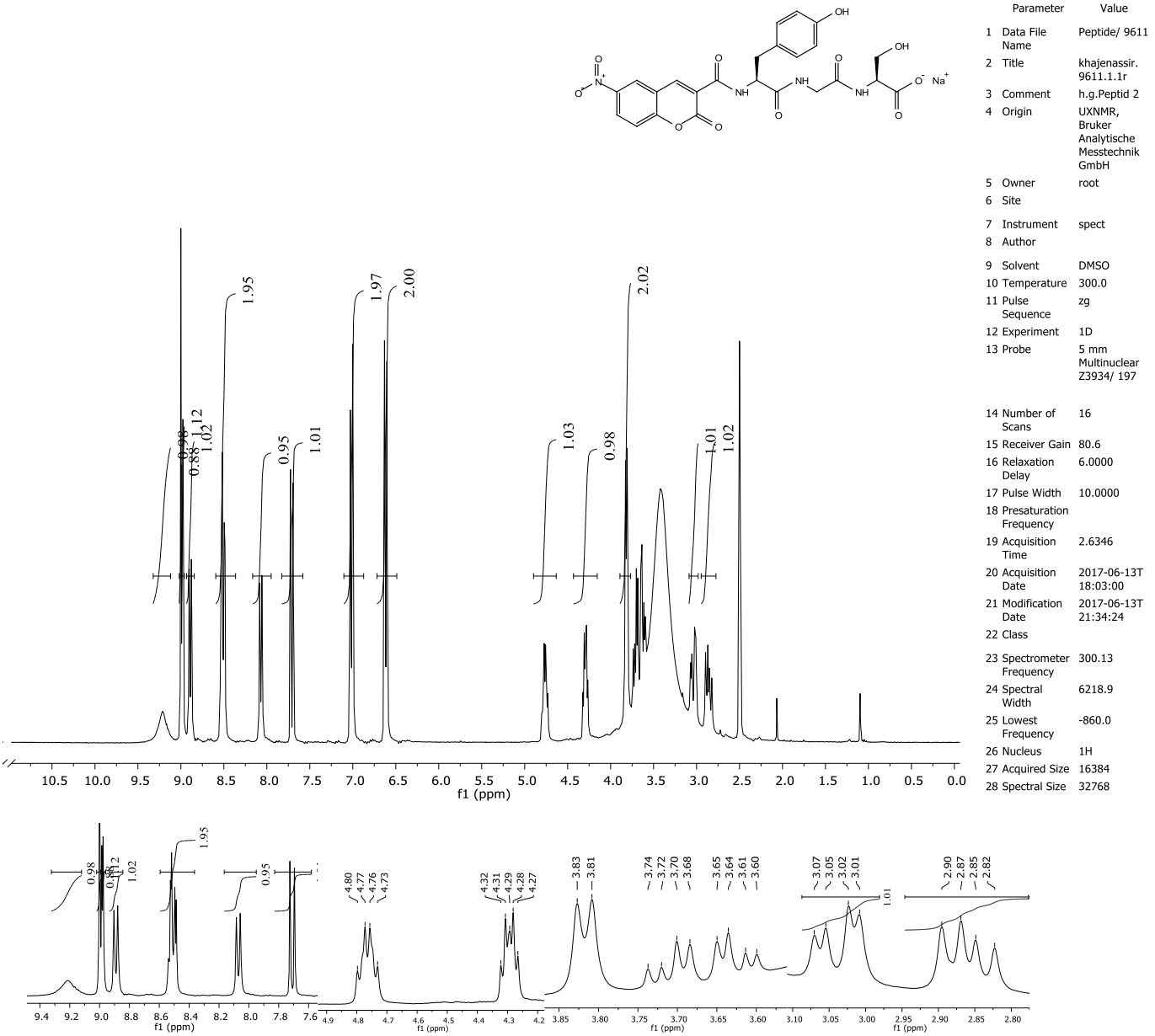
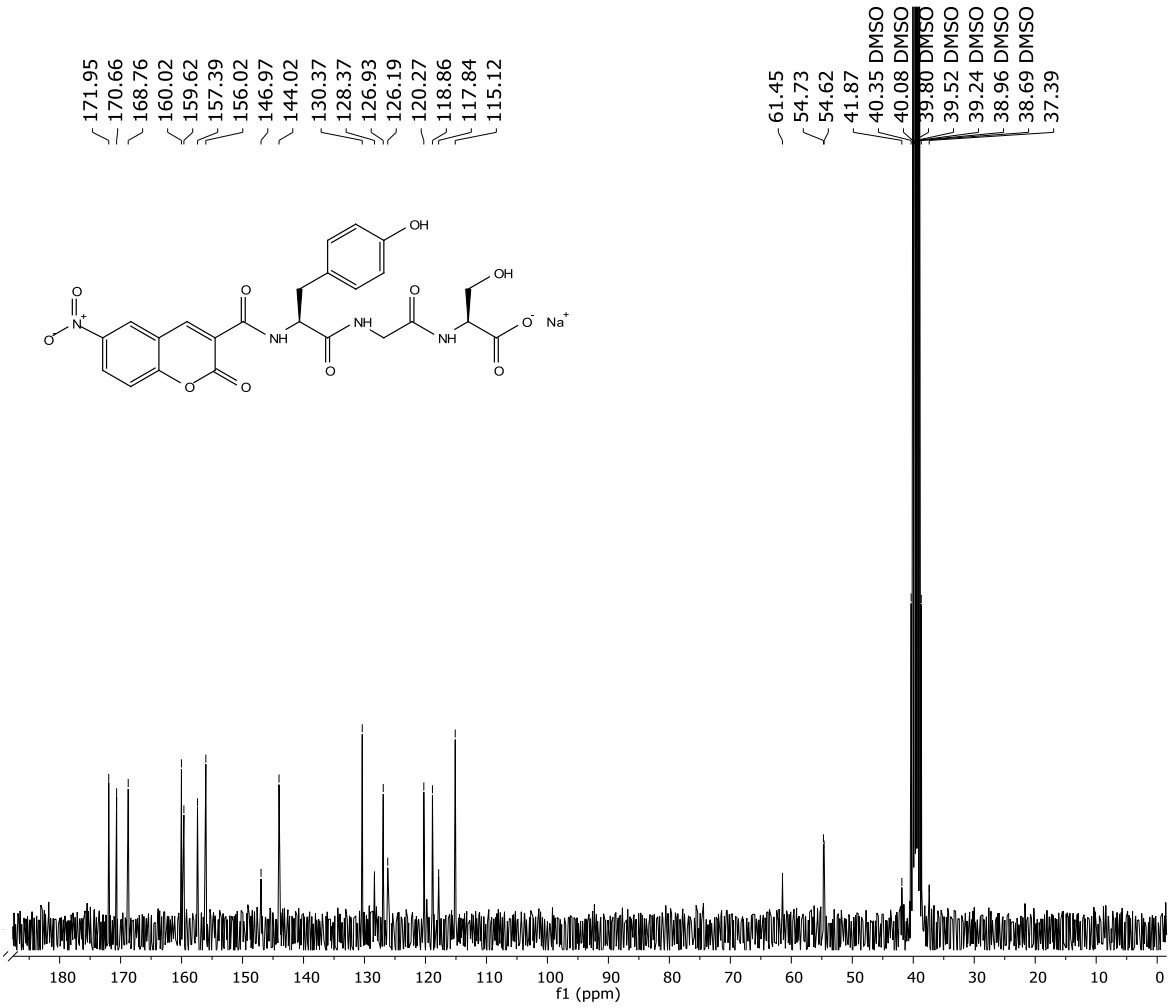
7	Instrument	spect
8	Author	
9	Solvent	DMSO
10	Temperature	300.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm Multinuclear Z3934/ 197
14	Number of Scans	1024
15	Receiver Gain	18390.4
16	Relaxation Delay	2.0000
17	Pulse Width	7.0000
18	Presaturation Frequency	
19	Acquisition Time	0.9110
20	Acquisition Date	2017-07-05T18:12:00
21	Modification Date	2017-07-05T22:30:24
22	Class	
23	Spectrometer Frequency	75.47
24	Spectral Width	17985.6
25	Lowest Frequency	-1477.0
26	Nucleus	13C
27	Acquired Size	16384
28	Spectral Size	65536

^{13}C NMR (75 MHz, DMSO-d_6) spectra of sodium (2-oxo-2H-chromene-3-carbonyl)-*L*-tyrosylglycyl-*L*-serinate (**11**)



^{1}H NMR (300 MHz, DMSO-d_6) spectra of sodium (6-nitro-2-oxo-2H-chromene-3-carbonyl)-*L*-tyrosylglycyl-*L*-serinate (**12**)



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5	Owner	root
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	DMSO
10	Temperature	300.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm Multinuclear Z3934/ 197
14	Number of Scans	1024
15	Receiver Gain	18390.4
16	Relaxation Delay	2.0000
17	Pulse Width	7.0000
18	Presaturation Frequency	
19	Acquisition Time	0.9110
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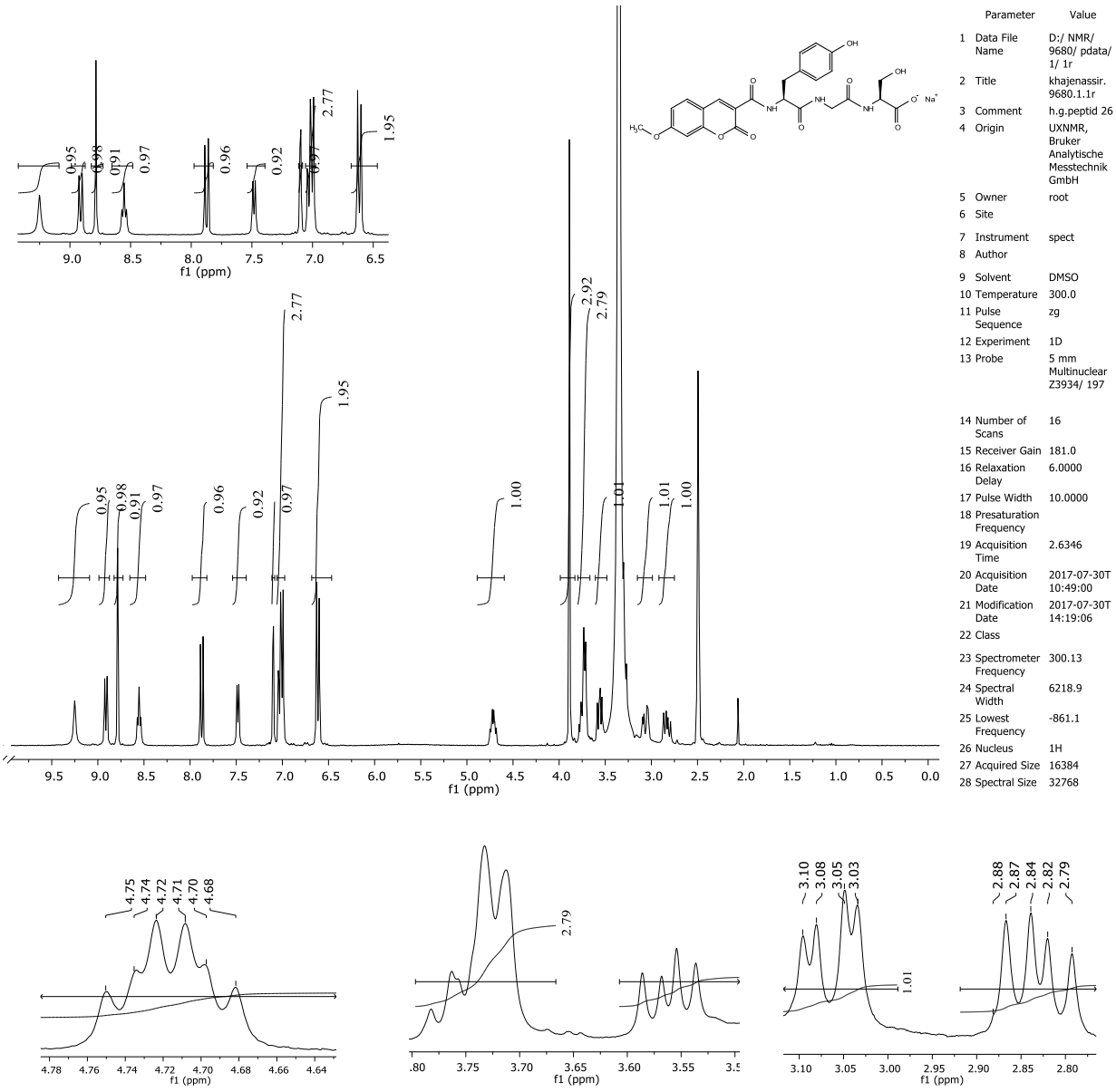
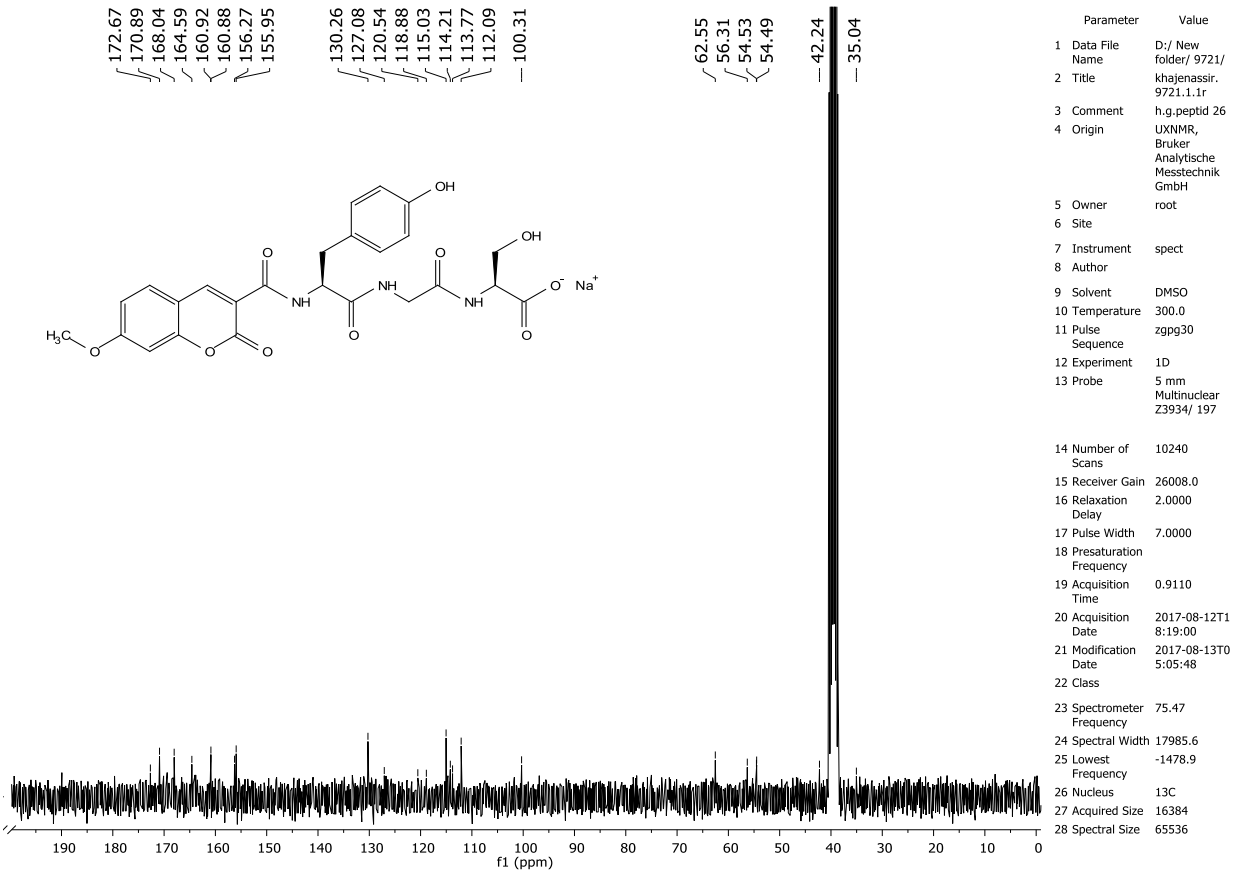
21	Modification Date	2017-07-05T21:36:38
22	Class	
23	Spectrometer Frequency	75.47
24	Spectral Width	17985.6
25	Lowest Frequency	-1474.0
26	Nucleus	13C
27	Acquired Size	16384
28	Spectral Size	65536

^{13}C NMR (75 MHz, DMSO-d_6) spectra of sodium (6-nitro-2-oxo-2H-chromene-3-carbonyl)-*L*-tyrosylglycyl-*L*-serinate (**12**)



^{1}H NMR (300 MHz, DMSO-d_6) spectra of sodium (7-methoxy-2-oxo-2H-chromene-3-carbonyl)-*L*-tyrosylglycyl-*L*-serinate (**13**)



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5	Owner	root
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	DMSO
10	Temperature	300.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm Multinuclear Z3934/ 197
14	Number of Scans	10240
15	Receiver Gain	26008.0
16	Relaxation Delay	2.0000
17	Pulse Width	7.0000
18	Presaturation Frequency	
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22	Class	
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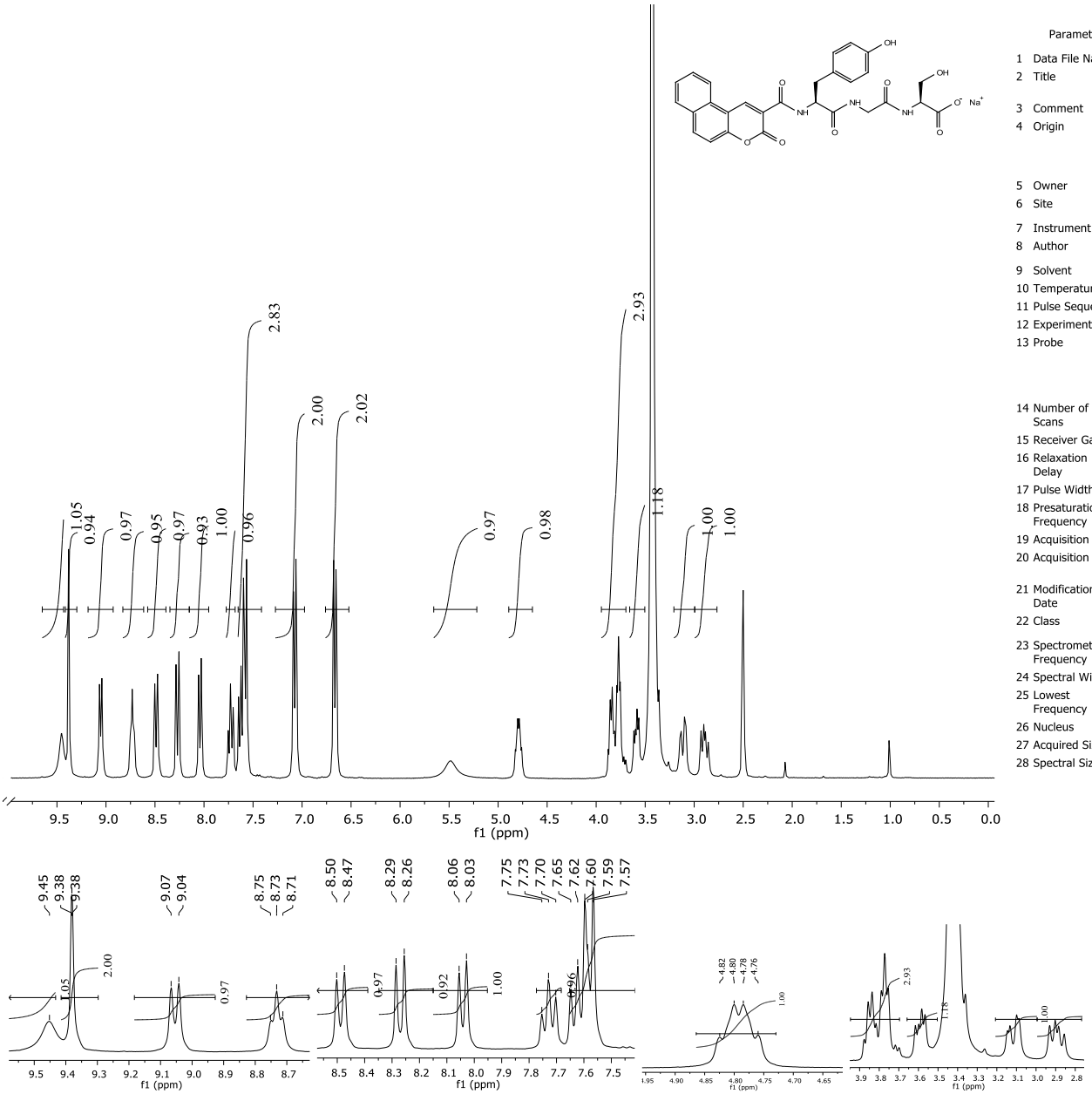
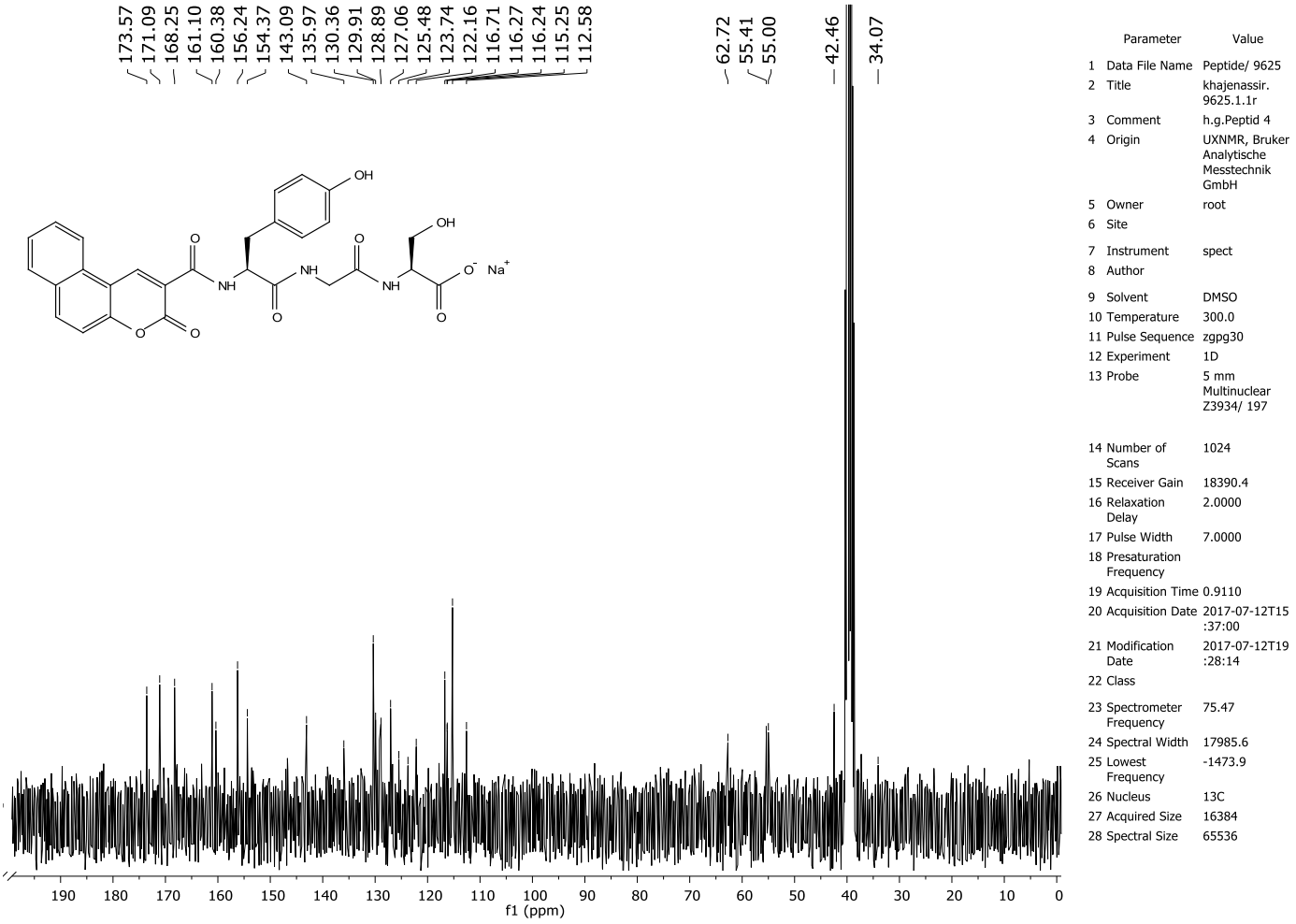
24	Spectral Width	17985.6
25	Lowest Frequency	-1478.9
26	Nucleus	13C
27	Acquired Size	16384
28	Spectral Size	65536

^{13}C NMR (75 MHz, DMSO-d_6) spectra of sodium (7-methoxy-2-oxo-2H-chromene-3-carbonyl)-*L*-tyrosylglycyl-*L*-serinate (**13**)



^{1}H NMR (300 MHz, DMSO-d_6) spectra of sodium (3-oxo-3H-benzo[*f*]chromene-2-carbonyl)-*L*-tyrosylglycyl-*L*-serinate (**14**)



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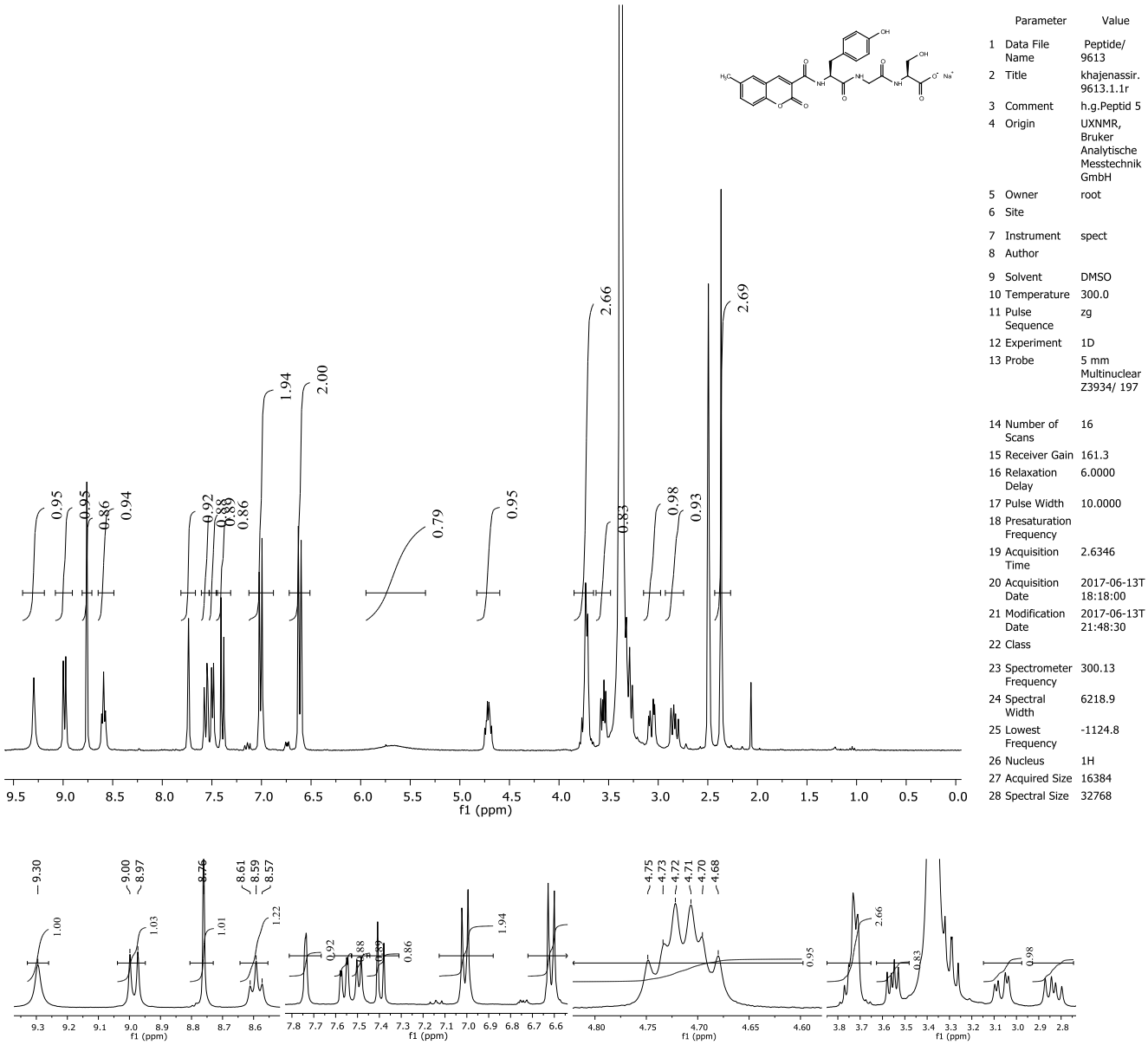
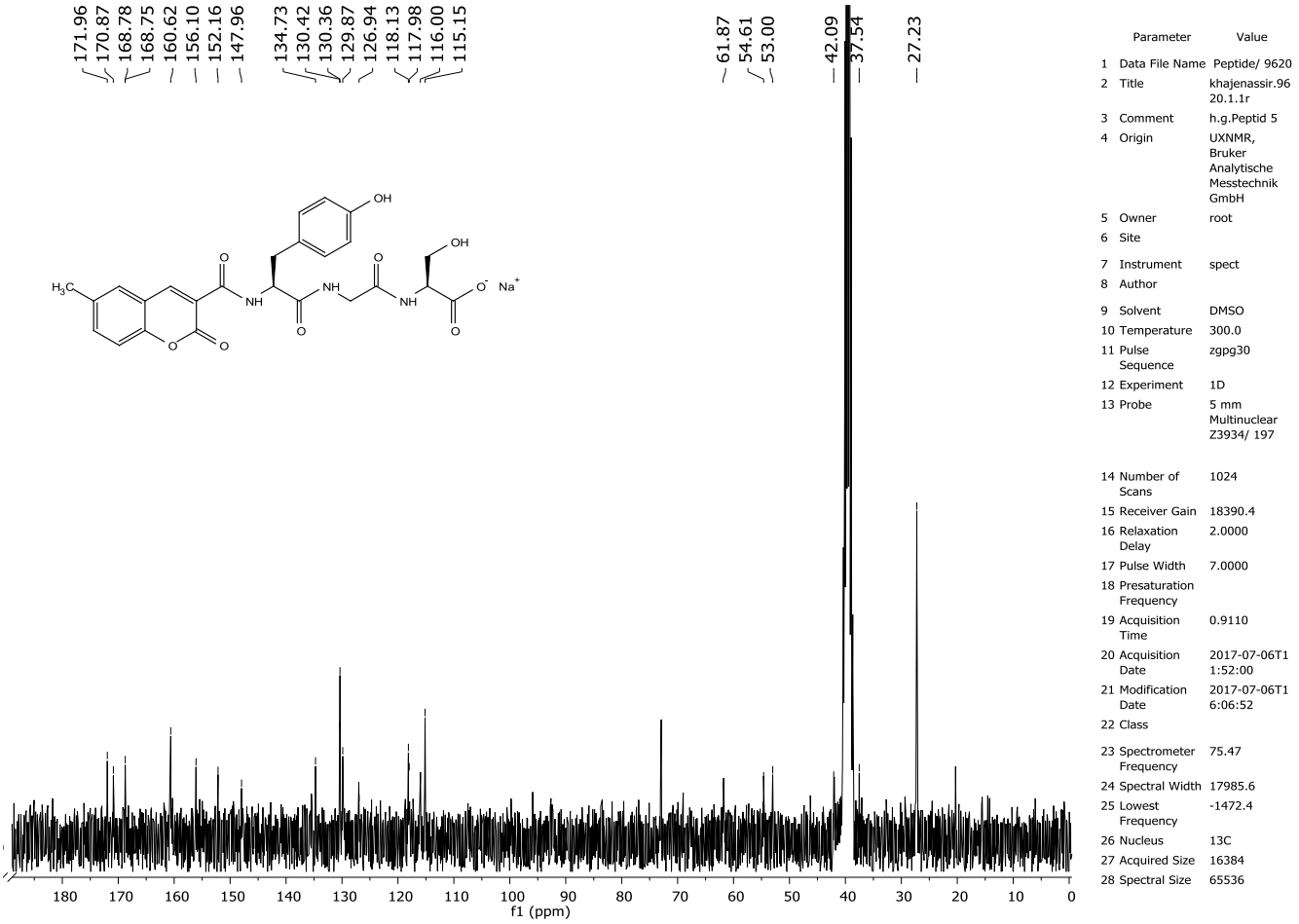
5	Owner	root
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	DMSO
10	Temperature	300.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm Multinuclear Z3934/ 197
14	Number of Scans	1024
15	Receiver Gain	18390.4
16	Relaxation Delay	2.0000
17	Pulse Width	7.0000
18	Presaturation Frequency	
19	Acquisition Time	0.9110
20	Acquisition Date	2017-07-12T15 :37:00
21	Modification Date	2017-07-12T19 :28:14
22	Class	
23	Spectrometer Frequency	75.47
24	Spectral Width	17985.6
25	Lowest Frequency	-1473.9
26	Nucleus	13C
27	Acquired Size	16384
28	Spectral Size	65536

^{13}C NMR (75 MHz, DMSO-d_6) spectra of sodium (3-oxo-3H-benzo[f]chromene-2-carbonyl)-*L*-tyrosylglycyl-*L*-serinate (**14**)



^{1}HNMR (300 MHz, DMSO-d_6) spectra of sodium (6-methyl-2-oxo-2H-chromene-3-carbonyl)-*L*-tyrosylglycyl-*L*-serinate (**15**)



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7	Instrument	spect
8	Author	
9	Solvent	DMSO
10	Temperature	300.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm Multinuclear Z3934/ 197
14	Number of Scans	1024
15	Receiver Gain	18390.4
16	Relaxation Delay	2.0000
17	Pulse Width	7.0000
18	Presaturation Frequency	
19	Acquisition Time	0.9110
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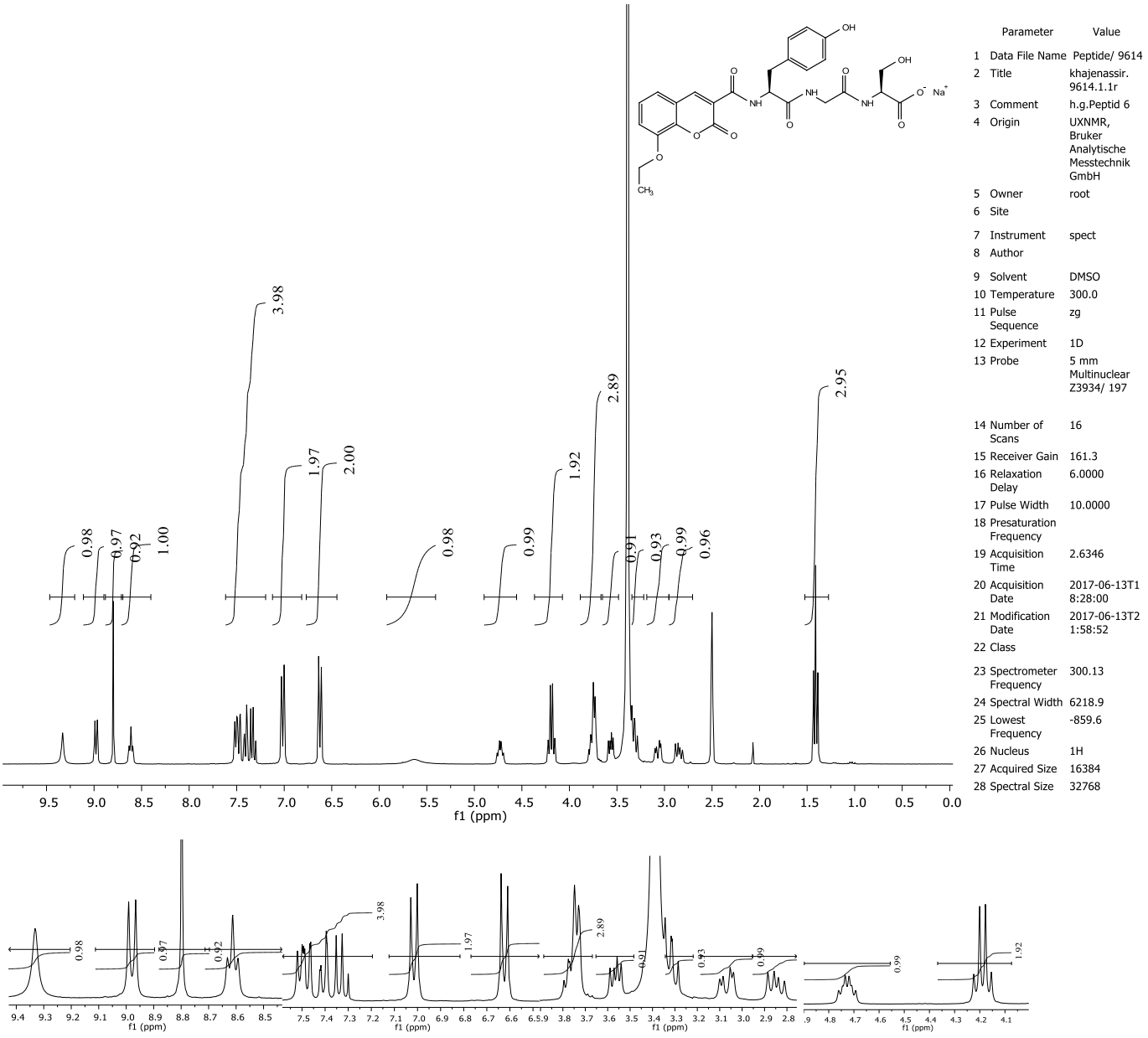
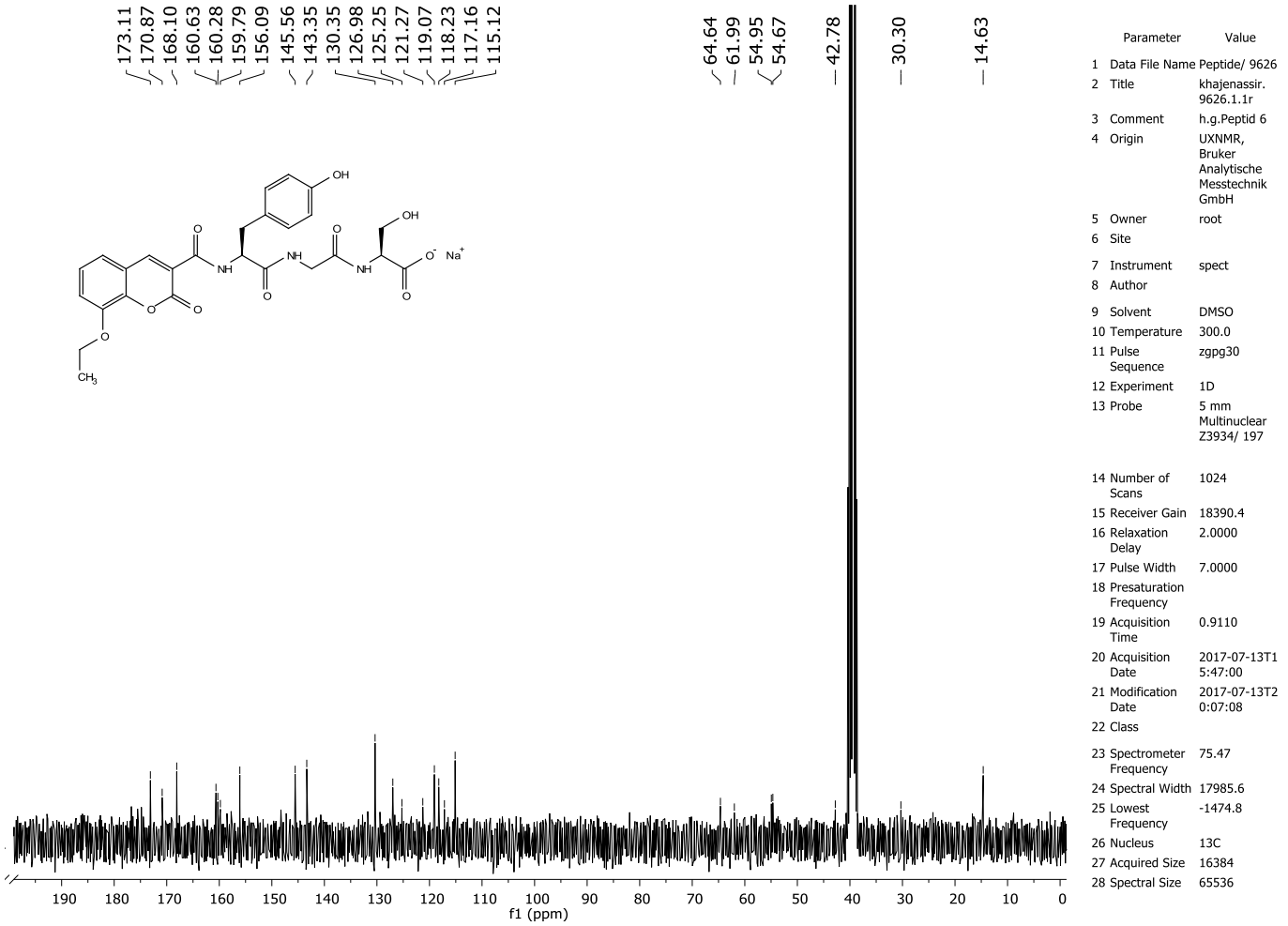
21	Modification Date	2017-07-06T16:06:52
22	Class	
23	Spectrometer Frequency	75.47
24	Spectral Width	17985.6
25	Lowest Frequency	-1472.4
26	Nucleus	13C
27	Acquired Size	16384
28	Spectral Size	65536

