Supporting Information for

The Meta-Position of Phe[4] in Leu-Enkephalin Regulates Potency, Selectivity, Functional Activity, and Bias at the Delta and Mu Opioid Receptors

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Table S1: Efficacy of cAMP inhibiton of Meta-substituted Phe[4] Analogs of Leu-enkephalin at δOR and μOR.

cAMP	**δOR**	**μOR**
Compound	Efficacy (%+SD)	Efficacy (%+SD)
1a (F)	95 ± 6	98 ± 6
1b (Cl)	94 ± 5	99 ± 7
1c (Br)	96 ± 4	104 ± 11
1d (I)	97 ± 4	94 ± 11
1e (Me)	92 ± 8	85 ± 10
1f (OMe)	98 ± 10	87 ± 5
1g (CF_3)	92 ± 8	90 ± 4
1h (CN)	100 ± 3	92 ± 13
1i (NO_2)	99 ± 6	105 ± 12
1j (2-pyr)	100 ± 8	99 ± 5
1k (3-pyr)	97 ± 8	100 ± 7
1l (4-pyr)	99 ± 10	99 ± 6
DADLE	97 ± 4	98 ± 6
Leu-enkephalin	100	100 ± 9
DAMGO	98 ± 4	100

Table S2: LogR values for Meta-substituted Phe[4] Analogs of Leu-enkephalin at δOR and μOR in the cAMP and β-arrestin 2 (β-arr2) assays. 95% confidence intervals are presented between parentheses.

	LogR (δOR)		LogR (μOR)	
Compound	cAMP	β-arr2	cAMP	β-arr2
1a (F)	9.4 (9.1-9.6)	8.1 (7.9-8.3)	8.0 (7.7-8.3)	5.8 (5.6-6.1)
1b (Cl)	10.6 (10.3-10.9)	9.0 (8.8-9.3)	7.5 (7.1-7.8)	7.2 (6.9-7.4)
1c (Br)	10.5 (10.2-10.9)	9.4 (9.1-9.6)	8.1 (7.8-8.5)	7.2 (6.9-7.4)
1d (I)	10.6 (10.3-10.9)	9.0 (8.8-9.3)	8.0 (7.6-8.4)	6.6 (6.4-6.9)
1e (Me)	10 (9.7-10.3)	8.3 (8.1-8.5)	8.1 (7.7-8.4)	6.1 (5.8-6.4)
1f (OMe)	9.8 (9.5-10.1)	7.9 (7.7-8.1)	7.4 (7.0-7.7)	5.6 (5.3-5.8)
1g (CF_3)	9.7 (9.4-10)	8.3 (8.1-8.6)	8.1 (7.8-8.4)	6.6 (6.4-6.9)
1h (CN)	9.3 (9.0-9.5)	7.4 (7.2-7.7)	7.5 (7.2-7.7)	5.9 (5.6-6.1)
1i (NO_2)	9.0 (8.8-9.3)	7.2 (6.9-7.4)	7.2 (6.9-7.5)	5.3 (5.0-5.5)
1j (2-pyr)	8.2 (8.0-8.5)	6.6 (6.3-6.9)	7.4 (7.1-7.7)	5.3 (5.0-5.6)
1k (3-pyr)	7.3 (7.0-7.6)	5.4 (5.1-5.8)	6.6 (6.3-6.9)	3.2 (2.7-3.6)
1l (4-pyr)	7.5 (7.3-7.8)	6.2 (5.9-6.4)	6.6 (6.3-6.8)	3.9 (3.6-4.2)
DADLE	9.0 (8.8-9.3)	8.3 (8.0-8.6)	7.6 (7.3-7.9)	6.4 (6.3-6.5)
Leu-enkephalin	8.9 (8.7-9.2)	7.8 (7.7-8.0)	7.0 (6.8-7.3)	5.5 (5.2-5.7)
DAMGO	5.9 (5.6-6.2)	-	7.8 (7.6-8.0)	6.9 (6.8-7.1)

SI-3 Characterization of Peptides

H_2N-Tyr-Gly-Gly-(*meta*-F)Phe-Leu-OH (1a). Yield 52.6%, 60.0 mg colorless solid. ^{1}H NMR (500 MHz, MeOD-d_4) δ 7.29 (q, *J* = 7.8 Hz, 1H), 7.16 – 7.06 (m, 4H), 6.95 (t, *J* = 8.6 Hz, 1H), 6.81 (d, *J* = 8.4 Hz, 2H), 4.74 (dd, *J* = 9.8, 4.6 Hz, 1H), 4.38 (t, *J* = 7.3 Hz, 1H), 4.15 – 4.09 (m, 1H), 4.00 – 3.91 (m, 2H), 3.80 – 3.72 (m, 2H), 3.24 – 3.14 (m, 2H), 3.03 – 2.98 (m, 2H), 1.77 – 1.61 (m, 3H), 0.96 (d, *J* = 6.2 Hz, 3H), 0.92 (d, *J* = 6.2 Hz, 3H). ^{13}C NMR (126 MHz, MeOD-d_4) δ 173.9, 171.9, 170.1, 169.8, 169.7, 162.8 (d, *J* = 244.0 Hz), 156.9, 139.8 (d, *J* = 7.6 Hz), 130.1, 129.6 (d, *J* = 8.2 Hz), 124.9 (d, *J* = 2.8 Hz), 124.6, 115.7 (d, *J* = 21.6 Hz), 115.5, 113.0 (d, *J* = 21.3 Hz), 54.7, 54.0, 51.4, 42.6, 41.8, 40.3, 37.2 (d, *J* = 1.8 Hz), 36.3, 24.5, 22.0, 20.5. ^{19}F NMR (471 MHz, MeOD-d_4) δ –115.0. HRMS (ESI$^+$) mass calculated for $[M+H]^+$ ($C_{28}H_{36}FN_5O_7$) m/z 574.2677, found m/z 574.2669; purity ≥95%, rt 2.76 min (protocol A).

H_2N-Tyr-Gly-Gly-(*meta*-Cl)Phe-Leu-OH (1b). Yield 50.9%, 60.2 mg colorless solid. ^{1}H NMR (500 MHz, MeOD-d_4) δ 7.37 (s, 1H), 7.31 – 7.20 (m, 3H), 7.13 (d, *J* = 8.4 Hz, 2H), 6.81 (d, *J* = 8.5 Hz, 2H), 4.72 (dd, *J* = 9.8, 4.6 Hz, 1H), 4.39 (t, *J* = 7.4 Hz, 1H), 4.18 – 4.06 (m, 1H), 4.00 – 4.10 (m, 2H), 3.80 – 3.73 (m, 2H), 3.78 (d, *J* = 22.5 Hz, 1H), 3.75 (d, *J* = 23.1 Hz, 1H), 3.21 – 3.16 (m, 2H), 3.02 – 2.96 (m, 2H), 1.76 – 1.59 (m, 3H), 0.97 (d, *J* = 6.2 Hz, 3H), 0.92 (d, *J* = 6.1 Hz, 3H). ^{13}C NMR (126 MHz, MeOD-d_4) δ 174.8, 171.9, 170.0, 169.8, 169.7, 156.9, 139.3, 133.7, 130.1, 129.5, 129.0, 127.5, 126.5, 124.5, 115.5, 54.7, 54.0, 51.3, 42.6, 41.8, 40.3, 37.1, 36.3, 24.5, 22.0, 20.4. HRMS (ESI$^+$) mass calculated for $[M+H]^+$ ($C_{28}H_{36}ClN_5O_7$) m/z 590.2473, found m/z 590.2431; purity ≥95%, rt 1.65 min (protocol B).

H_2N-Tyr-Gly-Gly-(*meta*-Br)Phe-Leu-OH (1c). Yield 47.6%, 60.5 mg colorless solid. ^{1}H NMR (500 MHz, MeOD-d_4) δ 7.54 (s, 1H), 7.38 (d, *J* = 7.9 Hz, 1H), 7.29 (d, *J* = 7.6 Hz, 1H), 7.21 (t, *J* = 7.8 Hz, 1H), 7.14 (d, *J* = 8.2 Hz, 2H), 6.81 (d, *J* = 8.2 Hz, 2H), 4.71 (dd, *J* = 10.1, 4.4 Hz, 1H), 4.33 (t, *J* = 7.3 Hz, 1H), 4.12 (t, *J* = 7.3 Hz, 1H), 3.99 (d, *J* = 26.6 Hz, 1H), 3.95 (d, *J* = 27.1 Hz, 1H), 3.77 (d, *J* = 24.5 Hz, 1H), 3.73 (d, *J* = 25.0 Hz, 1H), 3.19 (ddd, *J* = 15.3, 10.5, 5.4 Hz, 2H), 3.24 – 2.94 (m, 2H), 1.83 – 1.55 (m, 3H), 0.96 (d, *J* = 6.2 Hz, 3H), 0.92 (d, *J* = 6.1 Hz, 3H). ^{13}C NMR (126 MHz, MeOD-d_4) δ 171.8, 170.0, 170.0, 169.8, 156.9, 139.7, 132.0, 130.1, 129.7, 129.4, 127.9, 124.6, 121.9, 115.5, 54.8, 54.1, 52.0, 48.1, 47.9, 42.7, 41.8, 40.5, 37.0, 36.4, 24.6,

22.0, 20.5. HRMS (ESI^+) mass calculated for $[M+H]^+$ ($C_{28}H_{36}BrN_5O_7$) m/z 656.1696, found m/z 656.1711; purity ≥95%, rt 2.8 min (protocol A).

H_2N-Tyr-Gly-Gly-(*meta*-I)Phe-Leu-OH (1d). Yield 55.2%, 75.0 mg colorless solid. ^1H NMR (500 MHz, MeOD-d_4) δ 7.75 (s, 1H), 7.58 (d, *J* = 7.6 Hz, 1H), 7.33 (d, *J* = 7.7 Hz, 1H), 7.14 (d, *J* = 8.1 Hz, 2H), 7.07 (t, *J* = 7.8 Hz, 1H), 6.81 (d, *J* = 8.1 Hz, 2H), 4.68 (dd, *J* = 10.5, 4.1 Hz, 1H), 4.25 (dd, *J* = 9.1, 5.3 Hz, 1H), 4.12 (t, *J* = 7.2 Hz, 1H), 4.03 – 3.94 (m, 2H), 3.77 – 3.67 (m, 2H), 3.74 (d, *J* = 31.4 Hz, 1H), 3.70 (d, *J* = 32.0 Hz, 1H), 3.23 – 3.13 (m, 2H), 2.97 (ddd, *J* = 21.8, 14.0, 9.4 Hz, 2H), 1.76 – 1.54 (m, 3H), 0.96 (d, *J* = 6.1 Hz, 3H), 0.92 (d, *J* = 6.0 Hz, 3H). ^{13}C NMR (126 MHz, MeOD-d_4) δ 174.3, 171.7, 170.5, 170.1, 169.8, 156.9, 139.9, 138.0, 135.5, 130.1, 129.8, 128.4, 124.7, 115.5, 93.5, 54.8, 54.3, 53.2, 42.9, 41.8, 40.9, 36.9, 36.5, 24.7, 22.2, 20.7. HRMS (ESI^+) mass calculated for $[M+H]^+$ ($C_{28}H_{36}IN_5O_7$) m/z 682.1737, found m/z 681.1741; purity ≥95%, rt 2.97 min (protocol A).

H_2N-Tyr-Gly-Gly-(*meta*-Me)Phe-Leu-OH (1e). Yield 78.9%, 90.2 mg colorless solid. ^1H NMR (500 MHz, MeOD-d_4) δ 7.20 – 7.11 (m, 4H), 7.08 (d, *J* = 7.7 Hz, 1H), 7.03 (d, *J* = 7.5 Hz, 1H), 6.81 (d, *J* = 8.2 Hz, 2H), 4.69 (dd, *J* = 9.8, 4.6 Hz, 1H), 4.37 (t, *J* = 7.3 Hz, 1H), 4.12 (t, *J* = 7.3 Hz, 1H), 4.02 – 3.88 (m, 2H), 3.77 (d, *J* = 27.8 Hz, 1H), 3.74 (d, *J* = 28.2 Hz, 1H), 3.17 (ddd, *J* = 14.4, 9.3, 5.5 Hz, 2H), 2.97 (ddd, *J* = 23.4, 14.0, 9.0 Hz, 2H), 1.73 – 1.63 (m, 3H), 0.96 (d, *J* = 6.3 Hz, 3H), 0.92 (d, *J* = 6.2 Hz, 3H). ^{13}C NMR (126 MHz, MeOD-d_4) δ 175.2, 172.2, 170.0, 169.8, 169.7, 156.9, 137.7, 136.8, 130.1, 129.6, 127.9, 127.0, 126.0, 124.6, 115.4, 54.8, 54.5, 51.6, 42.6, 41.8, 40.4, 37.4, 36.3, 24.5, 22.0, 20.5, 20.0. HRMS (ESI^+) mass calculated for $[M+H]^+$ ($C_{29}H_{39}N_5O_7$) m/z 570.2927, found m/z 570.2923; purity ≥95%, rt 2.88 min (protocol A).

H_2N-Tyr-Gly-Gly-(*meta*-OMe)Phe-Leu-OH (1f). Yield 22.3%, 26.0 mg colorless solid. ^1H NMR (500 MHz, MeOD-d_4) δ 7.19 (t, *J* = 7.9 Hz, 1H), 7.13 (d, *J* = 8.3 Hz, 2H), 6.91 – 6.85 (m, 2H), 6.84 – 6.74 (m, 3H), 4.73 (dd, *J* = 9.6, 4.7 Hz, 1H), 4.43 (t, *J* = 7.4 Hz, 1H), 4.13 – 4.08 (m, 1H), 4.00 – 3.92 (m, 2H), 3.83 – 3.71 (m, 5H), 3.20-3.15 (m, 2H), 3.06 – 2.91 (m, 2H), 1.75 – 1.62 (m, 3H), 0.97 (d, *J* = 6.3 Hz, 3H), 0.92 (d, *J* = 6.4 Hz, 3H). ^{13}C NMR (126 MHz, MeOD-d_4) δ 174.2, 172.3, 170.0, 169.7, 169.6, 159.8, 156.9, 138.4, 130.1, 128.9, 124.5, 121.3, 115.4, 114.3, 112.1, 54.7, 54.2, 54.2, 50.7, 42.5, 41.8, 40.1, 37.5, 36.2, 24.5, 21.9, 20.4. HRMS (ESI^+) mass

calculated for $[M+H]^+$ ($C_{29}H_{39}N_5O_8$) m/z 586.2877, found m/z 585.2932; purity ≥95%, rt 1.57 min (protocol B).

H_2N-Tyr-Gly-Gly-(*meta*-CF_3)Phe-Leu-OH (1g). Yield 32.1%, 40.1 mg colorless solid. ^{1}H NMR (500 MHz, MeOD-d_4) δ 7.67 (s, 1H), 7.60 – 7.46 (m, 3H), 7.13 (d, *J* = 8.2 Hz, 2H), 6.80 (d, *J* = 8.2 Hz, 2H), 4.76 (dd, *J* = 9.8, 4.7 Hz, 1H), 4.41 (t, *J* = 7.4 Hz, 1H), 4.14 – 4.11 (m, 1H), 3.95 (t, *J* = 16.2 Hz, 1H), 3.76 (dd, *J* = 32.2, 16.8 Hz, 1H), 3.29 (dd, *J* = 14.0, 4.7 Hz, 1H), 3.18 (dd, *J* = 14.2, 6.5 Hz, 1H), 3.08 (dd, *J* = 14.0, 9.8 Hz, 1H), 3.00 (dd, *J* = 14.2, 8.1 Hz, 1H), 1.77 – 1.62 (m, 3H), 0.97 (d, *J* = 6.5 Hz, 1H), 0.92 (d, *J* = 6.2 Hz, 1H). ^{13}C NMR (126 MHz, MeOD-d_4) δ 174.5, 171.9, 170.0, 169.8, 169.7, 156.9, 138.4, 132.9, 130.2 (d, *J* = 31.8 Hz), 130.1, 128.7, 125.7 (q, *J* = 3.7 Hz), 124.5, 124.3 (q, *J* = 272.2 Hz), 123.1 (q, *J* = 4.0 Hz), 115.4, 54.7, 54.0, 51.0, 42.6, 41.7, 40.2, 37.3, 36.3, 24.5, 21.9, 20.4. ^{19}F NMR (471 MHz, MeOD-d_4) δ –63.3. HRMS (ESI^+) mass calculated for $[M+H]^+$ ($C_{29}H_{36}F_3N_5O_7$) m/z 624.2645, found m/z 624.2618; purity ≥95%, rt 2.89 min (protocol A).

H_2N-Tyr-Gly-Gly-(*meta*-CN)Phe-Leu-OH (1h). Yield 43.1%, 50.0 mg colorless solid. ^{1}H NMR (500 MHz, MeOD-d_4) δ 7.70 (s, 1H), 7.63 – 7.59 (m, 2H), 7.48 (t, *J* = 7.7 Hz, 1H), 7.14 (d, *J* = 8.0 Hz, 2H), 6.81 (d, *J* = 8.0 Hz, 2H), 4.75 (dd, *J* = 9.6, 4.8 Hz, 1H), 4.38 (dd, *J* = 9.0, 5.4 Hz, 1H), 4.13 (t, *J* = 7.4 Hz, 1H), 4.00-3.91 (m, 2H), 3.81-3.71 (m, 2H), 3.26 (dd, *J* = 14.0, 4.8 Hz, 1H), 3.19 (dd, *J* = 14.2, 6.4 Hz, 1H), 3.08-2.99 (m, 2H), 1.78 – 1.58 (m, 3H), 0.97 (d, *J* = 6.1 Hz, 3H), 0.92 (d, *J* = 6.0 Hz, 3H). ^{13}C NMR (126 MHz, MeOD-d_4) δ 173.9, 171.6, 170.0, 169.9, 169.7, 156.9, 138.8, 134.0, 132.8, 130.2, 130.1, 129.1, 124.6, 118.5, 115.5, 111.9, 54.8, 53.8, 51.5, 42.7, 41.8, 40.3, 37.0, 36.3, 24.6, 22.0, 20.4. HRMS (ESI^+) mass calculated for $[M+H]^+$ ($C_{29}H_{36}N_6O_7$) m/z 581.2723, found m/z 581.2755; purity ≥95%, rt 1.56 min (protocol B).

H_2N-Tyr-Gly-Gly-(*meta*-NO_2)Phe-Leu-OH (1i). Yield 66.7%, 80.3 mg colorless solid. ^{1}H NMR (400 MHz, MeOD-d_4) δ 8.30 (s, 1H), 8.11 (d, *J* = 8.2 Hz, 1H), 7.73 (d, *J* = 7.7 Hz, 1H), 7.54 (t, *J* = 7.9 Hz, 1H), 7.15 (d, *J* = 8.5 Hz, 2H), 6.81 (d, *J* = 8.5 Hz, 2H), 4.77 (dd, *J* = 10.6, 4.2 Hz, 1H), 4.25 (dd, *J* = 8.9, 5.5 Hz, 1H), 4.15 (dd, *J* = 8.3, 6.2 Hz, 1H), 3.96 (dd, *J* = 29.6, 16.7 Hz, 2H), 3.69 (dd, *J* = 45.1, 16.8 Hz, 2H), 3.37 (dd, *J* = 13.9, 4.3 Hz, 1H), 3.24 – 3.10 (m, 2H), 3.01 (dd, *J* = 14.2, 8.3 Hz, 1H), 1.73 – 160 (m, 3H), 0.96 (d, *J* = 6.1 Hz, 3H), 0.92 (d, *J* = 6.0 Hz, 3H). ^{13}C NMR (126 MHz, MeOD-d_4) δ 177.2, 171.4, 170.6, 170.0, 169.8, 156.9, 148.2, 139.5, 135.5, 130.1, 129.1, 124.7, 124.1, 121.3, 115.5, 54.9, 54.0, 53.2, 43.0, 41.8, 40.9, 37.0, 36.5,

24.7, 22.1, 20.6. HRMS (ESI^+) mass calculated for $[M+H]^+$ ($C_{29}H_{36}N_6O_9$) m/z 601.2606, found m/z 601.2622; purity ≥95%, rt 1.59 min (protocol B).

H_2N-Tyr-Gly-Gly-(2-pyridyl)Ala-Leu-OH (1j). Yield 10.8%, 12.1 mg colorless solid. ^1H NMR (500 MHz, MeOD-d_4) δ 8.63 (d, *J* = 5.4 Hz, 1H), 8.18 (t, *J* = 7.8 Hz, 1H), 7.73 (d, *J* = 7.9 Hz, 1H), 7.68 – 7.61 (m, 1H), 7.13 (d, *J* = 8.3 Hz, 2H), 6.80 (d, *J* = 8.2 Hz, 2H), 4.93 (dd, *J* = 8.5, 5.5 Hz, 1H), 4.44 – 4.38 (m, 1H), 4.11 (t, *J* = 7.2 Hz, 1H), 4.00 – 3.76 (m, 4H), 3.50 (dd, *J* = 14.3, 5.4 Hz, 1H), 3.38 – 3.27 (m, 1H), 3.17 (dd, *J* = 14.2, 6.5 Hz, 1H), 3.01 (dd, *J* = 14.2, 8.0 Hz, 1H), 1.78 – 1.58 (m, 3H), 0.97 (d, *J* = 6.0 Hz, 3H), 0.92 (d, *J* = 6.0 Hz, 3H). ^{13}C NMR (126 MHz, MeOD-d_4) δ 174.1, 170.8, 170.2, 169.8, 169.6, 156.9, 154.5, 144.7, 142.1, 130.1, 126.5, 124.5, 123.8, 115.4, 54.7, 52.4, 50.9, 42.4, 41.9, 39.9, 37.4, 36.2, 24.5, 21.9, 20.3. HRMS (ESI^+) mass calculated for $[M+H]^+$ ($C_{27}H_{36}N_6O_7$) m/z 557.2723, found m/z 557.2748; purity ≥95%, rt 2.46 min (protocol A).

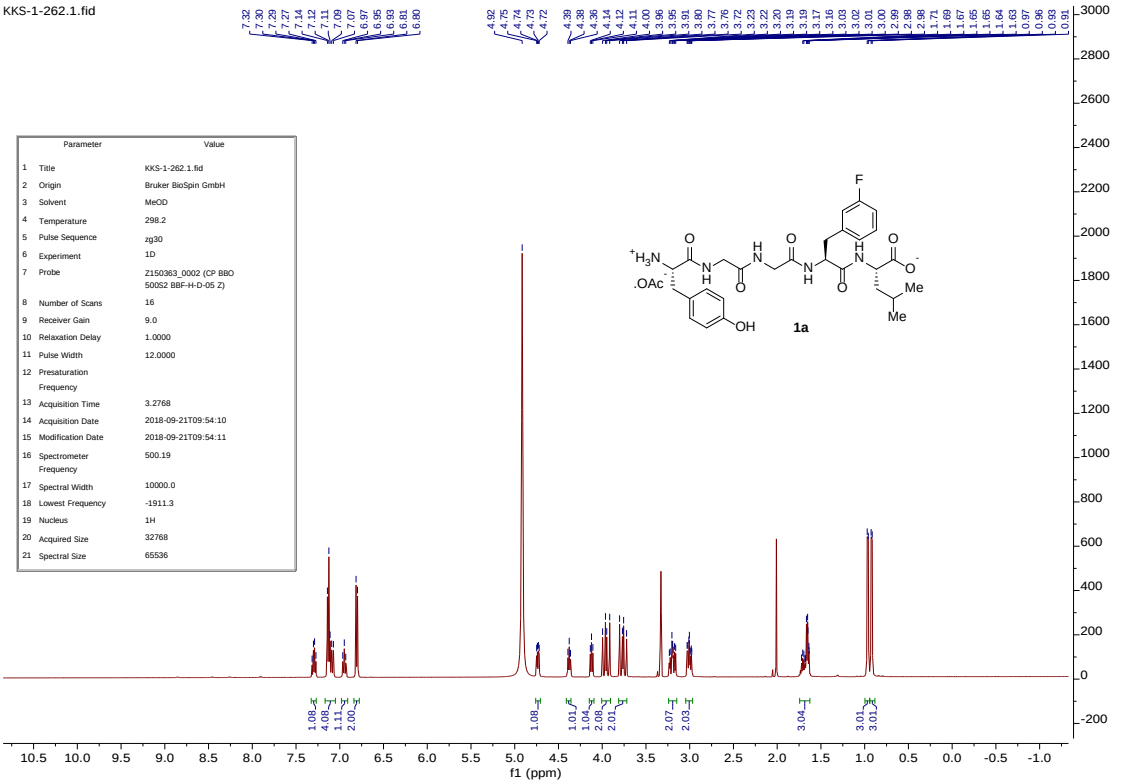
H_2N-Tyr-Gly-Gly-(3-pyridyl)Ala-Leu-OH (1k). Yield 62.9%, 70.0 mg colorless solid. ^1H NMR (400 MHz, MeOD-d_4) δ 8.49 (s, 1H), 8.42 (d, *J* = 3.8 Hz, 1H), 7.83 (d, *J* = 7.9 Hz, 1H), 7.40 (dd, *J* = 7.8, 5.0 Hz, 1H), 7.14 (d, *J* = 8.5 Hz, 2H), 6.81 (d, *J* = 8.5 Hz, 2H), 4.77 (dd, *J* = 9.3, 4.9 Hz, 1H), 4.45 – 4.33 (m, 1H), 4.12 (dd, *J* = 8.2, 6.4 Hz, 1H), 3.95 (dd, *J* = 27.3, 16.7 Hz, 2H), 3.78 (dd, *J* = 19.3, 16.7 Hz, 2H), 3.28 – 3.16 (m, 2H), 3.09 – 2.97 (m, 2H), 1.77 – 1.57 (m, 3H), 0.97 (d, *J* = 6.2 Hz, 3H), 0.92 (d, *J* = 6.1 Hz, 3H). ^{13}C NMR (126 MHz, MeOD-d_4) δ 174.6, 173.8, 171.5, 170.1, 169.7, 156.9, 149.2, 146.7, 138.3, 133.6, 130.1, 124.5, 123.8, 115.5, 54.7, 53.5, 51.1, 42.5, 41.8, 40.2, 36.3, 34.7, 24.6, 21.9, 20.4. HRMS (ESI^+) mass calculated for $[M+H]^+$ ($C_{27}H_{36}N_6O_7$) m/z 557.2723, found m/z 557.2659; purity ≥95%, rt 2.46 min (protocol A).