^{13}C NMR (75 MHz, DMSO-d_6) spectra of sodium (6-methyl-2-oxo-2H-chromene-3-carbonyl)-*L*-tyrosylglycyl-*L*-serinate (**15**)



^{1}HNMR (300 MHz, DMSO-d_6) spectra of sodium (8-ethoxy-2-oxo-2H-chromene-3-carbonyl)-*L*-tyrosylglycyl-*L*-serinate (**16**)



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7	Instrument	spect
8	Author	
9	Solvent	DMSO
10	Temperature	300.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm Multinuclear Z3934/ 197
14	Number of Scans	1024
15	Receiver Gain	18390.4
16	Relaxation Delay	2.0000
17	Pulse Width	7.0000
18	Presaturation Frequency	
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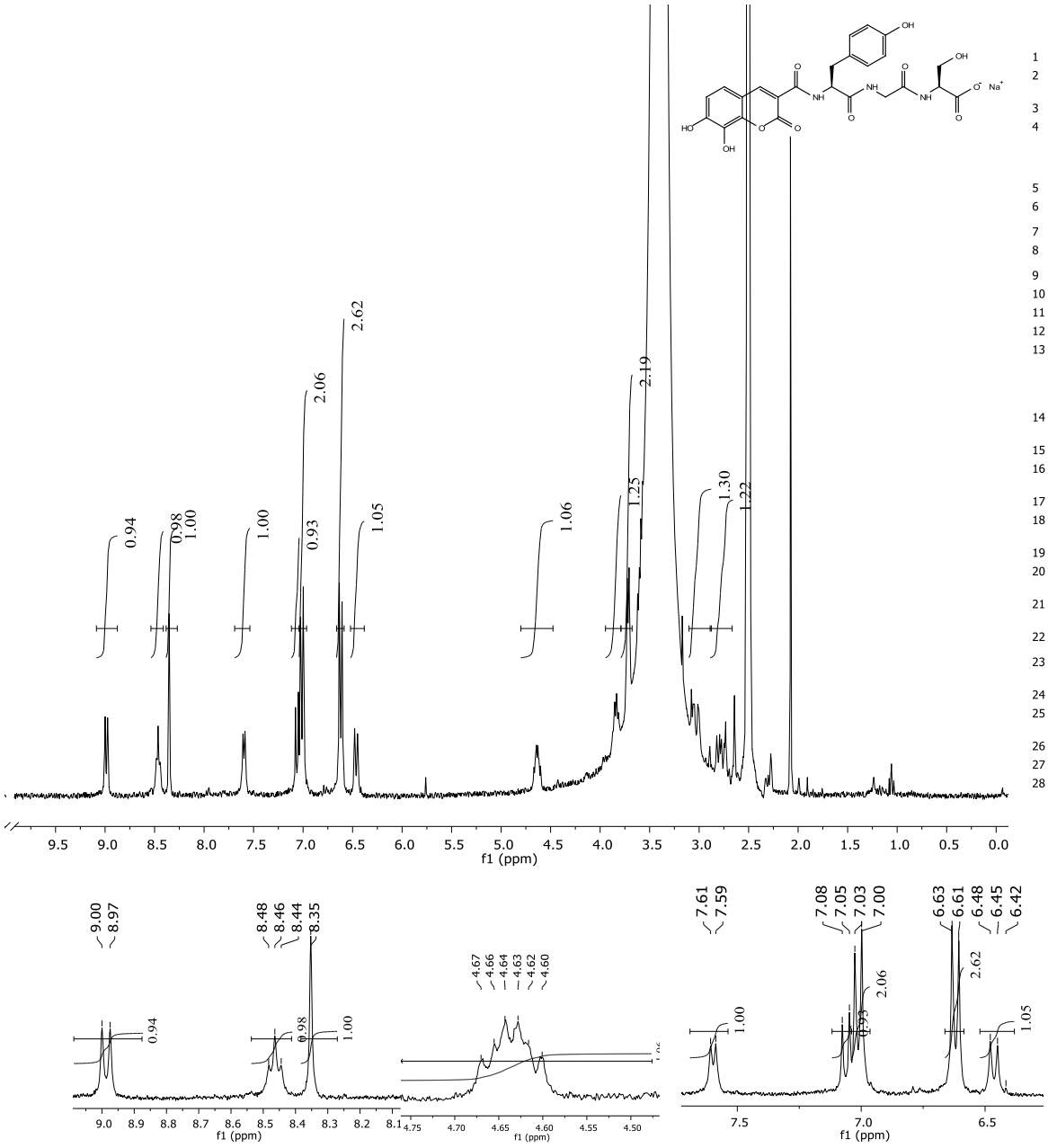
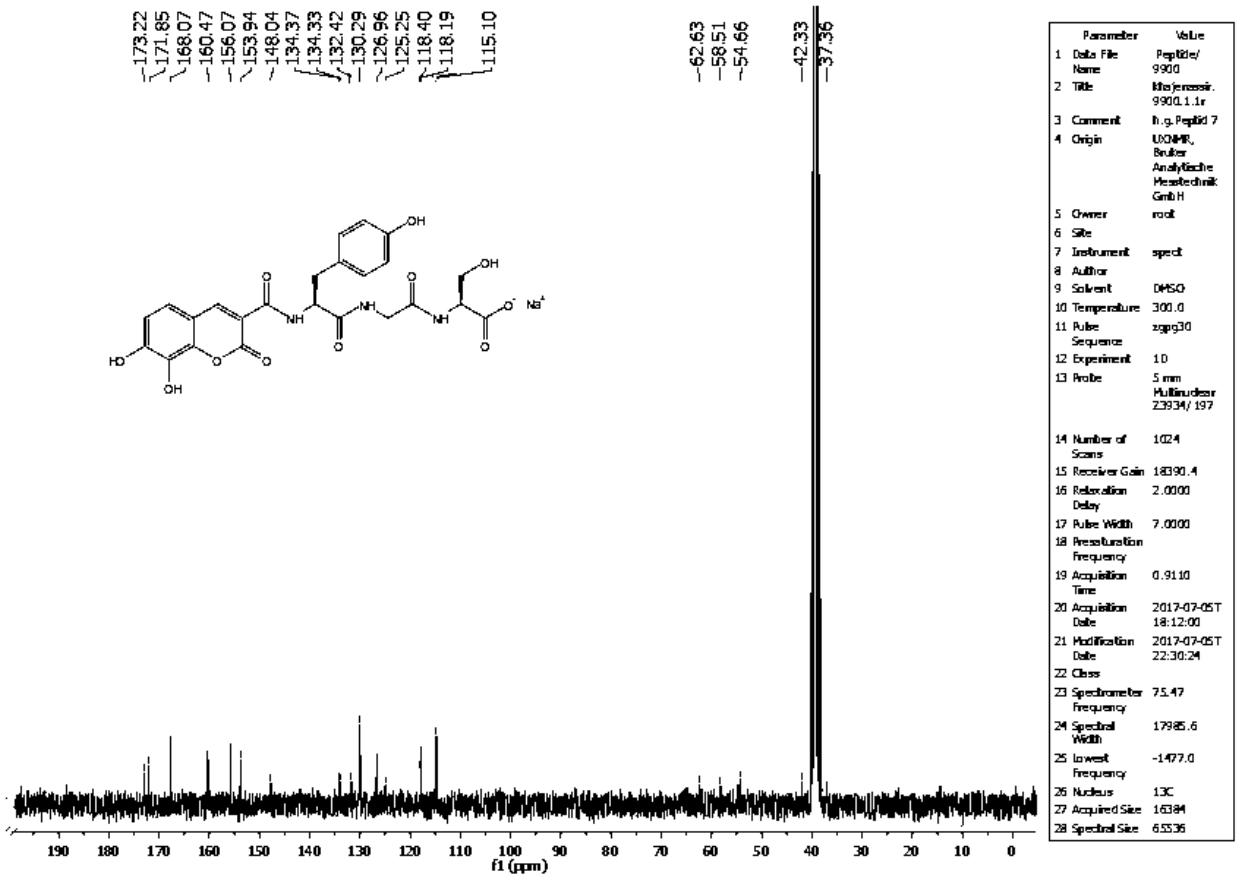
21	Modification Date	2017-07-13T20:07:08
22	Class	
23	Spectrometer Frequency	75.47
24	Spectral Width	17985.6
25	Lowest Frequency	-1474.8
26	Nucleus	13C
27	Acquired Size	16384
28	Spectral Size	65536

^{13}CNMR (75 MHz, DMSO-d_6) spectra of sodium (8-ethoxy-2-oxo-2H-chromene-3-carbonyl)-*L*-tyrosylglycyl-*L*-serinate (**16**)



^{1}H NMR (300 MHz, DMSO-d_6) of sodium (7, 8-dihydroxy-2-oxo-2H-chromene-3-carbonyl)-*L*-tyrosylglycyl-*L*-serinate (**17**)



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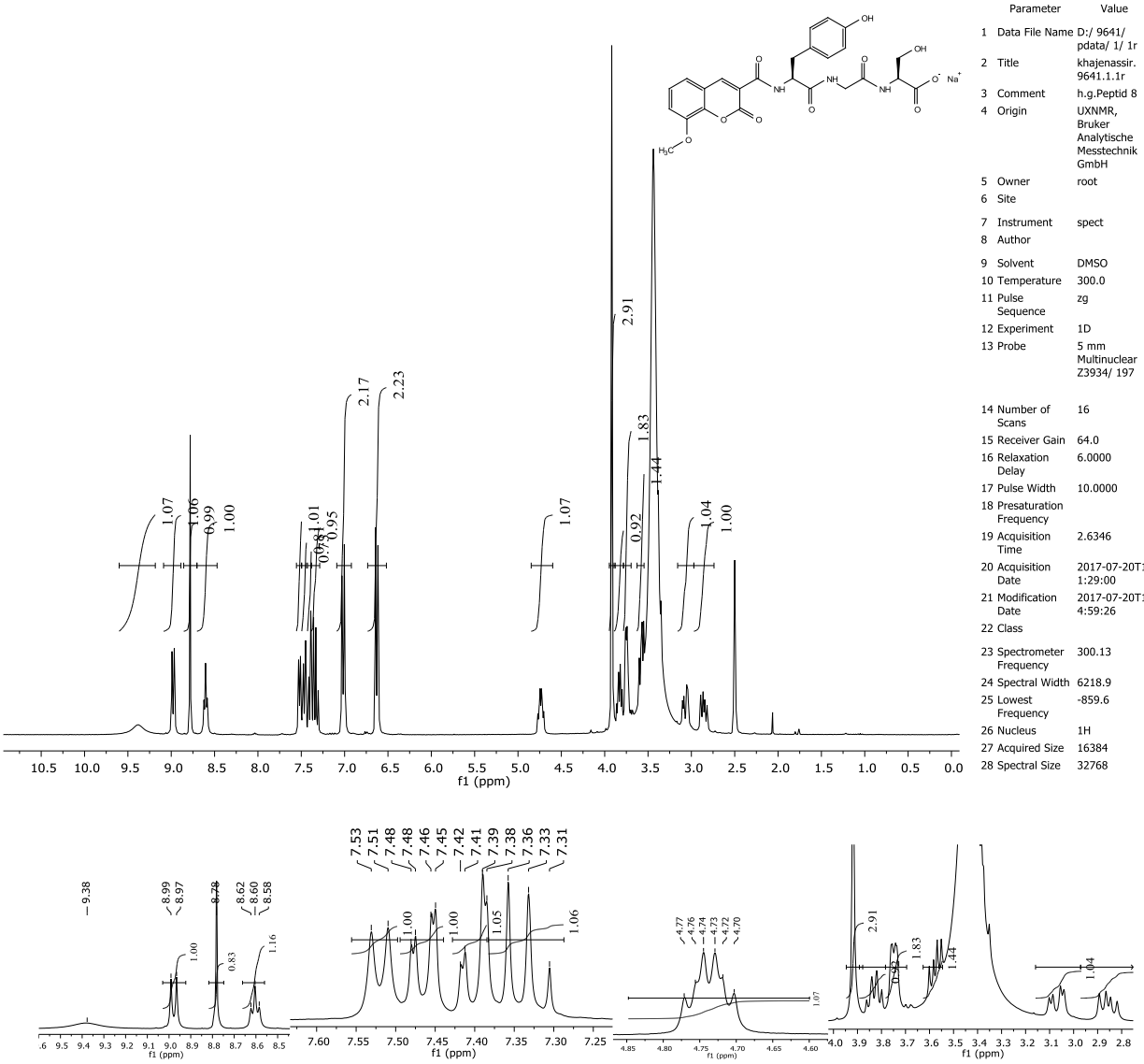
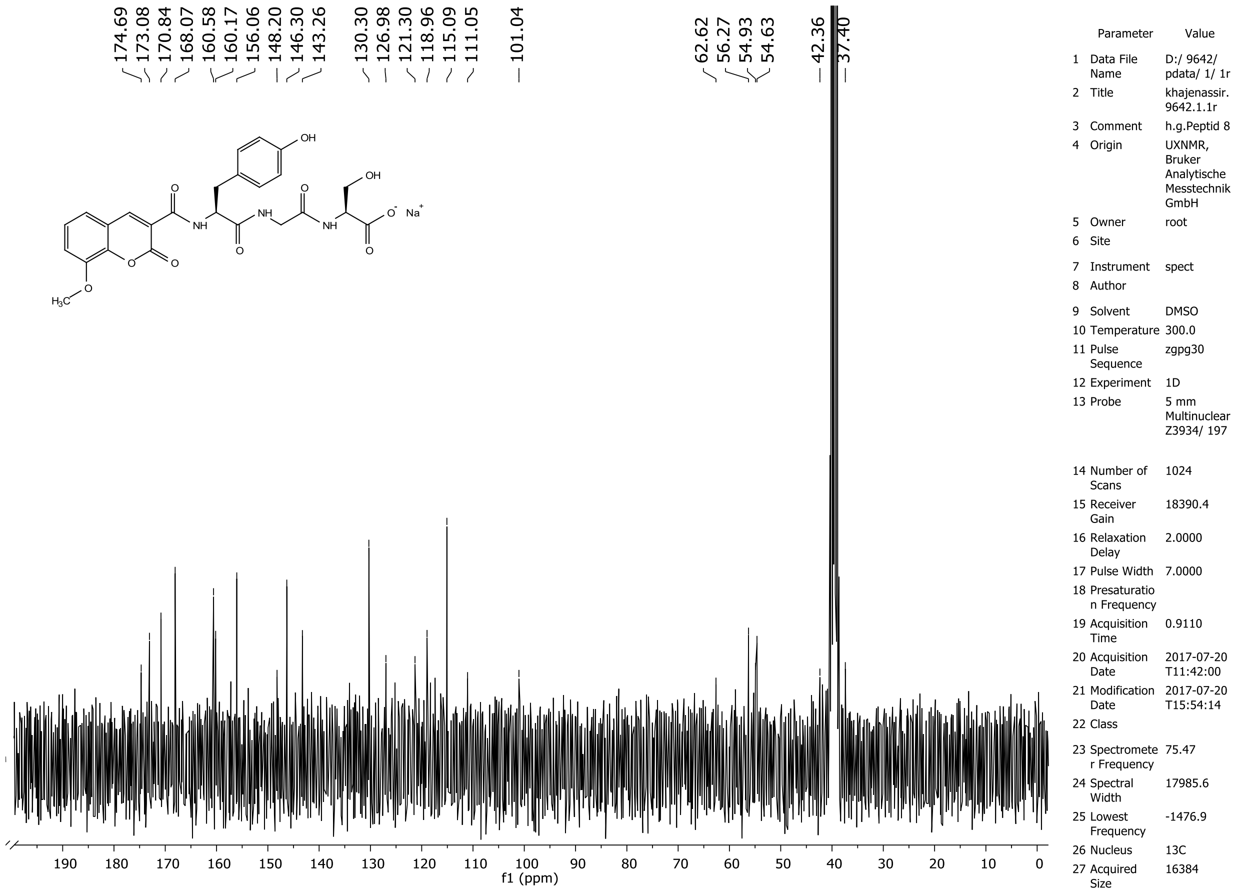
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	DMSO
10	Temperature	300.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm Multinuclear 23934/197
14	Number of Scans	1024
15	Receiver Gain	18390.4
16	Relaxation Delay	2.0000
17	Pulse Width	7.0000
18	Presaturation Frequency	
19	Acquisition Time	0.9110
20	Acquisition Date	2017-07-05T 18:12:00
21	Modification Date	2017-07-05T 22:30:24
22	Class	
23	Spectrometer Frequency	75.47
24	Spectral Width	17985.6
25	lowest Frequency	-1477.0
26	Nucleus	13C
27	Acquired Size	16384
28	Spectral Size	65536

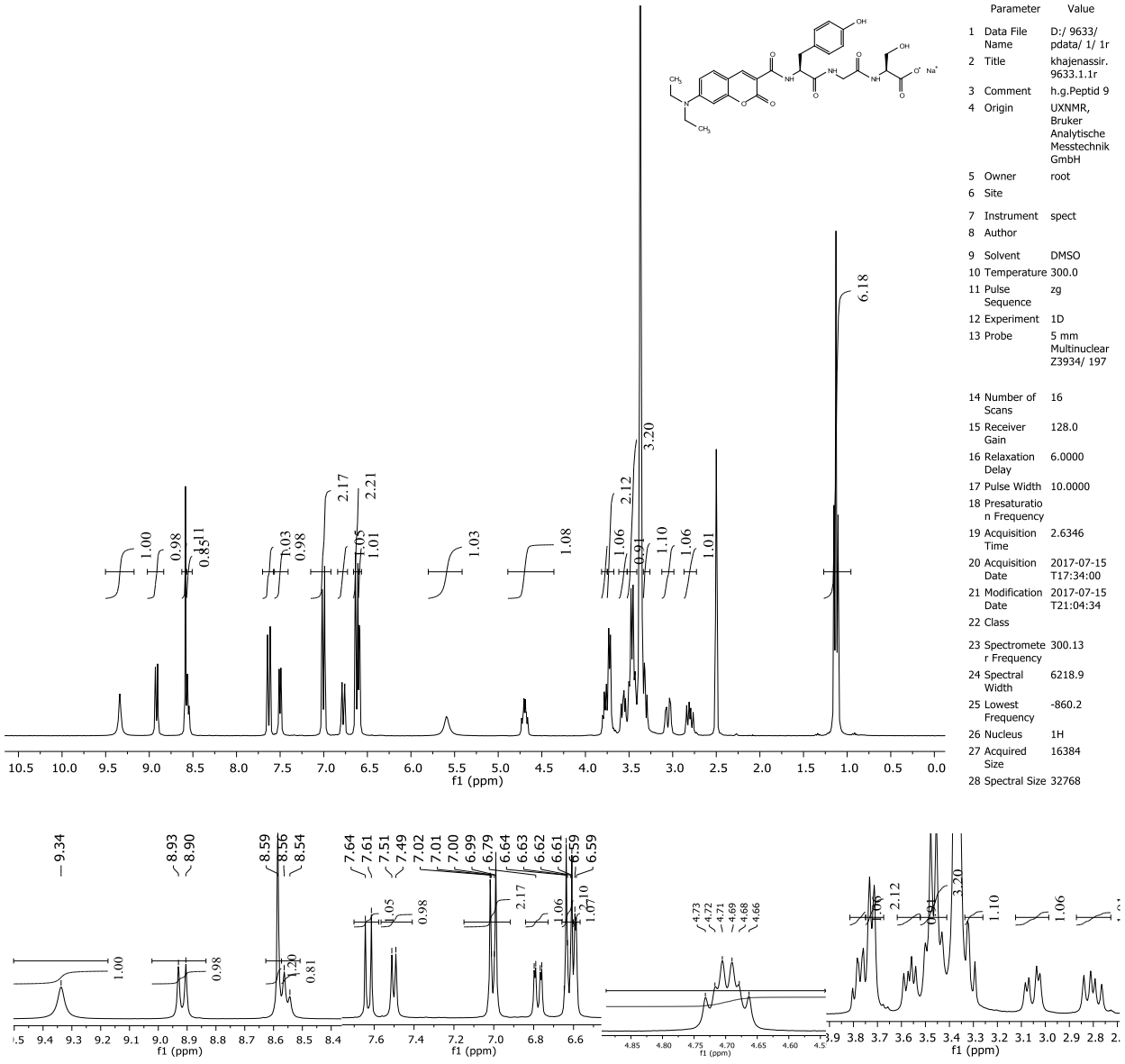
^{13}C NMR (75 MHz, DMSO-d_6) of sodium (7, 8-dihydroxy-2-oxo-2H-chromene-3-carbonyl)-*L*-tyrosylglycyl-*L*-serinate (**17**)



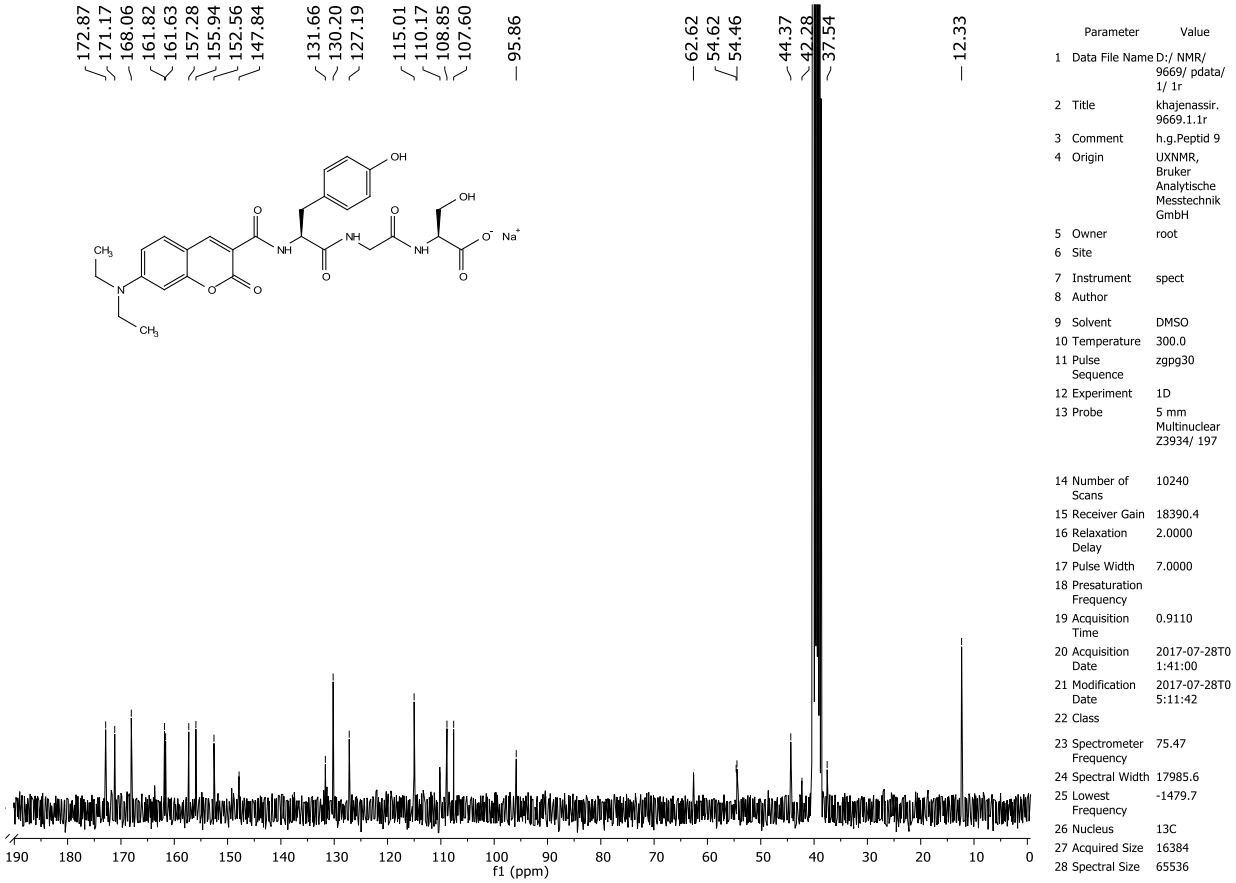
^{1}H NMR (300 MHz, DMSO-d_6) spectra of sodium (8-methoxy-2-oxo-2H-chromene-3-carbonyl)-*L*-tyrosylglycyl-*L*-serinate (**18**)



^{13}C NMR (75 MHz, DMSO-d_6) spectra of sodium (8-methoxy-2-oxo-2H-chromene-3-carbonyl)-*L*-tyrosylglycyl-*L*-serinate (**18**)



^{1}H NMR (300 MHz, DMSO-d_6) spectra of sodium (7-(diethylamino)-2-oxo-2H-chromene-3-carbonyl)-*L*-tyrosylglycyl-*L*-serinate (**19**)



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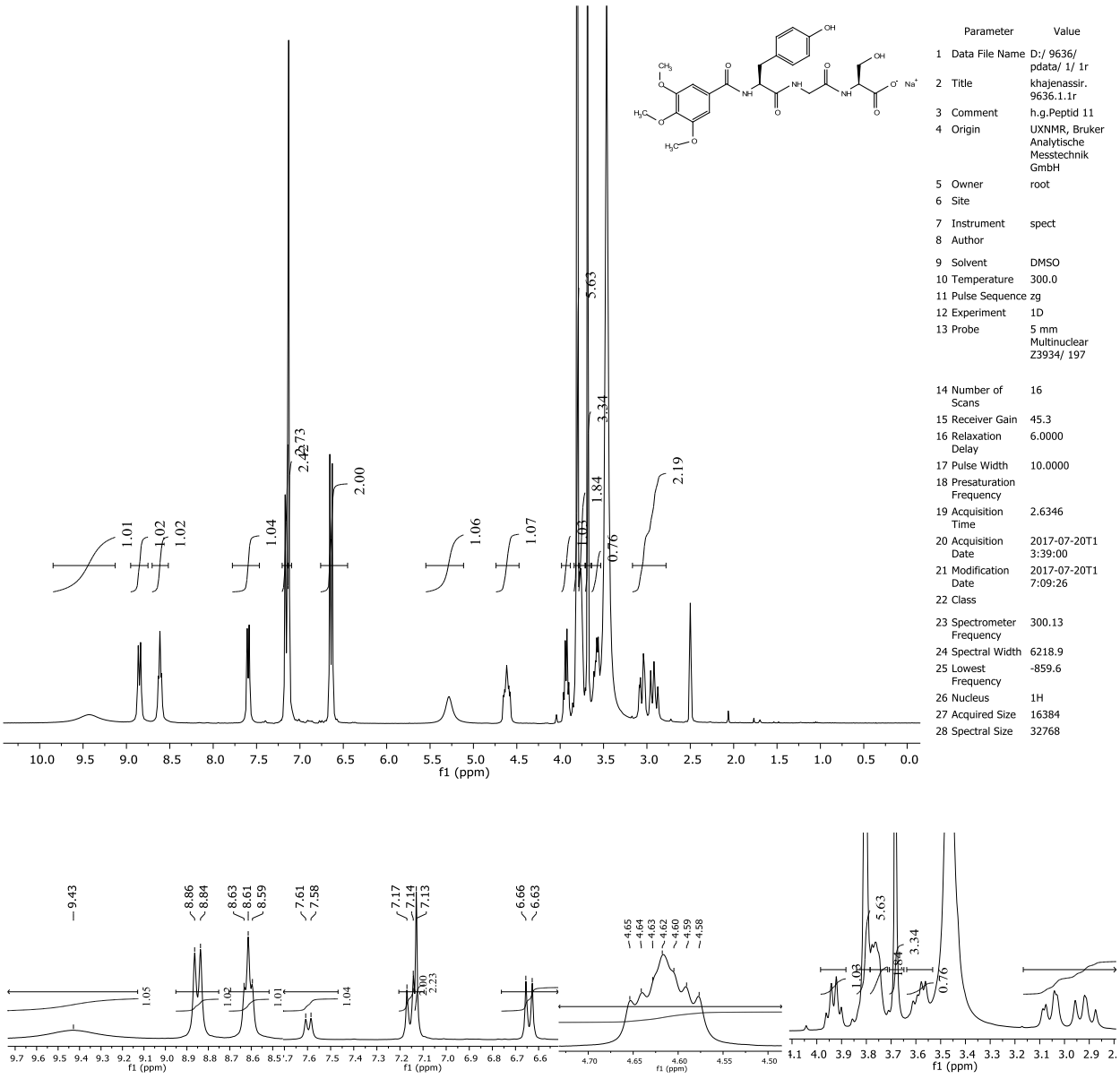
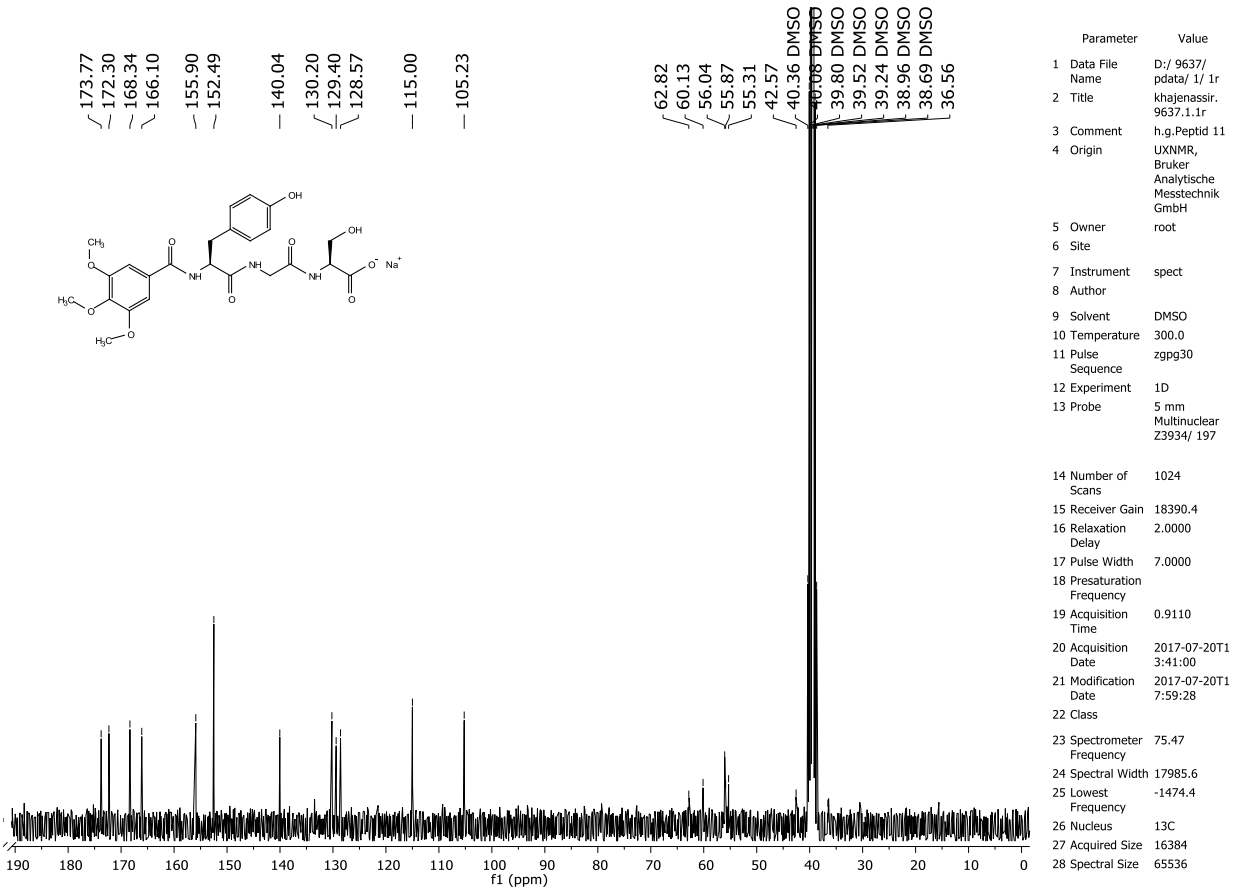
5	Owner	root
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	DMSO
10	Temperature	300.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm Multinuclear Z3934/ 197
14	Number of Scans	10240
15	Receiver Gain	18390.4
16	Relaxation Delay	2.0000
17	Pulse Width	7.0000
18	Presaturation Frequency	
19	Acquisition Time	0.9110
20	Acquisition Date	2017-07-28T01:41:00
21	Modification Date	2017-07-28T05:11:42
22	Class	
23	Spectrometer Frequency	75.47
24	Spectral Width	17985.6
25	Lowest Frequency	-1479.7
26	Nucleus	13C
27	Acquired Size	16384
28	Spectral Size	65536

^{13}C NMR (75 MHz, DMSO-d_6) spectra of sodium (7-(diethylamino)-2-oxo-2H-chromene-3-carbonyl)-*L*-tyrosylglycyl-*L*-serinate (**19**)



^{1}H NMR (300 MHz, DMSO-d_6) spectra of sodium (3, 4, 5-trimethoxybenzoyl)-*L*-tyrosylglycyl-*L*-serinate (**20**)



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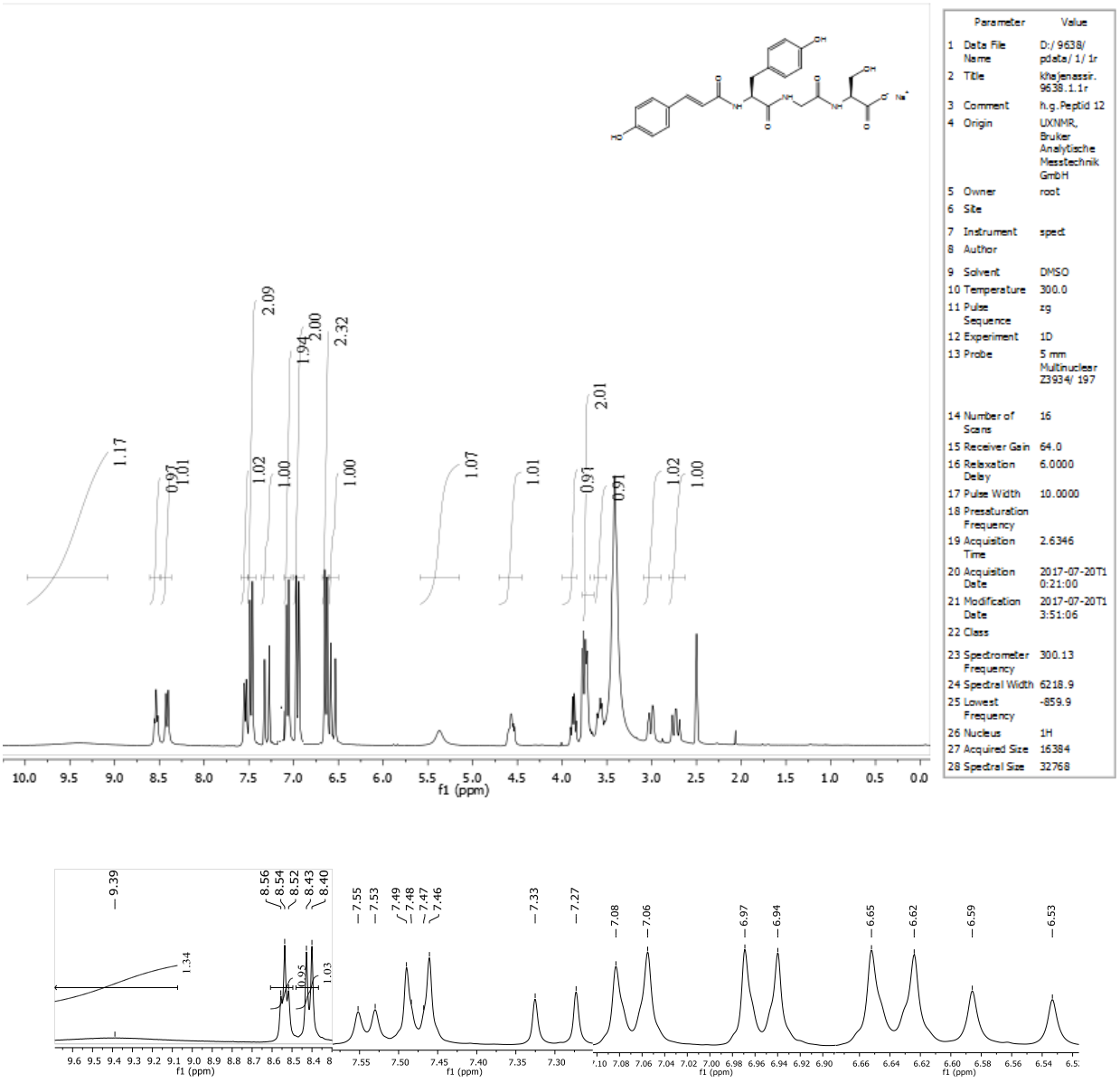
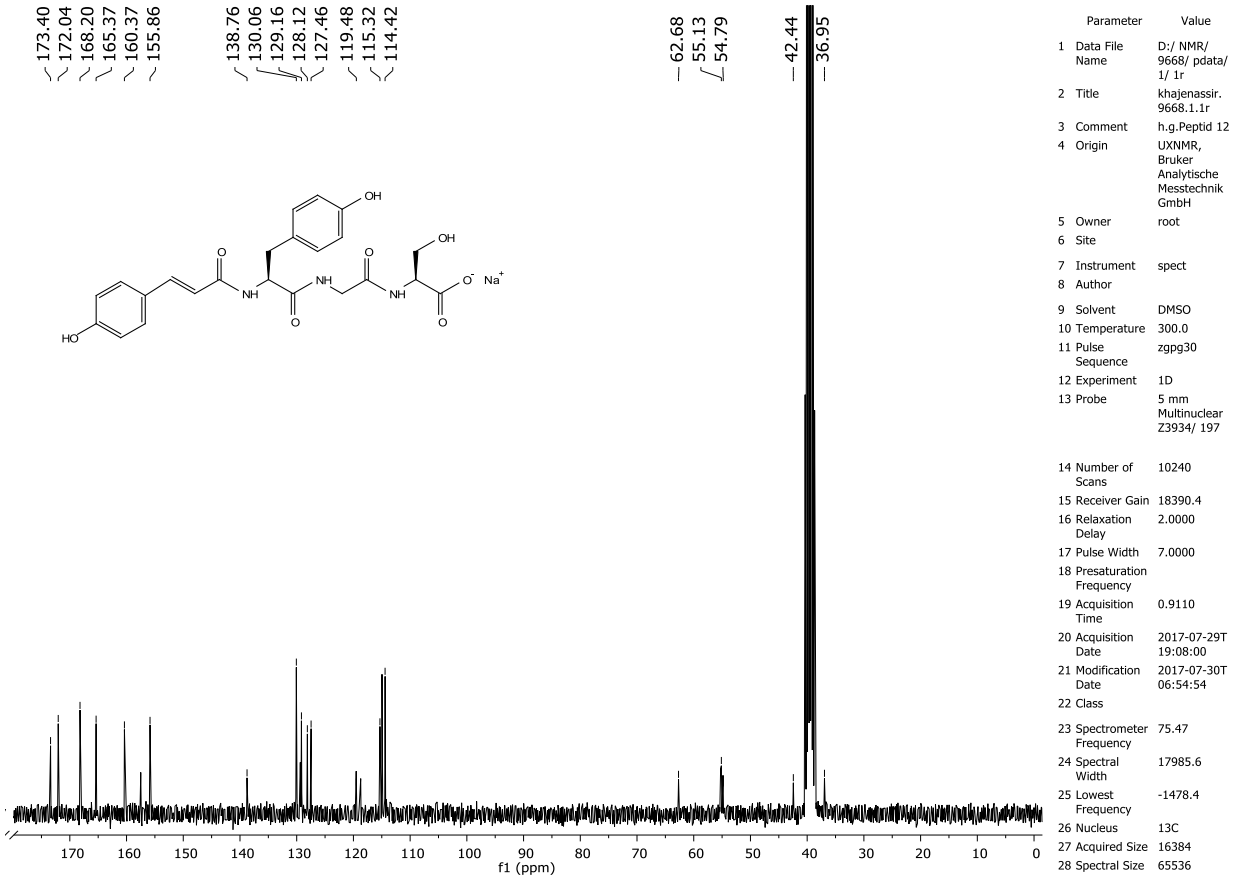
5	Owner	root
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	DMSO
10	Temperature	300.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm Multinuclear Z3934/ 197
14	Number of Scans	1024
15	Receiver Gain	18390.4
16	Relaxation Delay	2.0000
17	Pulse Width	7.0000
18	Presaturation Frequency	
19	Acquisition Time	0.9110
20	Acquisition Date	2017-07-20T13:41:00
21	Modification Date	2017-07-20T17:59:28
22	Class	
23	Spectrometer Frequency	75.47
24	Spectral Width	17985.6
25	Lowest Frequency	-1474.4
26	Nucleus	13C
27	Acquired Size	16384
28	Spectral Size	65536

^{13}C NMR (75 MHz, DMSO-d_6) spectra of sodium (3, 4, 5-trimethoxybenzoyl)-*L*-tyrosylglycyl-*L*-serinate (**20**)



^{1}H NMR (300 MHz, DMSO-d_6) spectra of sodium ((E)-3-(4-hydroxyphenyl) acryloyl)-*L*-tyrosylglycyl-*L*-serinate (**21**)