H_2N-Tyr-Gly-Gly-(4-pyridyl)Ala-Leu-OH (1l). Yield 32.4%, 36.1 mg colorless solid. ^1H NMR (500 MHz, MeOD-d_4) δ 8.51 (d, *J* = 5.3 Hz, 2H), 7.53 (d, *J* = 5.3 Hz, 2H), 7.13 (d, *J* = 8.2 Hz, 2H), 6.80 (d, *J* = 8.3 Hz, 2H), 4.84 (dd, *J* = 9.4, 4.9 Hz, 1H), 4.45 – 4.36 (m, 1H), 4.13 (dd, *J* = 8.1, 6.4 Hz, 1H), 3.94 (dd, *J* = 20.4, 16.7 Hz, 2H), 3.78 (dd, *J* = 30.3, 16.7 Hz, 2H), 3.33 – 3.27 (m, 1H), 3.21 – 3.08 (m, 2H), 3.01 (dd, *J* = 14.2, 8.1 Hz, 1H), 1.75 – 1.63 (m, 3H), 0.97 (d, *J* = 6.1 Hz, 3H), 0.92 (d, *J* = 6.1 Hz, 3H). ^{13}C NMR (126 MHz, MeOD-d_4) δ 174.3, 173.8, 171.2, 170.1, 169.7, 156.9, 150.2, 146.7, 130.1, 125.8, 124.5, 115.4, 54.7, 52.9, 50.9, 42.6, 41.8, 40.0,

37.1, 36.2, 24.5, 21.9, 20.3. HRMS (ESI^+) mass calculated for $[M+H]^+$ ($C_{27}H_{36}N_6O_7$) m/z 557.2723, found m/z 557.2729; purity ≥95%, rt 1.20 min (protocol B).

NMR Spectra of Peptides

KKS-1-262.1.fid



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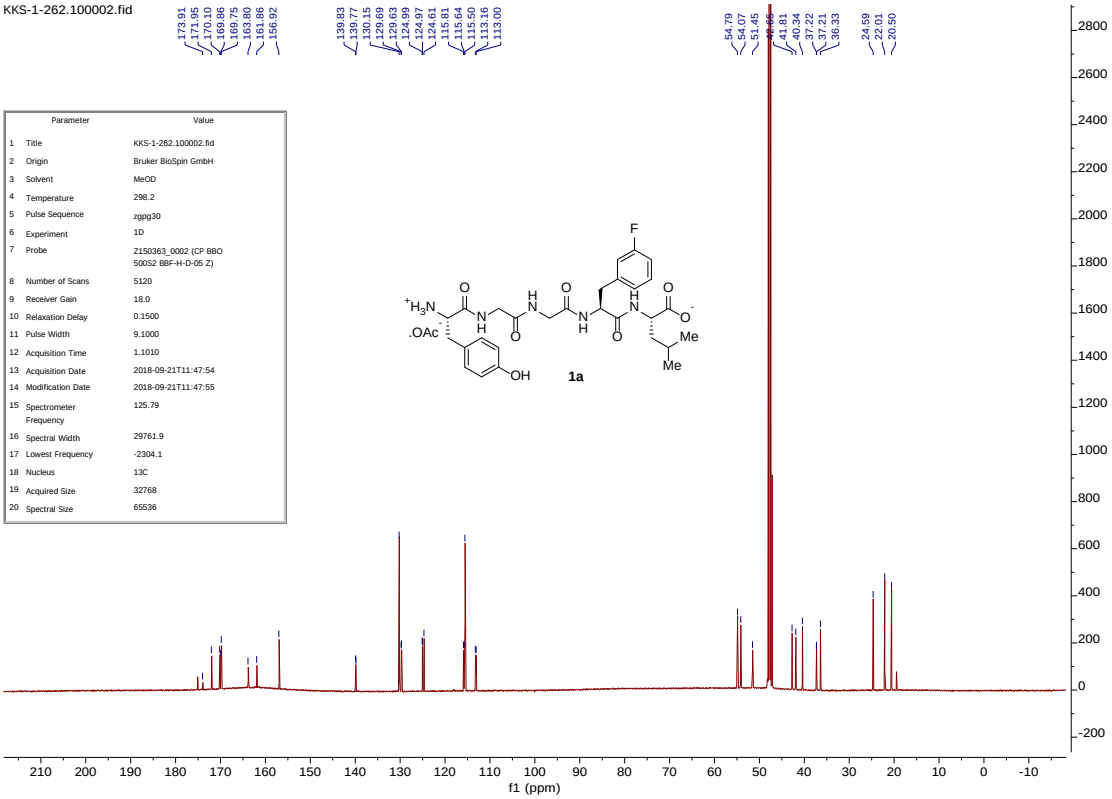
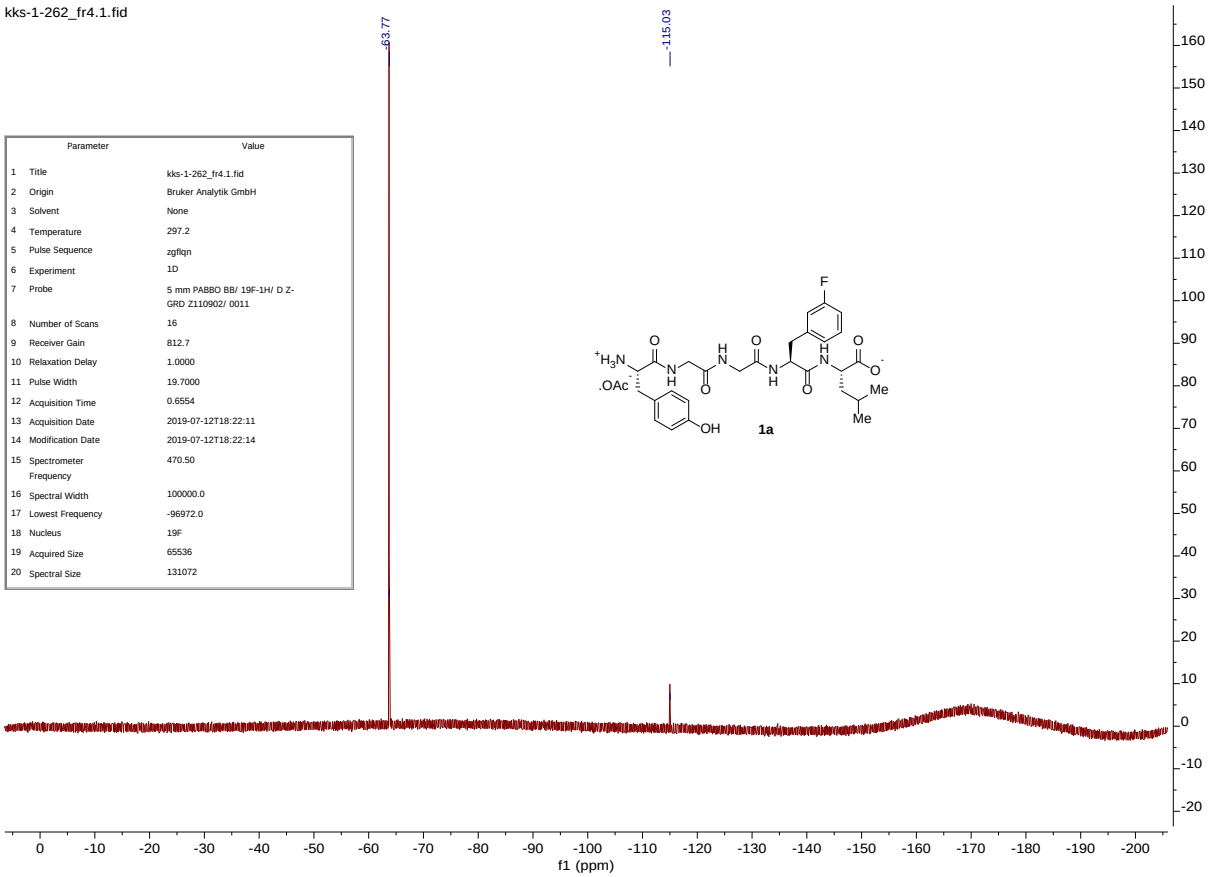
3	Solvent	MeOD
4	Temperature	298.2
5	Pulse Sequence	zg30
6	Experiment	1D
7	Probe	Z150363_0002 (CP BBO 500S2 BBF-H-D-05 Z)
8	Number of Scans	16
9	Receiver Gain	9.0
10	Relaxation Delay	1.0000
11	Pulse Width	12.0000
12	Presaturation Frequency	
13	Acquisition Time	3.2768
14	Acquisition Date	2018-09-21T09:54:10
15	Modification Date	2018-09-21T09:54:11
16	Spectrometer Frequency	500.19
17	Spectral Width	10000.0
18	Lowest Frequency	-1911.3
19	Nucleus	1H
20	Acquired Size	32768
21	Spectral Size	65536