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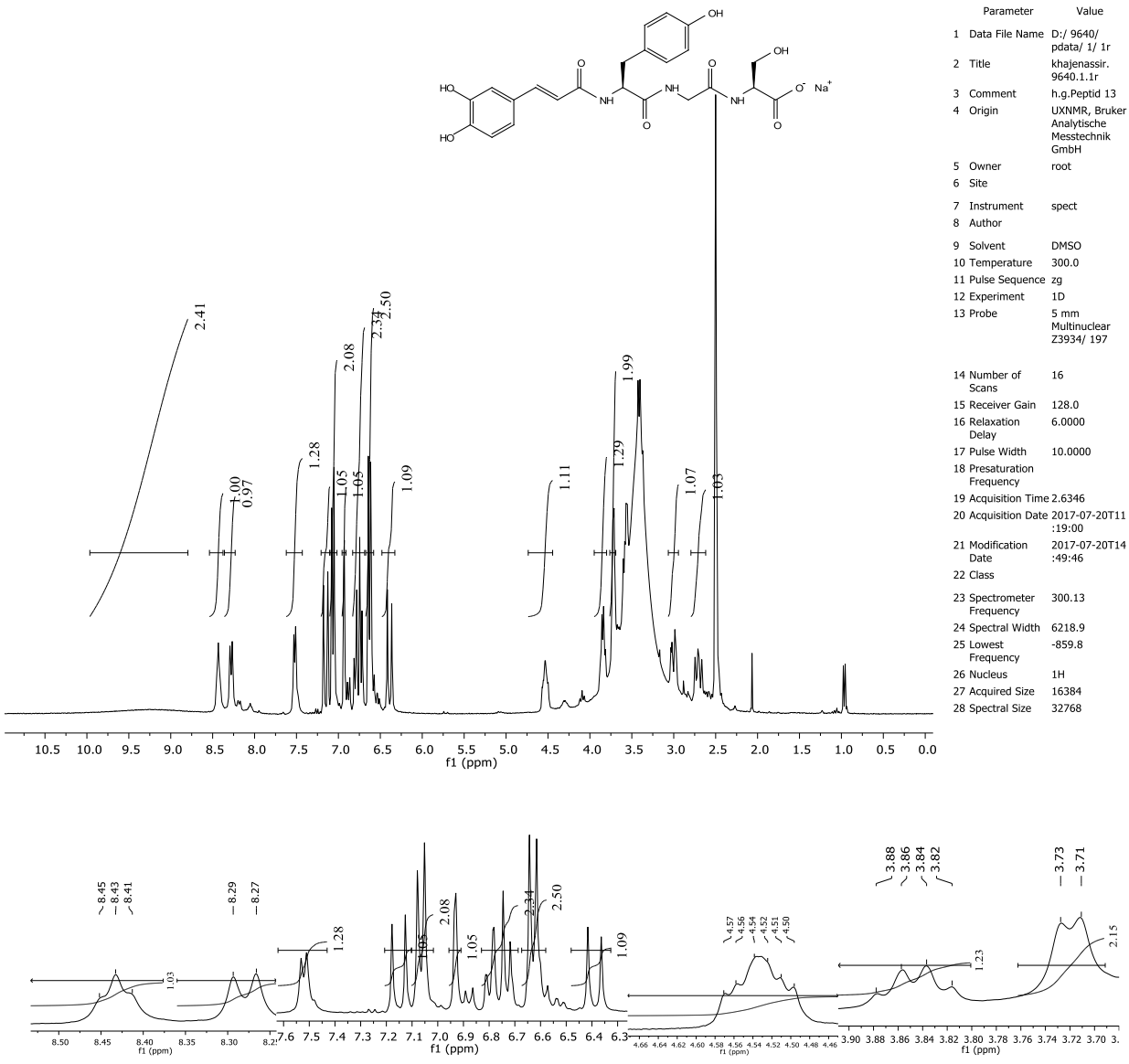
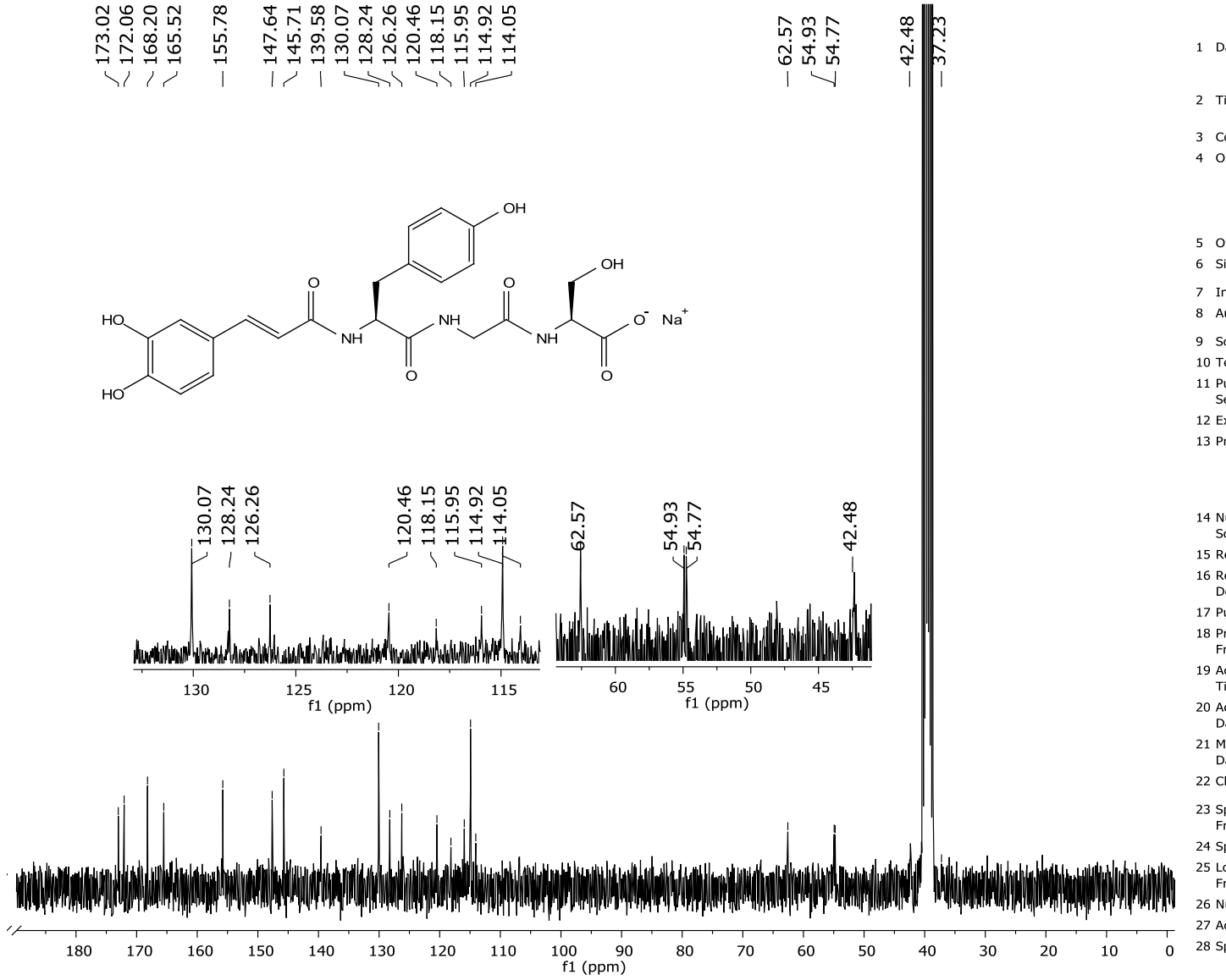
5	Owner	root
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	DMSO
10	Temperature	300.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm Multinuclear Z3934/ 197
14	Number of Scans	10240
15	Receiver Gain	18390.4
16	Relaxation Delay	2.0000
17	Pulse Width	7.0000
18	Presaturation Frequency	
19	Acquisition Time	0.9110
20	Acquisition Date	2017-07-29T 19:08:00
21	Modification Date	2017-07-30T 06:54:54
22	Class	
23	Spectrometer Frequency	75.47
24	Spectral Width	17985.6
25	Lowest Frequency	-1478.4
26	Nucleus	13C
27	Acquired Size	16384
28	Spectral Size	65536

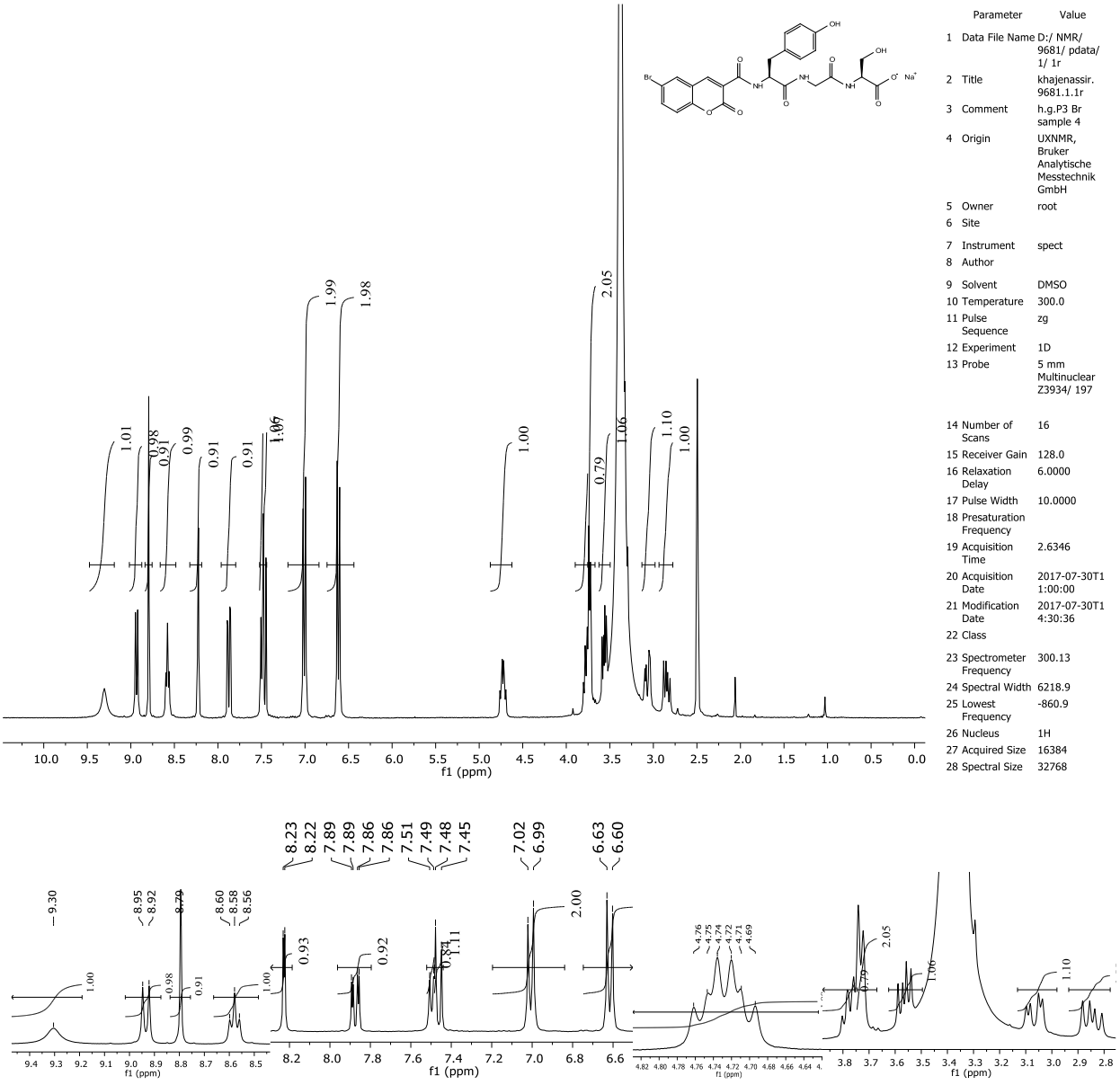
^{13}C NMR (75 MHz, DMSO-d_6) spectra of sodium ((*E*)-3-(4-hydroxyphenyl) acryloyl)-*L*-tyrosylglycyl-*L*-serinate (**21**)



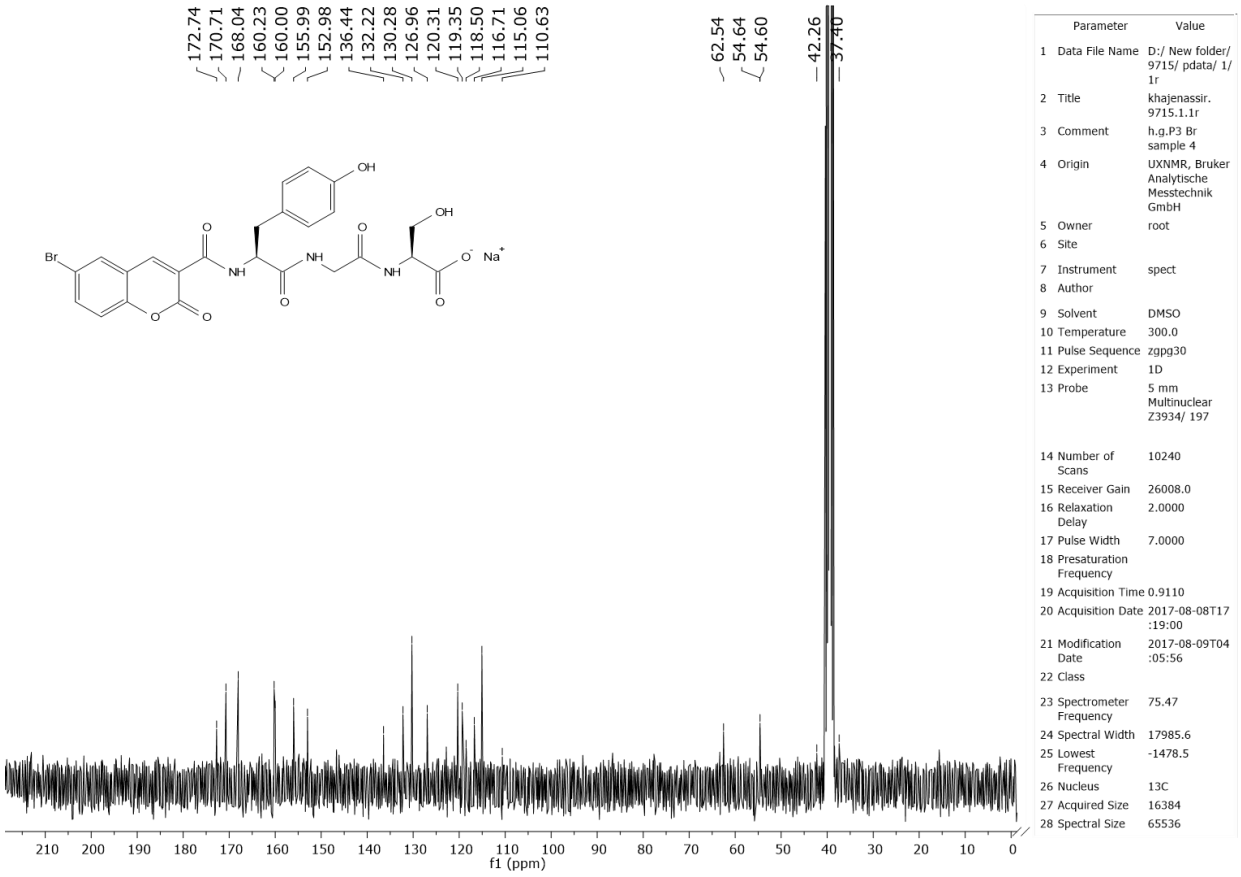
^{1}H NMR (300 MHz, DMSO-d_6) spectra of sodium ((*E*)-3-(3,4-Dihydroxyphenyl) acryloyl)-*L*-tyrosylglycyl-*L*-serinate (**22**)



^{13}C NMR (75 MHz, DMSO-d_6) spectra of sodium ((*E*)-3-(3,4-Dihydroxyphenyl) acryloyl)-*L*-tyrosylglycyl-*L*-serinate (**22**)



^{1}H NMR (300 MHz, DMSO-d_6) spectra of sodium (6-bromo-2-oxo-2H-chromene-3-carbonyl)-*L*-tyrosylglycyl-*L*-serinate (**23**)



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3	Comment	h.g.P3 Br sample 4
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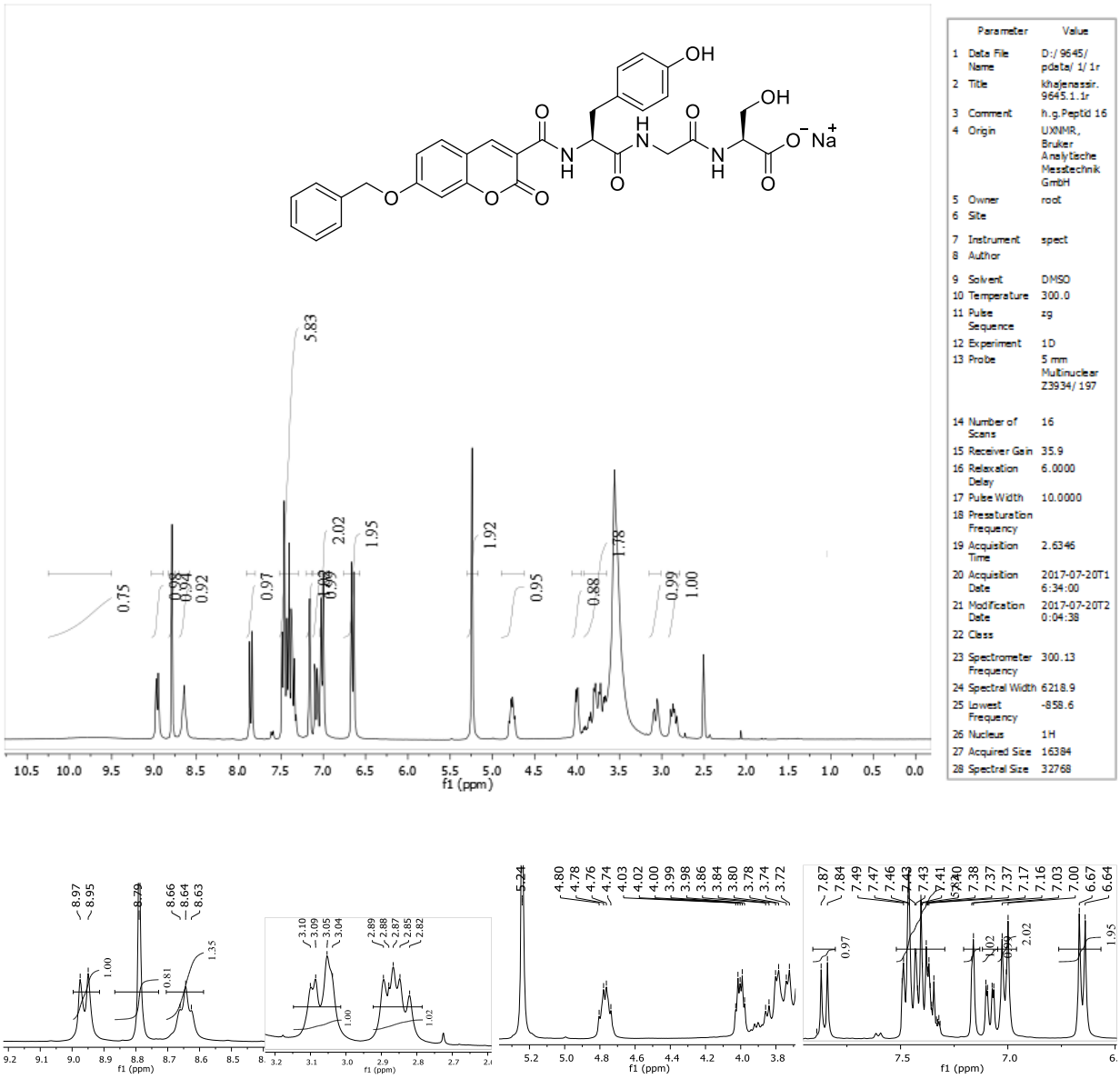
5	Owner	root
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	DMSO
10	Temperature	300.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm Multinuclear Z3934/ 197
14	Number of Scans	10240
15	Receiver Gain	26008.0
16	Relaxation Delay	2.0000
17	Pulse Width	7.0000
18	Presaturation Frequency	
19	Acquisition Time	0.9110
20	Acquisition Date	2017-08-08T17 :19:00
21	Modification Date	2017-08-09T04 :05:56
22	Class	
23	Spectrometer Frequency	75.47
24	Spectral Width	17985.6
25	Lowest Frequency	-1478.5
26	Nucleus	13C
27	Acquired Size	16384
28	Spectral Size	65536

^{13}C NMR (75 MHz, DMSO-d_6) spectra of sodium (6-bromo-2-oxo-2H-chromene-3-carbonyl)-*L*-tyrosylglycyl-*L*-serinate (**23**)



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3	Comment	h.g.Peptid 16
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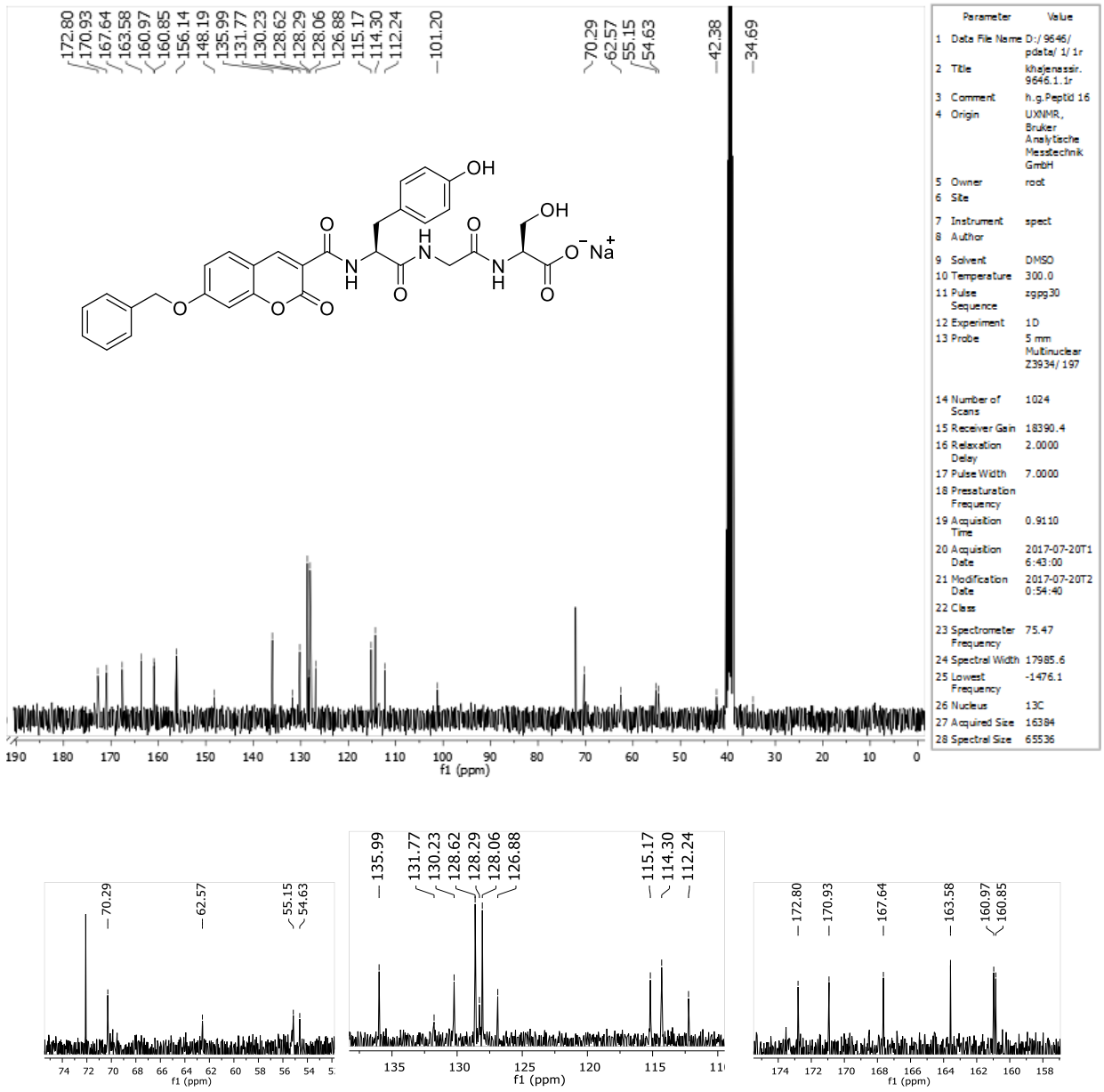
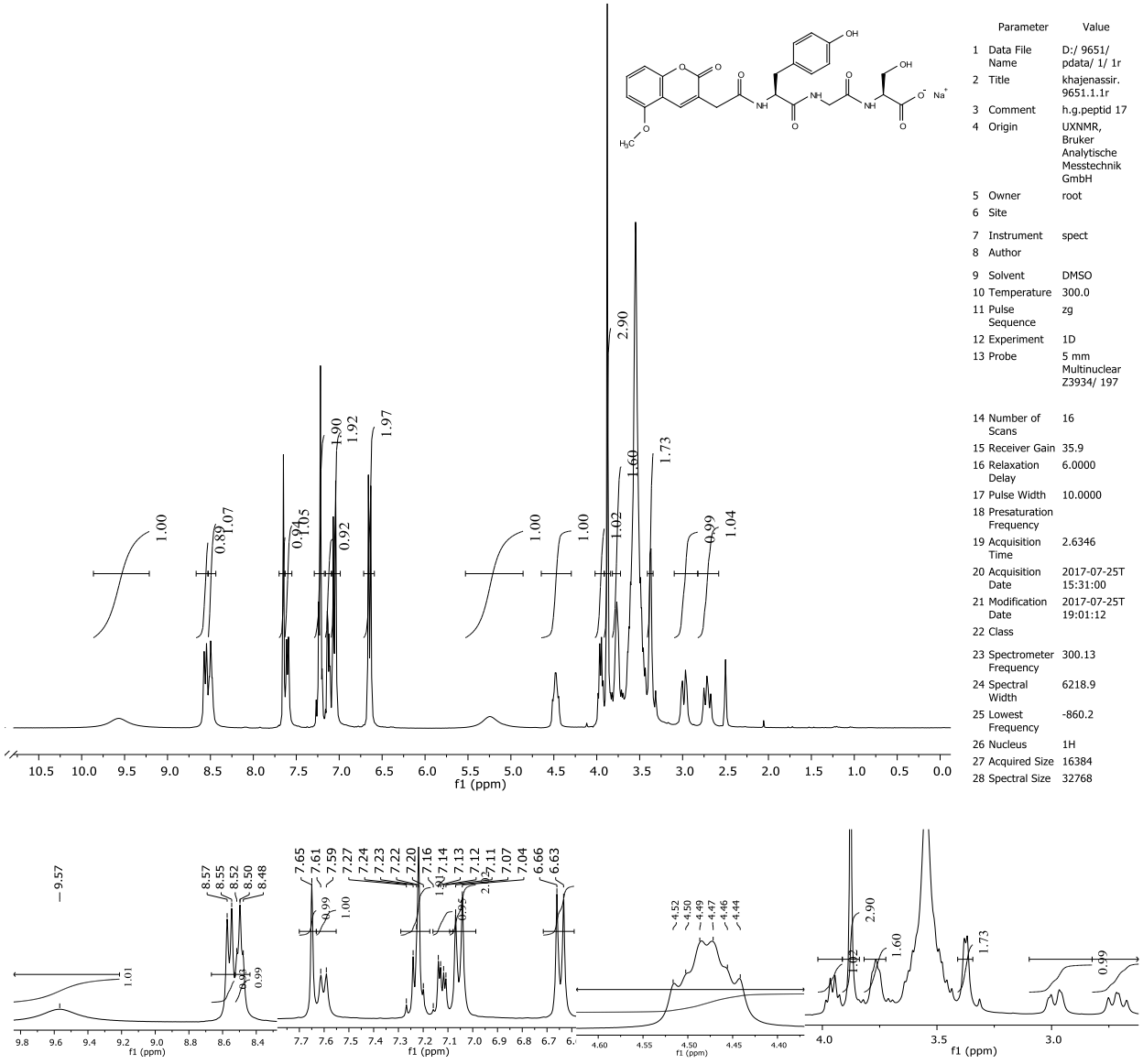
5	Owner	root
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	DMSO
10	Temperature	300.0
11	Pulse Sequence	zg
12	Experiment	1D
13	Probe	5 mm Multinuclear Z3934/197
14	Number of Scans	16
15	Receiver Gain	35.9
16	Relaxation Delay	6.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	2.6346
20	Acquisition Date	2017-07-20T16:34:00
21	Modification Date	2017-07-20T20:04:38
22	Class	
23	Spectrometer Frequency	300.13
24	Spectral Width	6218.9
25	Lowest Frequency	-858.6
26	Nucleus	1H
27	Acquired Size	16384
28	Spectral Size	32768

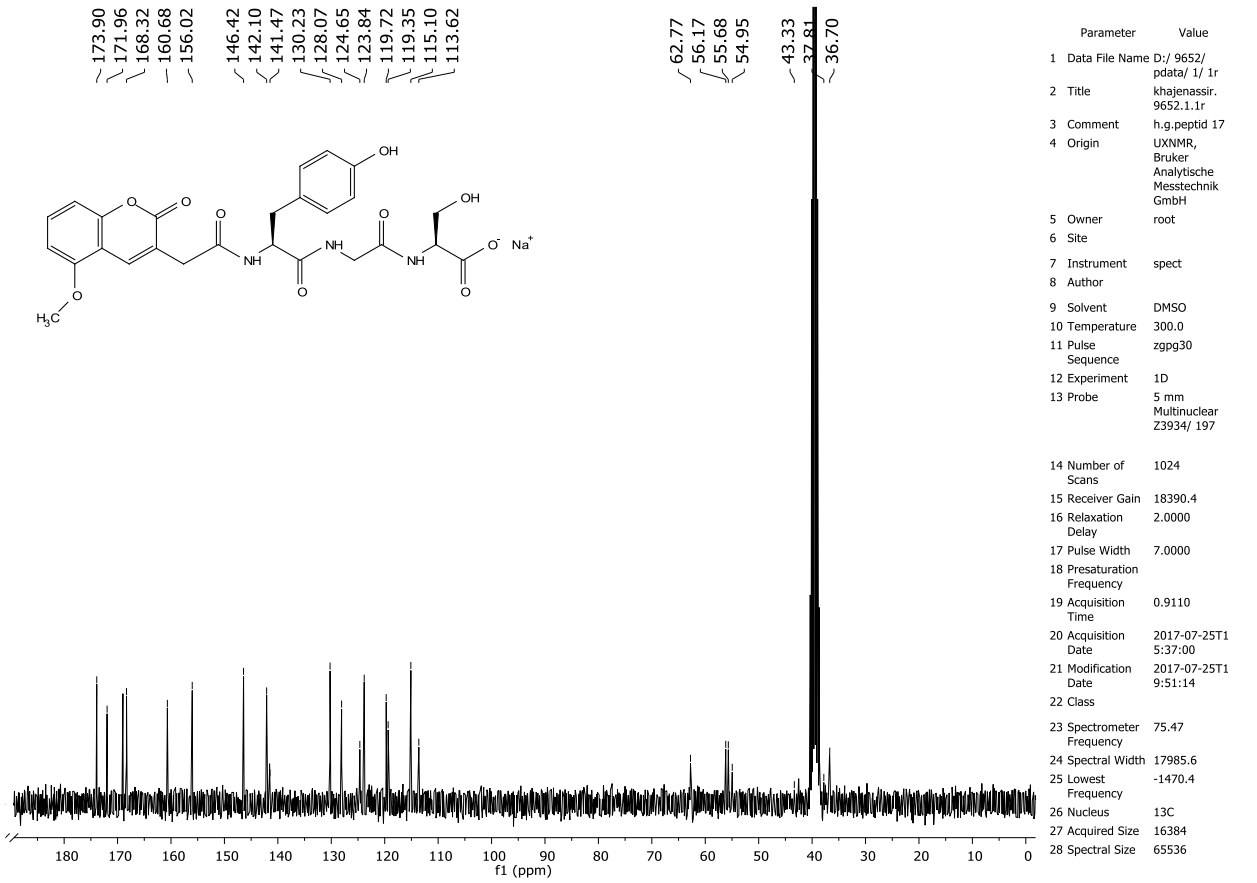
^{1}H NMR (300 MHz, DMSO-d_6) spectra of sodium (6-(benzyloxy)-2-oxo-2H-chromene-3-carbonyl)-*L*-tyrosylglycyl-*L*-serinate (**24**)



^{13}C NMR (75 MHz, DMSO-d_6) spectra of sodium (6-(benzyloxy)-2-oxo-2H-chromene-3-carbonyl)-*L*-tyrosylglycyl-*L*-serinate (**24**)



^{1}H NMR (300 MHz, DMSO-d_6) spectra of sodium (2-(5-methoxy-2-oxo-2H-chromen-3-yl) acetyl)-*L*-tyrosylglycyl-*L*-serinate (**25**)



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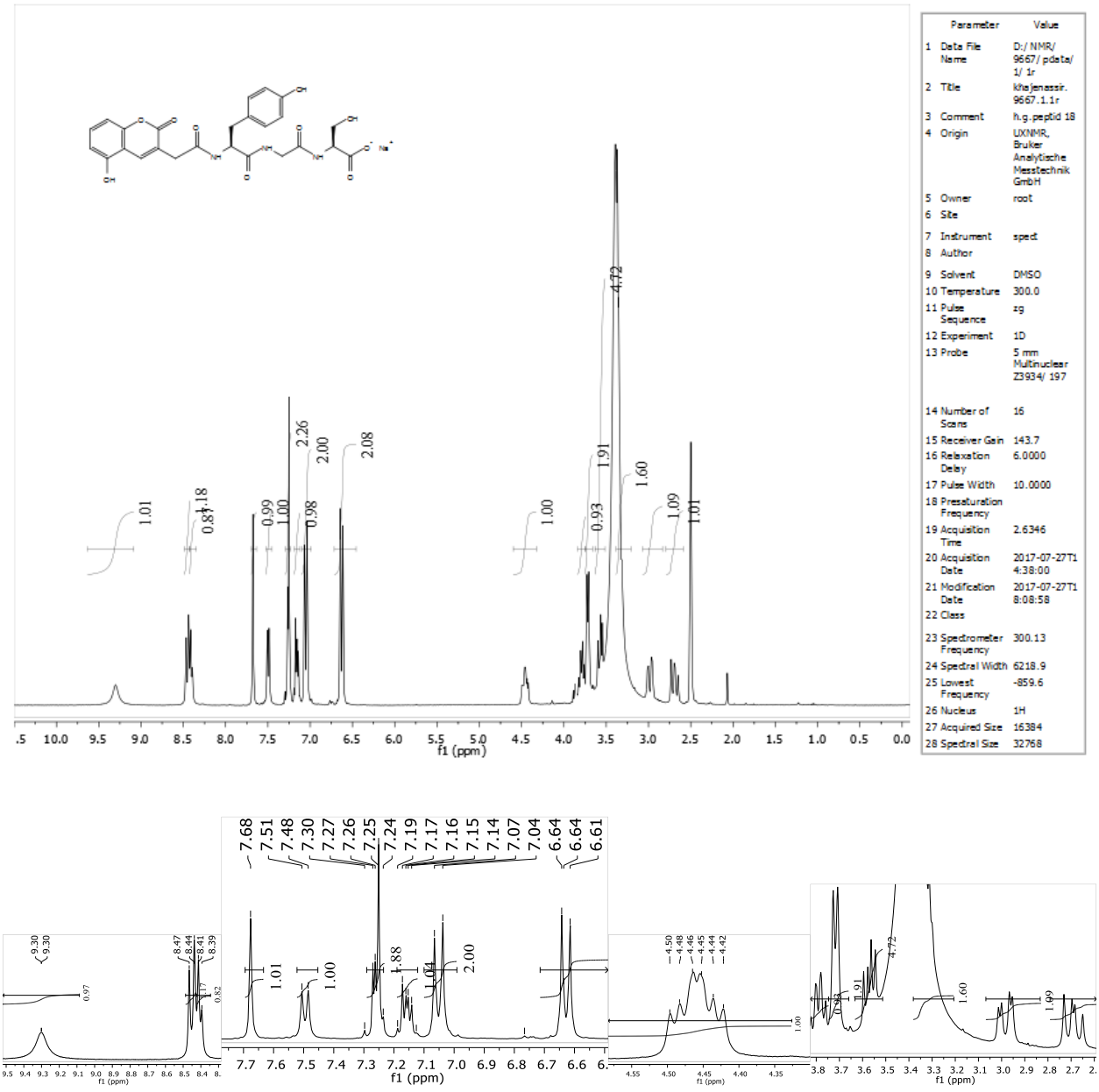
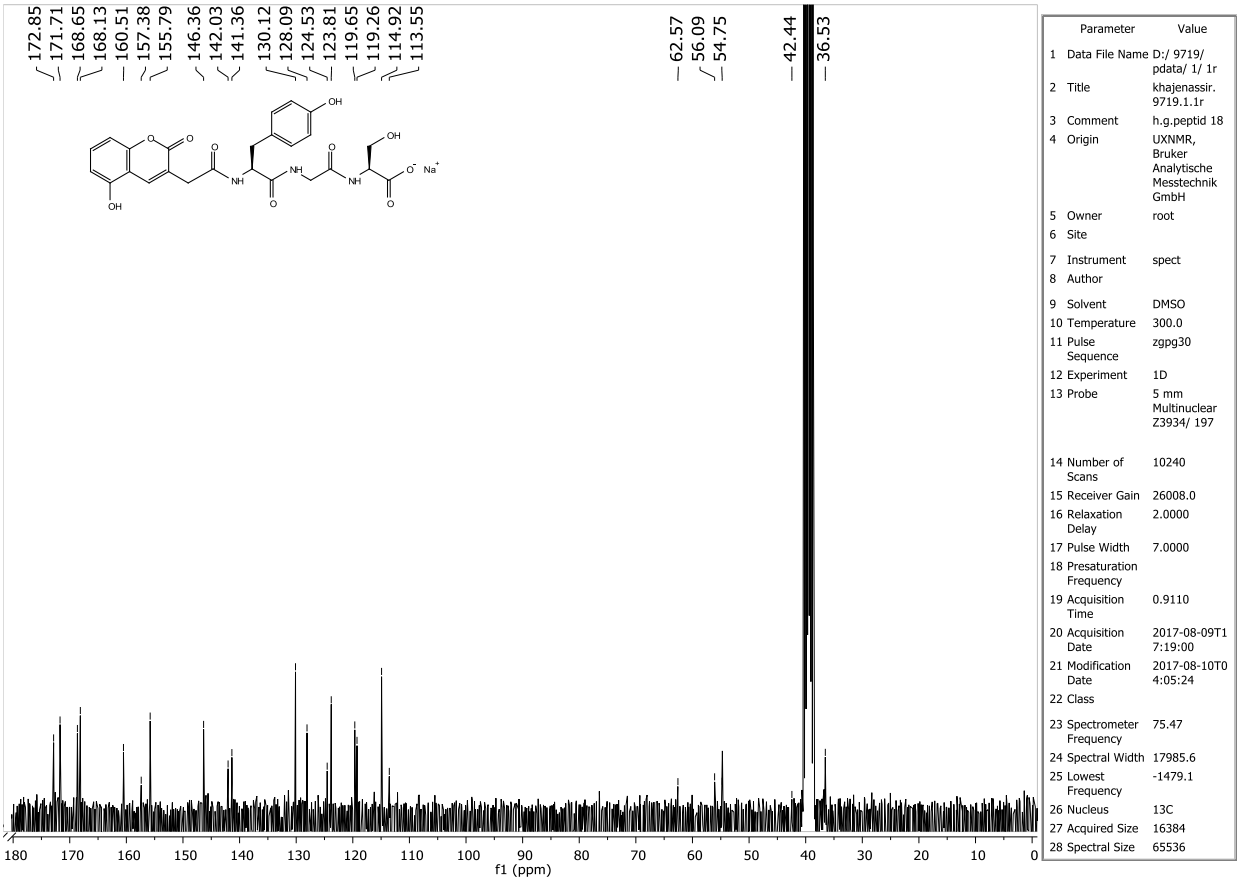
5	Owner	root
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	DMSO
10	Temperature	300.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm Multinuclear Z3934/ 197
14	Number of Scans	1024
15	Receiver Gain	18390.4
16	Relaxation Delay	2.0000
17	Pulse Width	7.0000
18	Presaturation Frequency	
19	Acquisition Time	0.9110
20	Acquisition Date	2017-07-25T15:37:00
21	Modification Date	2017-07-25T19:51:14
22	Class	
23	Spectrometer Frequency	75.47
24	Spectral Width	17985.6
25	Lowest Frequency	-1470.4
26	Nucleus	13C
27	Acquired Size	16384
28	Spectral Size	65536

^{13}C NMR (75 MHz, DMSO-d_6) spectra of sodium (2-(5-methoxy-2-oxo-2H-chromen-3-yl) acetyl)-*L*-tyrosylglycyl-*L*-serinate (**25**)



^{1}H NMR (300 MHz, DMSO-d_6) spectra of sodium (2-(5-hydroxy-2-oxo-2H-chromen-3-yl) acetyl)-*L*-tyrosylglycyl-*L*-serinate (**26**)



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3	Comment	h.g.peptid 18
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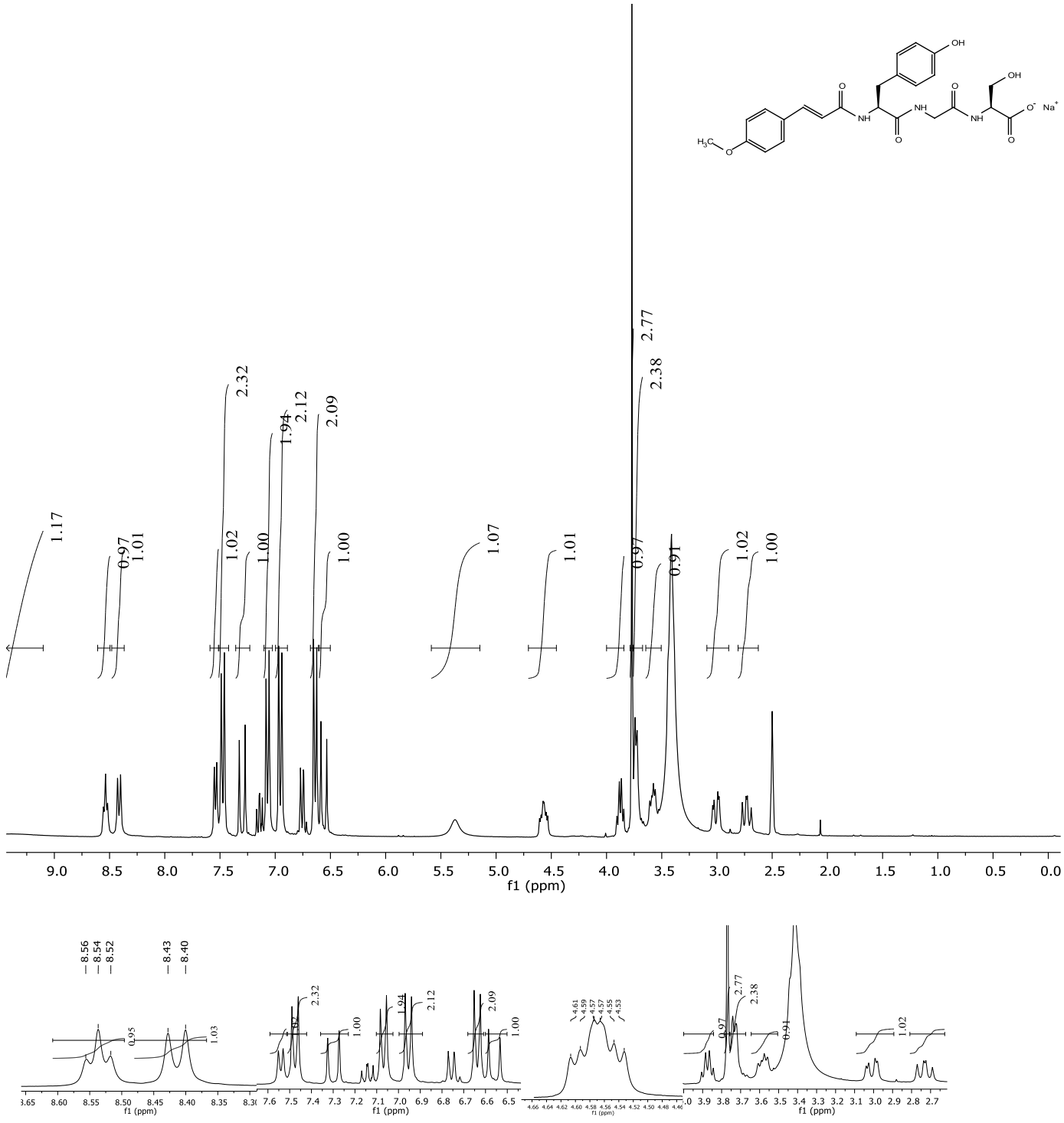
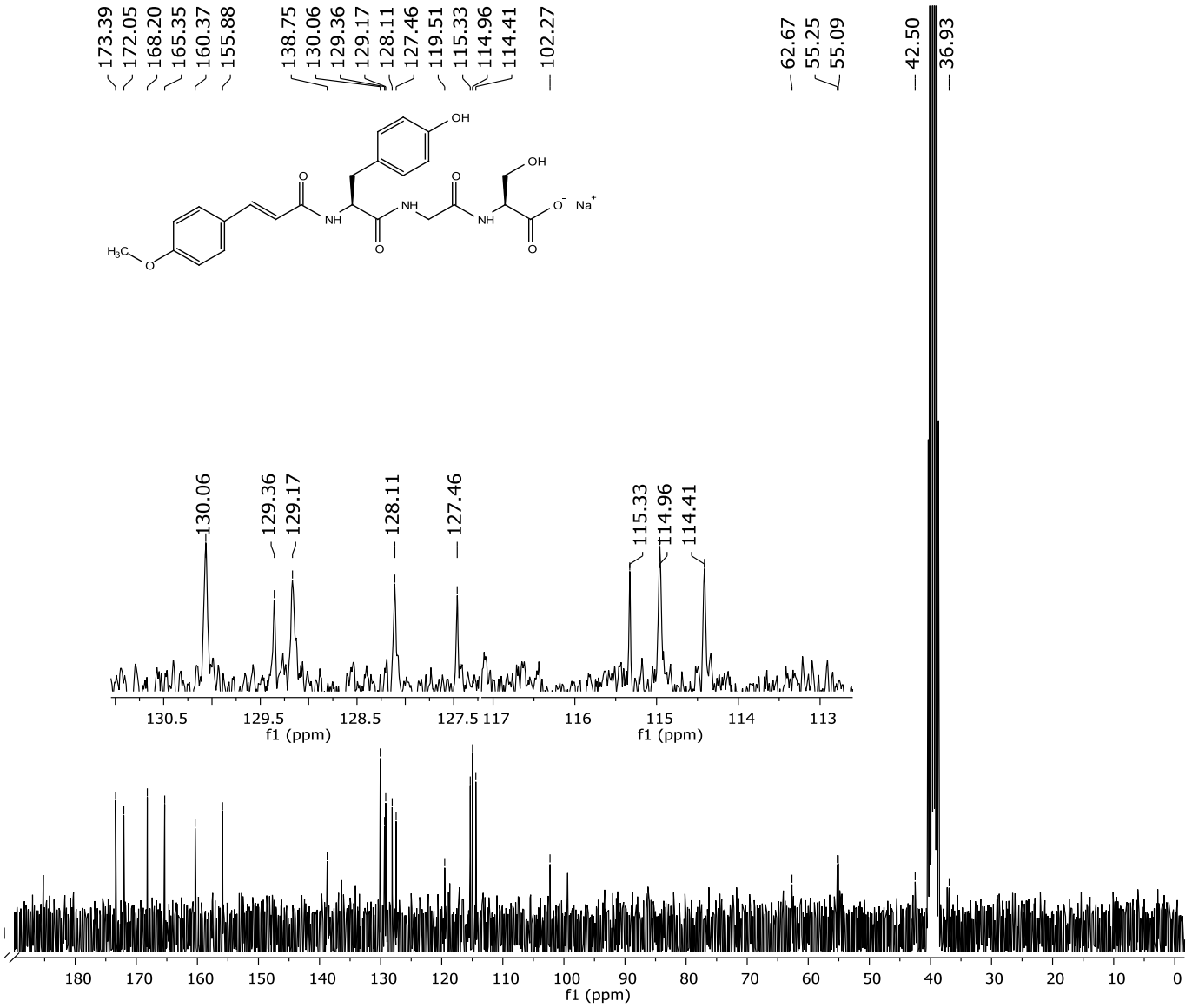
5	Owner	root
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	DMSO
10	Temperature	300.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm Multinuclear Z3934/ 197
14	Number of Scans	10240
15	Receiver Gain	26008.0
16	Relaxation Delay	2.0000
17	Pulse Width	7.0000
18	Presaturation Frequency	
19	Acquisition Time	0.9110
20	Acquisition Date	2017-08-09T17:19:00
21	Modification Date	2017-08-10T04:05:24
22	Class	
23	Spectrometer Frequency	75.47
24	Spectral Width	17985.6
25	Lowest Frequency	-1479.1
26	Nucleus	13C
27	Acquired Size	16384
28	Spectral Size	65536

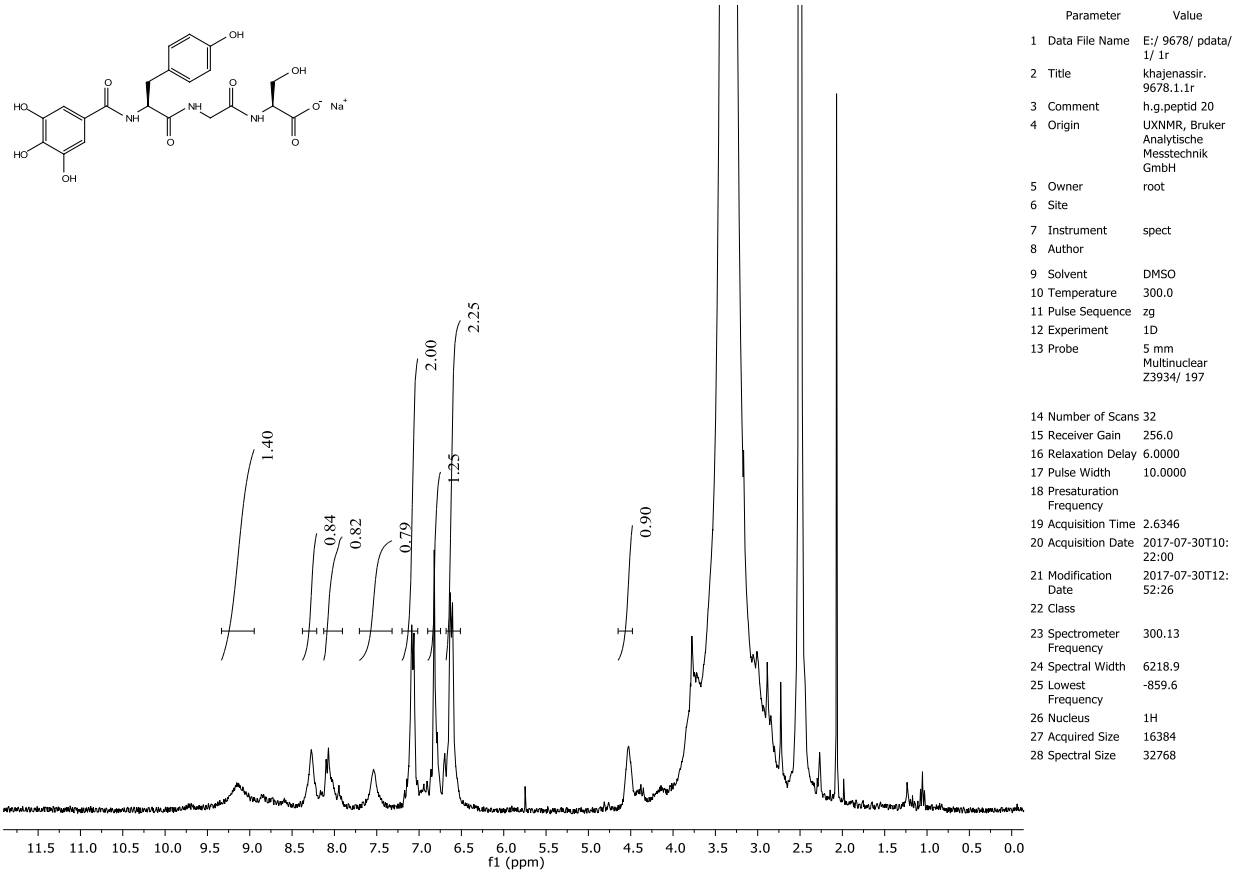
^{13}C NMR (75 MHz, DMSO-d_6) spectra of sodium (2-(5-hydroxy-2-oxo-2H-chromen-3-yl) acetyl)-*L*-tyrosylglycyl-*L*-serinate (**26**)



^{1}H NMR (300 MHz, DMSO-d_6) spectra of sodium ((*E*)-3-(4-methoxyphenyl) acryloyl)-*L*-tyrosylglycyl-*L*-serinate (**27**)



^{13}C NMR (75 MHz, DMSO-d_6) spectra of sodium ((*E*)-3-(4-methoxyphenyl) acryloyl)-*L*-tyrosylglycyl-*L*-serinate (**27**)



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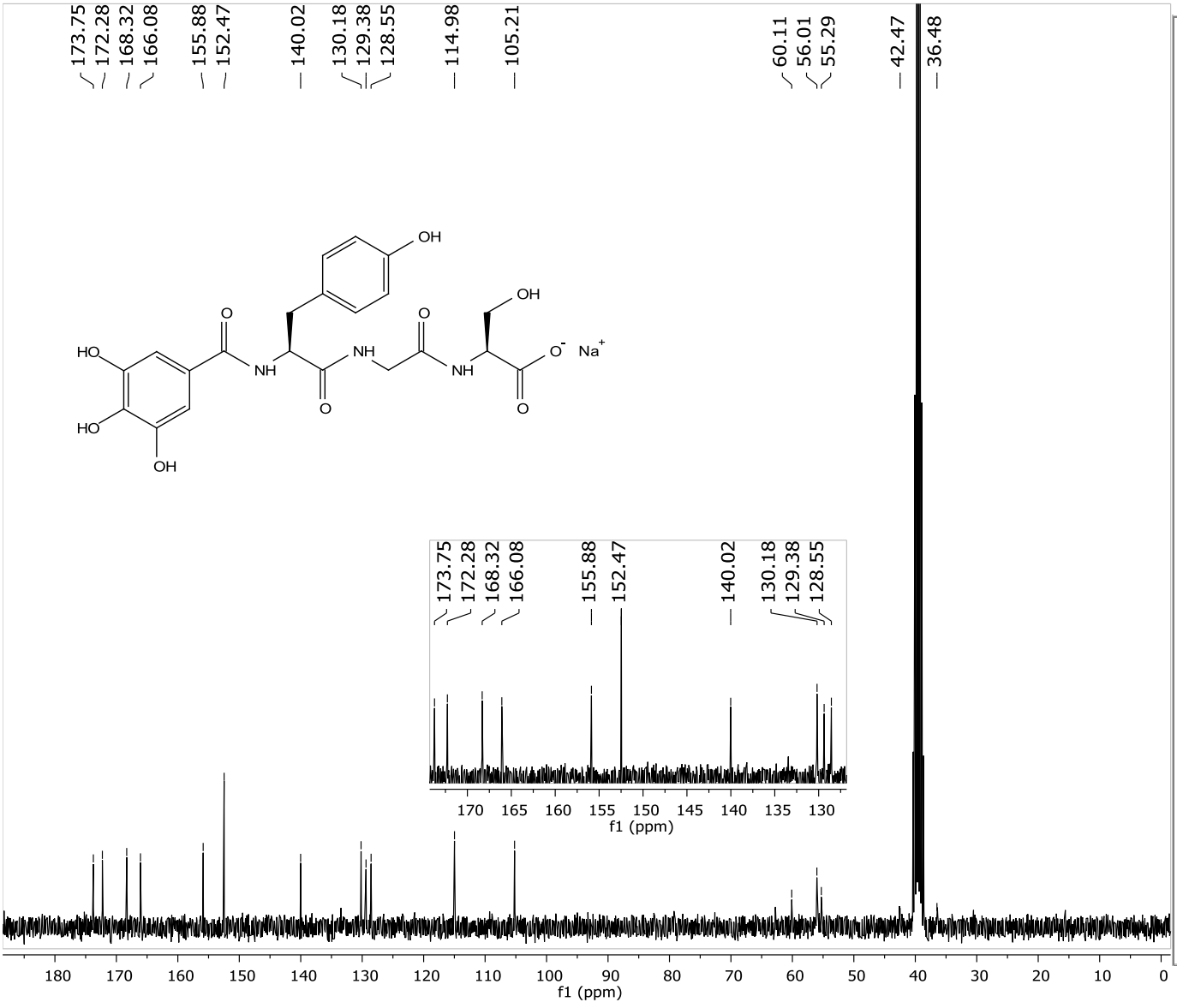
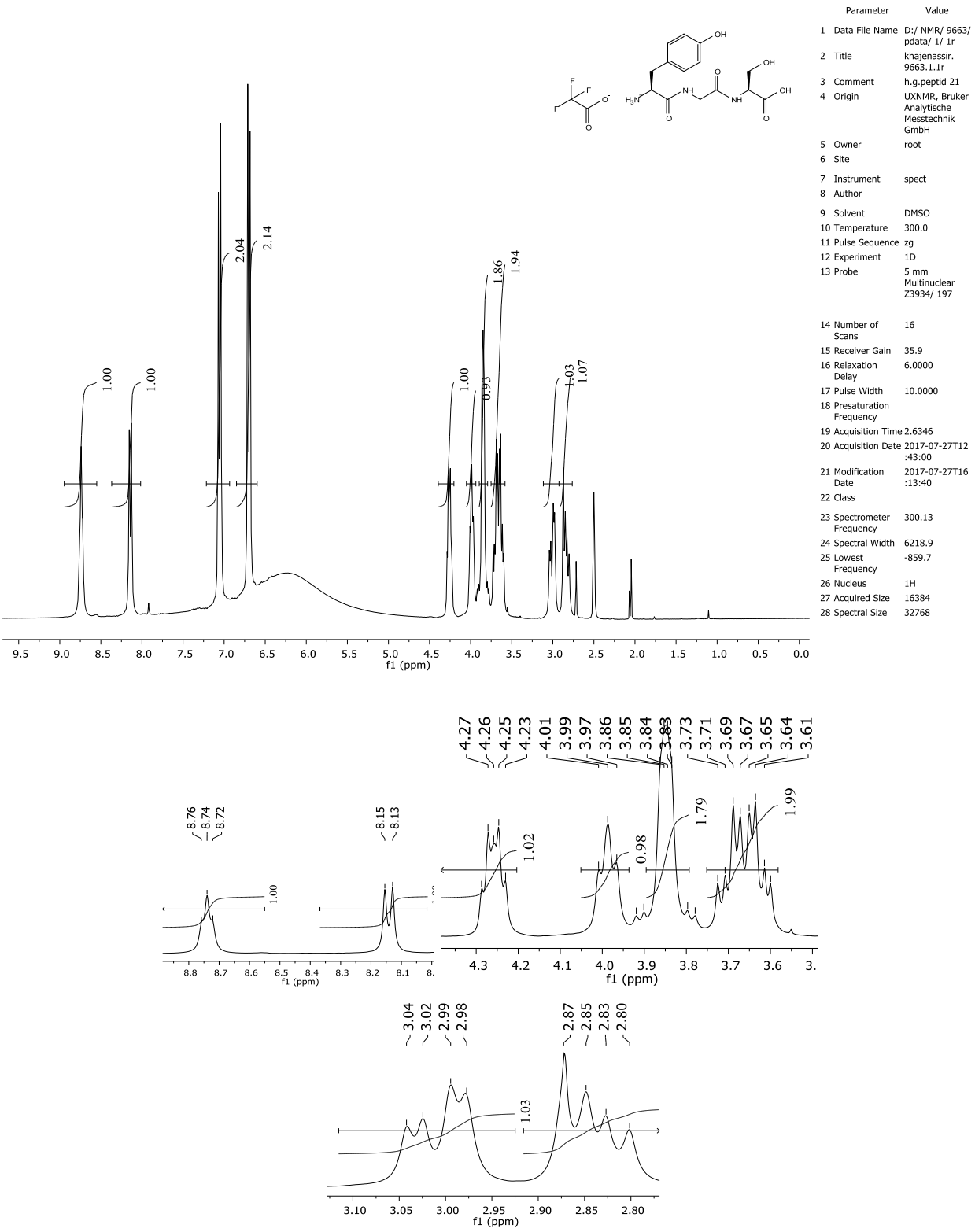
5	Owner	root
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	DMSO
10	Temperature	300.0
11	Pulse Sequence	zg
12	Experiment	1D
13	Probe	5 mm Multinuclear Z3934/ 197
14	Number of Scans	32
15	Receiver Gain	256.0
16	Relaxation Delay	6.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	2.6346
20	Acquisition Date	2017-07-30T10: 22:00
21	Modification Date	2017-07-30T12: 52:26
22	Class	
23	Spectrometer Frequency	300.13
24	Spectral Width	6218.9
25	Lowest Frequency	-859.6
26	Nucleus	1H
27	Acquired Size	16384
28	Spectral Size	32768

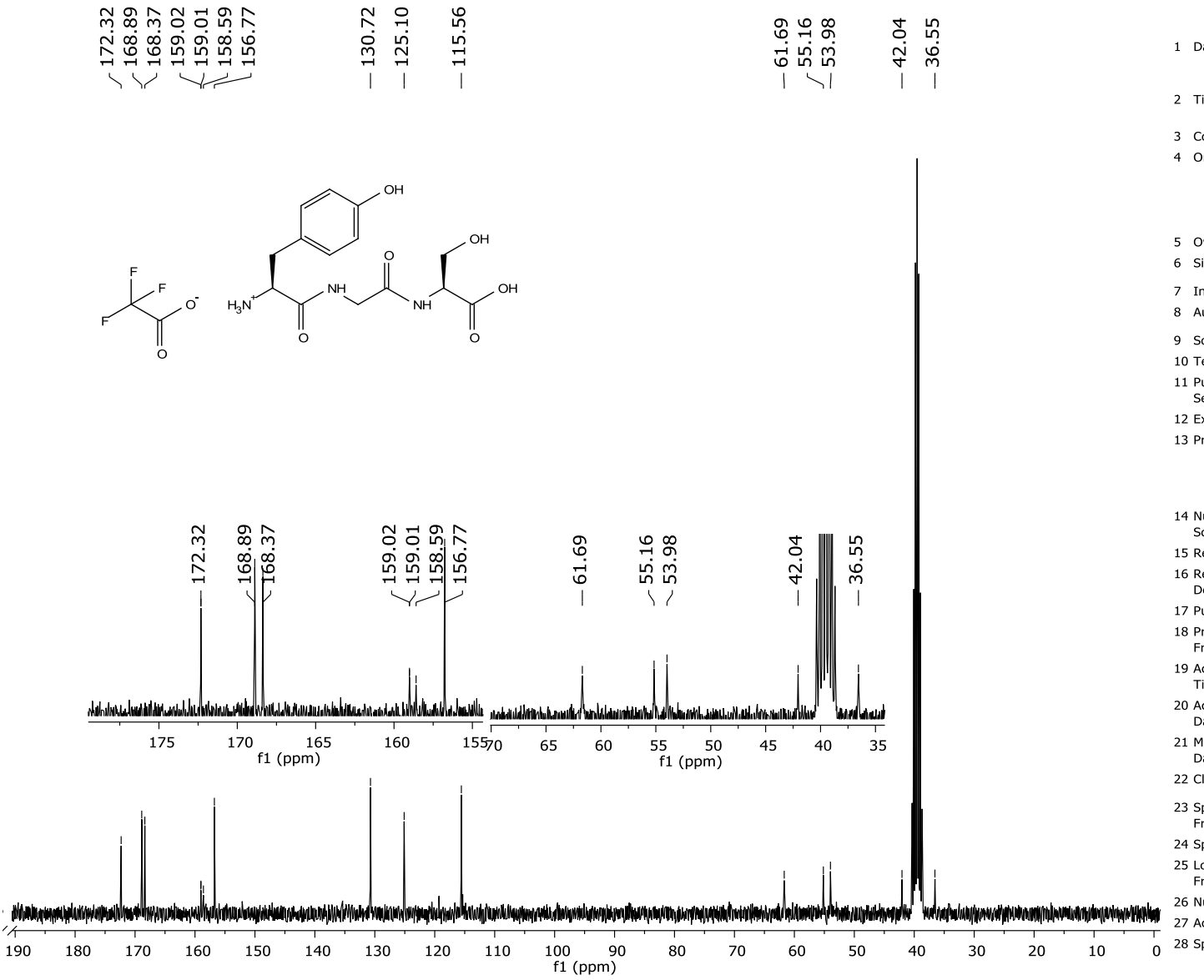
^{1}H NMR (300 MHz, DMSO-d_6) spectra of sodium (3, 4, 5-trihydroxybenzoyl)-*L*-tyrosylglycyl-*L*-serinate (**28**)



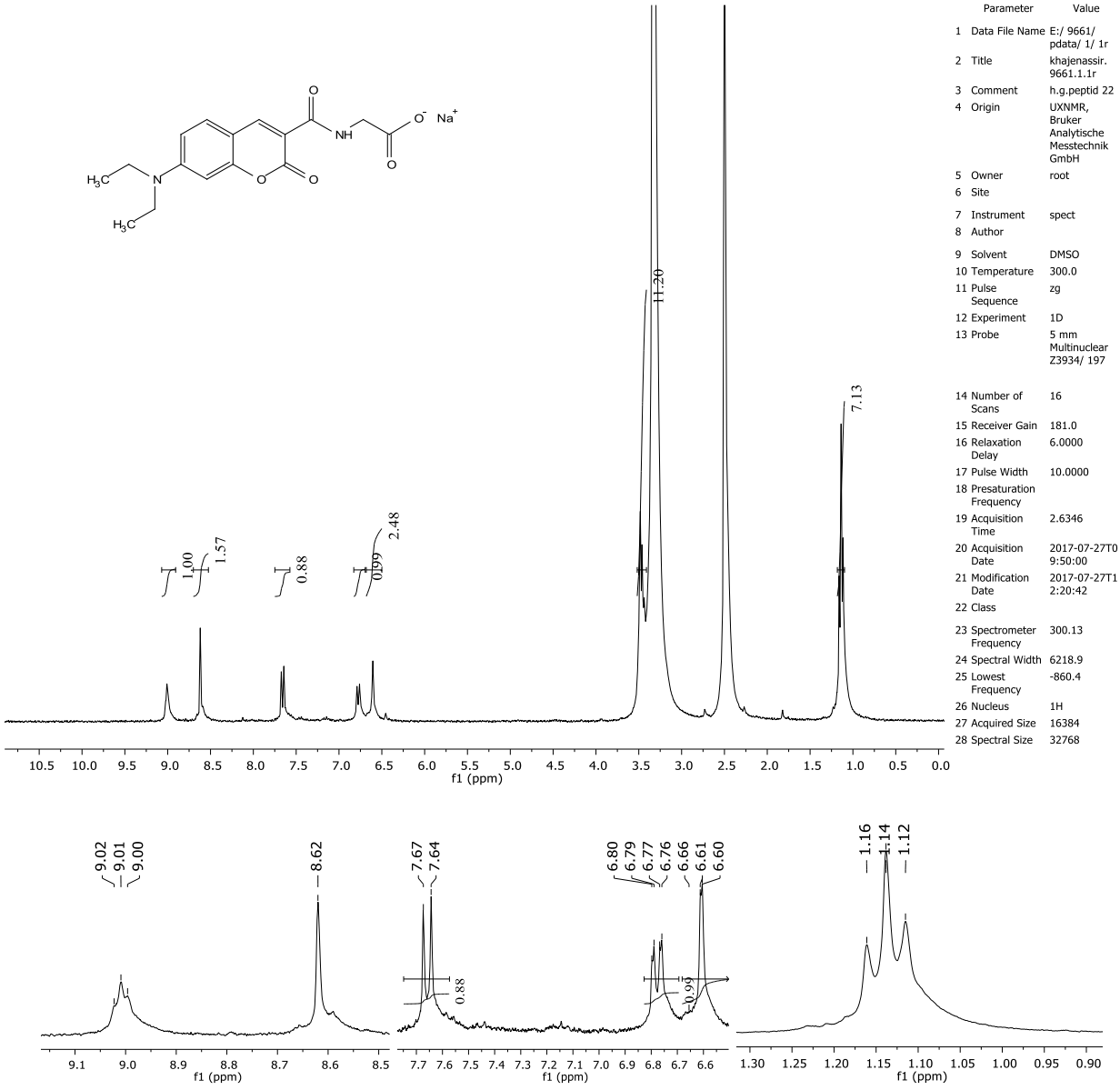
^{13}C NMR (75 MHz, DMSO-d_6) spectra of sodium (3, 4, 5-trihydroxybenzoyl)-*L*-tyrosylglycyl-*L*-serinate (**28**)



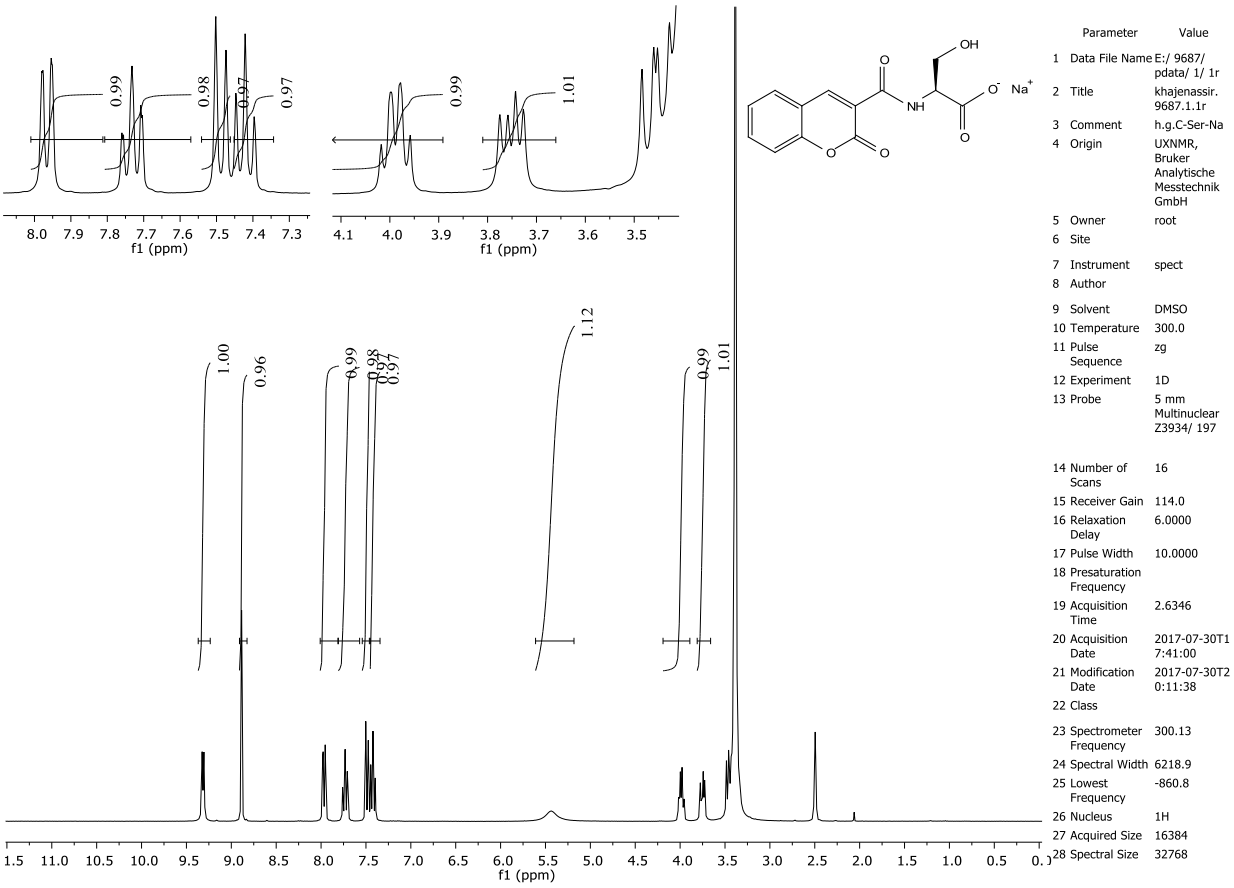
^{1}H NMR (300 MHz, DMSO-d_6) spectra of (*S*)-1-((2-(((*S*)-1-carboxy-2-hydroxyethyl) amino)-2-oxoethyl) amino)-3-(4-hydroxyphenyl)-1-oxopropan-2-aminium 2,2,2-trifluoroacetate (**29**)



^{13}C NMR (75 MHz, DMSO-d_6) spectra of (*S*)-1-((2-(((*S*)-1-carboxy-2-hydroxyethyl) amino)-2-oxoethyl) amino)-3-(4-hydroxyphenyl)-1-oxopropan-2-aminium 2,2,2-trifluoroacetate (**29**)



^{1}H NMR (300 MHz, DMSO-d_6) spectra of sodium (7-(diethylamino)-2-oxo-2H-chromene-3-carbonyl) glycinate (**30**)



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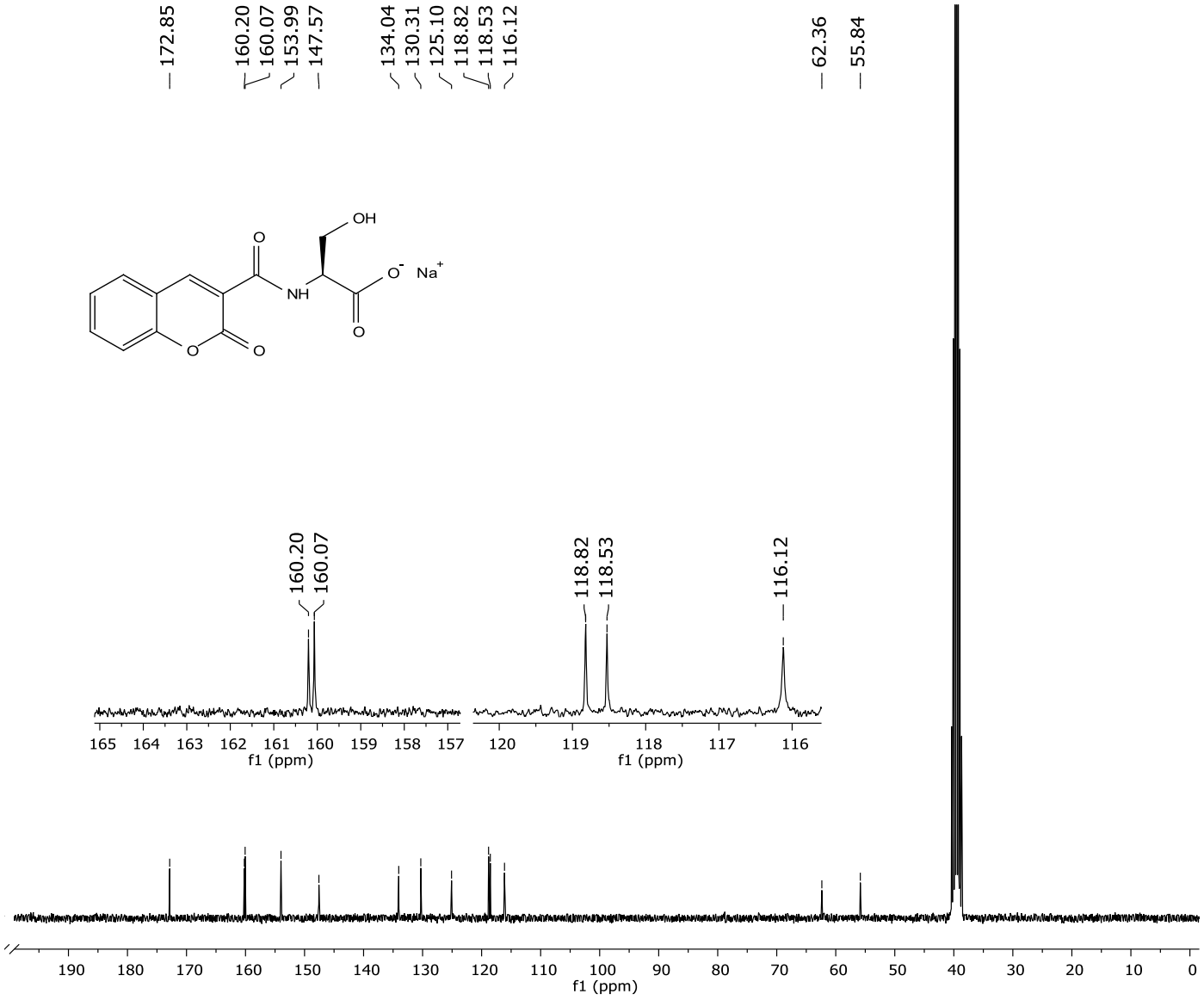
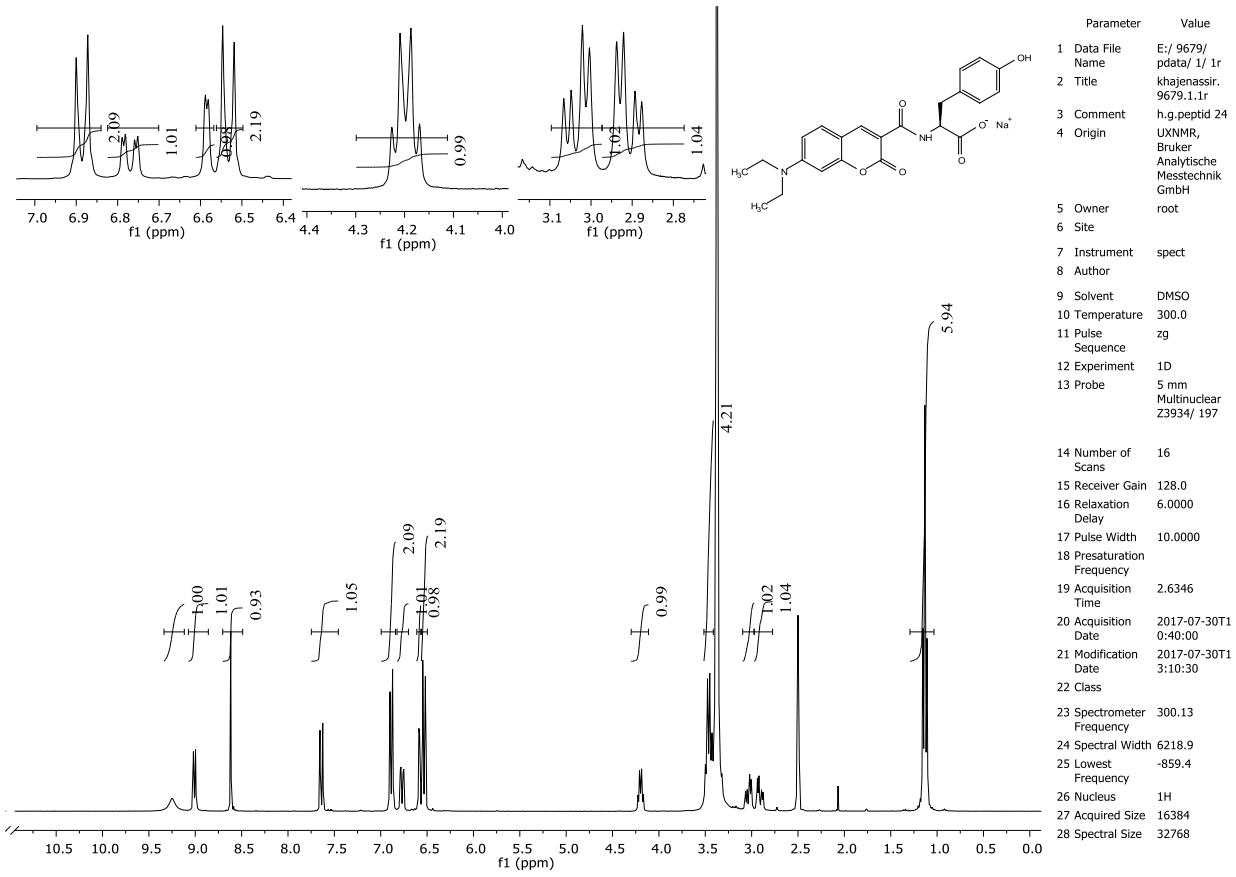
5	Owner	root
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	DMSO
10	Temperature	300.0
11	Pulse Sequence	zg
12	Experiment	1D
13	Probe	5 mm Multinuclear Z3934/ 197
14	Number of Scans	16
15	Receiver Gain	114.0
16	Relaxation Delay	6.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	2.6346
20	Acquisition Date	2017-07-30T17:41:00
21	Modification Date	2017-07-30T20:11:38
22	Class	
23	Spectrometer Frequency	300.13
24	Spectral Width	6218.9
25	Lowest Frequency	-860.8
26	Nucleus	1H
27	Acquired Size	16384
28	Spectral Size	32768

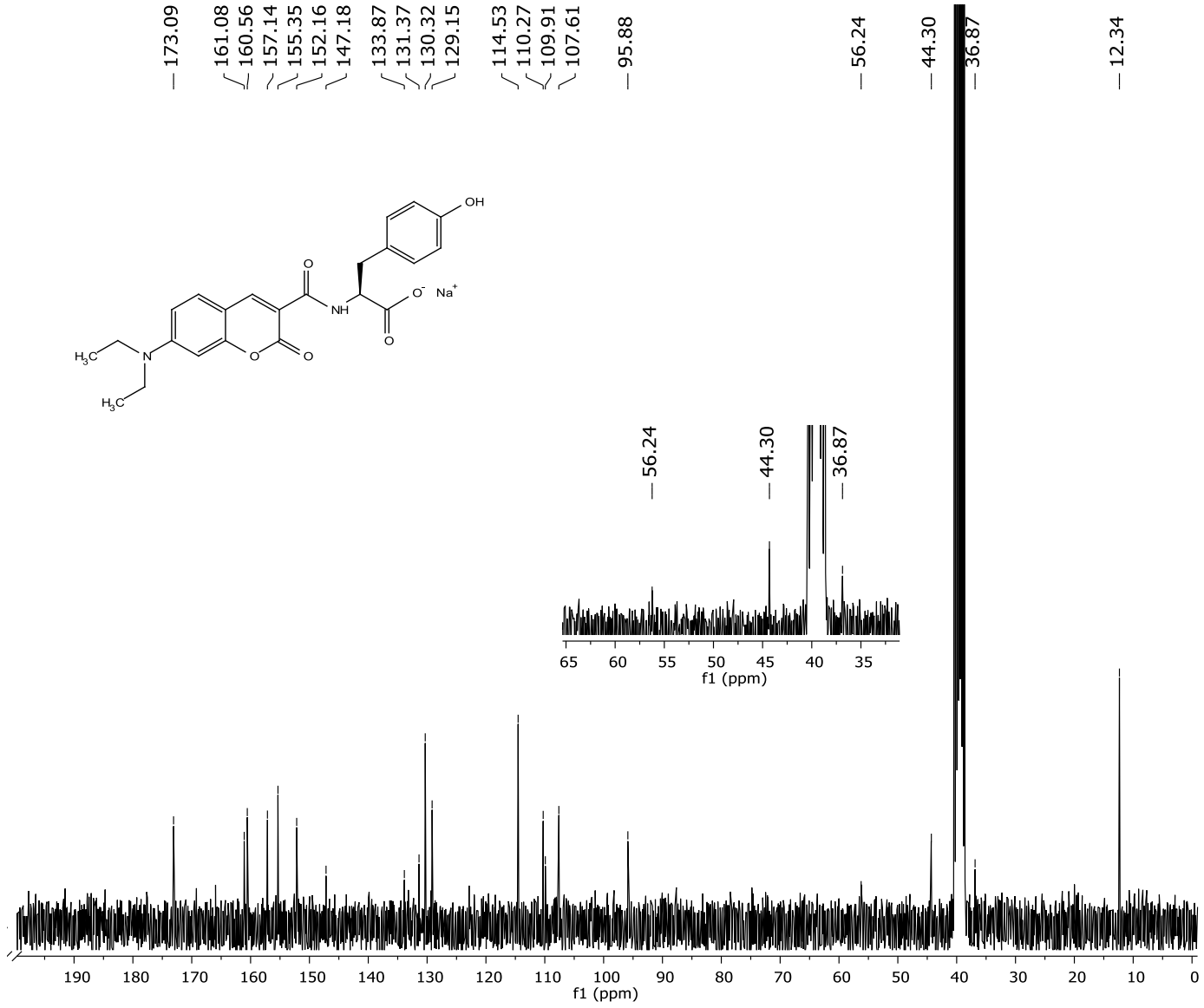
^{1}H NMR (300 MHz, DMSO-d_6) spectra of sodium (2-oxo-2H-chromene-3-carbonyl)-*L*-serinate (**31**)