KKS-1-262.100002.fid



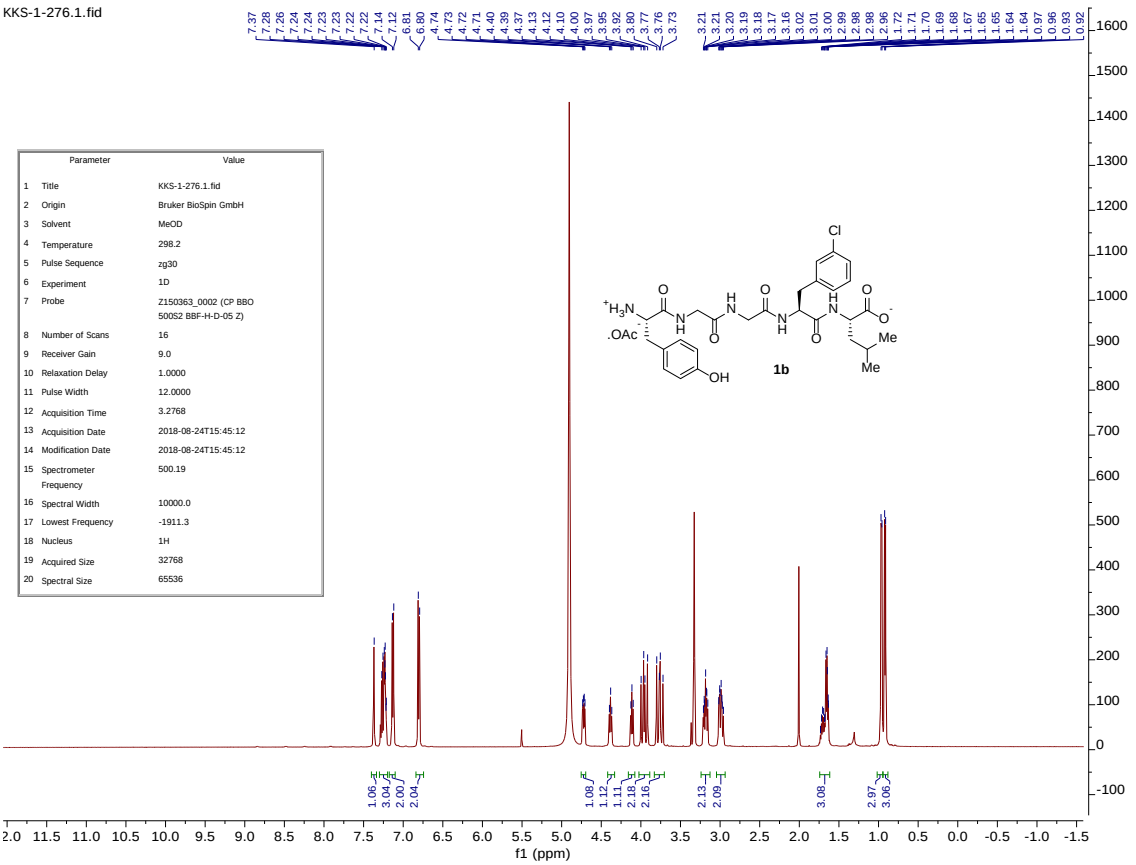
	Parameter	Value
1	Title	KKS-1-262.100002.fid
2	Origin	Bruker BioSpin GmbH
3	Solvent	MeOD
4	Temperature	298.2
5	Pulse Sequence	zgpg30
6	Experiment	1D
7	Probe	Z150363_0002 (CP BBO 500S2 BBF-H-D-05 Z)
8	Number of Scans	5120
9	Receiver Gain	18.0
10	Relaxation Delay	0.1500
11	Pulse Width	9.1000
12	Acquisition Time	1.1010
13	Acquisition Date	2018-09-21T11:47:54
14	Modification Date	2018-09-21T11:47:55
15	Spectrometer Frequency	125.79
16	Spectral Width	29761.9
17	Lowest Frequency	-2304.1
18	Nucleus	13C
19	Acquired Size	32768
20	Spectral Size	65536

kks-1-262_fr4.1.fid

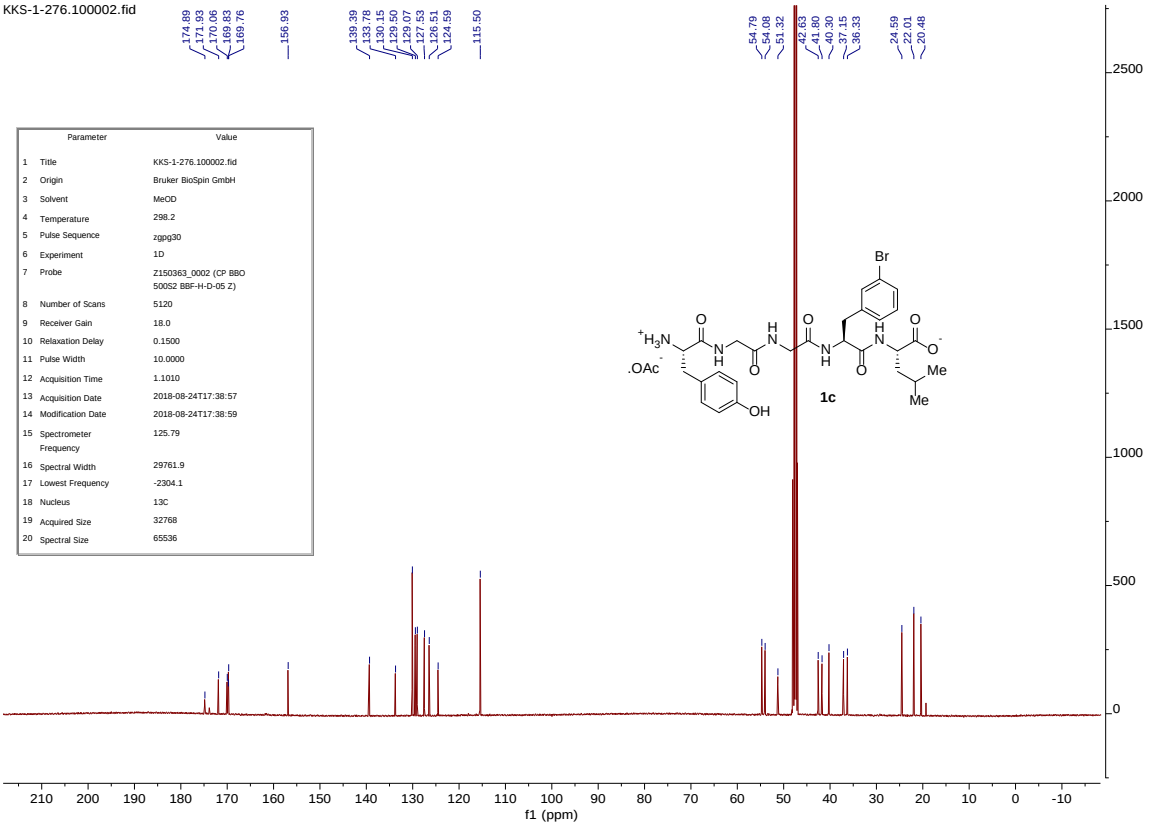


	Parameter	Value
1	Title	kks-1-262_fr4.1.fid
2	Origin	Bruker Analytik GmbH
3	Solvent	None
4	Temperature	297.2
5	Pulse Sequence	zgflqn
6	Experiment	1D
7	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z110902/ 0011
8	Number of Scans	16
9	Receiver Gain	812.7
10	Relaxation Delay	1.0000
11	Pulse Width	19.7000
12	Acquisition Time	0.6554
13	Acquisition Date	2019-07-12T18:22:11
14	Modification Date	2019-07-12T18:22:14
15	Spectrometer Frequency	470.50
16	Spectral Width	100000.0
17	Lowest Frequency	-96972.0
18	Nucleus	19F
19	Acquired Size	65536
20	Spectral Size	131072

1a

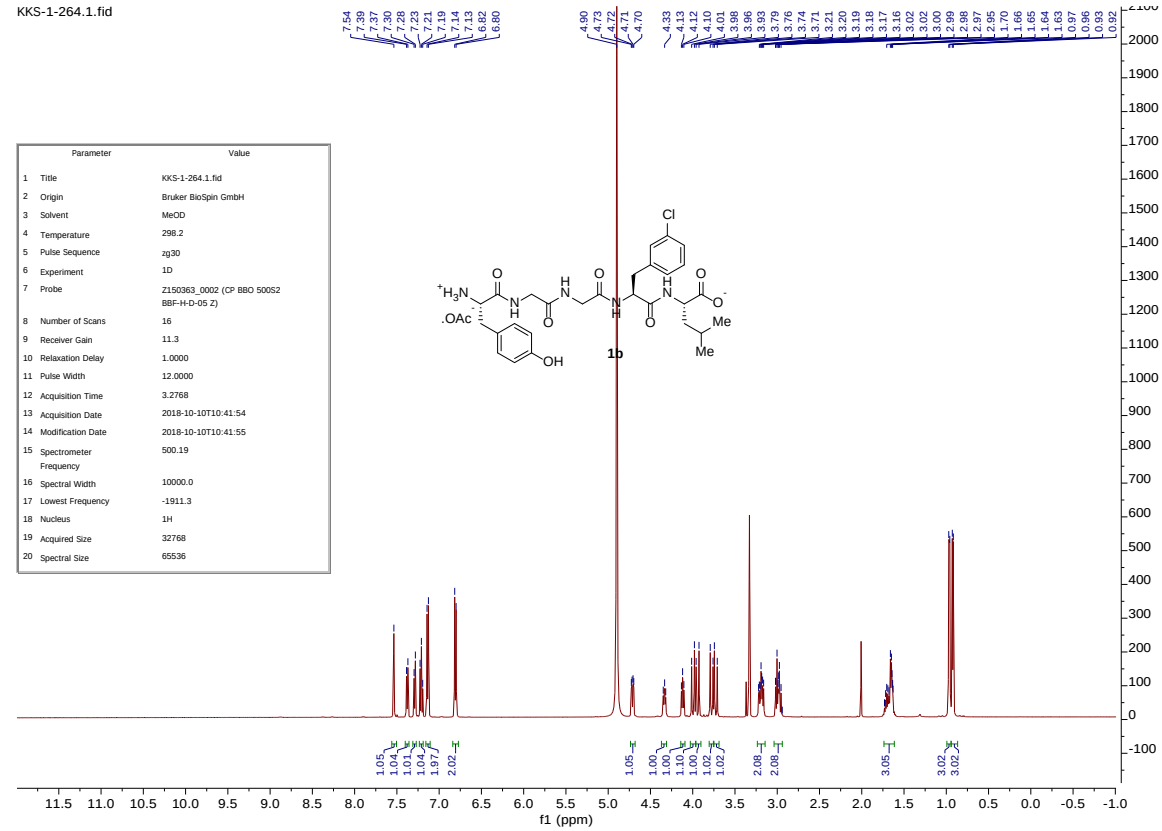

KKS-1-276.1.fid
Parameter Value
1 Title KKS-1-276.1.fid
2 Origin Bruker BioSpin GmbH
3 Solvent MeOD
4 Temperature 298.2
5 Pulse Sequence zg30
6 Experiment 1D
7 Probe Z150363_0002 (CP BBO 500S2 BBF-H-D-05 Z)
8 Number of Scans 16
9 Receiver Gain 9.0
10 Relaxation Delay 1.0000
11 Pulse Width 12.0000
12 Acquisition Time 3.2768
13 Acquisition Date 2018-08-24T15:45:12
14 Modification Date 2018-08-24T15:45:12
15 Spectrometer Frequency 500.19
16 Spectral Width 10000.0
17 Lowest Frequency -1911.3
18 Nucleus 1H
19 Acquired Size 32768
20 Spectral Size 65536
1b
f1 (ppm)