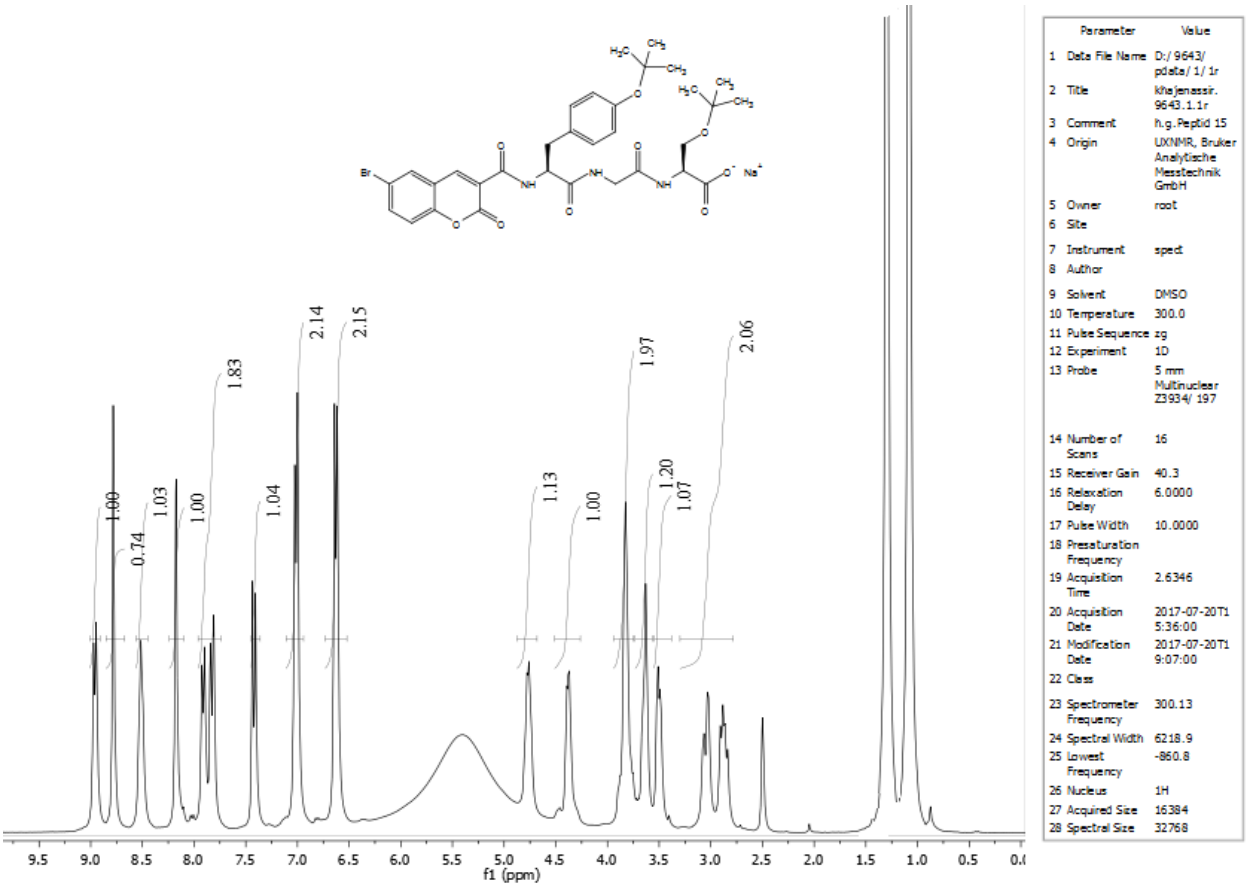
^{13}C NMR (75 MHz, DMSO-d_6) spectra of sodium (2-oxo-2H-chromene-3-carbonyl)-*L*-serinate (**31**)



^{1}H NMR (300 MHz, DMSO-d_6) spectra of sodium (7-(diethylamino)-2-oxo-2H-chromene-3-carbonyl)-*L*-tyrosinate (**32**)



^{13}C NMR (75 MHz, DMSO-d_6) spectra of sodium (7-(diethylamino)-2-oxo-2H-chromene-3-carbonyl)-*L*-tyrosinate (**32**)



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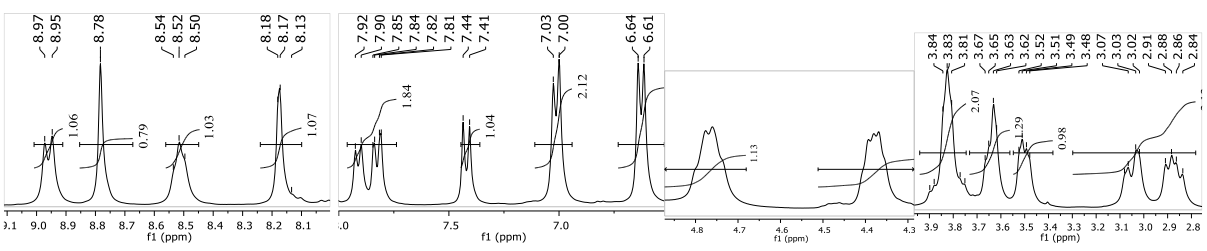
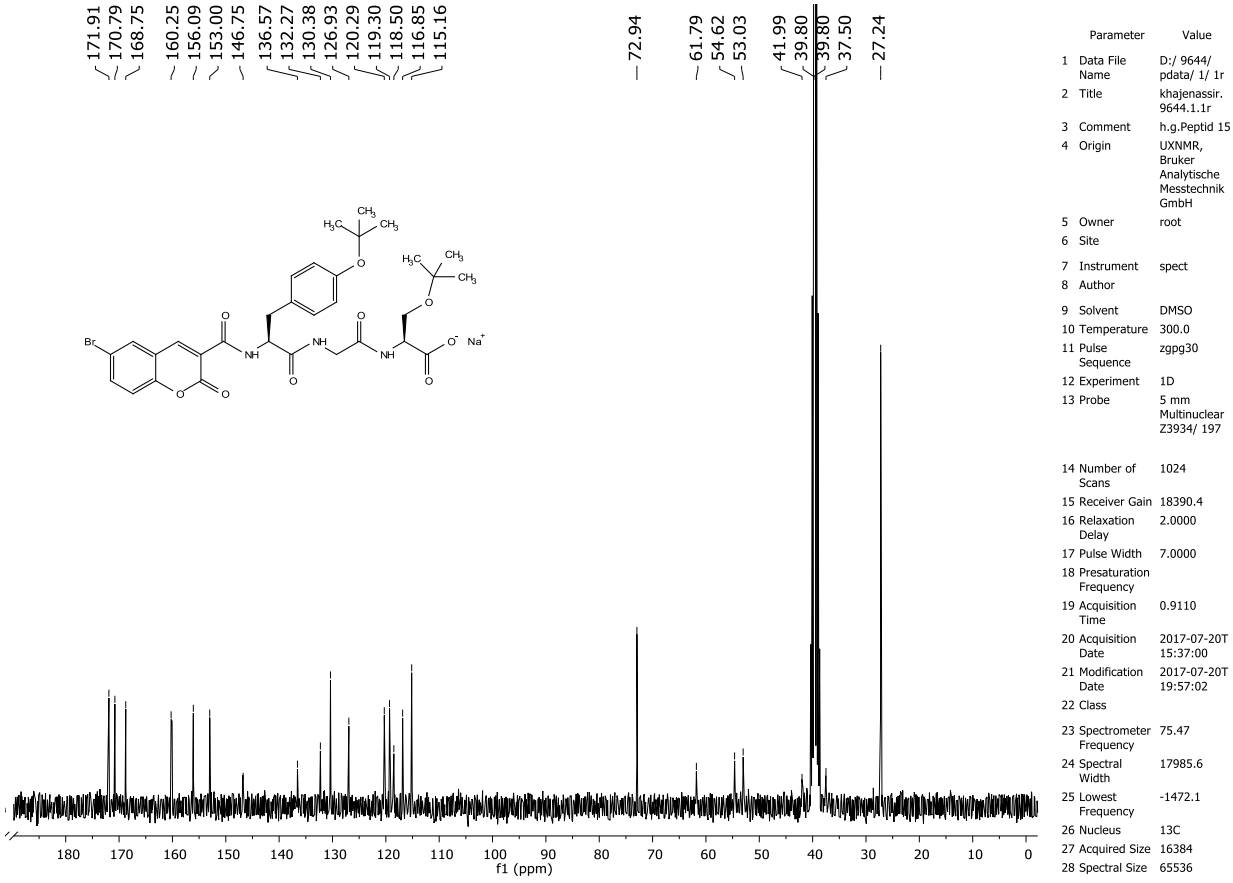
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	DMSO
10	Temperature	300.0
11	Pulse Sequence	zg
12	Experiment	1D
13	Probe	5 mm Multinuclear Z3934/197
14	Number of Scans	16
15	Receiver Gain	40.3
16	Relaxation Delay	6.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	2.6346
20	Acquisition Date	2017-07-20T15:36:00
21	Modification Date	2017-07-20T19:07:00
22	Class	
23	Spectrometer Frequency	300.13
24	Spectral Width	6218.9
25	Lowest Frequency	-860.8
26	Nucleus	1H
27	Acquired Size	16384
28	Spectral Size	32768



^{1}H NMR (300 MHz, DMSO-*d*$_6$) spectra of sodium *N*-(((*S*)-2-(6-bromo-2-oxo-2H-chromene-3-carboxamido)-3-(4- (tert butoxy) phenyl) propanoyl)glycyl)-*O*-(tert-butyl)-*L*-serinate



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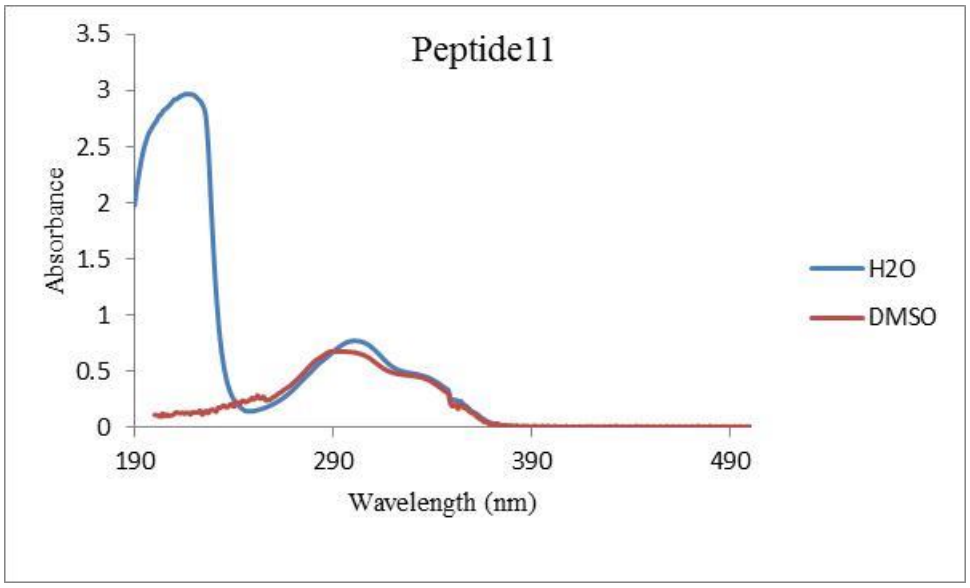
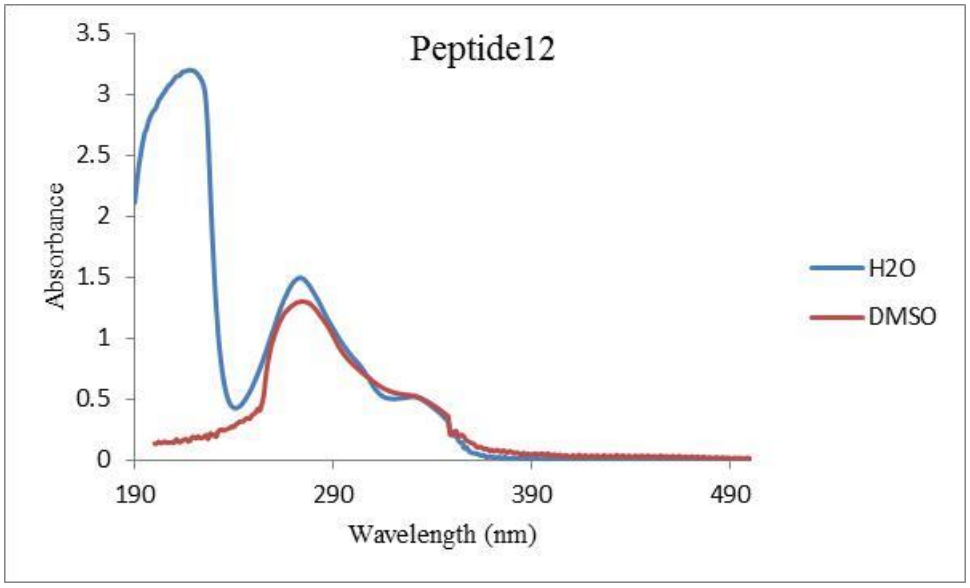
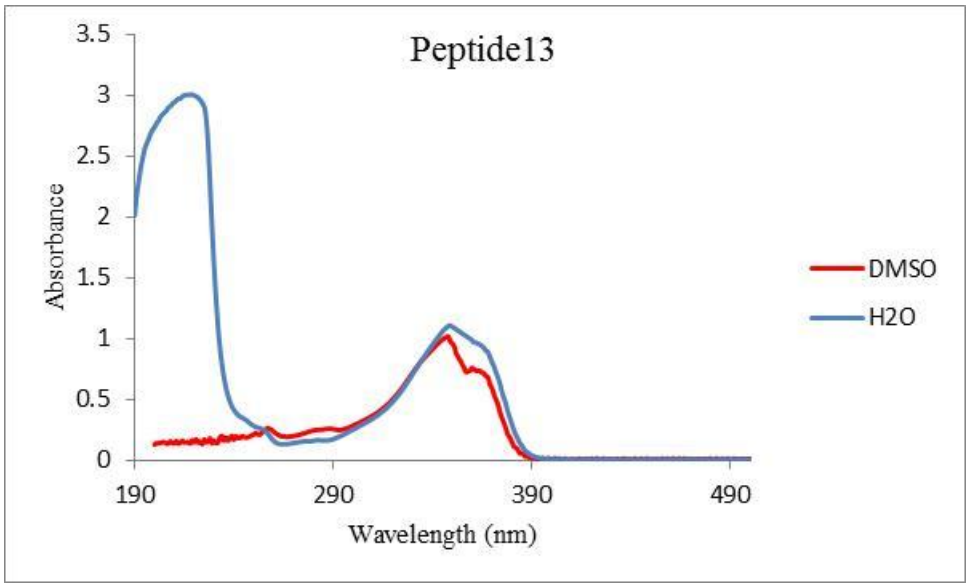
5	Owner	root
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	DMSO
10	Temperature	300.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm Multinuclear Z3934/ 197
14	Number of Scans	1024
15	Receiver Gain	18390.4
16	Relaxation Delay	2.0000
17	Pulse Width	7.0000
18	Presaturation Frequency	
19	Acquisition Time	0.9110
20	Acquisition Date	2017-07-20T 15:37:00
21	Modification Date	2017-07-20T 19:57:02
22	Class	
23	Spectrometer Frequency	75.47
24	Spectral Width	17985.6
25	Lowest Frequency	-1472.1
26	Nucleus	13C
27	Acquired Size	16384
28	Spectral Size	65536

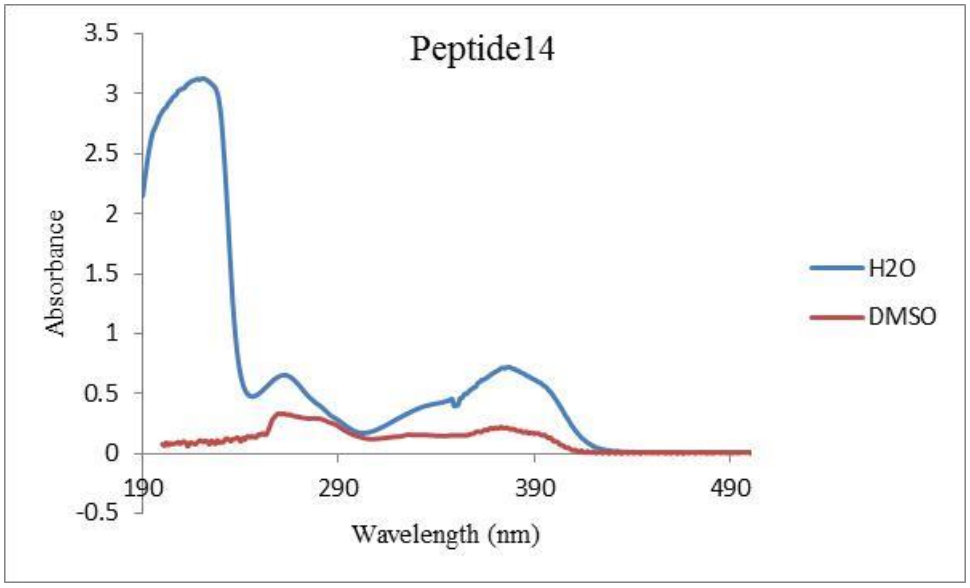
^{13}C NMR (75 MHz, DMSO-*d*$_6$) spectra of sodium *N*-(((*S*)-2-(6-bromo-2-oxo-2H-chromene-3-carboxamido)-3-(4- (tert butoxy) phenyl) propanoyl) glycyl)-*O*-(tert-butyl)-*L*-serinate

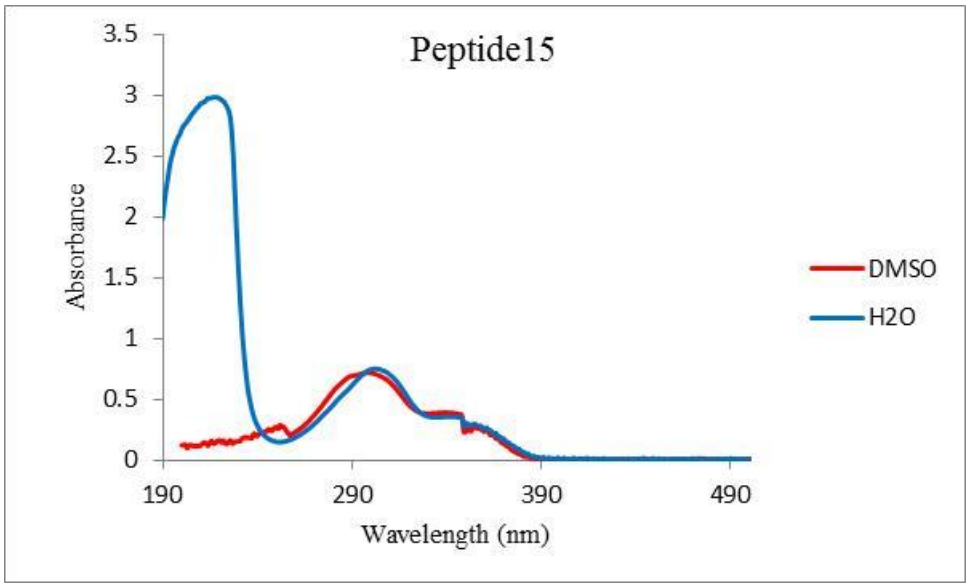
Fluorescence and absorbtion Spectra:

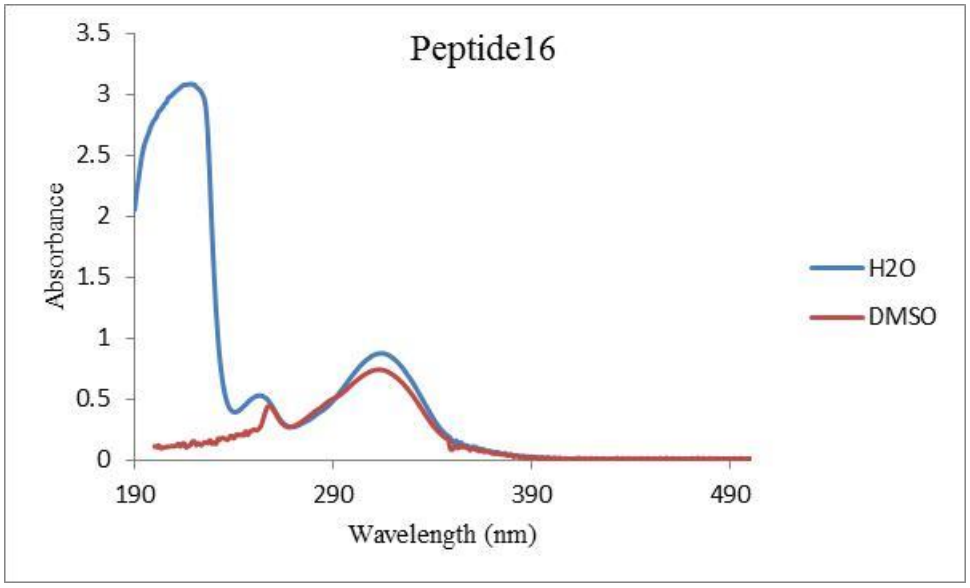


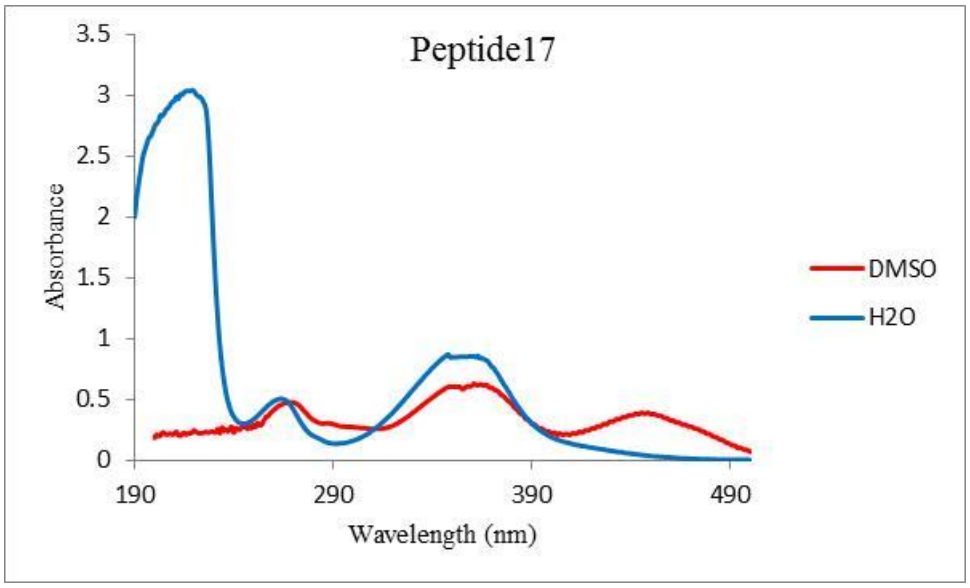

Peptide12
Absorbance
3.5
3
2.5
2
1.5
1
0.5
0
190
290
390
490
Wavelength (nm)
H2O
DMSO

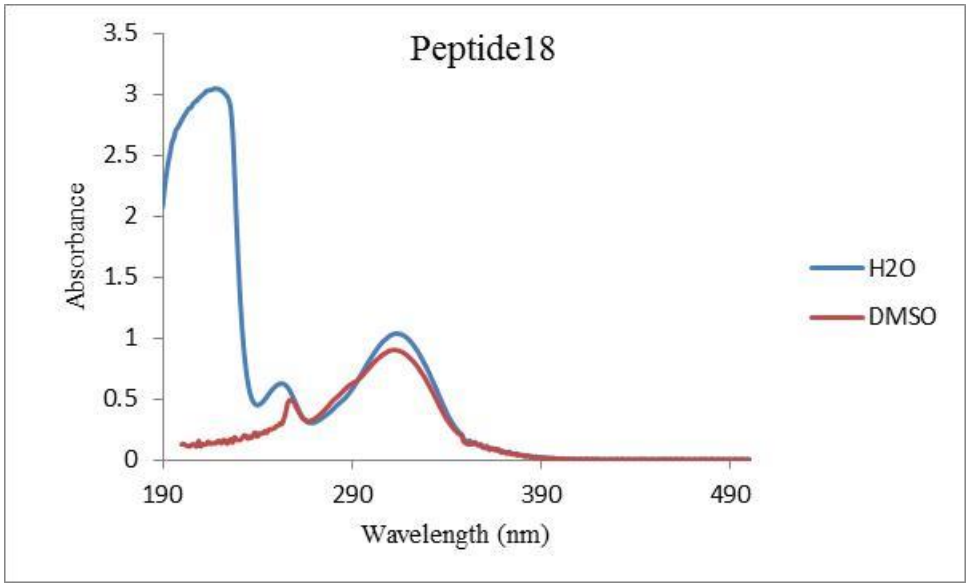

Peptide13
Absorbance
3.5
3
2.5
2
1.5
1
0.5
0
190
290
390
490
Wavelength (nm)
DMSO
H2O

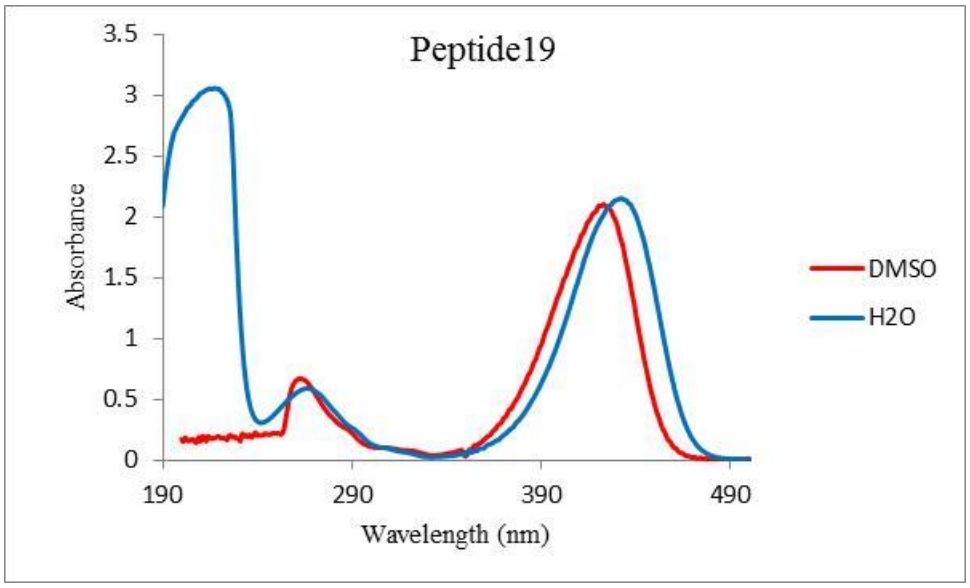

Peptide14
Absorbance
Wavelength (nm)
3.5
3
2.5
2
1.5
1
0.5
0
-0.5
190
290
390
490
H2O
DMSO

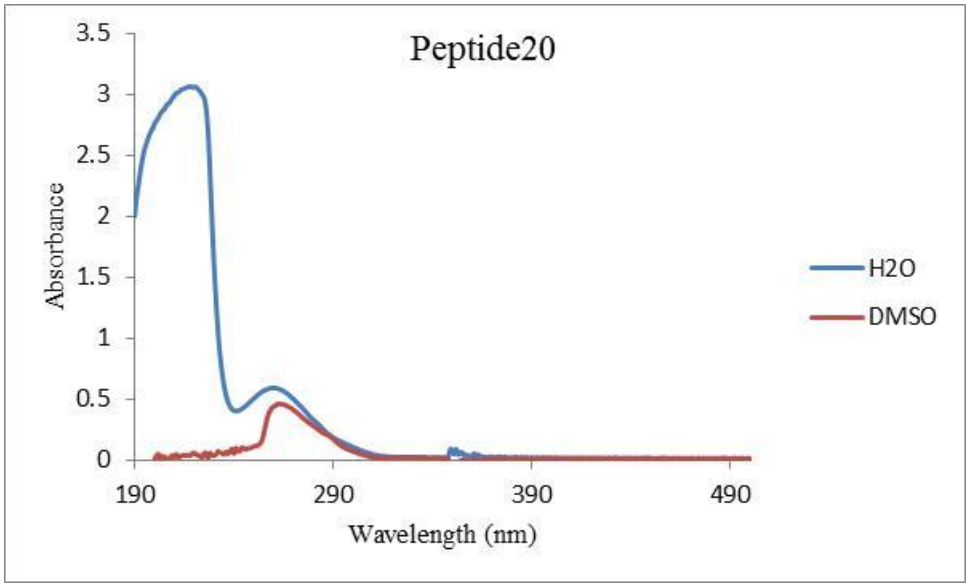

Peptide15
Absorbance
Wavelength (nm)
3.5
3
2.5
2
1.5
1
0.5
0
190
290
390
490
DMSO
H2O


Peptide16
Absorbance
3.5
3
2.5
2
1.5
1
0.5
0
190
290
390
490
Wavelength (nm)
H2O
DMSO


Peptide17
Absorbance
3.5
3
2.5
2
1.5
1
0.5
0
190
290
390
490
Wavelength (nm)
DMSO
H2O


Peptide18
Absorbance
Wavelength (nm)
H2O
DMSO
3.5
3
2.5
2
1.5
1
0.5
0
190
290
390
490


Peptide19
Absorbance
Wavelength (nm)
DMSO
H2O
3.5
3
2.5
2
1.5
1
0.5
0
190
290
390
490


Peptide20
Absorbance
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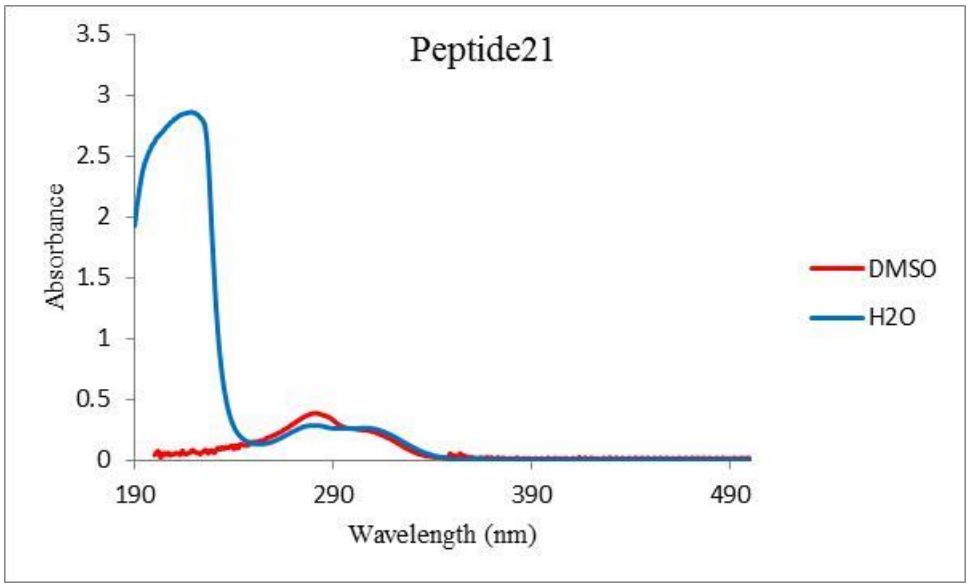
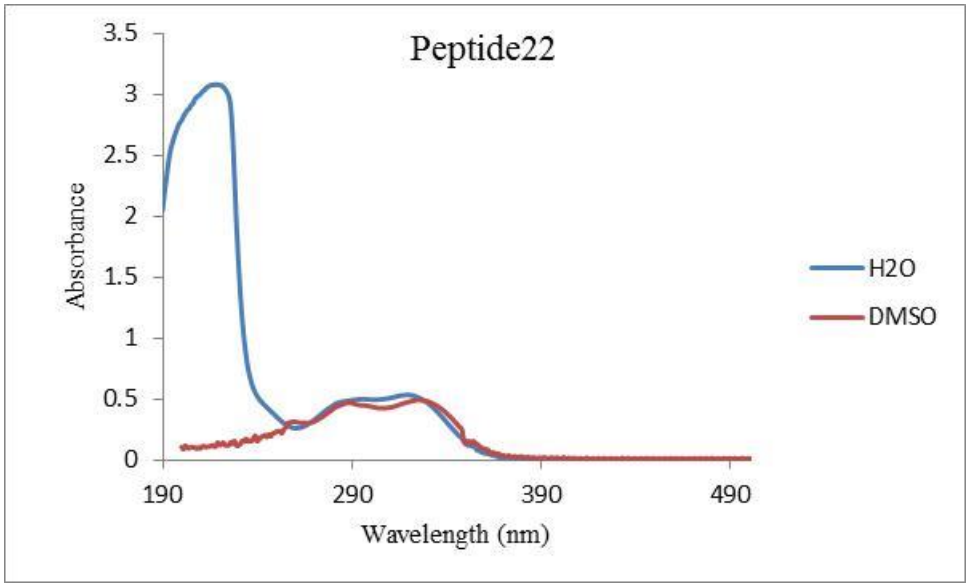
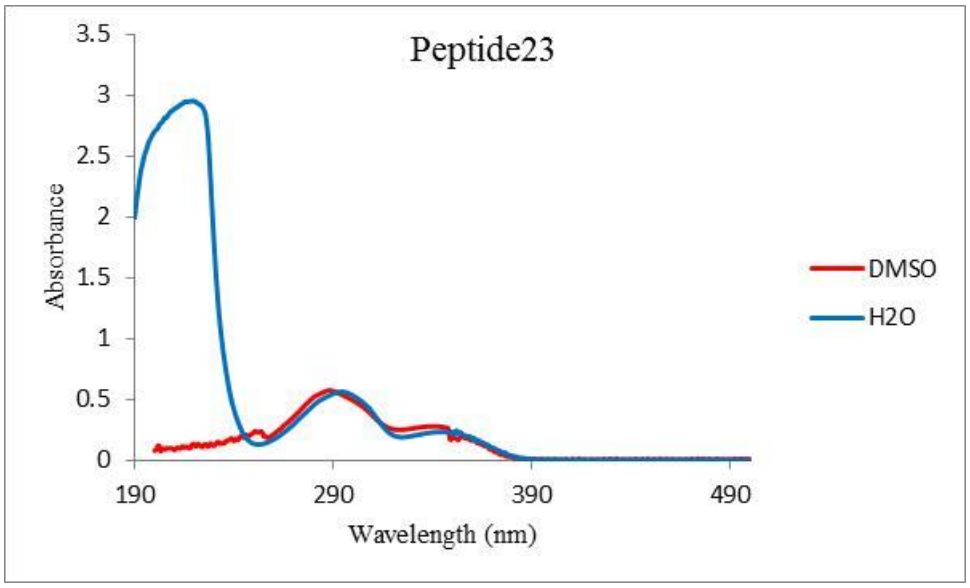
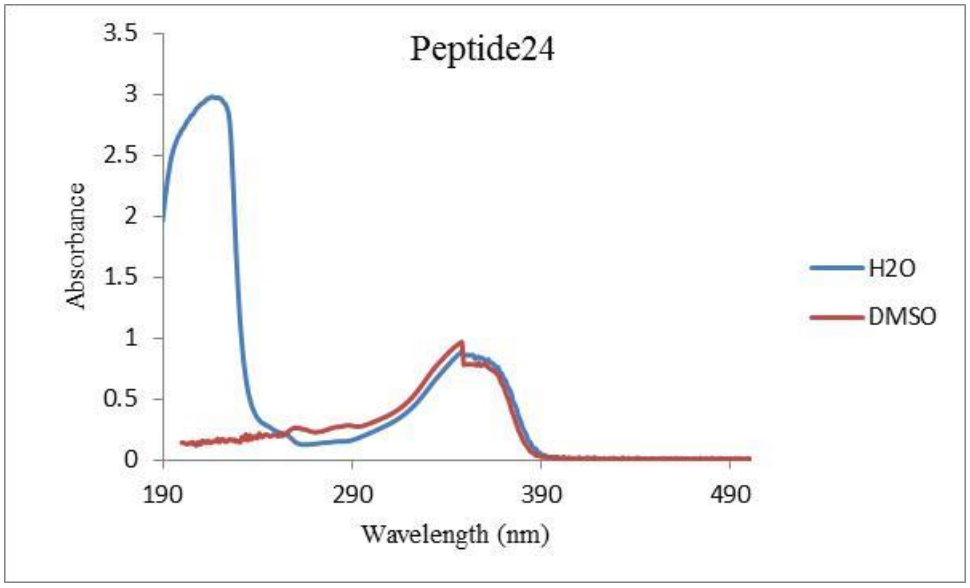
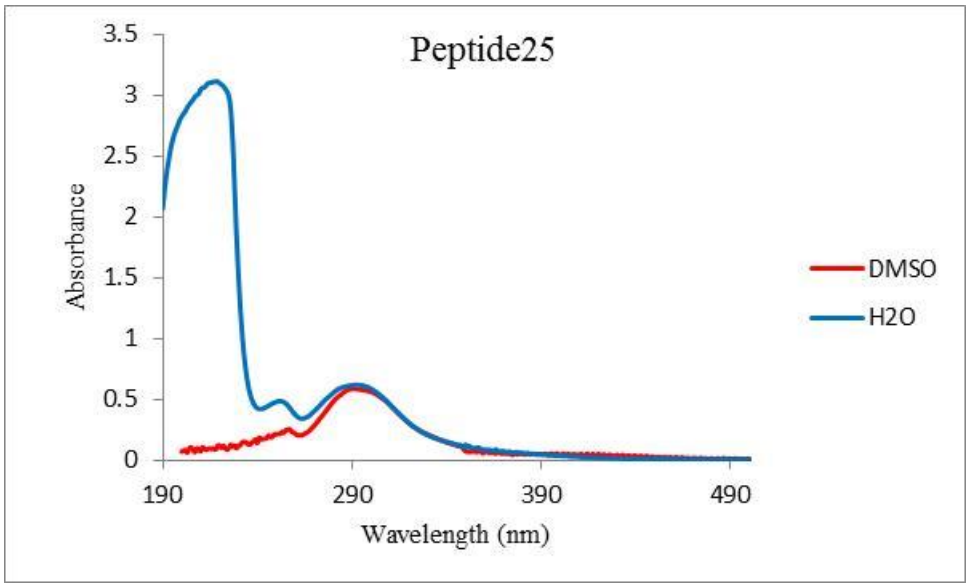
3
2.5
2
1.5
1
0.5
0
190
290
390
490
Wavelength (nm)
H2O
DMSO

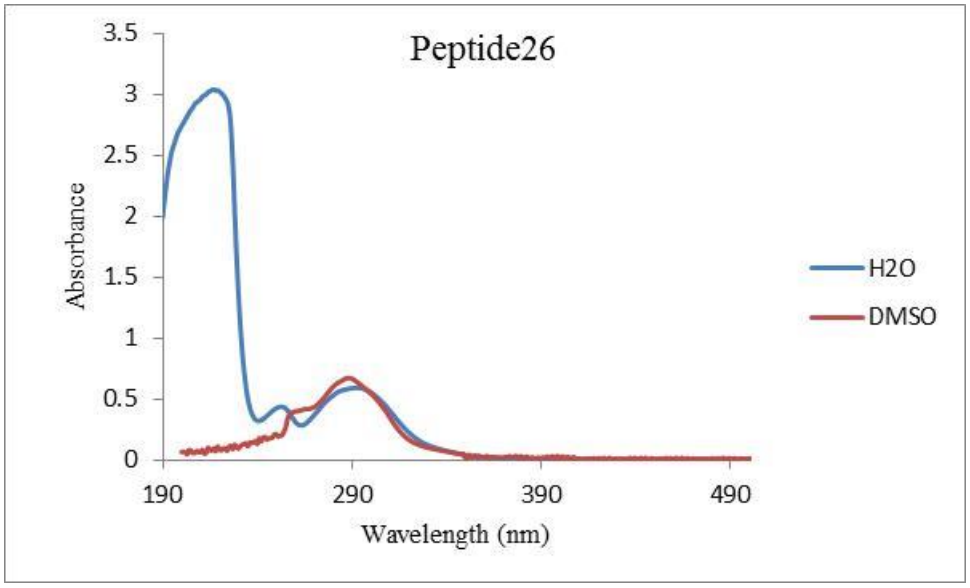

Peptide21
Absorbance
3.5
3
2.5
2
1.5
1
0.5
0
190
290
390
490
Wavelength (nm)
DMSO
H2O