KKS-1-276.100002.fid

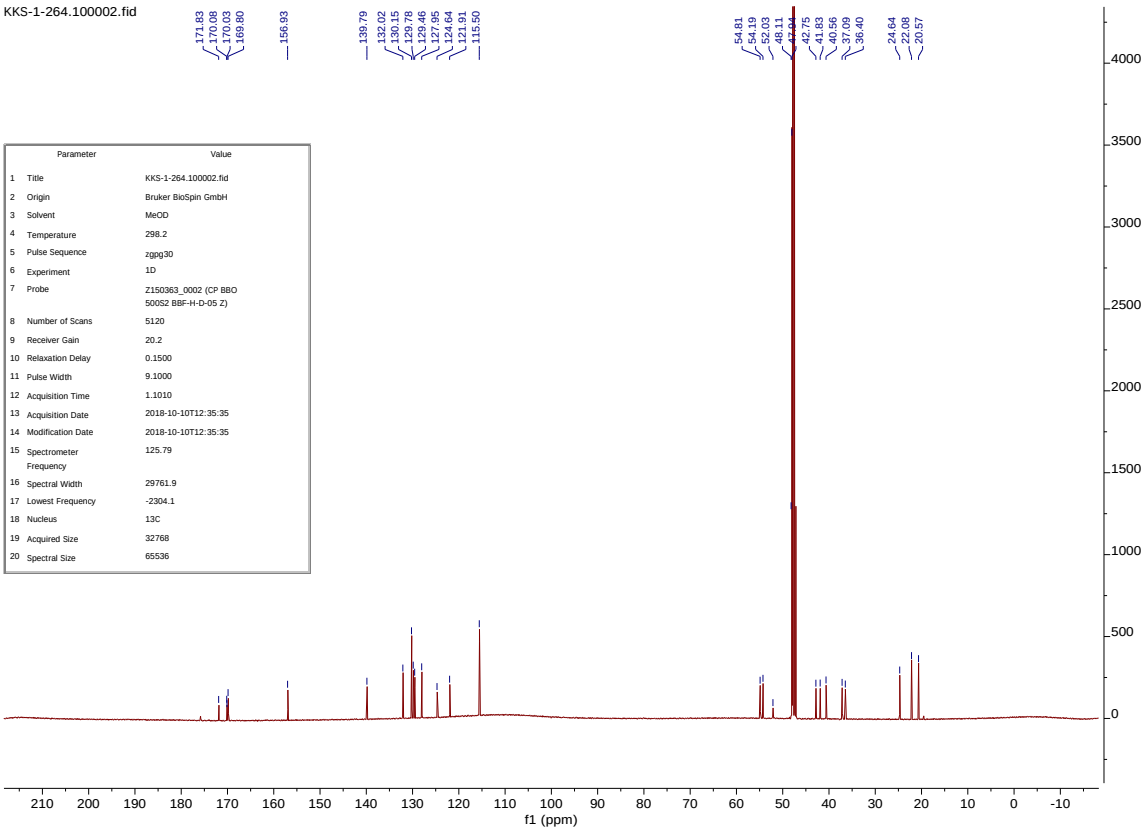


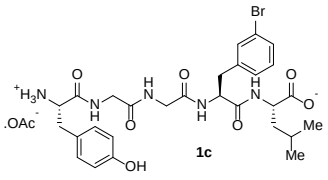
	Parameter	Value
1	Title	KKS-1-276.100002.fid
2	Origin	Bruker BioSpin GmbH
3	Solvent	MeOD
4	Temperature	298.2
5	Pulse Sequence	zgpg30
6	Experiment	1D
7	Probe	Z150363_0002 (CP BBO 500S2 BBF-H-D-05 Z)
8	Number of Scans	5120
9	Receiver Gain	18.0
10	Relaxation Delay	0.1500
11	Pulse Width	10.0000
12	Acquisition Time	1.1010
13	Acquisition Date	2018-08-24T17:38:57
14	Modification Date	2018-08-24T17:38:59
15	Spectrometer Frequency	125.79
16	Spectral Width	29761.9
17	Lowest Frequency	-2304.1
18	Nucleus	13C
19	Acquired Size	32768
20	Spectral Size	65536

KKS-1-264.1.fid



	Parameter	Value
1	Title	KKS-1-264.1.fid
2	Origin	Bruker BioSpin GmbH
3	Solvent	MeOD
4	Temperature	298.2
5	Pulse Sequence	zg30
6	Experiment	1D
7	Probe	Z150363_0002 (CP BBO 500S2 BBF-H-D-05 Z)
8	Number of Scans	16
9	Receiver Gain	11.3
10	Relaxation Delay	1.0000
11	Pulse Width	12.0000
12	Acquisition Time	3.2768
13	Acquisition Date	2018-10-10T10:41:54
14	Modification Date	2018-10-10T10:41:55
15	Spectrometer Frequency	500.19
16	Spectral Width	10000.0
17	Lowest Frequency	-1911.3
18	Nucleus	1H
19	Acquired Size	32768
20	Spectral Size	65536

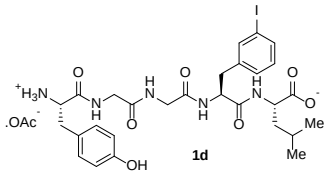

KKS-1-264.100002.fid
171.83
170.08
170.03
169.80
156.93
139.79
132.02
130.15
129.78
129.46
127.95
124.64
121.91
115.50
54.81
54.19
52.03
48.11
47.04
42.75
41.83
40.56
37.09
36.40
24.64
22.08
20.57
Parameter Value
1 Title KKS-1-264.100002.fid
2 Origin Bruker BioSpin GmbH
3 Solvent MeOD
4 Temperature 298.2
5 Pulse Sequence zgpg30
6 Experiment 1D
7 Probe Z150363_0002 (CP BBO 500S2 BBF-H-D-05 Z)
8 Number of Scans 5120
9 Receiver Gain 20.2
10 Relaxation Delay 0.1500
11 Pulse Width 9.1000
12 Acquisition Time 1.1010
13 Acquisition Date 2018-10-10T12:35:35
14 Modification Date 2018-10-10T12:35:35
15 Spectrometer Frequency 125.79
16 Spectral Width 29761.9
17 Lowest Frequency -2304.1
18 Nucleus 13C
19 Acquired Size 32768
20 Spectral Size 65536
4000
3500
3000
2500
2000
1500
1000
500
0
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


Br
+H3N
.OAc-
OH
Me
Me

1c

KKS-1-286.1.fid

	Parameter	Value
1	Title	KKS-1-286.1.fid
2	Origin	Bruker BioSpin GmbH
3	Solvent	MeOD
4	Temperature	298.2
5	Pulse Sequence	zg30
6	Experiment	1D
7	Probe	Z150363_0002 (CP BBO 500S2 BBF-H-D-05 Z)
8	Number of Scans	16
9	Receiver Gain	11.3
10	Relaxation Delay	1.0000
11	Pulse Width	12.0000
12	Acquisition Time	3.2768
13	Acquisition Date	2018-09-24T07:09:40
14	Modification Date	2018-09-24T07:09:40
15	Spectrometer Frequency	500.19
16	Spectral Width	10000.0
17	Lowest Frequency	-1911.3
18	Nucleus	1H
19	Acquired Size	32768
20	Spectral Size	65536

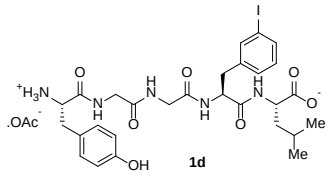


1d

f1 (ppm)

KKS-1-286.100002.fid

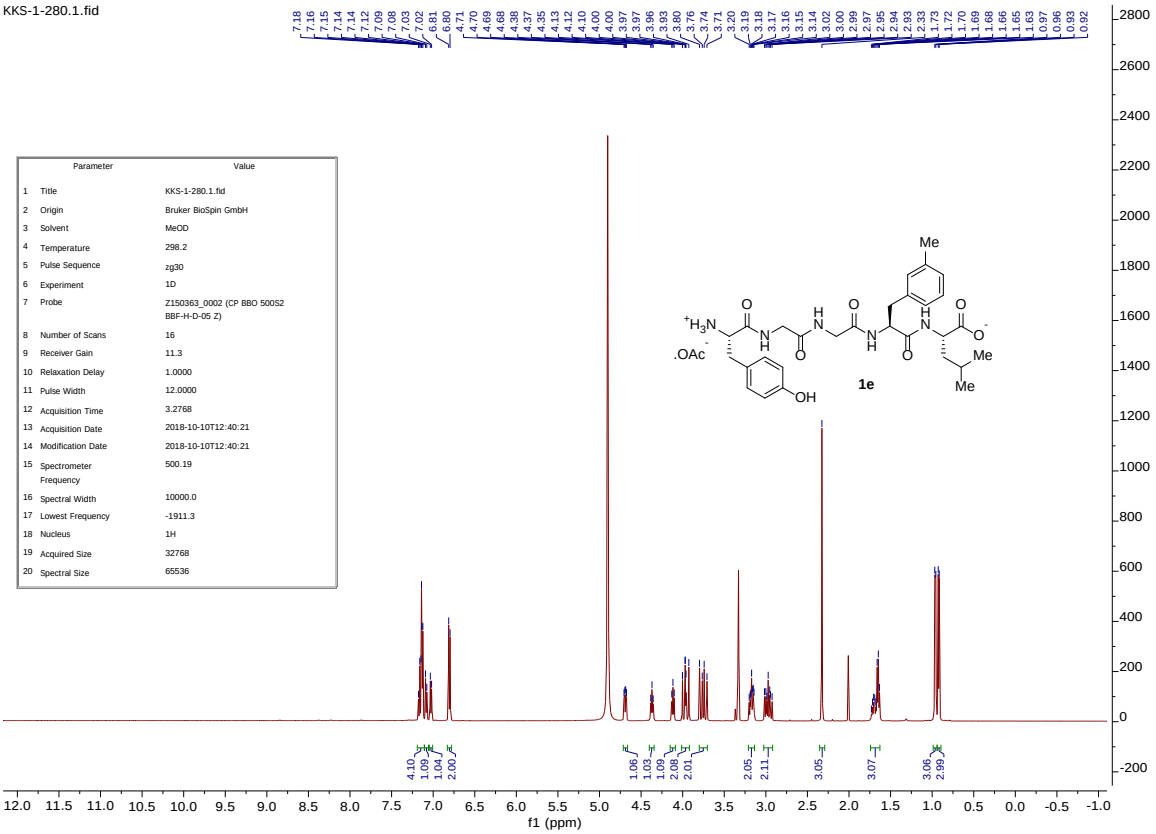
	Parameter	Value
1	Title	KKS-1-286.100002.fid
2	Origin	Bruker BioSpin GmbH
3	Solvent	MeOD
4	Temperature	298.2
5	Pulse Sequence	zgpg30
6	Experiment	1D
7	Probe	Z150363_0002 (CP BBO 500S2 BBF-H-D-05 Z)
8	Number of Scans	5120
9	Receiver Gain	16.0
10	Relaxation Delay	0.1500
11	Pulse Width	9.1000
12	Acquisition Time	1.1010
13	Acquisition Date	2018-09-24T09:03:20
14	Modification Date	2018-09-24T09:03:20
15	Spectrometer Frequency	125.79
16	Spectral Width	29761.9
17	Lowest Frequency	-2304.1
18	Nucleus	13C
19	Acquired Size	32768
20	Spectral Size	65536



1d

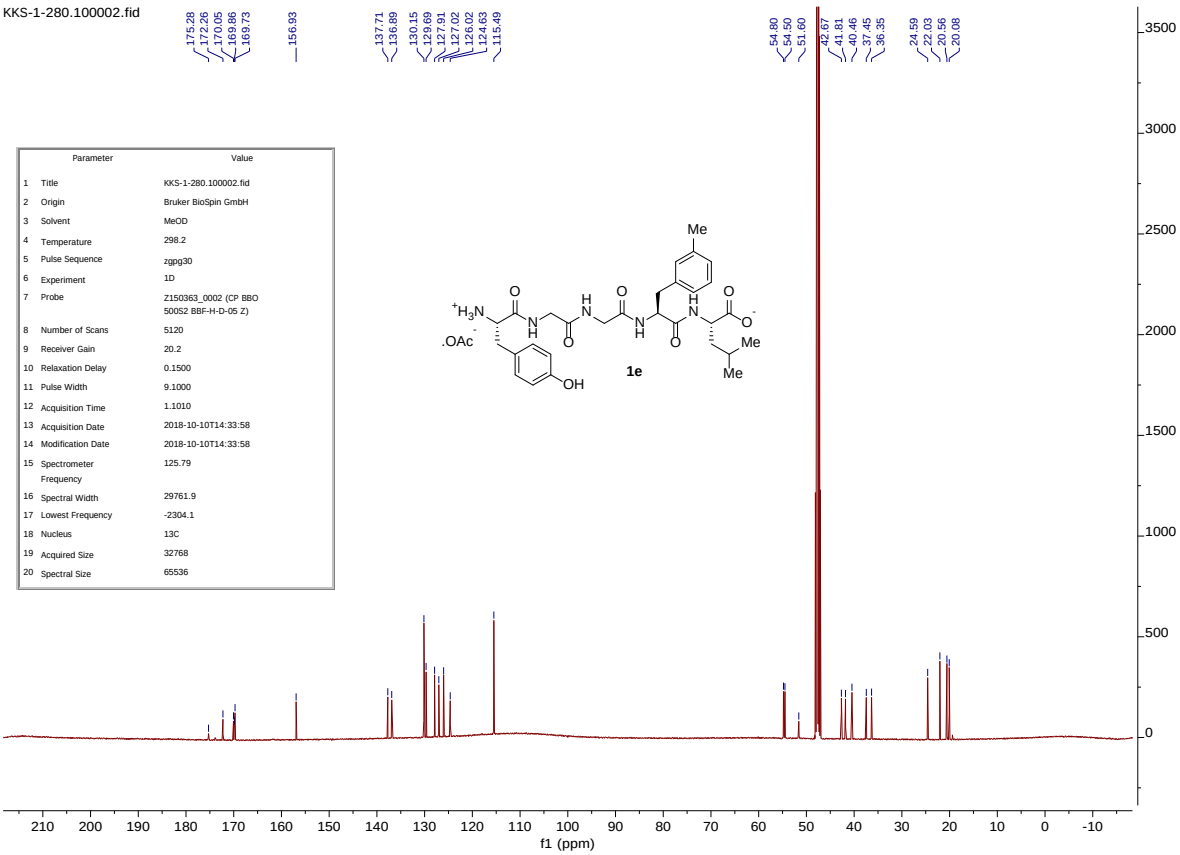
f1 (ppm)