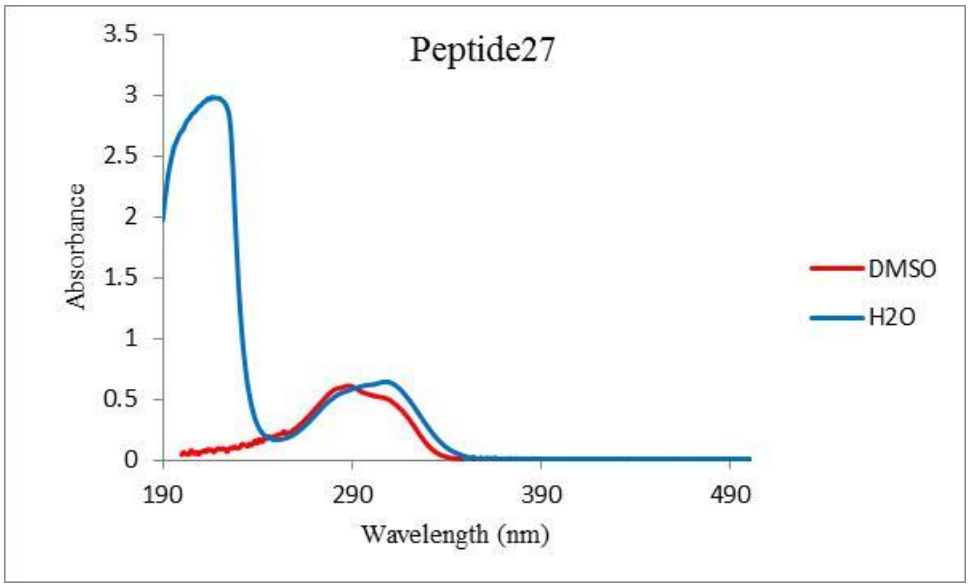

Peptide22
Absorbance
Wavelength (nm)
H2O
DMSO
3.5
3
2.5
2
1.5
1
0.5
0
190
290
390
490

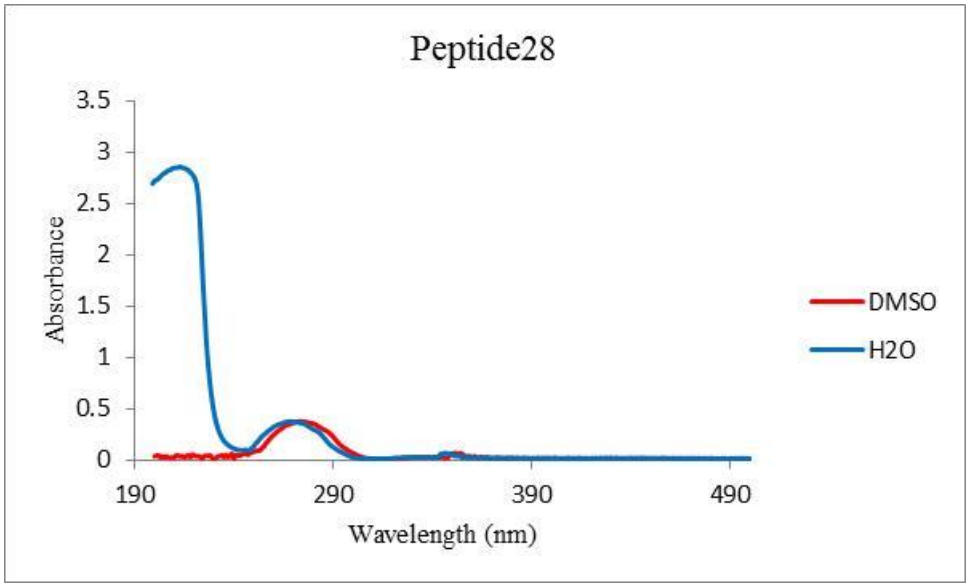

Peptide23
Absorbance
Wavelength (nm)
DMSO
H2O
3.5
3
2.5
2
1.5
1
0.5
0
190
290
390
490

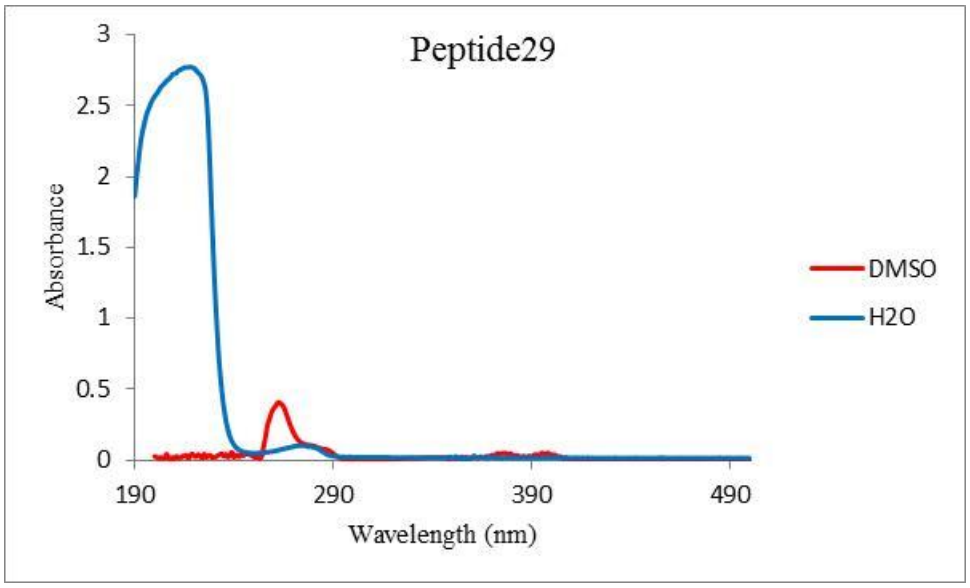

Peptide24
Absorbance
3.5
3
2.5
2
1.5
1
0.5
0
190
290
390
490
Wavelength (nm)
H2O
DMSO

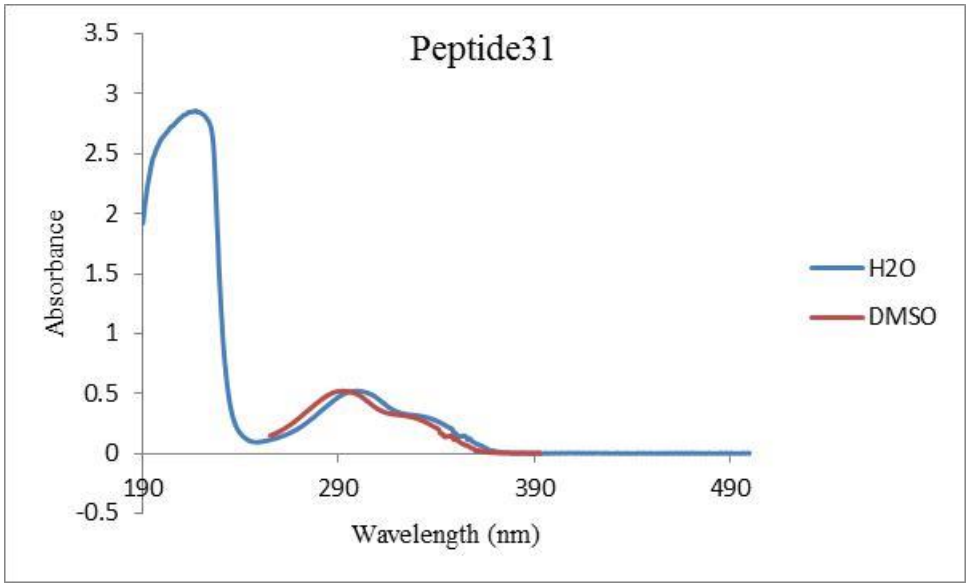

Peptide25
Absorbance
3.5
3
2.5
2
1.5
1
0.5
0
190
290
390
490
Wavelength (nm)
DMSO
H2O

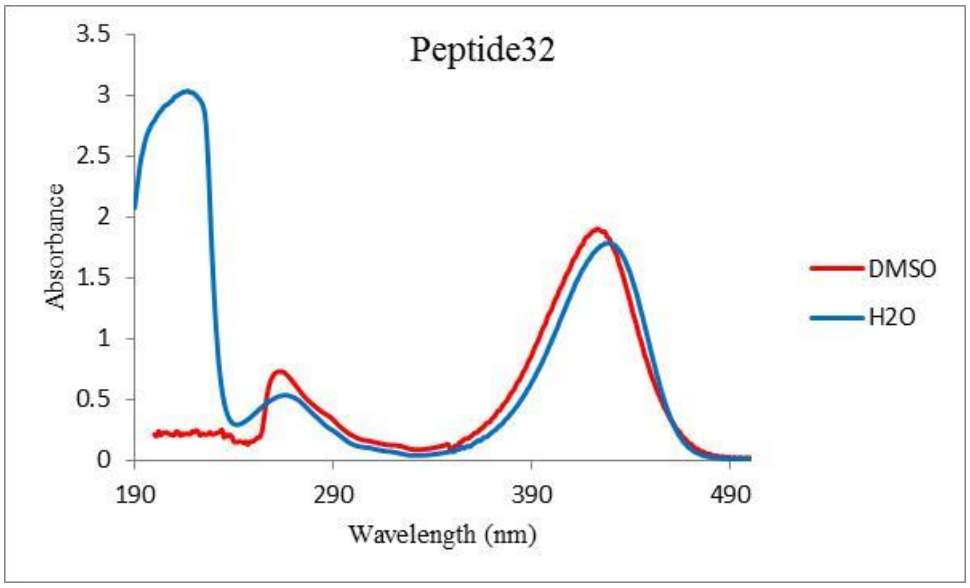

Peptide26
Absorbance
3.5
3
2.5
2
1.5
1
0.5
0
190
290
390
490
Wavelength (nm)
H2O
DMSO

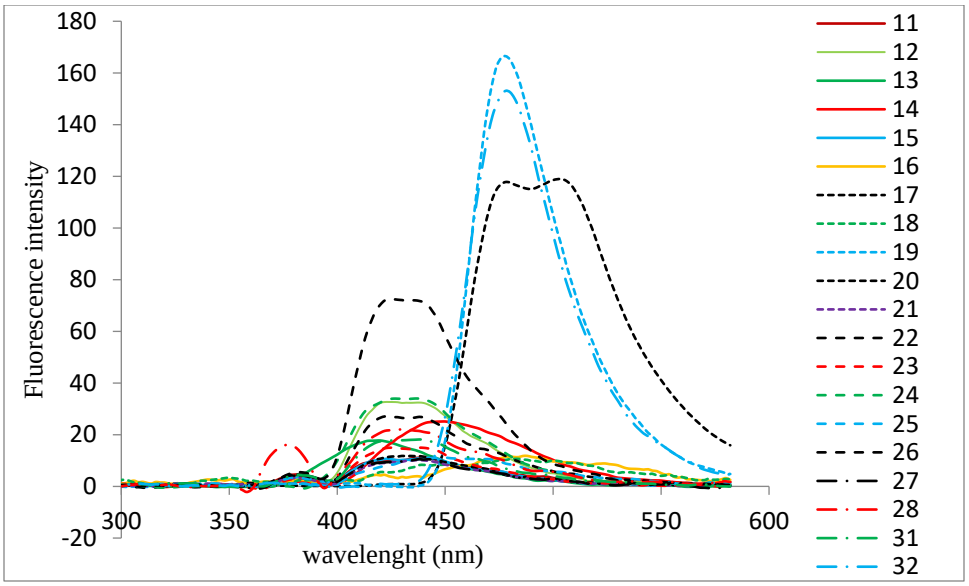

Peptide27
Absorbance
3.5
3
2.5
2
1.5
1
0.5
0
190
290
390
490
Wavelength (nm)
DMSO
H2O


Peptide28
3.5
3
2.5
2
1.5
1
0.5
0
Absorbance
190
290
390
490
Wavelength (nm)
DMSO
H2O

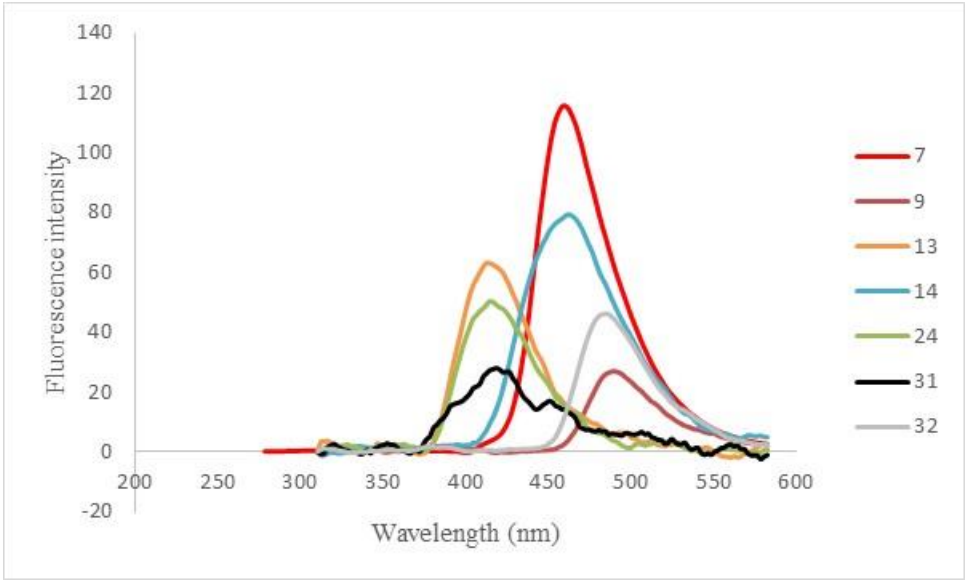

Peptide29
3
2.5
2
1.5
1
0.5
0
Absorbance
190
290
390
490
Wavelength (nm)
DMSO
H2O


Peptide31
3.5
3
2.5
2
1.5
1
0.5
0
-0.5
Absorbance
190
290
390
490
Wavelength (nm)
H2O
DMSO

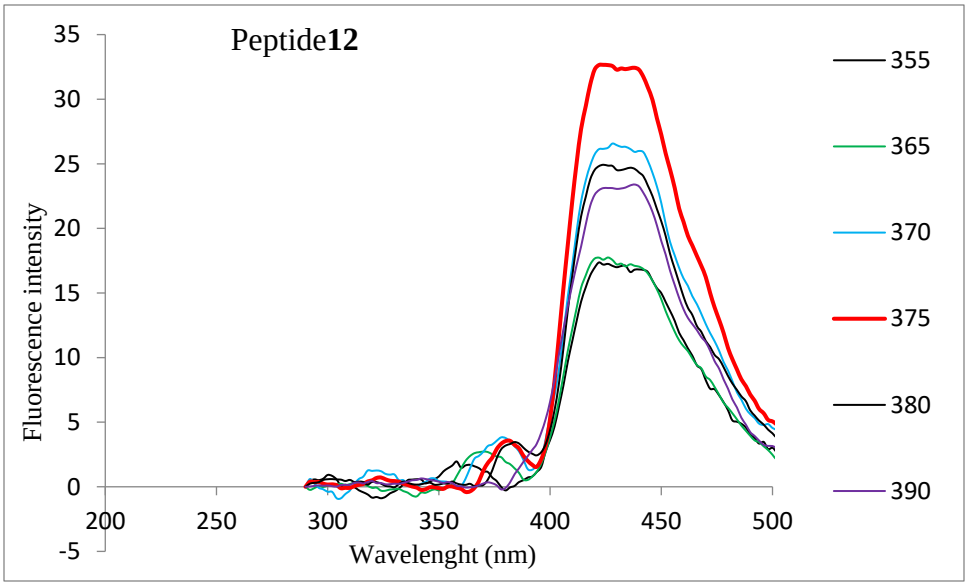

Peptide32
3.5
3
2.5
2
1.5
1
0.5
0
Absorbance
190
290
390
490
Wavelength (nm)
DMSO
H2O

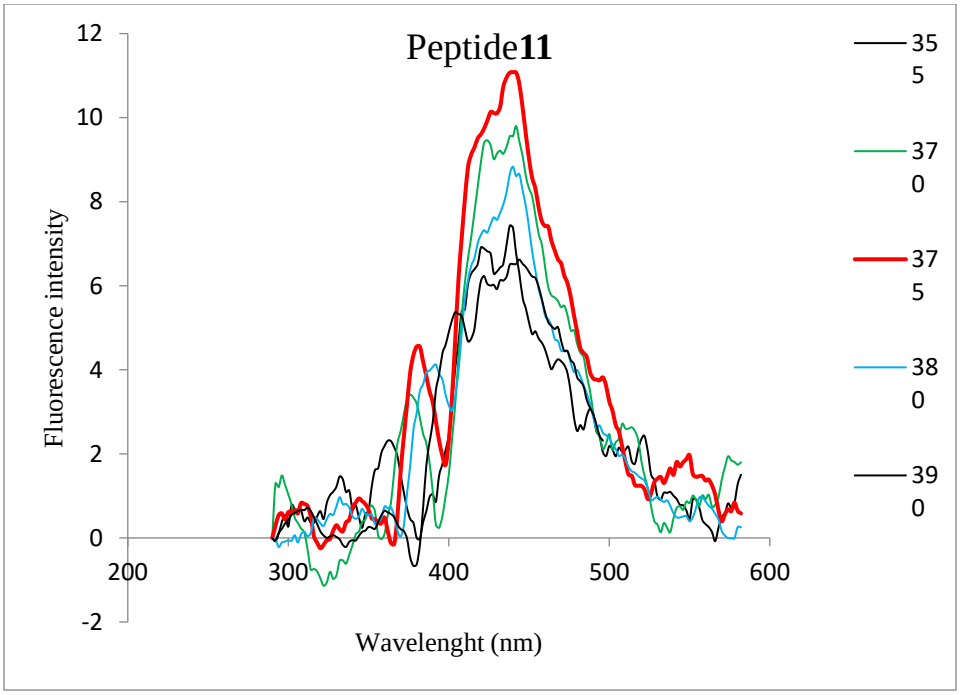


Fluorescence emission spectra of compounds in DMSO



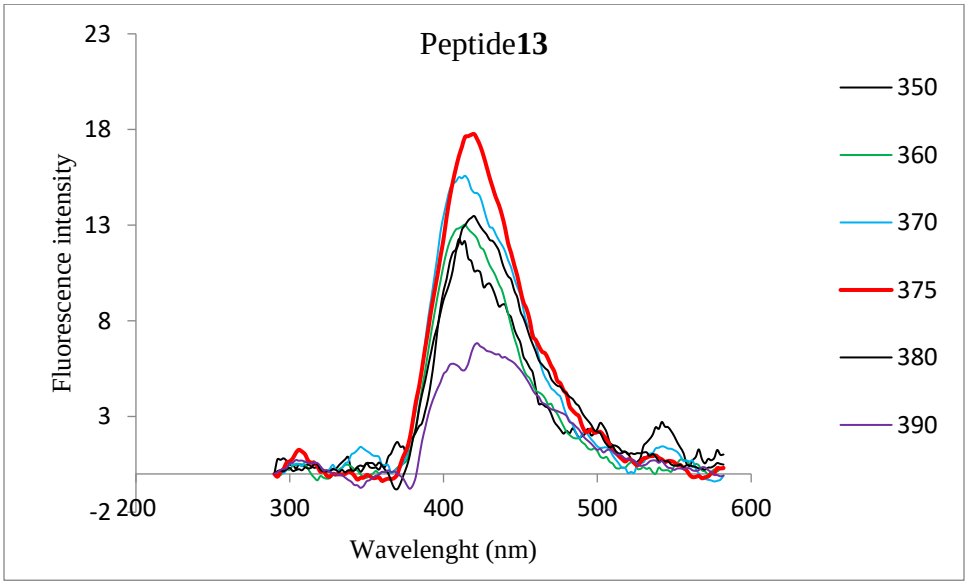
Fluorescence emission spectra of compounds in H_2O



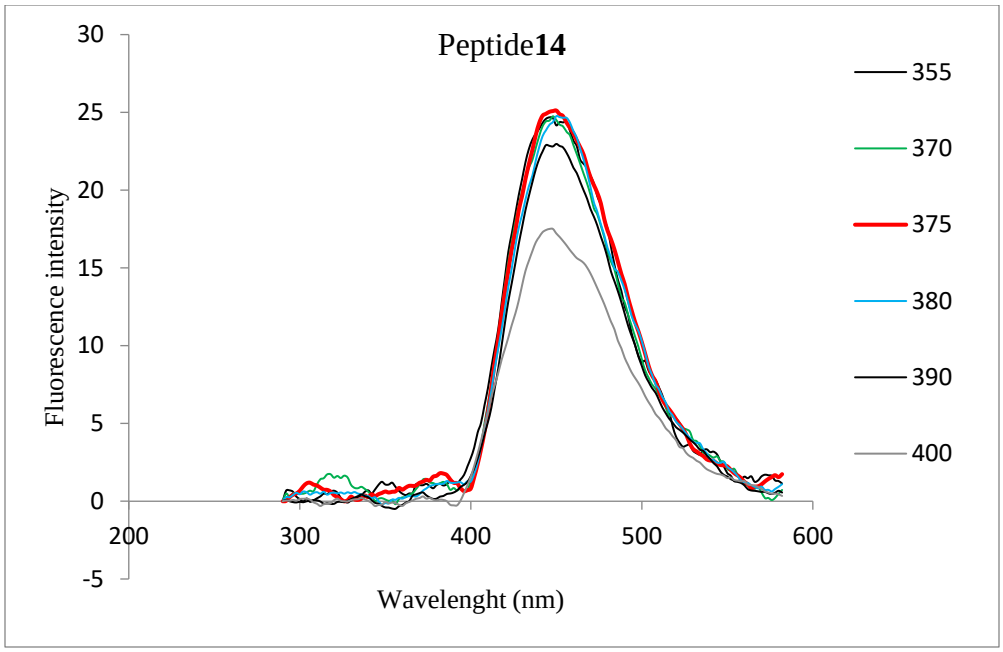


Fluorescence Spectra of **11** in DMSO

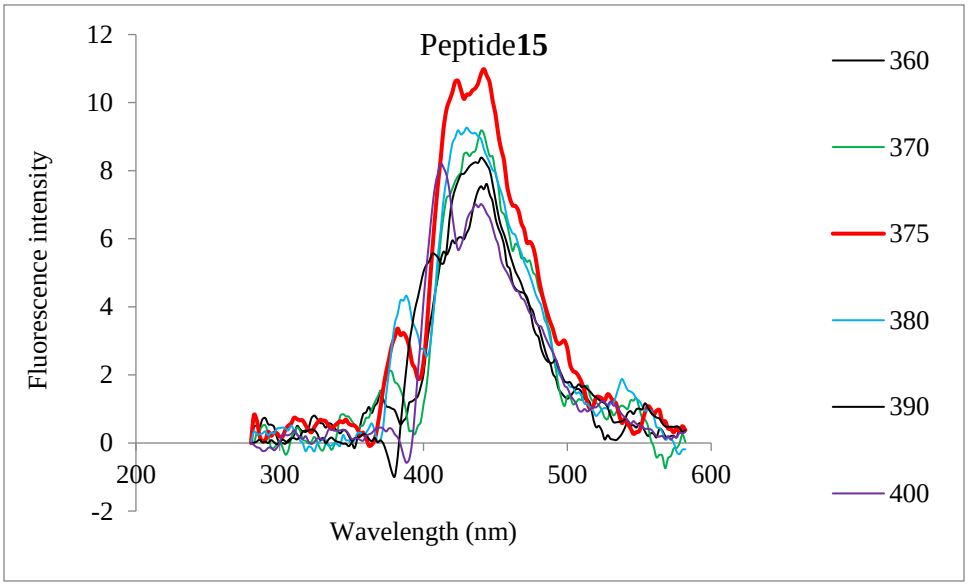
Fluorescence Spectra of **12** in DMSO



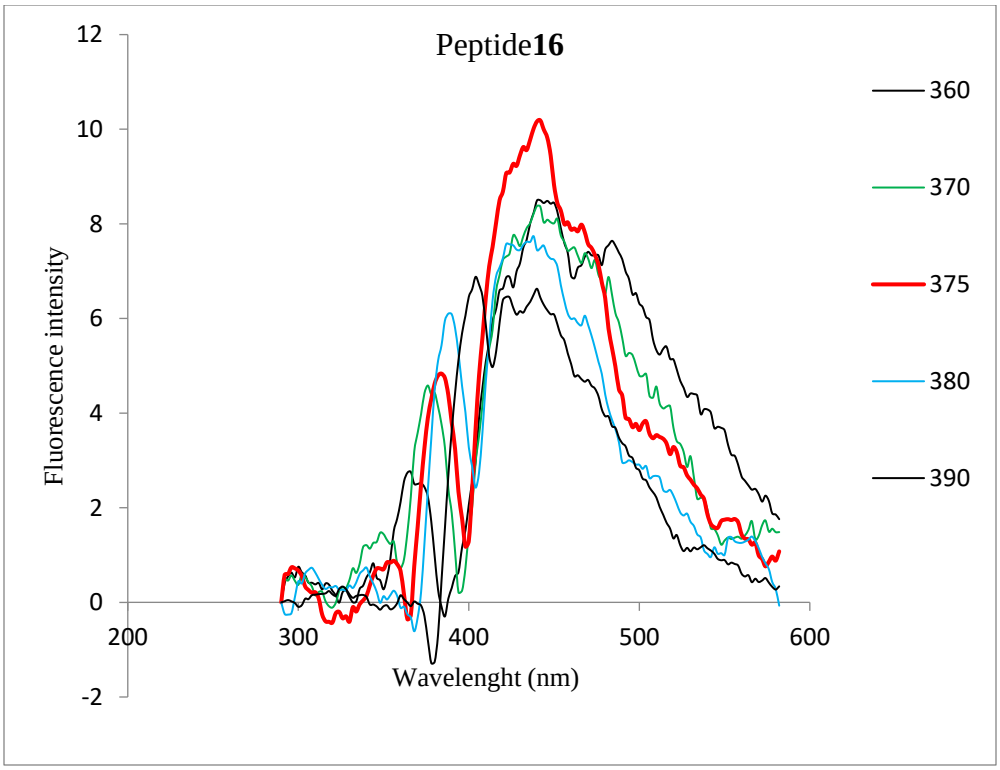
Fluorescence Spectra of **13** in DMSO



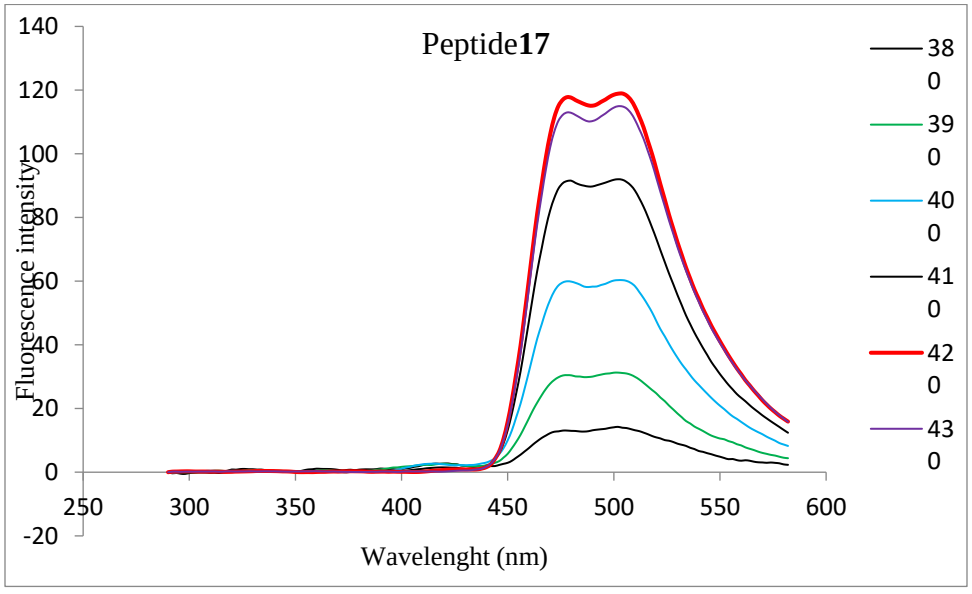
Fluorescence Spectra of **14** in DMSO



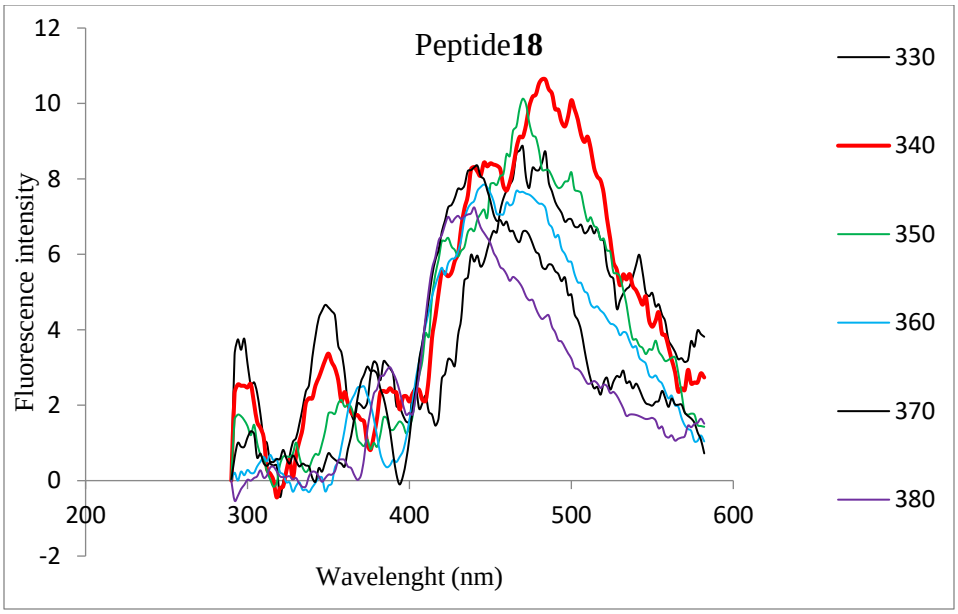
Fluorescence Spectra of **15** in DMSO



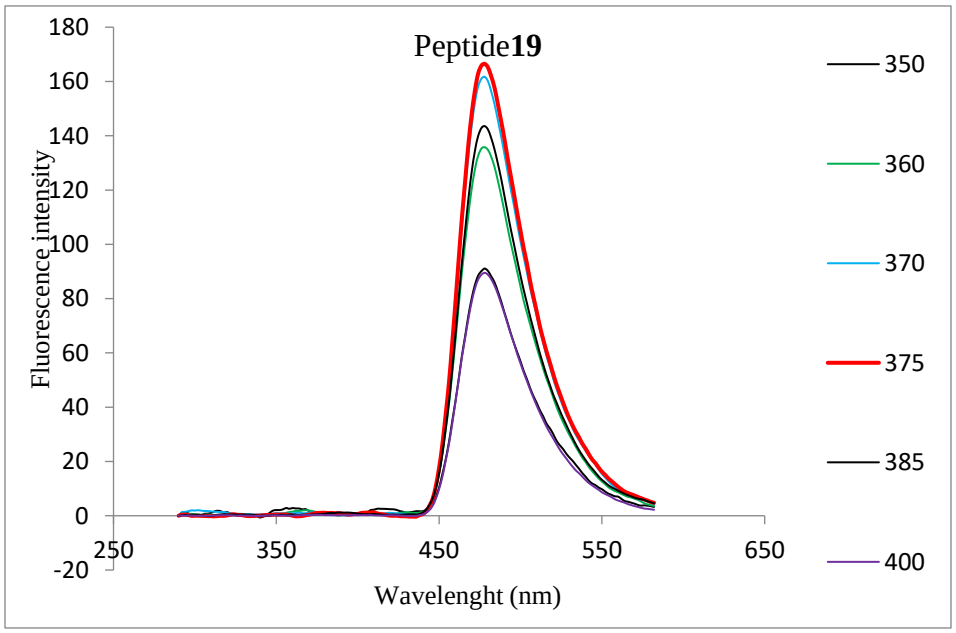
Fluorescence Spectra of **16** in DMSO



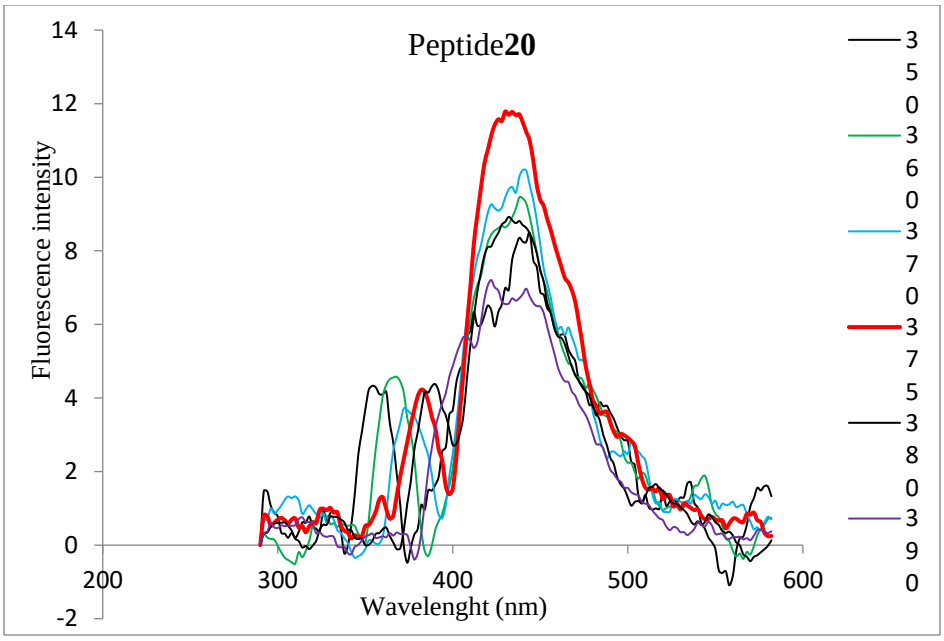
Fluorescence Spectra of **17** in DMSO



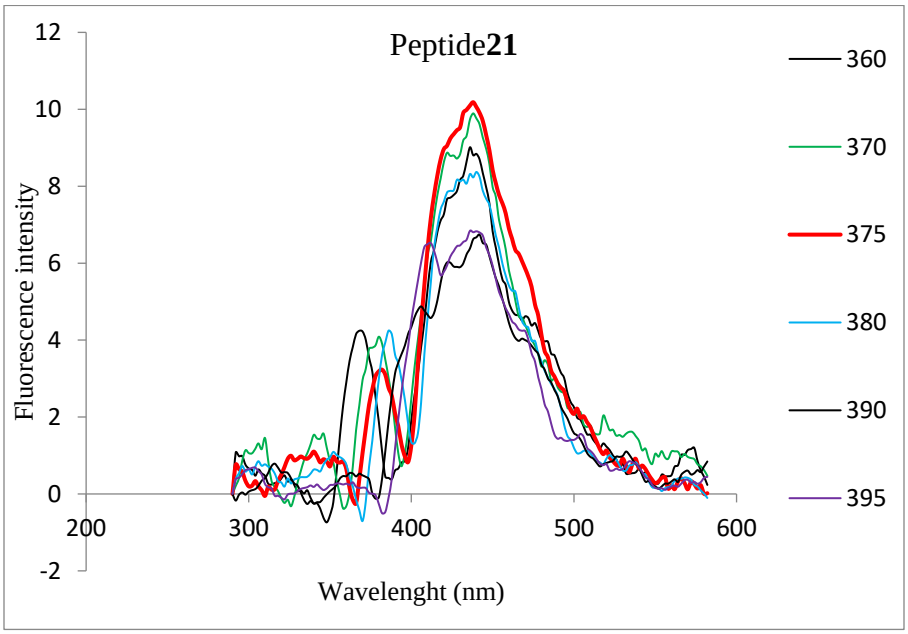
Fluorescence Spectra of **18** in DMSO



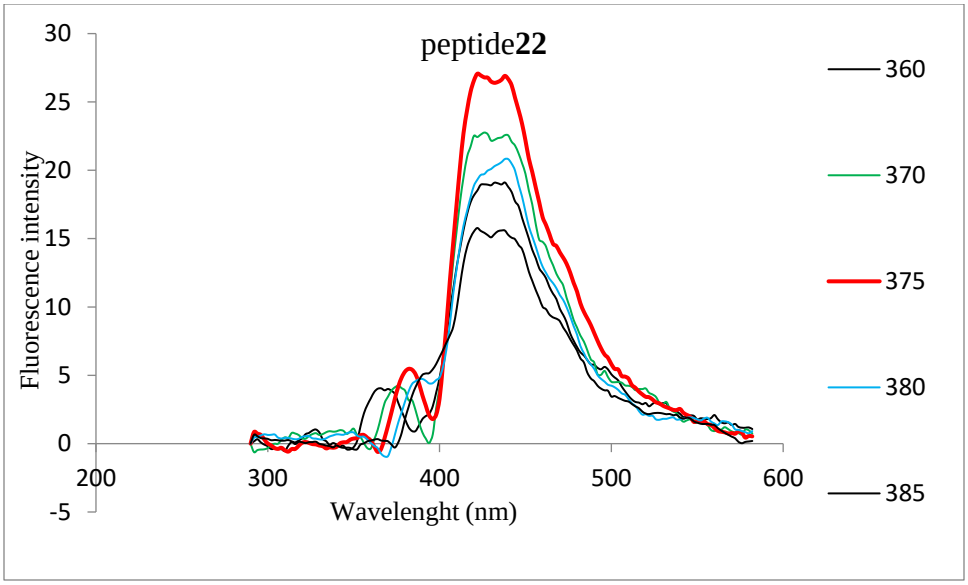
Fluorescence Spectra of **19** in DMSO



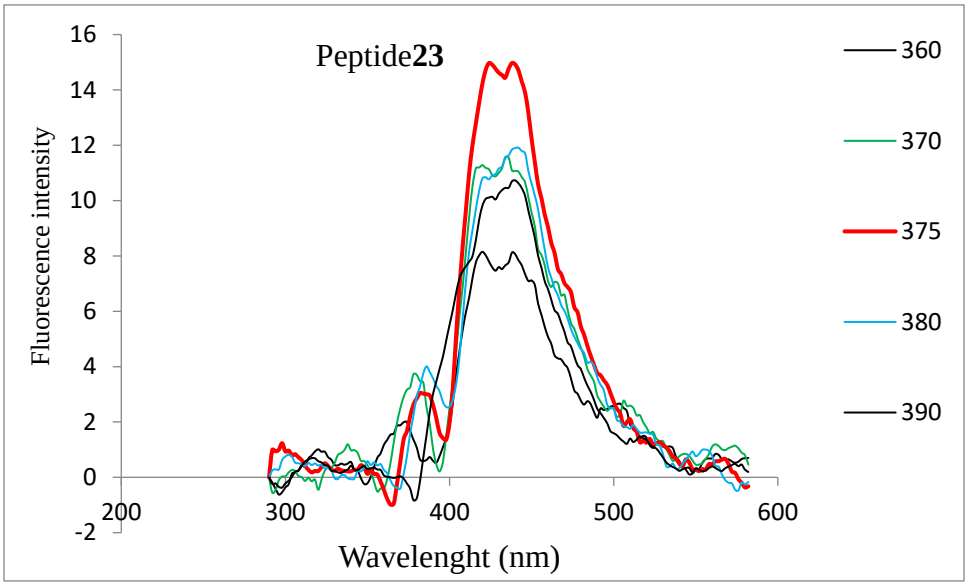
Fluorescence Spectra of **20** in DMSO



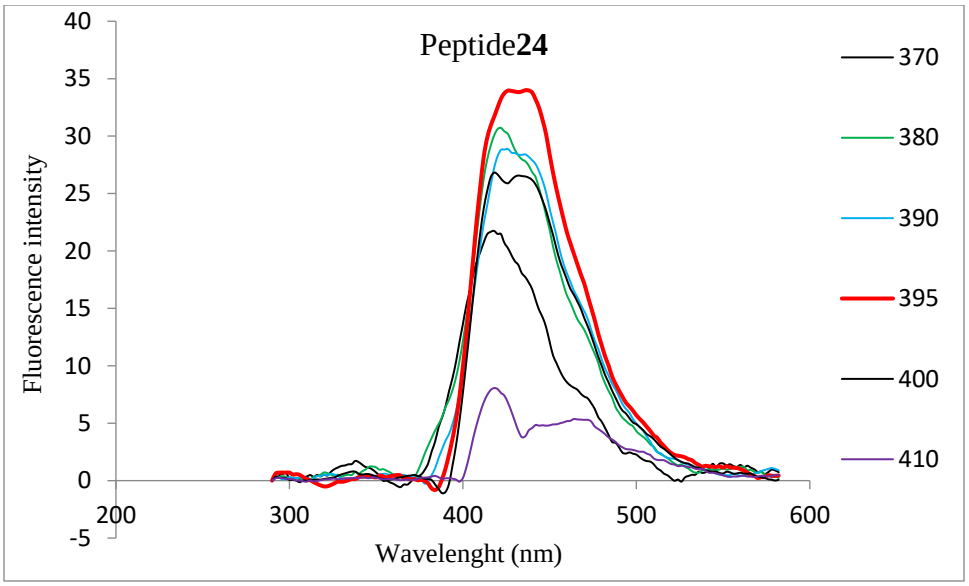
Fluorescence Spectra of **21** in DMSO



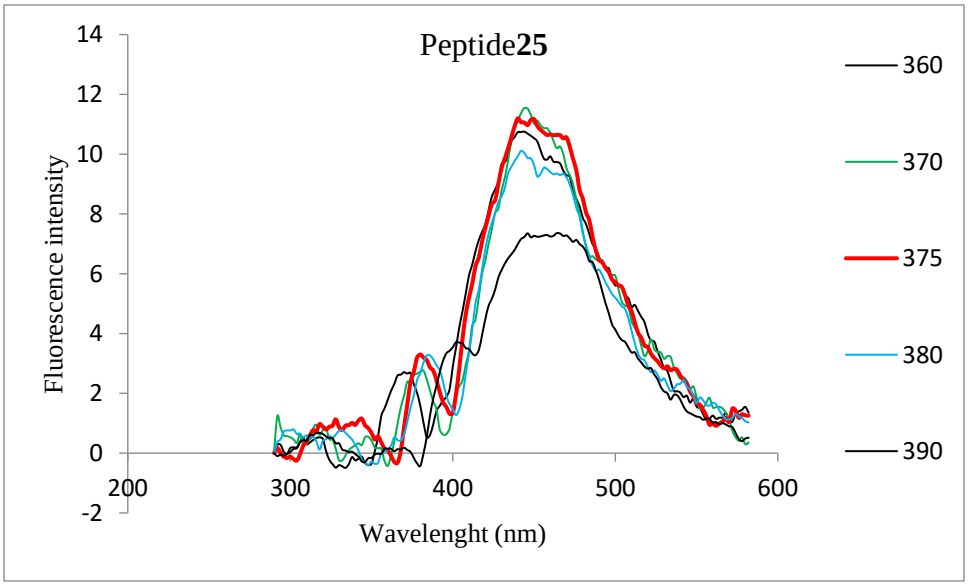
Fluorescence Spectra of **22** in DMSO



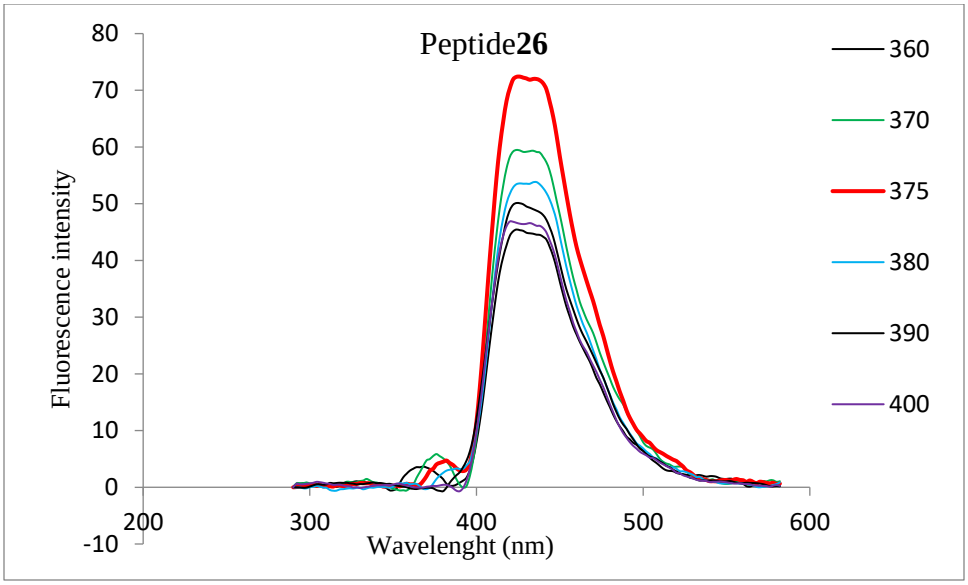
Fluorescence Spectra of **23** in DMSO



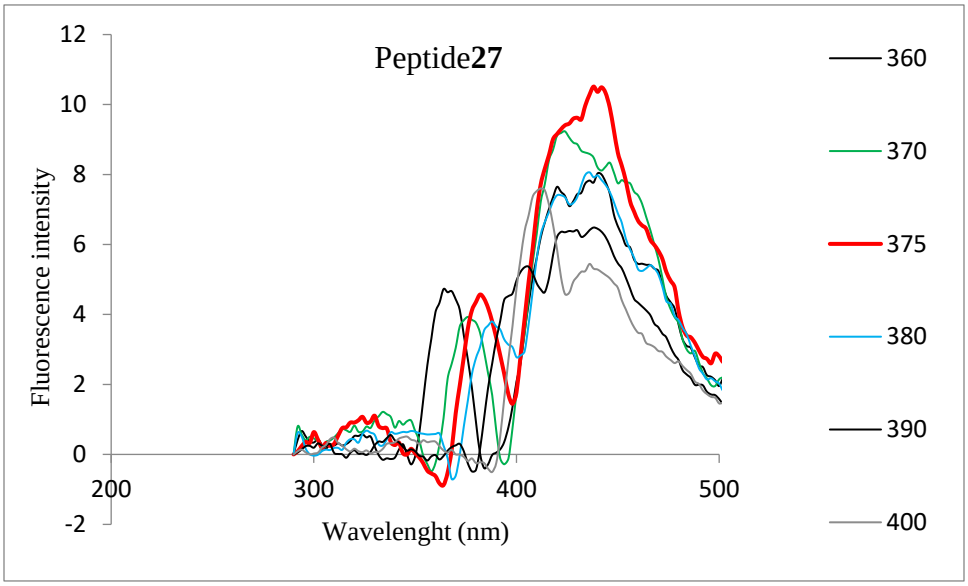
Fluorescence Spectra of **24** in DMSO



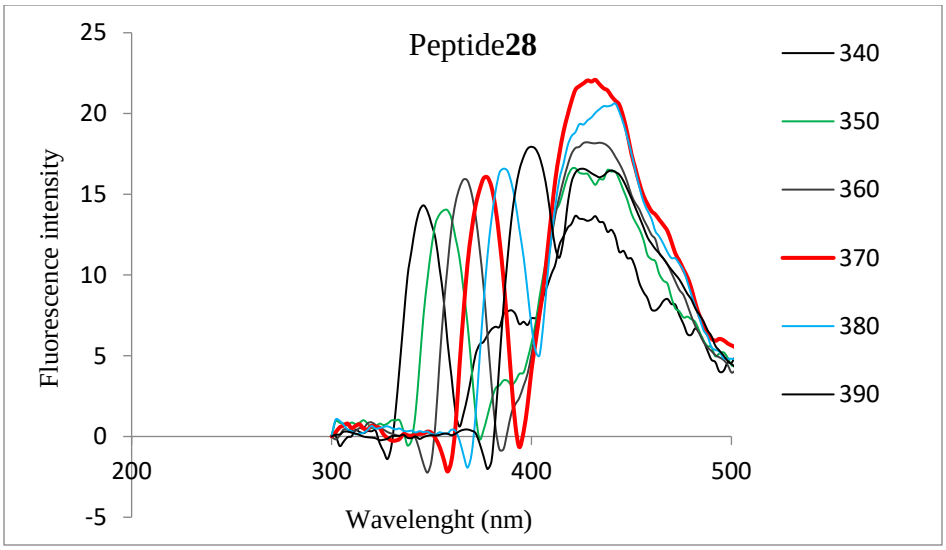
Fluorescence Spectra of **25** in DMSO



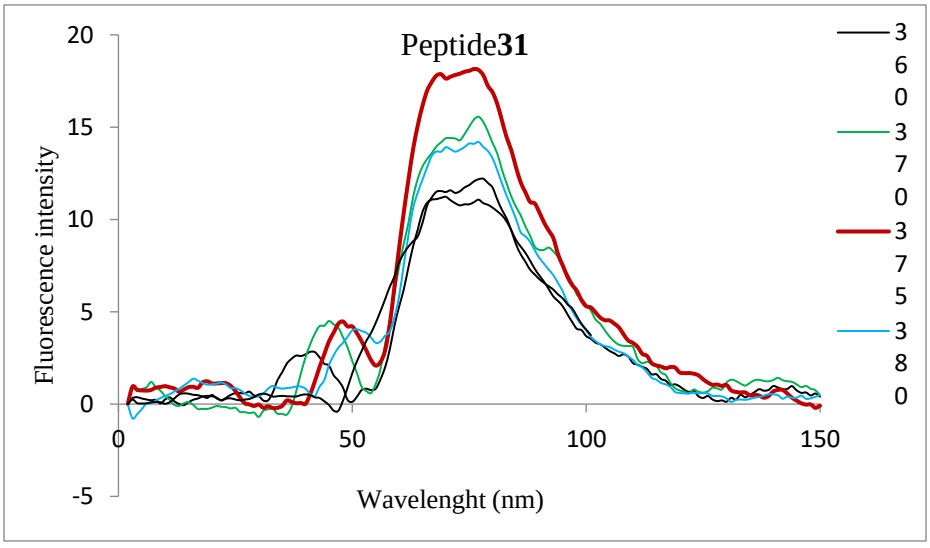
Fluorescence Spectra of **26** in DMSO



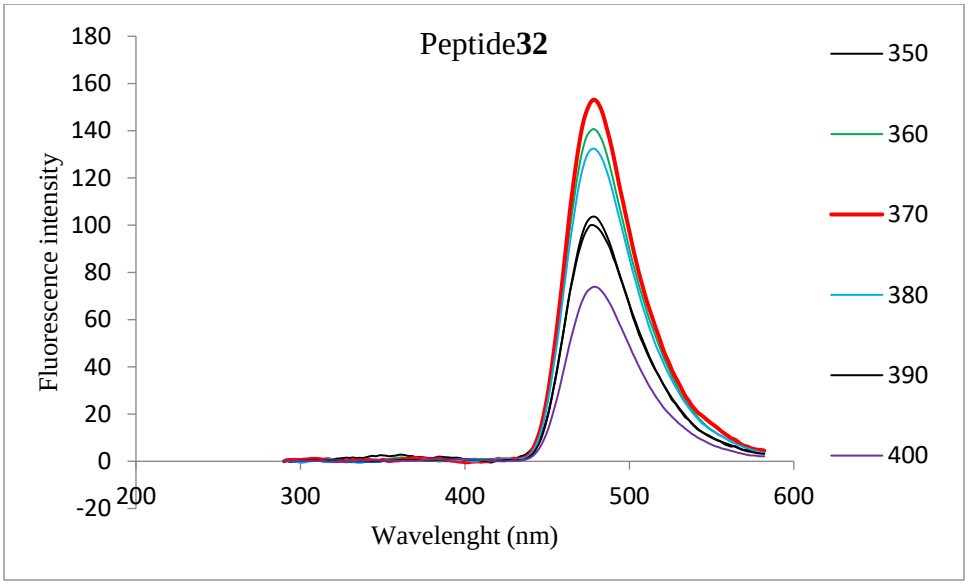
Fluorescence Spectra of **27** in DMSO



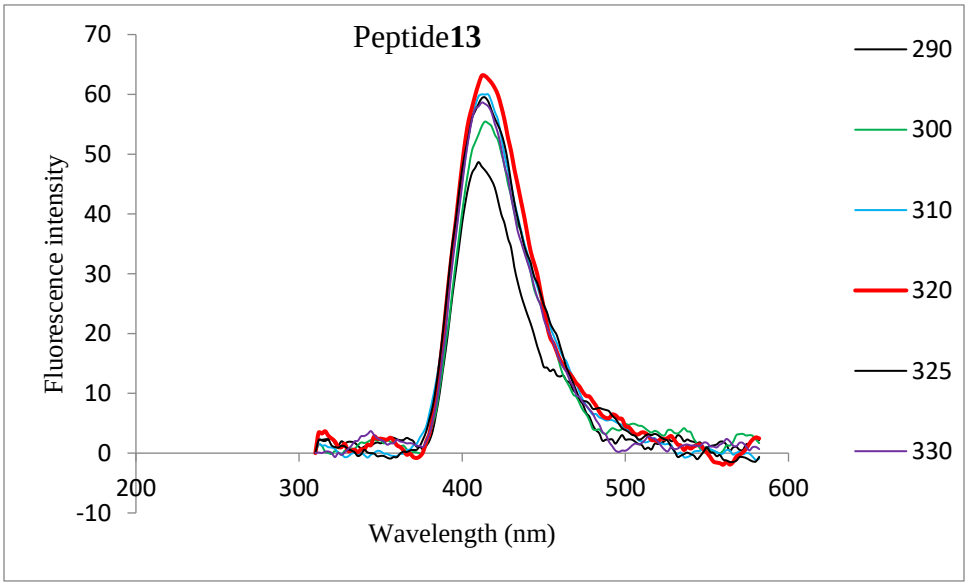
Fluorescence Spectra of **28** in DMSO



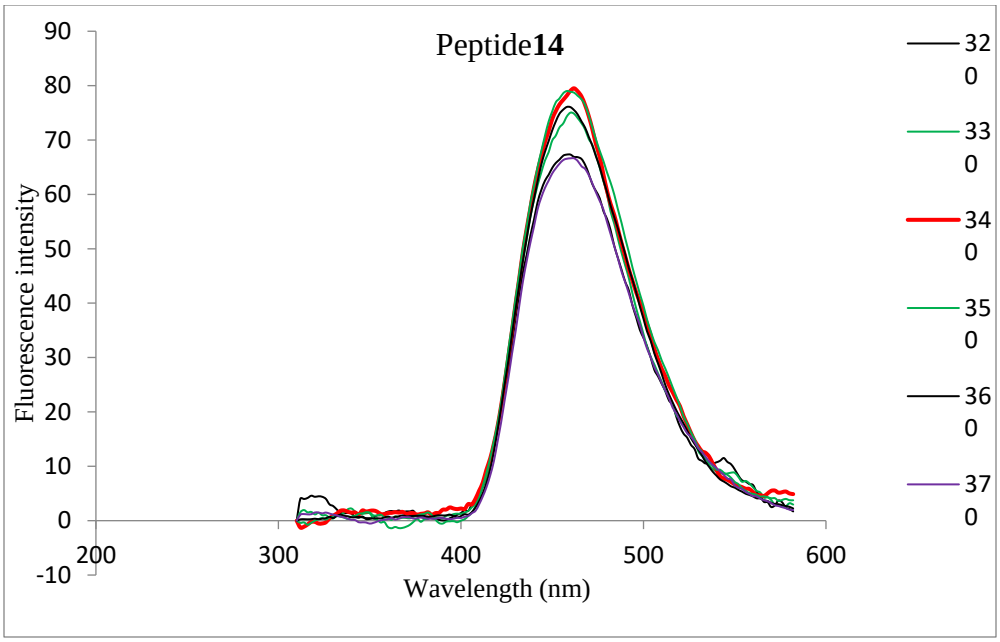
Fluorescence Spectra of **31** in DMSO



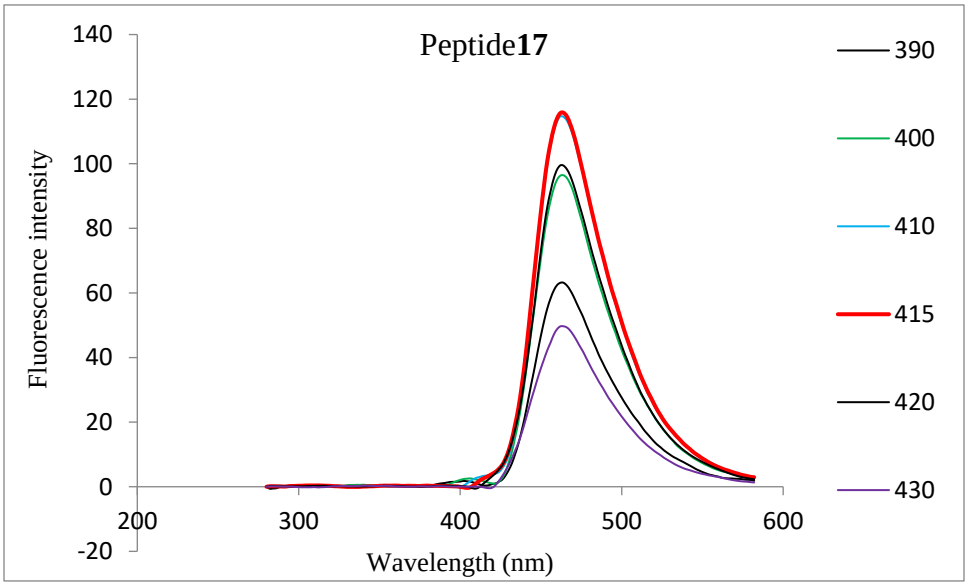
Fluorescence Spectra of **32** in DMSO



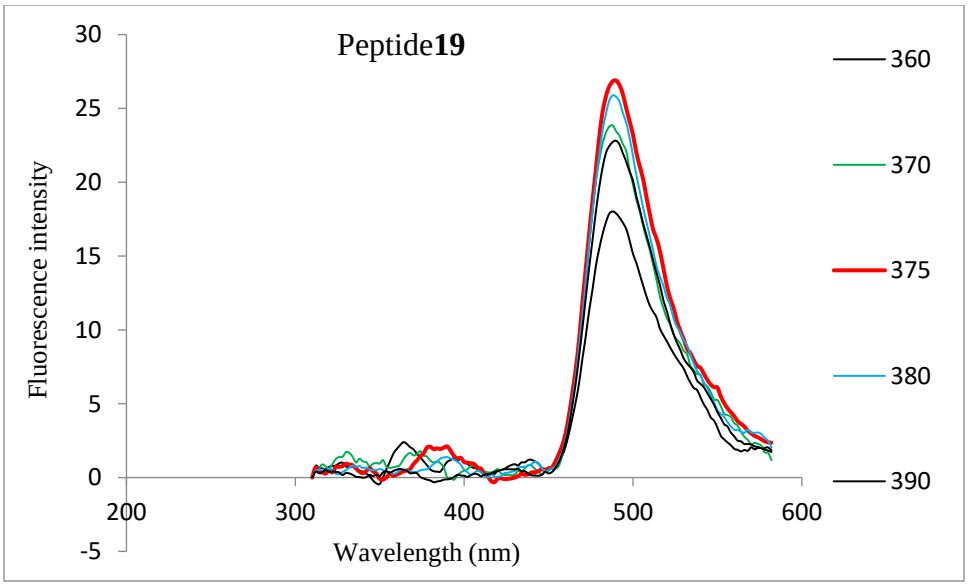
Fluorescence Spectra of **13** in H_2O



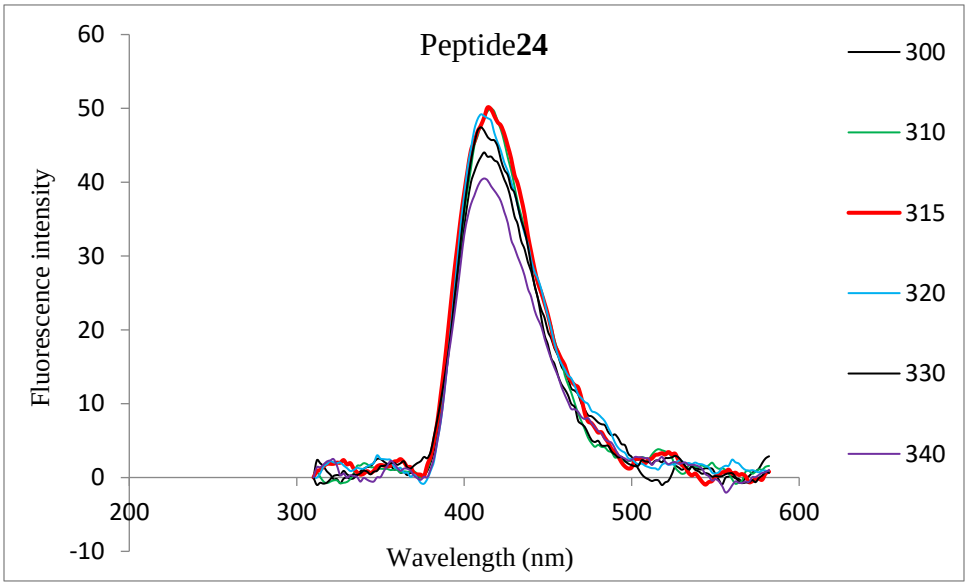
Fluorescence Spectra of **14** in H_2O



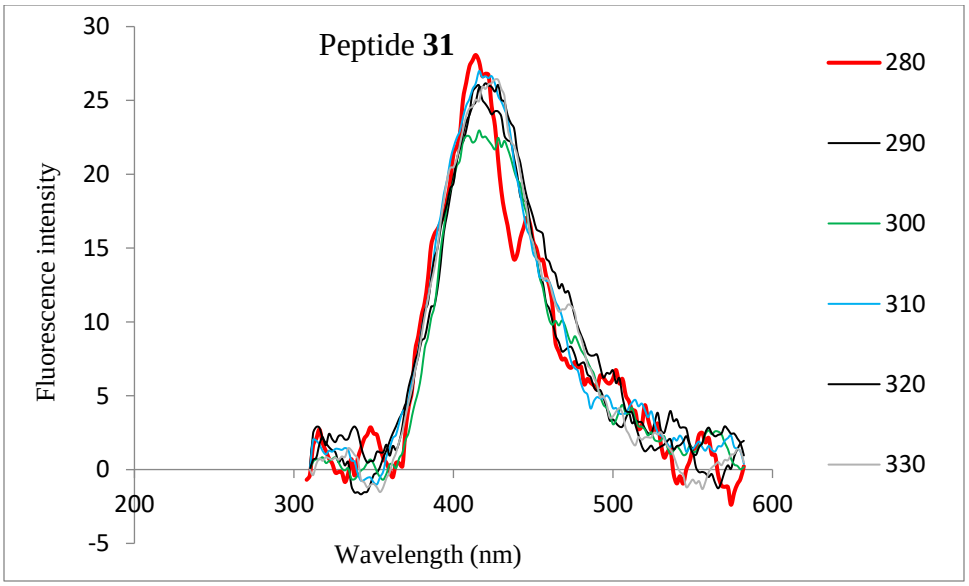
Fluorescence Spectra of **17** in H_2O



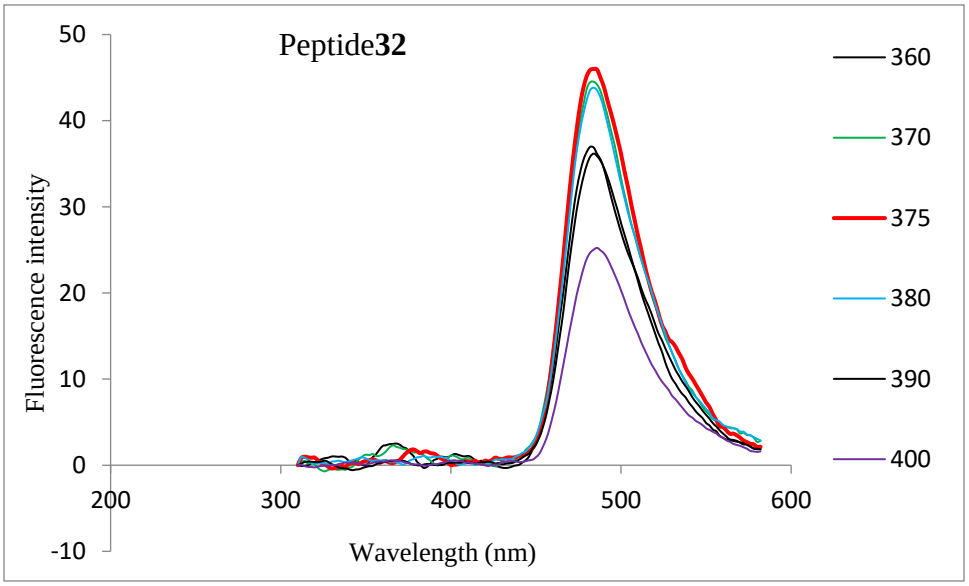
Fluorescence Spectra of **19** in H_2O



Fluorescence Spectra of **24** in H_2O

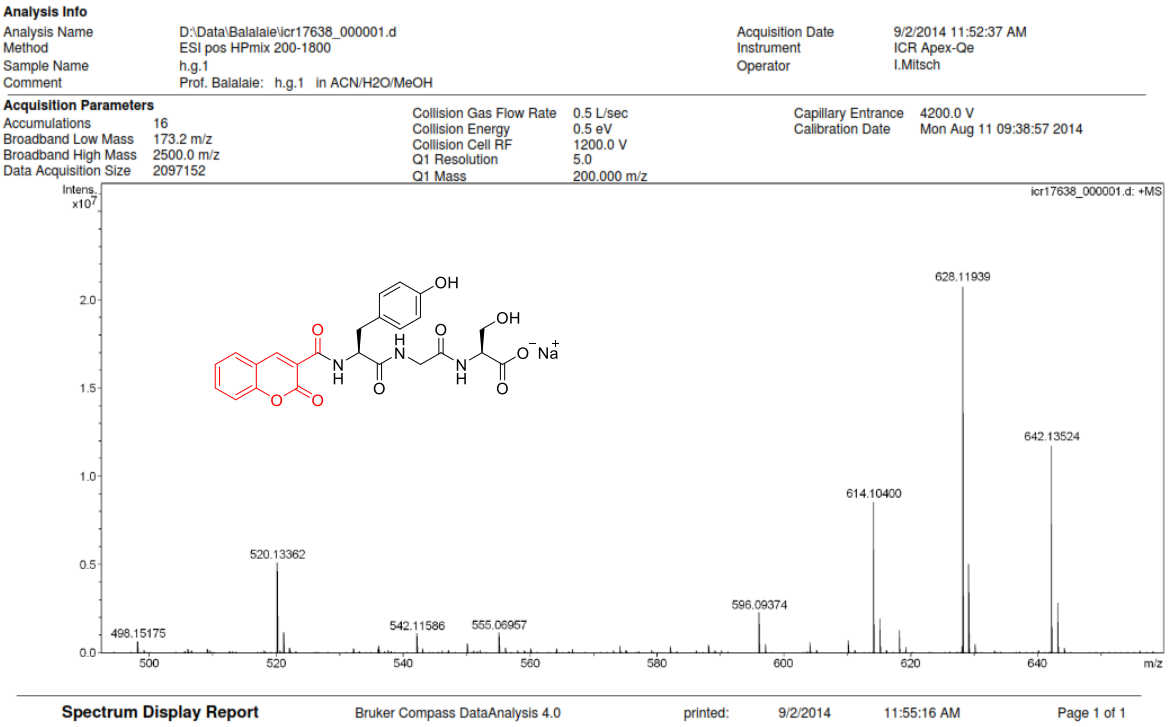


Fluorescence Spectra of **31** in H_2O

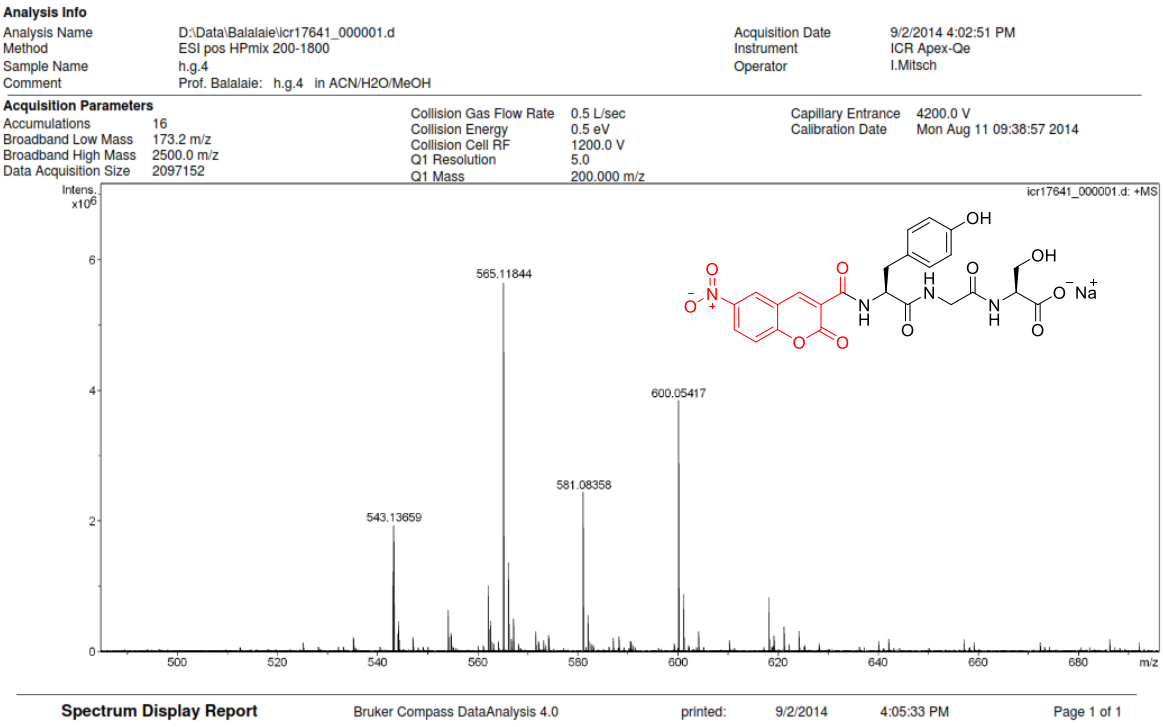


Fluorescence Spectra of **32** in H_2O

HR-MS spectra:



HR-MS spectra of **11**



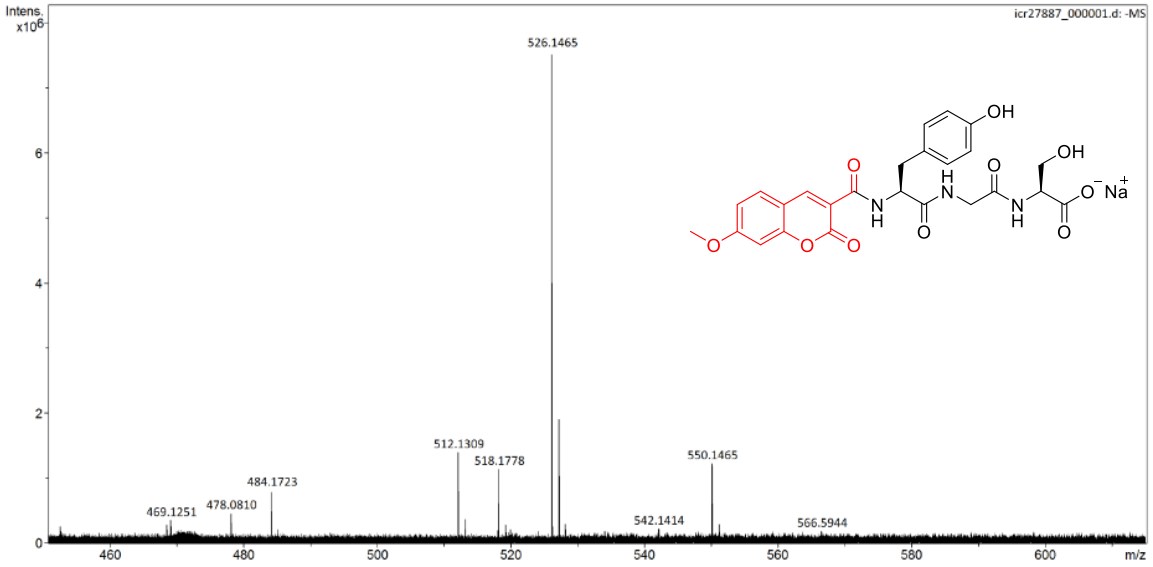
HR-MS spectra of **12**

Analysis Info

Analysis Name	D:\Data\Balalaie\icr27887_000001.d	Acquisition Date	7/12/2017 1:48:14 PM
Method	ESI neg HPmix 200-1800	Instrument	ICR Apex-Qe
Sample Name	1-Peptide3	Operator	I.Mitsch
Comment	Prof. Balalaie: 1-Peptide3 in H2O/MeOH		

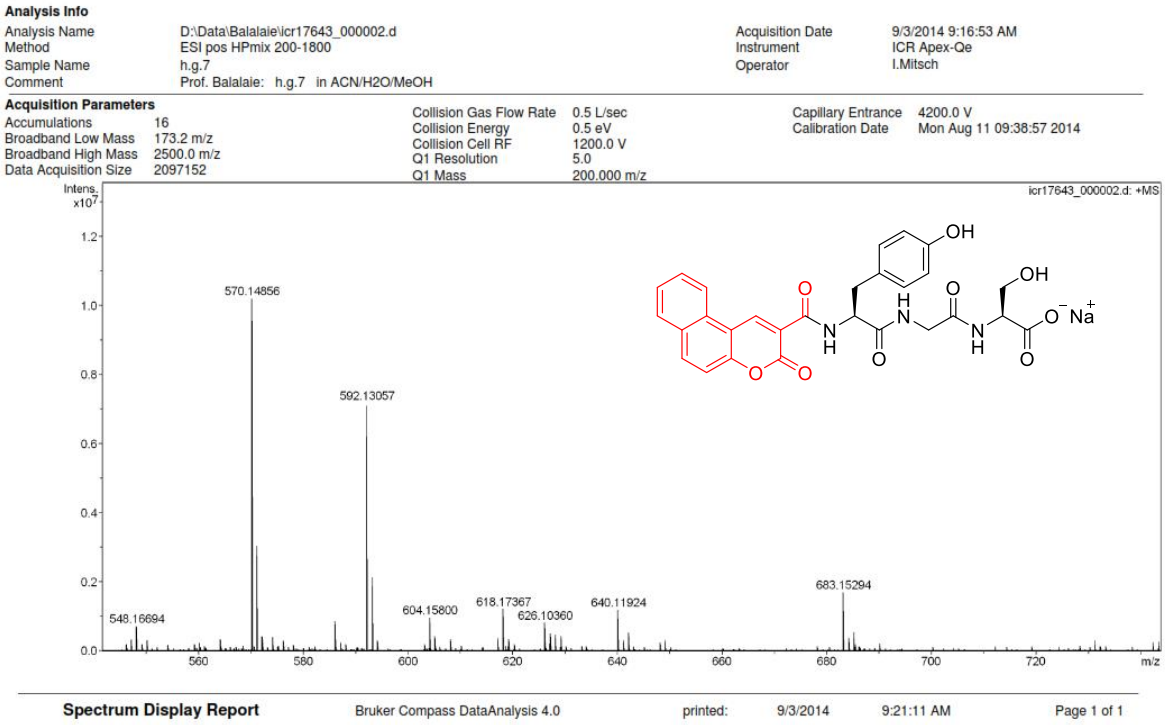
Acquisition Parameters

Accumulations	16	Collision Gas Flow Rate	0.3 L/sec	Capillary Entrance	3900.0 V
Broadband Low Mass	173.2 m/z	Collision Energy	0.0 eV	Calibration Date	Wed Jun 21 08:27:51 2017
Broadband High Mass	2300.0 m/z	Collision Cell RF	1100.0 V		
Data Acquisition Size	2097152	Q1 Resolution	6.0		
		Q1 Mass	200.000 m/z		

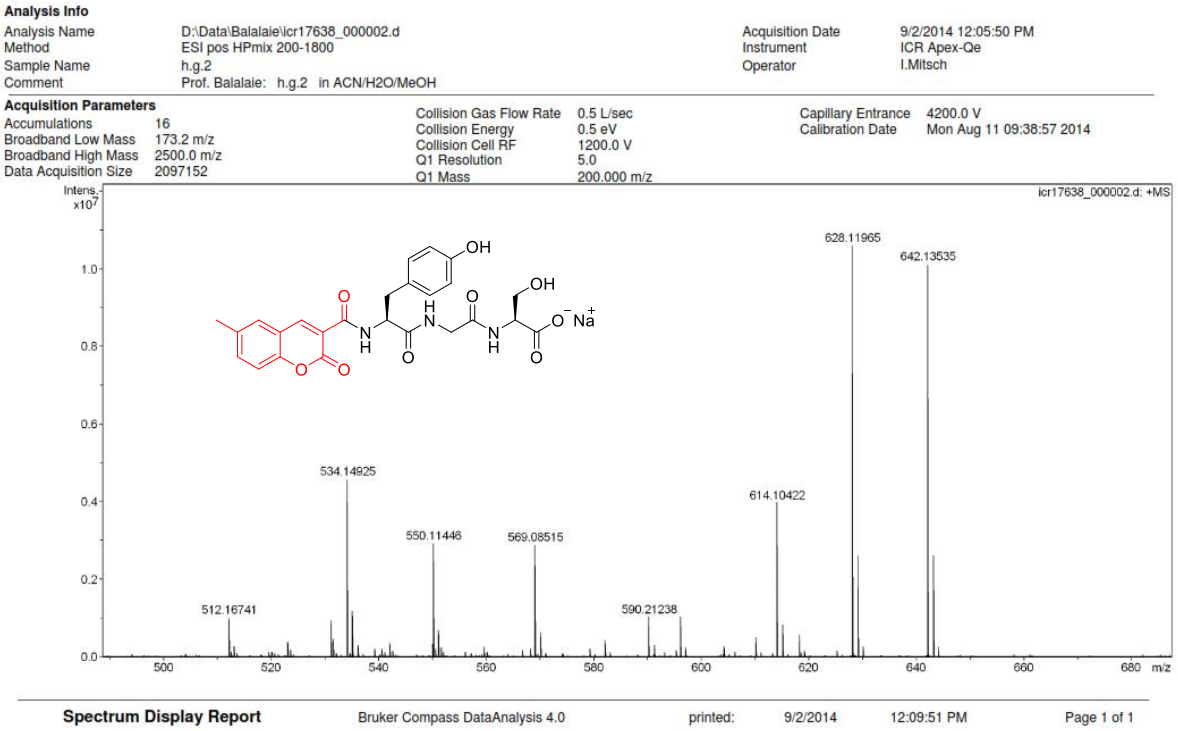


Spectrum Display Report Bruker Compass DataAnalysis 4.3 printed: 7/12/2017 1:50:53 PM Page 1 of 1

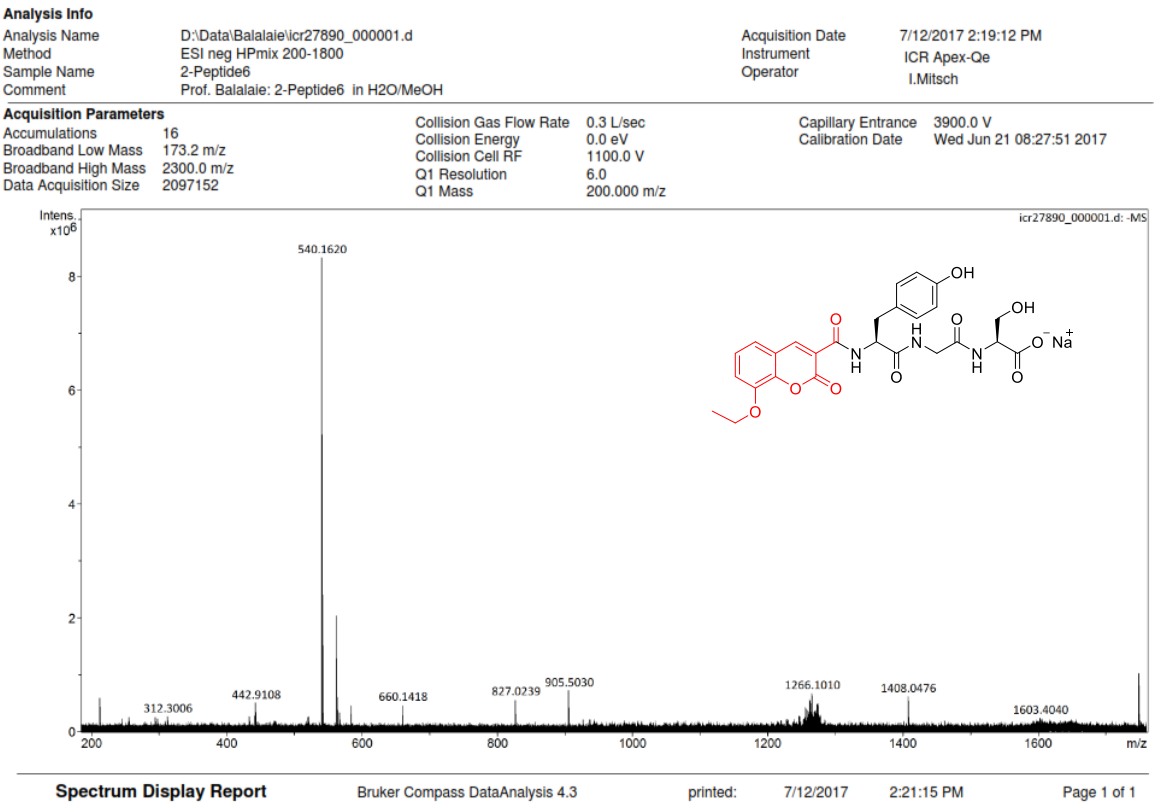
HR-MS spectra of **13**



HR-MS spectra of **14**



HR-MS spectra of **15**



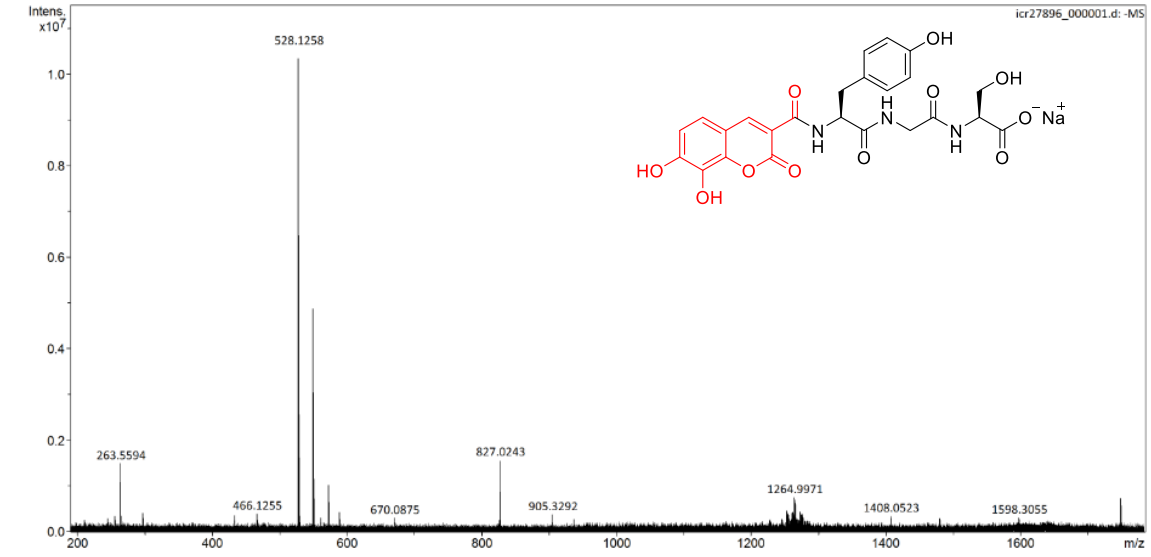
HR-MS spectra of **16**

Analysis Info

Analysis Name	D:\Data\Balalaie\icr27896_000001.d	Acquisition Date	7/13/2017 9:33:18 AM
Method	ESI neg HPmix 200-1800	Instrument	ICR Apex-Qe
Sample Name	3-Peptide7	Operator	I.Mitsch
Comment	Prof. Balalaie: 3-Peptide7 in H2O/MeOH		