KKS-1-280.1.fid



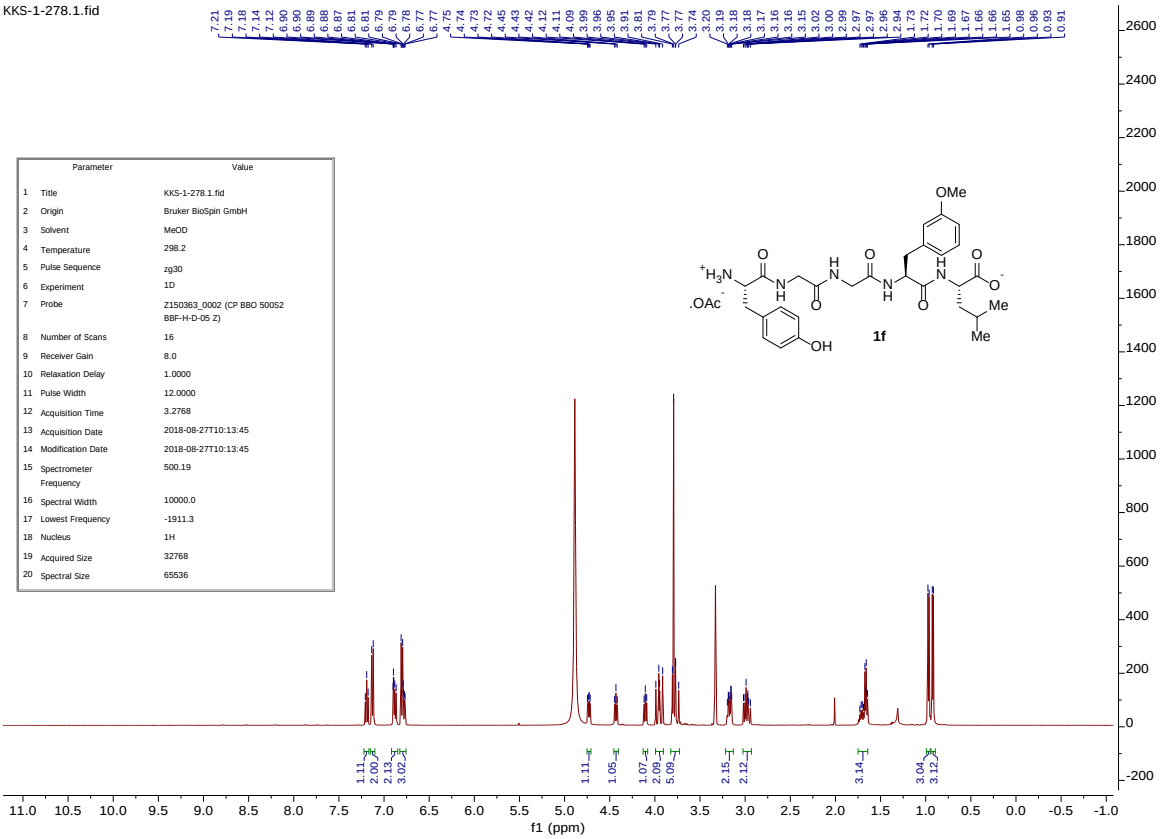
	Parameter	Value
1	Title	KKS-1-280.1.fid
2	Origin	Bruker BioSpin GmbH
3	Solvent	MeOD
4	Temperature	298.2
5	Pulse Sequence	zg30
6	Experiment	1D
7	Probe	Z150363_0002 (CP BBO 500S2 BBF-H-D-05 Z)
8	Number of Scans	16
9	Receiver Gain	11.3
10	Relaxation Delay	1.0000
11	Pulse Width	12.0000
12	Acquisition Time	3.2768
13	Acquisition Date	2018-10-10T12:40:21
14	Modification Date	2018-10-10T12:40:21
15	Spectrometer Frequency	500.19
16	Spectral Width	10000.0
17	Lowest Frequency	-1911.3
18	Nucleus	1H
19	Acquired Size	32768
20	Spectral Size	65536

KKS-1-280.100002.fid



	Parameter	Value
1	Title	KKS-1-280.100002.fid
2	Origin	Bruker BioSpin GmbH
3	Solvent	MeOD
4	Temperature	298.2
5	Pulse Sequence	zgpg30
6	Experiment	1D
7	Probe	Z150363_0002 (CP BBO 500S2 BBF-H-D-05 Z)
8	Number of Scans	5120
9	Receiver Gain	20.2
10	Relaxation Delay	0.1500
11	Pulse Width	9.1000
12	Acquisition Time	1.1010
13	Acquisition Date	2018-10-10T14:33:58
14	Modification Date	2018-10-10T14:33:58
15	Spectrometer Frequency	125.79
16	Spectral Width	29761.9
17	Lowest Frequency	-2304.1
18	Nucleus	13C
19	Acquired Size	32768
20	Spectral Size	65536

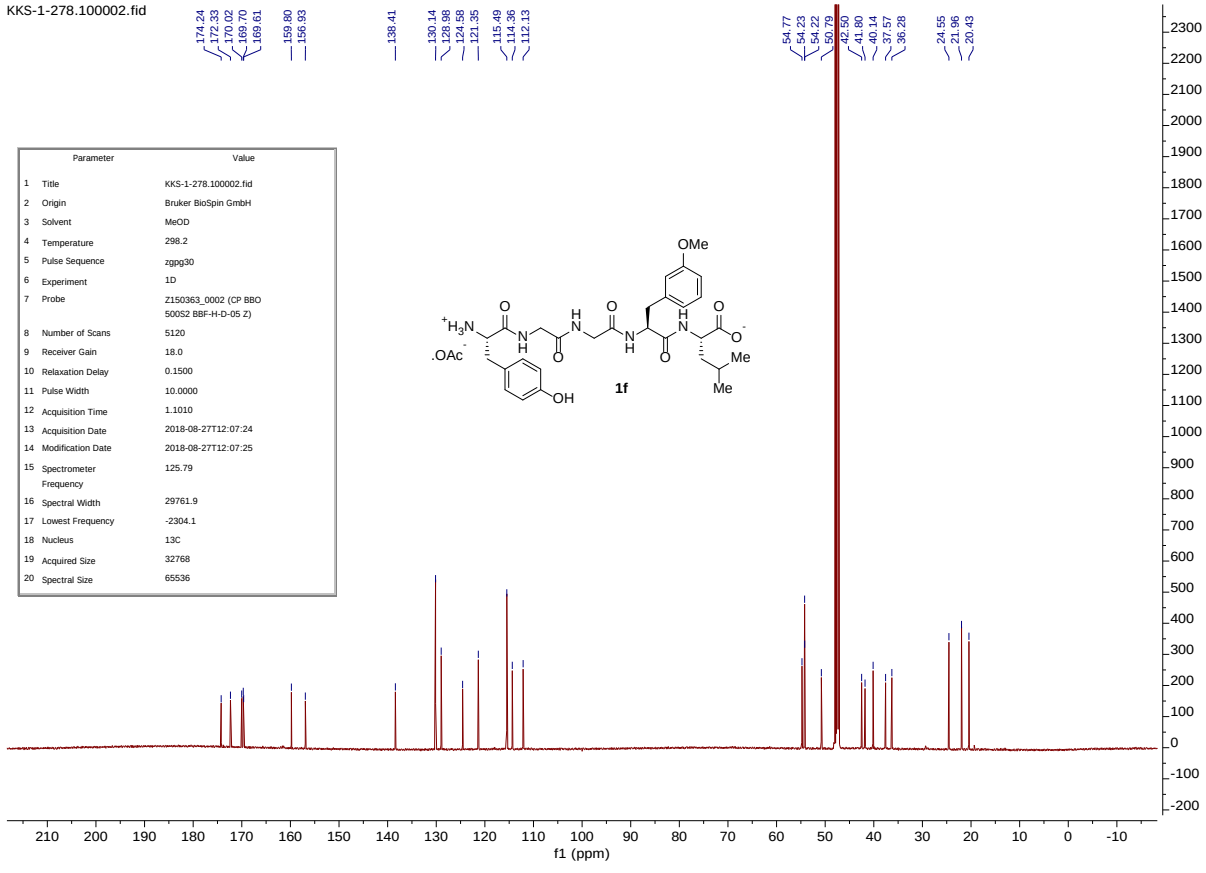
KKS-1-278.1.fid



	Parameter	Value
1	Title	KKS-1-278.1.fid
2	Origin	Bruker BioSpin GmbH
3	Solvent	MeOD
4	Temperature	298.2
5	Pulse Sequence	zg30
6	Experiment	1D
7	Probe	Z150363_0002 (CP BBO 500S2 BBF-H-D-05 Z)
8	Number of Scans	16
9	Receiver Gain	8.0
10	Relaxation Delay	1.0000
11	Pulse Width	12.0000
12	Acquisition Time	3.2768
13	Acquisition Date	2018-08-27T10:13:45
14	Modification Date	2018-08-27T10:13:45
15	Spectrometer Frequency	500.19
16	Spectral Width	10000.0
17	Lowest Frequency	-1911.3
18	Nucleus	1H
19	Acquired Size	32768
20	Spectral Size	65536

1f

KKS-1-278.100002.fid

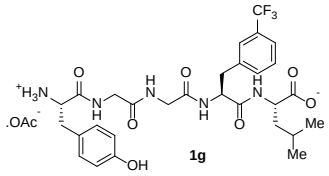


	Parameter	Value
1	Title	KKS-1-278.100002.fid
2	Origin	Bruker BioSpin GmbH
3	Solvent	MeOD
4	Temperature	298.2
5	Pulse Sequence	zgpg30
6	Experiment	1D
7	Probe	Z150363_0002 (CP BBO 500S2 BBF-H-D-05 Z)
8	Number of Scans	5120
9	Receiver Gain	18.0
10	Relaxation Delay	0.1500
11	Pulse Width	10.0000
12	Acquisition Time	1.1010
13	Acquisition Date	2018-08-27T12:07:24
14	Modification Date	2018-08-27T12:07:25
15	Spectrometer Frequency	125.79
16	Spectral Width	29761.9
17	Lowest Frequency	-2304.1
18	Nucleus	13C
19	Acquired Size	32768
20	Spectral Size	65536

1f

KKS-1-290.1.fid

	Parameter	Value
1	Title	KKS-1-290.1.fid
2	Origin	Bruker BioSpin GmbH
3	Solvent	MeOD
4	Temperature	298.2
5	Pulse Sequence	zg30
6	Experiment	1D
7	Probe	Z150363_0002 (CP BBO 500S2 BBF-H-D-05 Z)
8	Number of Scans	16
9	Receiver Gain	9.0
10	Relaxation Delay	1.0000
11	Pulse Width	12.0000
12	Acquisition Time	3.2768
13	Acquisition Date	2018-09-20T09:57:18
14	Modification Date	2018-09-20T09:57:18
15	Spectrometer Frequency	500.19
16	Spectral Width	10000.0
17	Lowest Frequency	-1911.3
18	Nucleus	1H
19	Acquired Size	32768
20	Spectral Size	65536

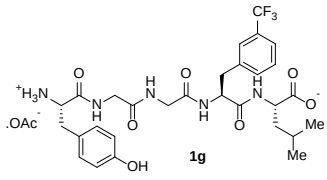


1g

f1 (ppm)

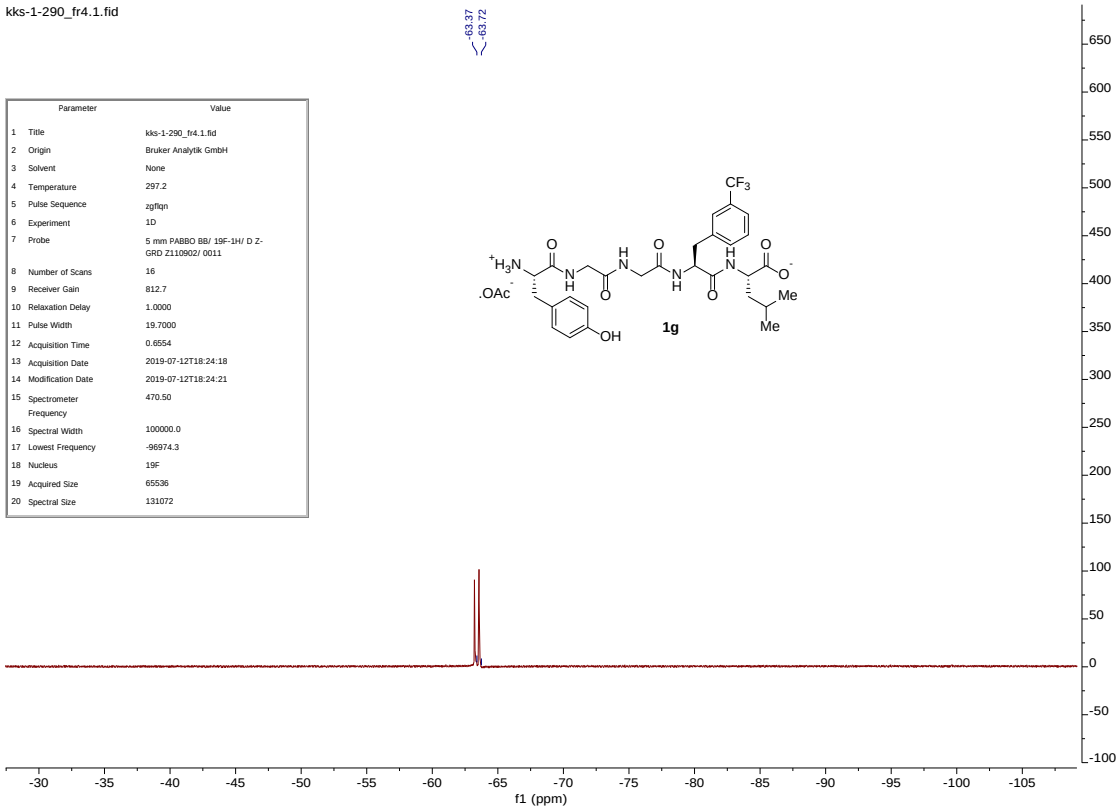
KKS-1-290.100002.fid

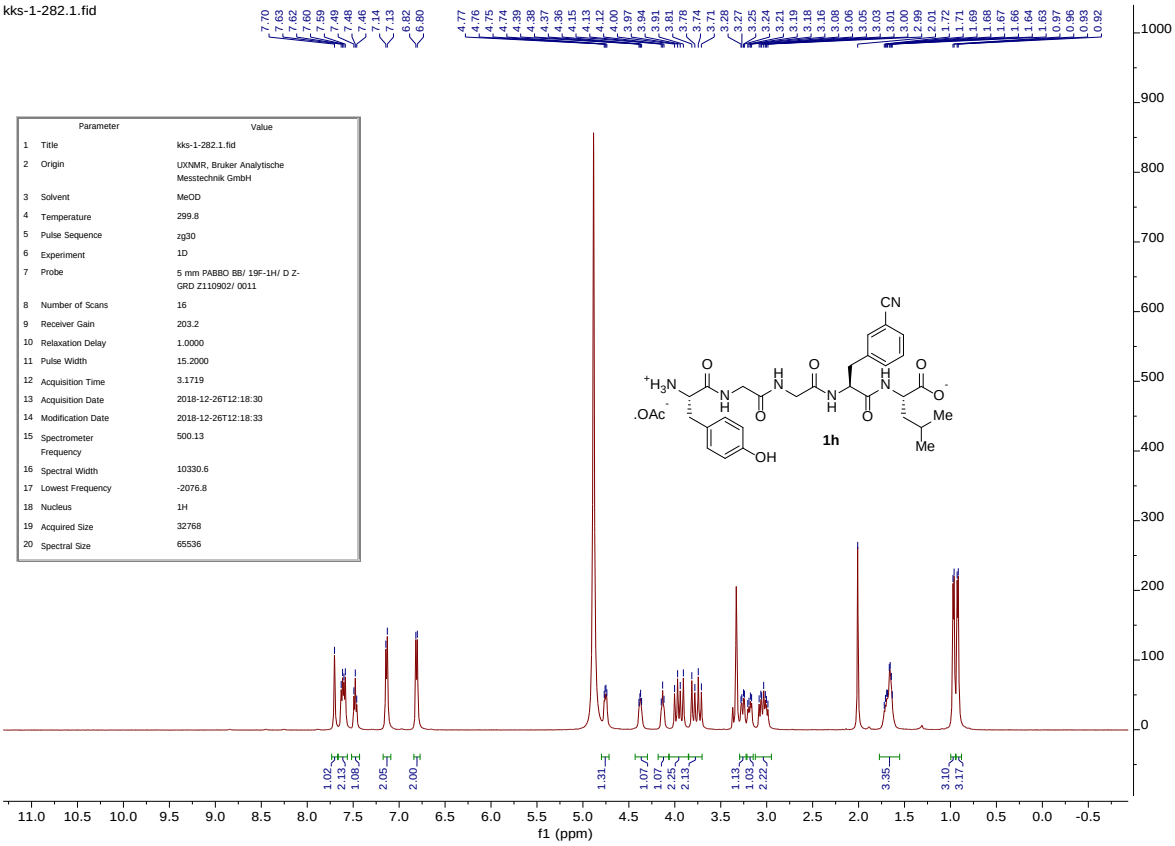
	Parameter	Value
1	Title	KKS-1-290.100002.fid
2	Origin	Bruker BioSpin GmbH
3	Solvent	MeOD
4	Temperature	298.2
5	Pulse Sequence	zgpg30
6	Experiment	1D
7	Probe	Z150363_0002 (CP BBO 500S2 BBF-H-D-05 Z)
8	Number of Scans	5120
9	Receiver Gain	18.0
10	Relaxation Delay	0.1500
11	Pulse Width	9.1000
12	Acquisition Time	1.1010
13	Acquisition Date	2018-09-20T11:51:08
14	Modification Date	2018-09-20T11:51:08
15	Spectrometer Frequency	125.79
16	Spectral Width	29761.9
17	Lowest Frequency	-2304.1
18	Nucleus	13C
19	Acquired Size	32768
20	Spectral Size	65536