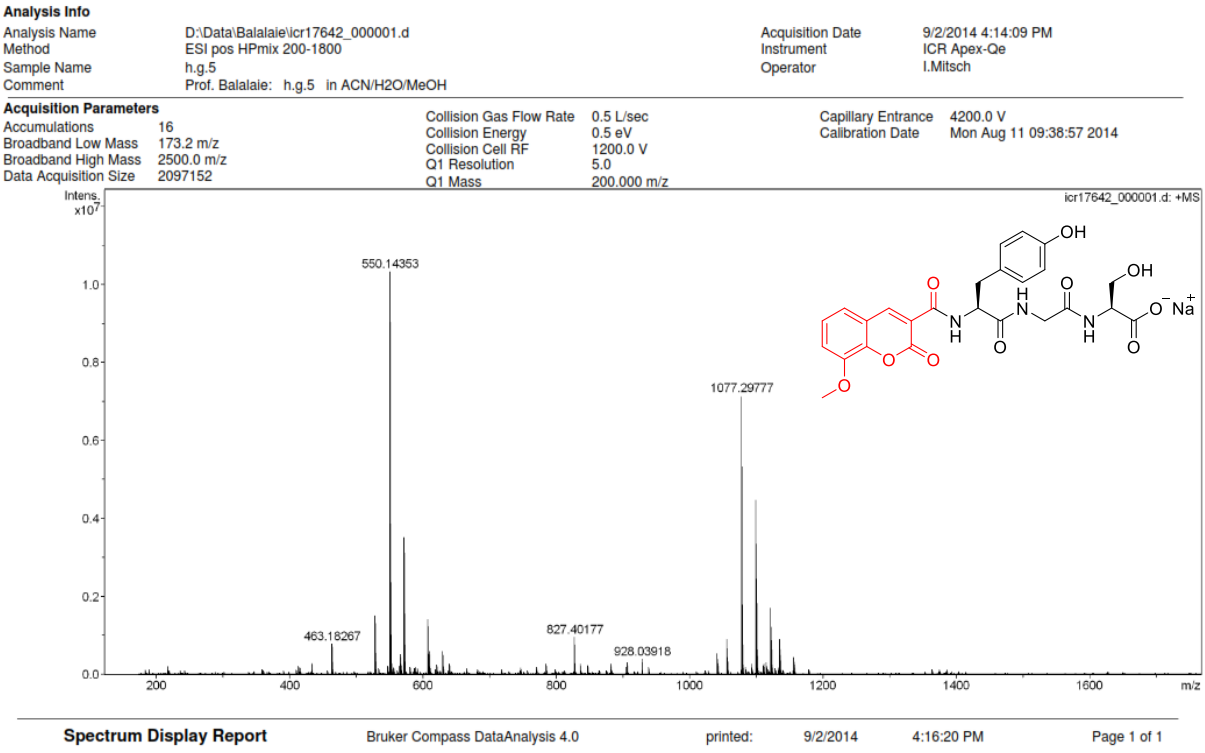
Acquisition Parameters

Accumulations	16	Collision Gas Flow Rate	0.3 L/sec	Capillary Entrance	3900.0 V
Broadband Low Mass	173.2 m/z	Collision Energy	0.0 eV	Calibration Date	Wed Jun 21 08:27:51 2017
Broadband High Mass	2300.0 m/z	Collision Cell RF	1100.0 V		
Data Acquisition Size	2097152	Q1 Resolution	6.0		
		Q1 Mass	200.000 m/z		

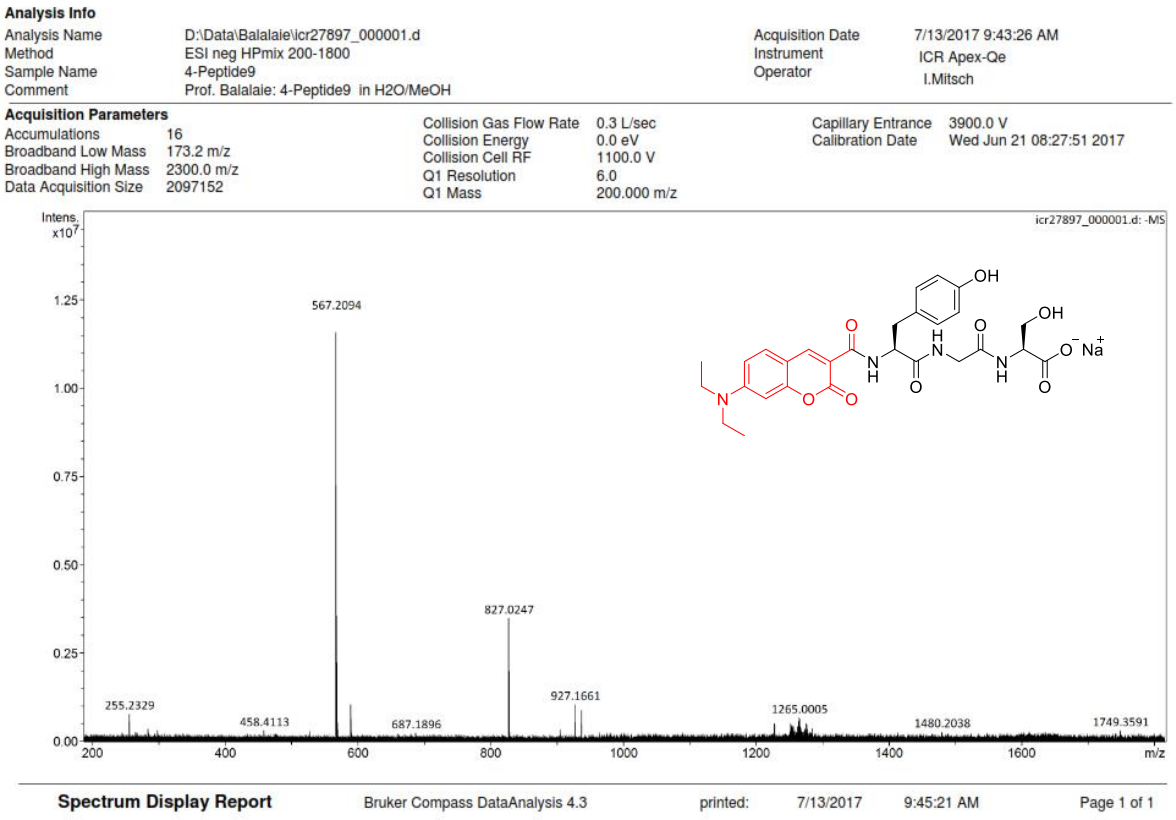


Spectrum Display Report Bruker Compass DataAnalysis 4.3 printed: 7/13/2017 9:35:31 AM Page 1 of 1

HR-MS spectra of **17**



HR-MS spectra of **18**



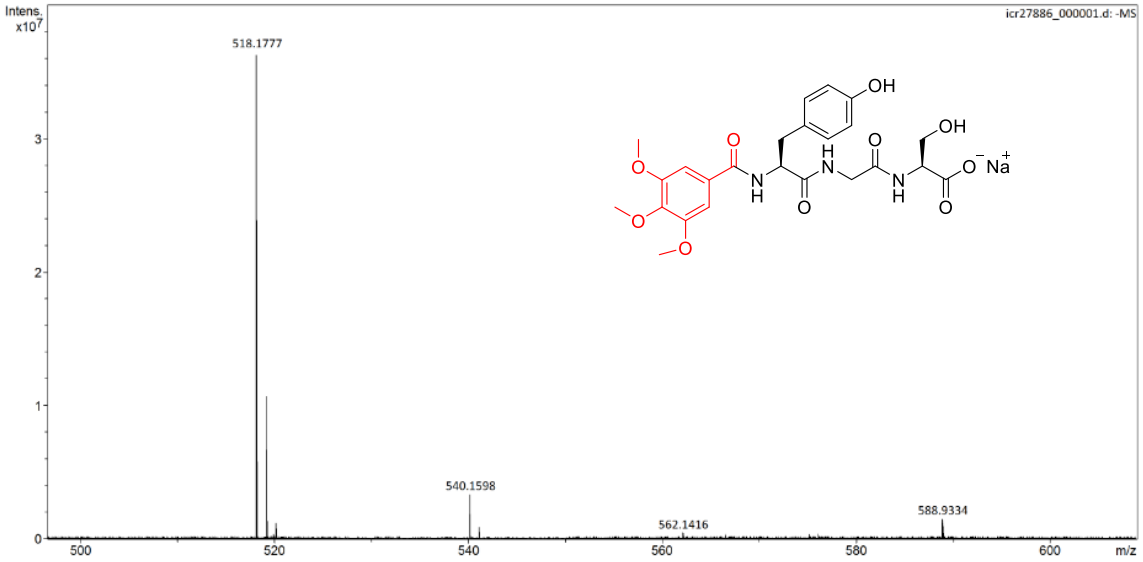
HR-MS spectra of **19**

Analysis Info

Analysis Name	D:\Data\Balalaie\icr27886_000001.d	Acquisition Date	7/12/2017 1:38:32 PM
Method	ESI neg HPmix 200-1800	Instrument	ICR Apex-Qe
Sample Name	6-Peptide11	Operator	I.Mitsch
Comment	Prof. Balalaie: 6-Peptide11 in H2O/MeOH		

Acquisition Parameters

Accumulations	16	Collision Gas Flow Rate	0.3 L/sec	Capillary Entrance	3900.0 V
Broadband Low Mass	173.2 m/z	Collision Energy	0.0 eV	Calibration Date	Wed Jun 21 08:27:51 2017
Broadband High Mass	2300.0 m/z	Collision Cell RF	1100.0 V		
Data Acquisition Size	2097152	Q1 Resolution	6.0		
		Q1 Mass	200.000 m/z		



Spectrum Display Report Bruker Compass DataAnalysis 4.3 printed: 7/12/2017 1:41:37 PM Page 1 of 1

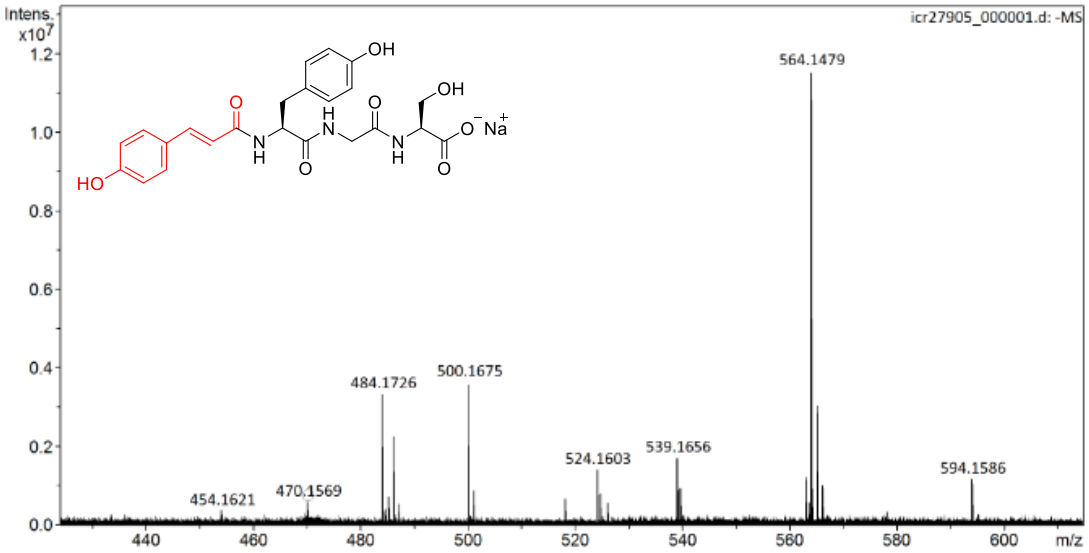
HR-MS spectra of **20**

Mass Spectrum Formula Report

Analysis Info Acquisition Date 7/14/2017 8:49:47 AM

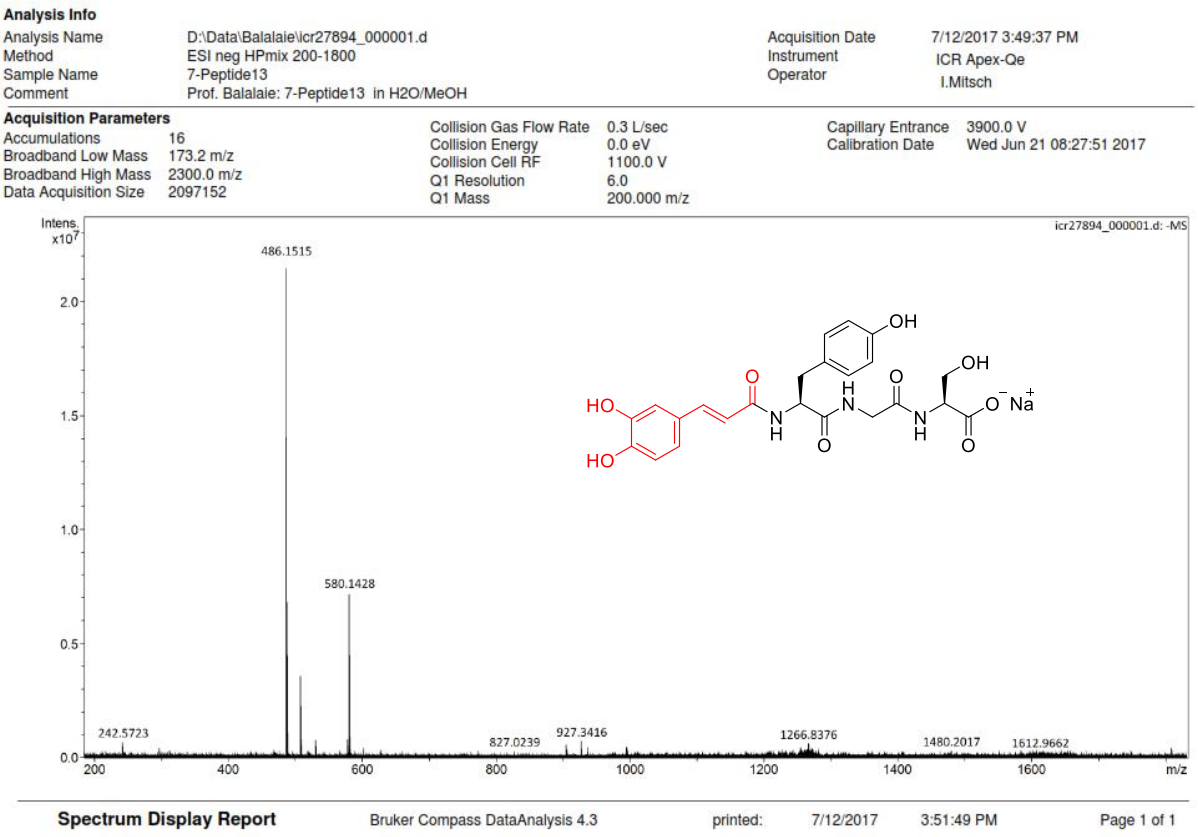
Analysis Name D:\Data\Balalaie\icr27905_000001.d

Comment Prof. Balalaie: 22-peptide12 in H2O/MeOH



Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
470.1569	C23H24N3O8	470.1569	-0.1	n.a.	13.5	even	ok
	C22H18N10O3	470.1569	-0.1	n.a.	19.0	odd	ok
	C7H14N22O4	470.1574	0.9	n.a.	12.0	odd	ok
	C8H20N15O9	470.1574	1.0	n.a.	6.5	even	ok
	C9H26N8O14	470.1574	1.0	n.a.	1.0	odd	ok
	C6H18N18O8	470.1560	-1.9	n.a.	7.0	odd	ok
	C5H12N25O3	470.1560	-1.9	n.a.	12.5	even	ok

HR-MS spectra of **21**



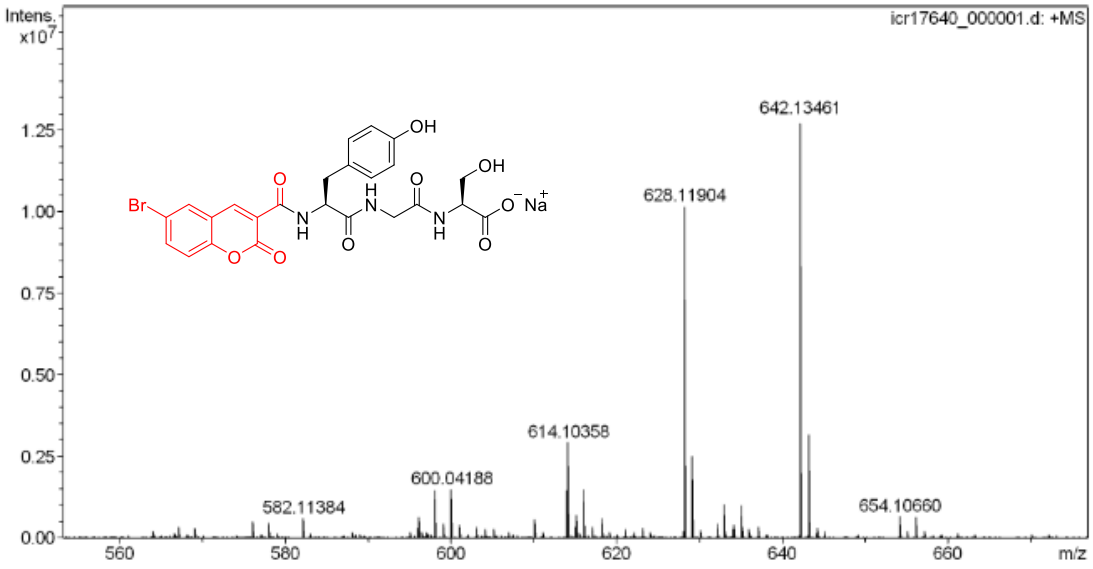
HR-MS spectra of **22**

Mass Spectrum Formula Report

Analysis Info Acquisition Date 9/2/2014 12:24:37 PM

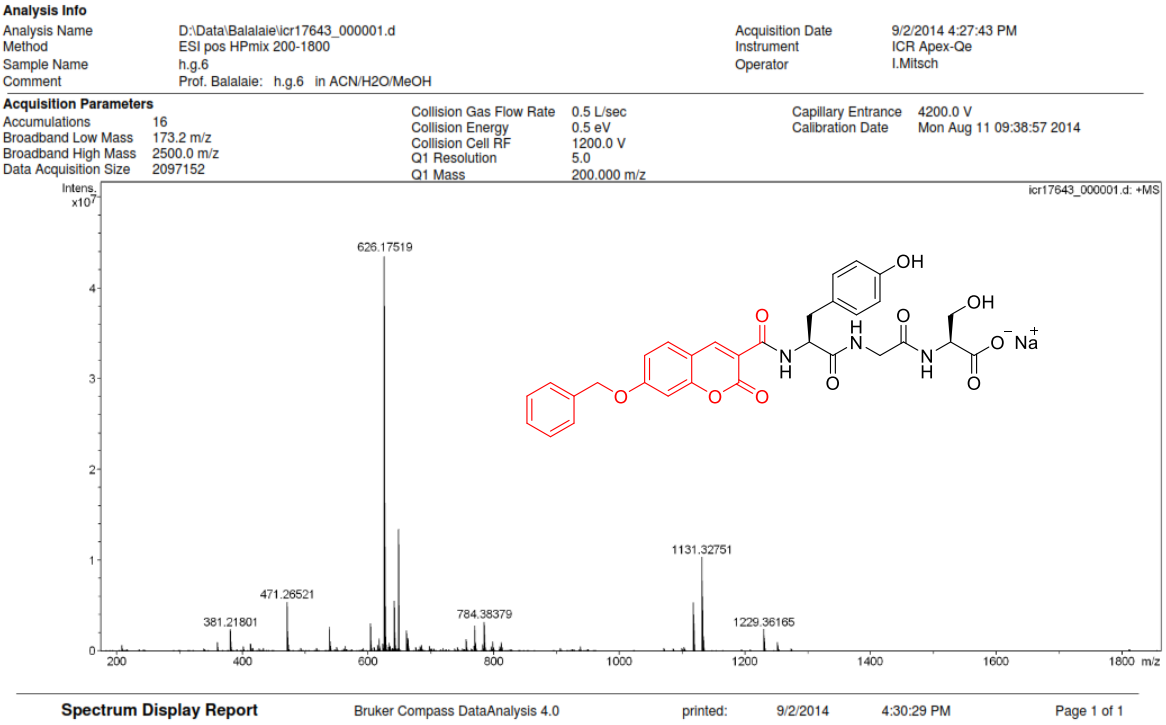
Analysis Name D:\Data\Balalaie\icr17640_000001.d

Comment Prof. Balalaie: h.g.3 in ACN/H2O/MeOH

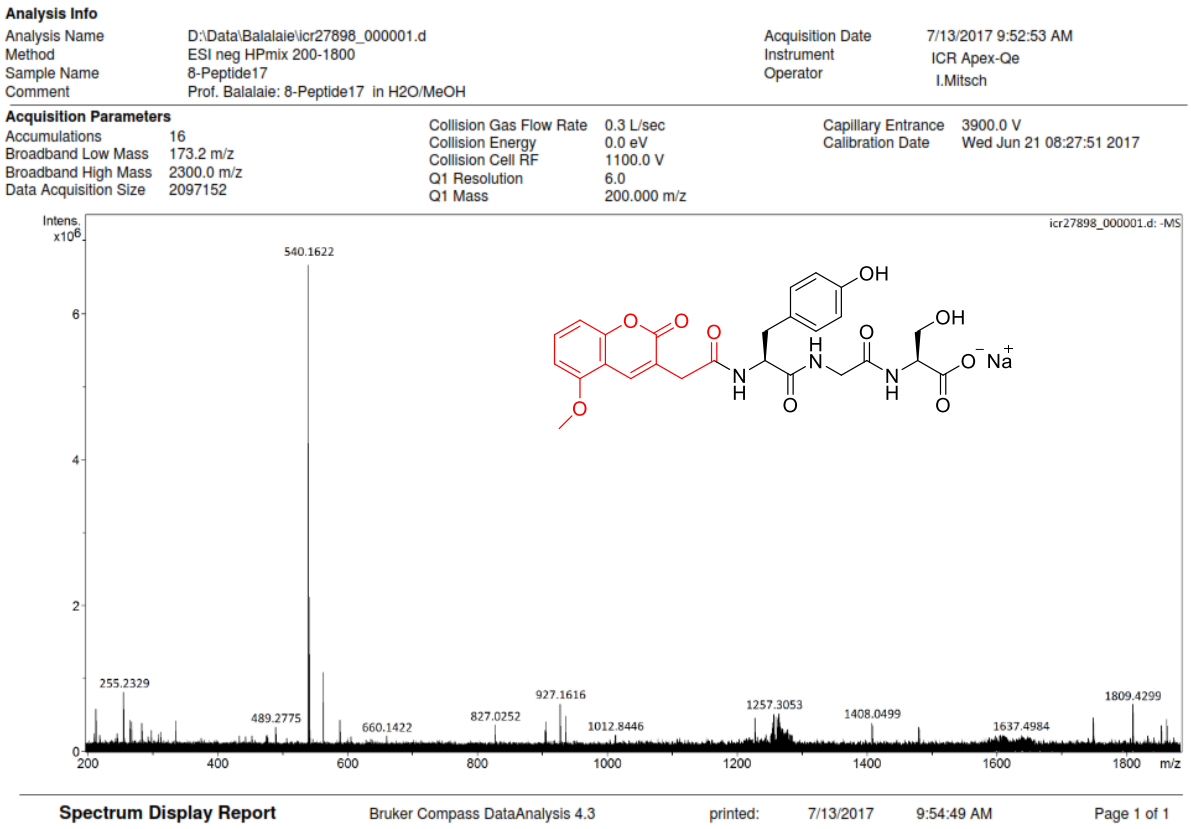


Meas. m/z	Formula	m/z	err [mDa]	err [ppm]	mSigma	rdb	N-Rule	e⁻ Conf
576.06205	C 24 H 18 N O 16	576.06201	-0.0	-0.1	138.9	16.5	ok	even
	C 25 H 14 N 5 O 12	576.06335	1.3	2.3	150.4	21.5	ok	even
	C 24 H 8 N 12 O 7	576.06334	1.3	2.3	154.7	27.0	ok	odd
	C 27 H 16 N 2 O 13	576.06469	2.6	4.6	156.4	21.0	ok	odd
	C 26 H 10 N 9 O 8	576.06468	2.6	4.6	160.5	26.5	ok	even
	C 25 H 4 N 16 O 3	576.06468	2.6	4.6	193.1	32.0	ok	odd
	C 35 H 8 N 6 O 4	576.06015	-1.9	-3.3	205.0	35.0	ok	odd
	C 37 H 10 N 3 O 5	576.06150	-0.5	-1.0	210.9	34.5	ok	even
	C 39 H 12 O 6	576.06284	0.8	1.4	216.8	34.0	ok	odd
	C 36 H 4 N 10	576.06149	-0.6	-1.0	217.7	40.0	ok	odd
	C 38 H 6 N 7 O	576.06283	0.8	1.4	223.4	39.5	ok	even
	C 40 H 8 N 4 O 2	576.06418	2.1	3.7	229.5	39.0	ok	odd
598.04396	C 24 H 7 N 12 Na O 7	598.04529	1.3	2.2	29.4	27.0	ok	odd
	C 26 H 9 N 9 Na O 8	598.04663	2.7	4.5	33.1	26.5	ok	even

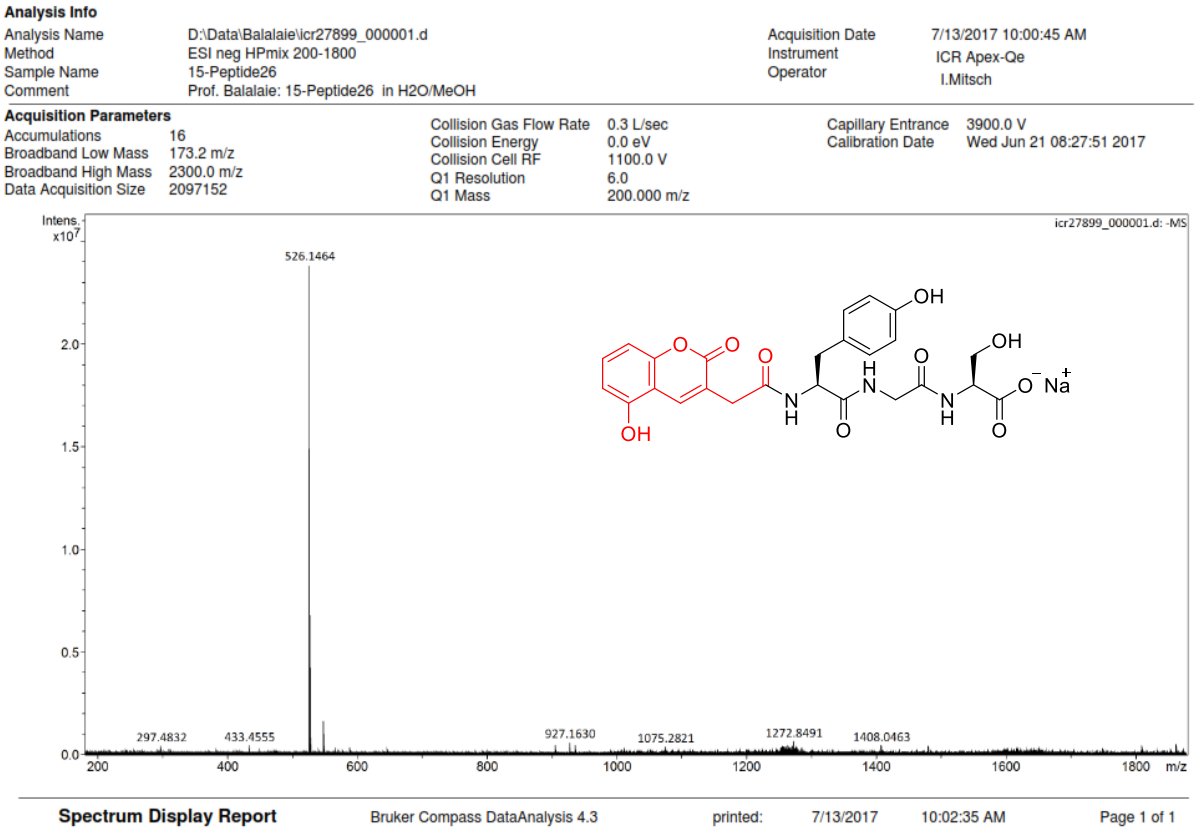
HR-MS spectra of **23**



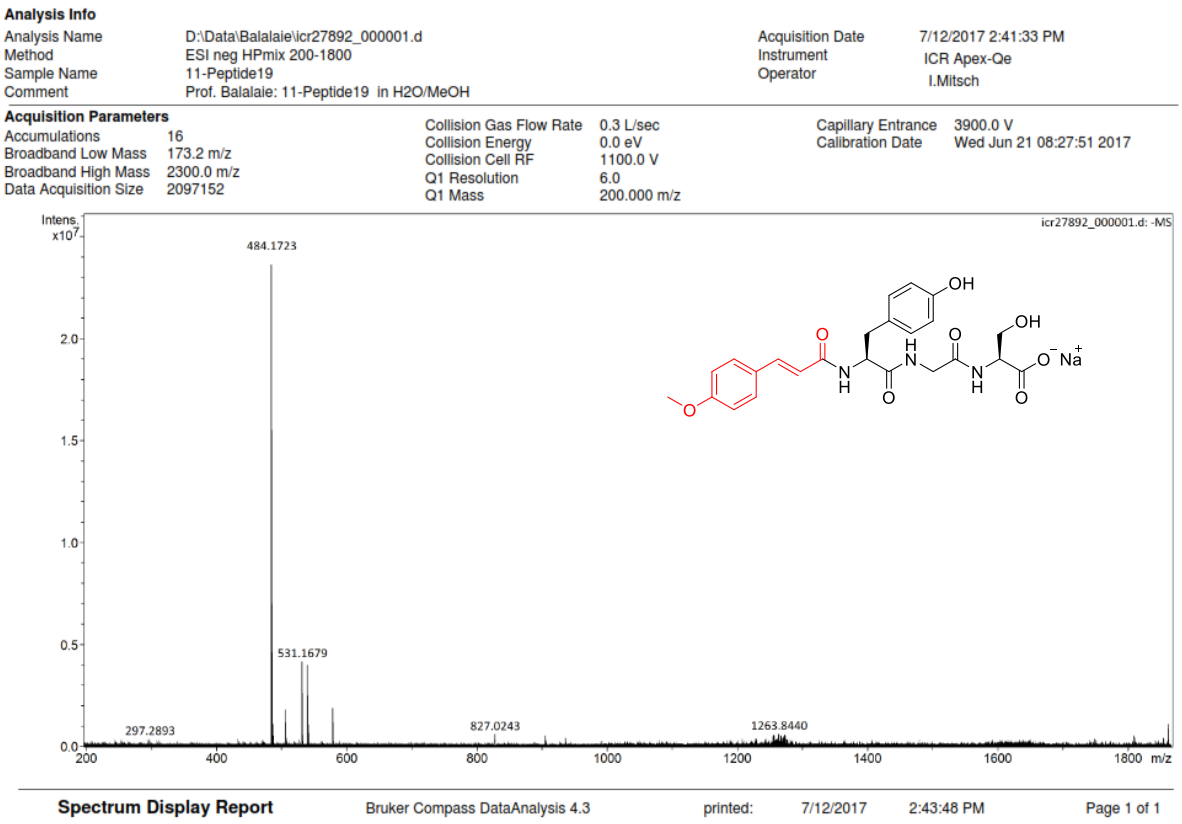
HR-MS spectra of **24**



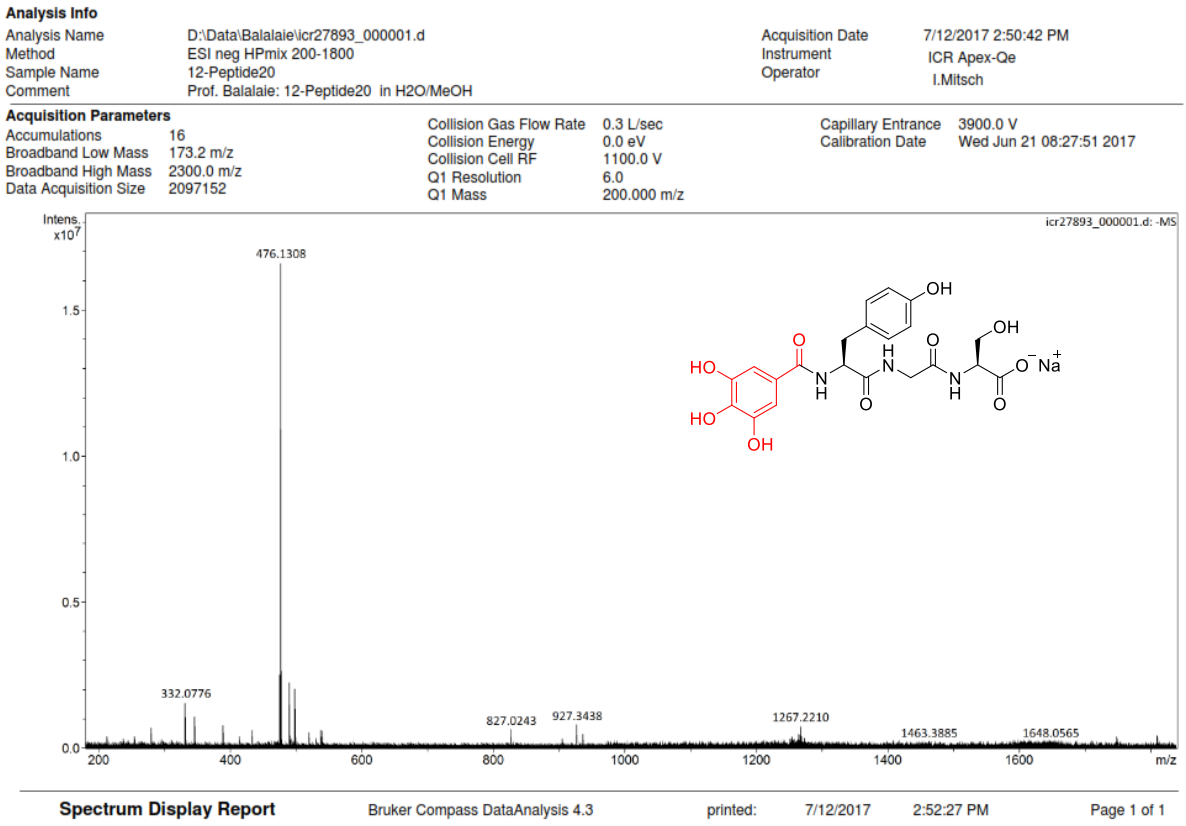
HR-MS spectra of **25**



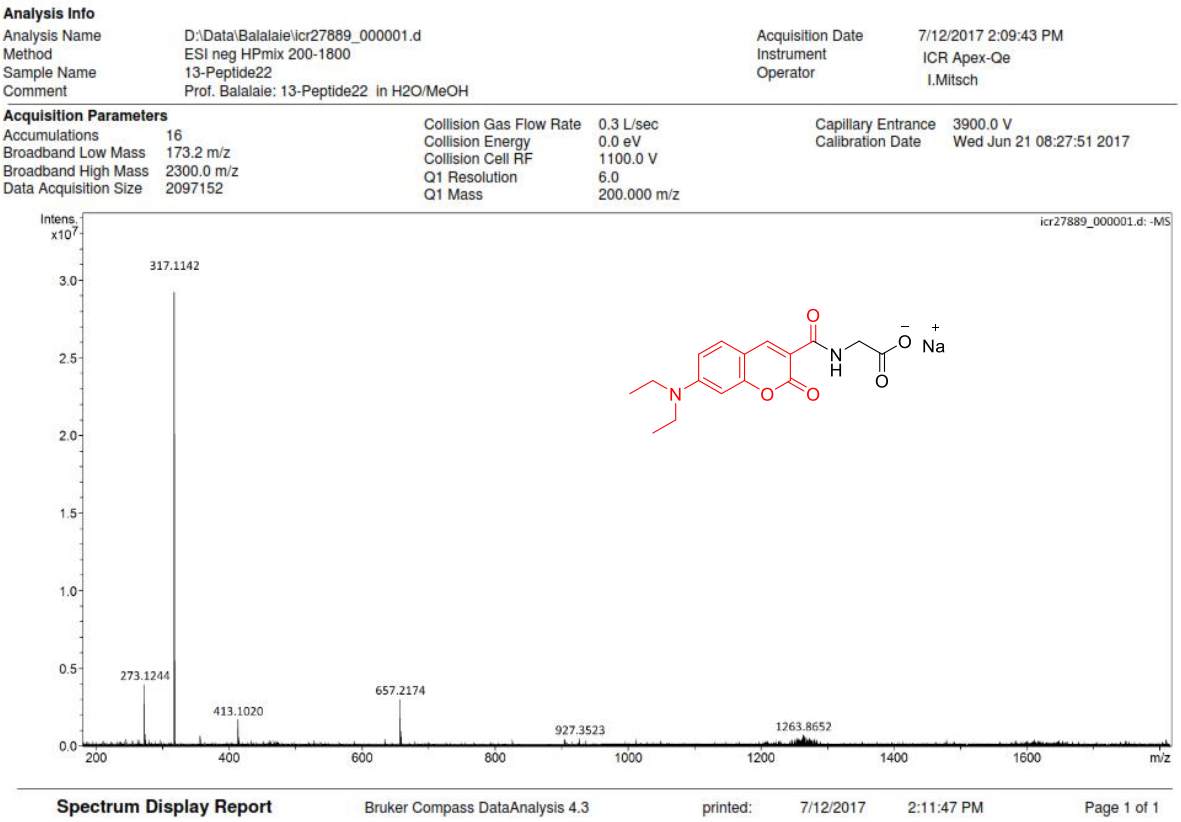
HR-MS spectra of **26**



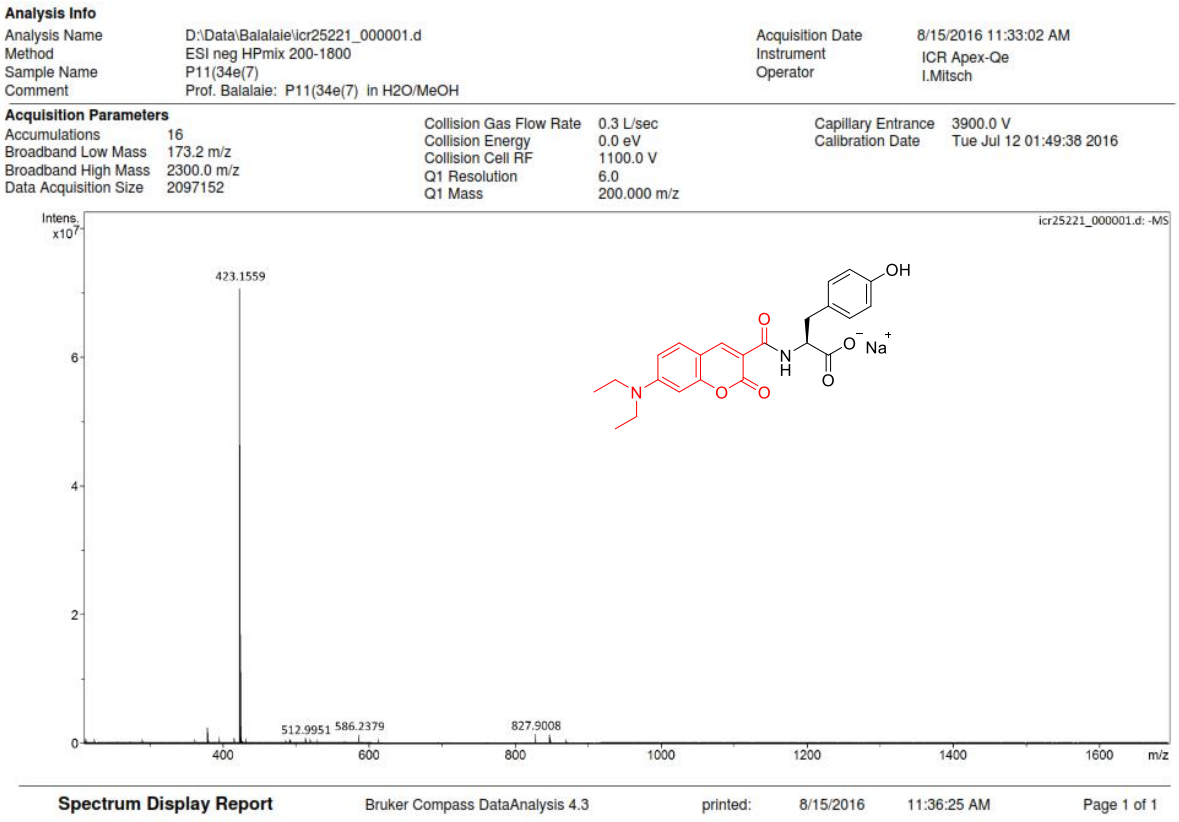
HR-MS spectra of **27**



HR-MS spectra of **28**



HR-MS spectra of **30**



HR-MS spectra of **32**

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