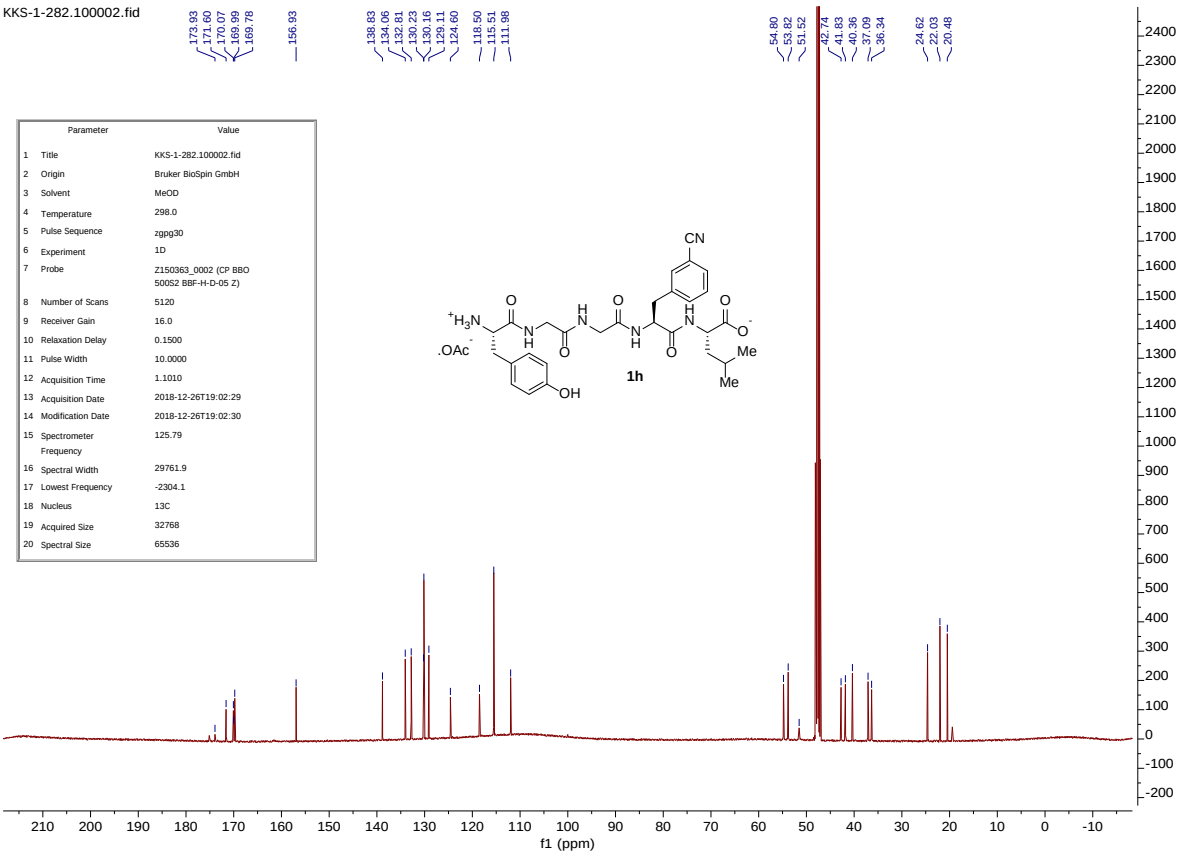


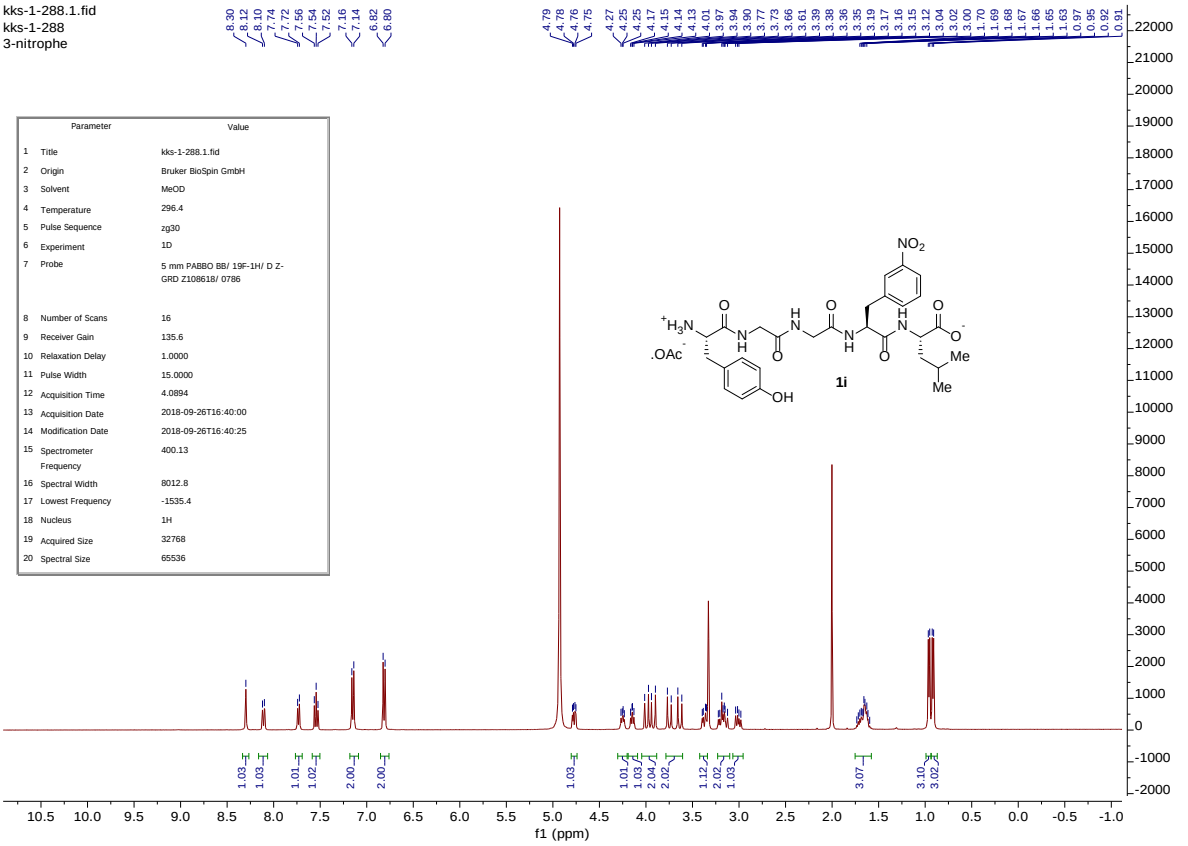
1g

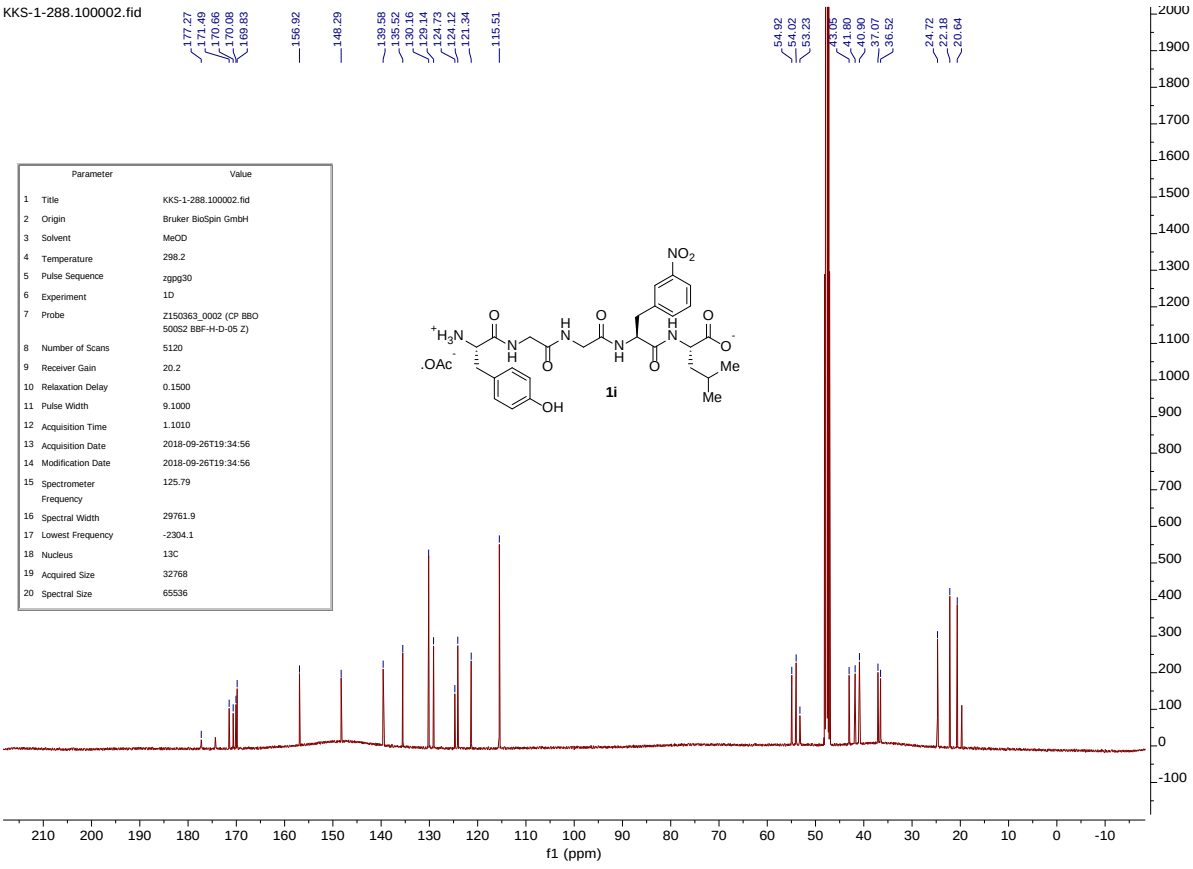
f1 (ppm)


kks-1-290_fr4.1.fid
-63.37
-63.72
Parameter Value
1 Title kks-1-290_fr4.1.fid
2 Origin Bruker Analytik GmbH
3 Solvent None
4 Temperature 297.2
5 Pulse Sequence zgflqn
6 Experiment 1D
7 Probe 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z110902/ 0011
8 Number of Scans 16
9 Receiver Gain 812.7
10 Relaxation Delay 1.0000
11 Pulse Width 19.7000
12 Acquisition Time 0.6554
13 Acquisition Date 2019-07-12T18:24:18
14 Modification Date 2019-07-12T18:24:21
15 Spectrometer Frequency 470.50
16 Spectral Width 100000.0
17 Lowest Frequency -96974.3
18 Nucleus 19F
19 Acquired Size 65536
20 Spectral Size 131072
CF3
+H3N
.OAc
OH
Me
Me
1g
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
-100
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
-105
f1 (ppm)

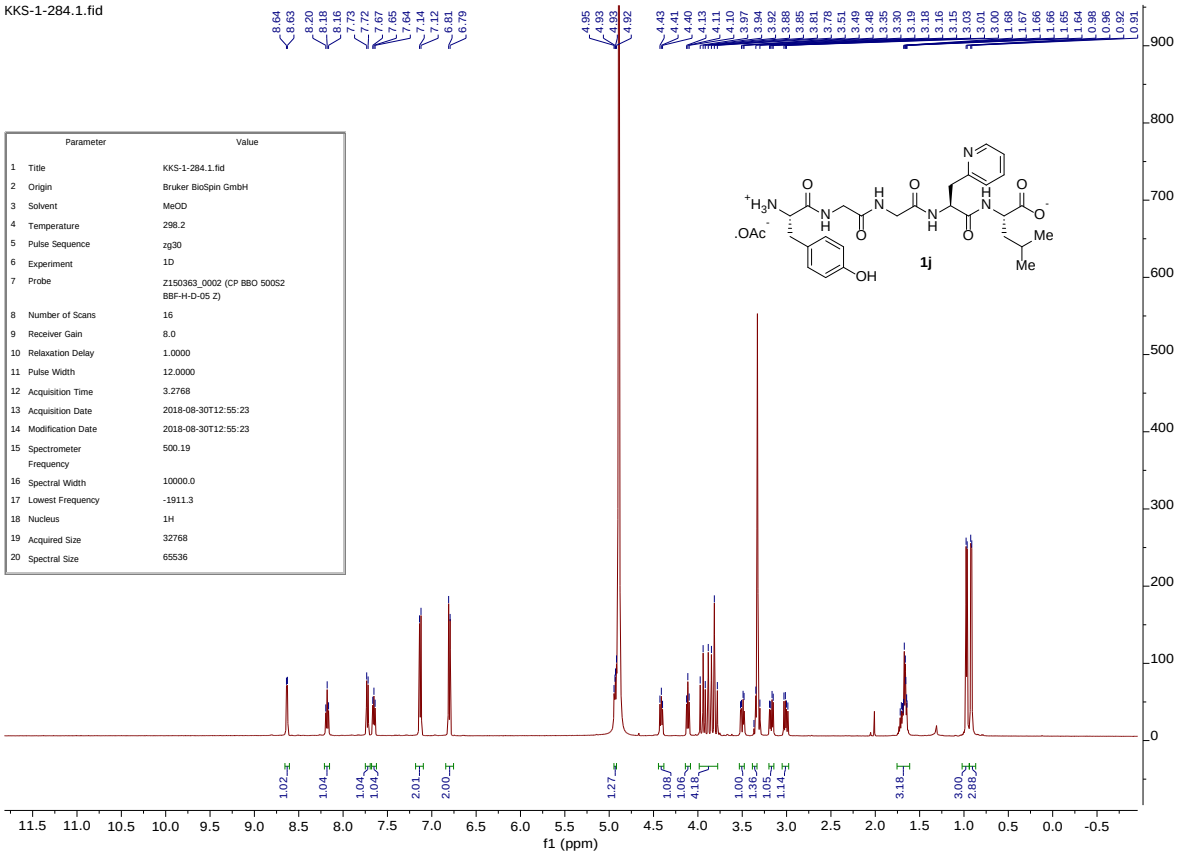

kks-1-282.1.fid
7.70 7.63 7.62 7.60 7.59 7.49 7.48 7.46 7.14 7.13 6.82 6.80
4.77 4.76 4.75 4.74 4.39 4.38 4.37 4.36 4.15 4.13 4.12 4.00 3.97 3.94 3.91 3.81 3.78 3.74 3.71 3.28 3.27 3.25 3.24 3.21 3.19 3.18 3.16 3.08 3.06 3.05 3.03 3.01 3.00 2.99 2.01 1.72 1.71 1.69 1.68 1.67 1.66 1.64 1.63 0.97 0.96 0.93 0.92
Parameter Value
1 Title kks-1-282.1.fid
2 Origin UXNMR, Bruker Analytische Messtechnik GmbH
3 Solvent MeOD
4 Temperature 299.8
5 Pulse Sequence zg30
6 Experiment 1D
7 Probe 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z110902/ 0011
8 Number of Scans 16
9 Receiver Gain 203.2
10 Relaxation Delay 1.0000
11 Pulse Width 15.2000
12 Acquisition Time 3.1719
13 Acquisition Date 2018-12-26T12:18:30
14 Modification Date 2018-12-26T12:18:33
15 Spectrometer Frequency 500.13
16 Spectral Width 10330.6
17 Lowest Frequency -2076.8
18 Nucleus 1H
19 Acquired Size 32768
20 Spectral Size 65536
CN
+H3N
.OAc
OH
Me
Me
1h
1.02 2.13 1.08 2.05 2.00 1.31 1.07 1.07 2.25 2.13 1.13 1.03 2.22 3.35 3.10 3.17
f1 (ppm)


KKS-1-282.100002.fid
173.93 171.60 170.07 169.99 169.78 156.93 138.83 134.06 131.81 130.23 130.16 129.11 124.60 118.50 115.51 111.98 54.80 53.82 51.52 42.74 41.83 40.36 37.09 36.34 24.62 22.03 20.48
Parameter Value
1 Title KKS-1-282.100002.fid
2 Origin Bruker BioSpin GmbH
3 Solvent MeOD
4 Temperature 298.0
5 Pulse Sequence zgpg30
6 Experiment 1D
7 Probe Z150363_0002 (CP BBO 500S2 BBF-H-D-05 Z)
8 Number of Scans 5120
9 Receiver Gain 16.0
10 Relaxation Delay 0.1500
11 Pulse Width 10.0000
12 Acquisition Time 1.1010
13 Acquisition Date 2018-12-26T19:02:29
14 Modification Date 2018-12-26T19:02:30
15 Spectrometer Frequency 125.79
16 Spectral Width 29761.9
17 Lowest Frequency -2304.1
18 Nucleus 13C
19 Acquired Size 32768
20 Spectral Size 65536
CN
+H3N
.OAc
OH
Me
Me
1h
f1 (ppm)


kks-1-288.1.fid
kks-1-288
3-nitrophe
8.30 8.12 8.10 7.74 7.72 7.56 7.54 7.52 7.16 7.14 6.82 6.80
4.79 4.78 4.76 4.75 4.27 4.25 4.25 4.17 4.15 4.14 4.13 4.01 3.97 3.94 3.90 3.77 3.73 3.66 3.61 3.39 3.38 3.36 3.35 3.19 3.17 3.16 3.15 3.12 3.04 3.02 3.00 1.70 1.69 1.68 1.67 1.66 1.65 1.63 0.97 0.95 0.92 0.91
Parameter Value
1 Title kks-1-288.1.fid
2 Origin Bruker BioSpin GmbH
3 Solvent MeOD
4 Temperature 296.4
5 Pulse Sequence zg30
6 Experiment 1D
7 Probe 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0786
8 Number of Scans 16
9 Receiver Gain 135.6
10 Relaxation Delay 1.0000
11 Pulse Width 15.0000
12 Acquisition Time 4.0894
13 Acquisition Date 2018-09-26T16:40:00
14 Modification Date 2018-09-26T16:40:25
15 Spectrometer Frequency 400.13
16 Spectral Width 8012.8
17 Lowest Frequency -1535.4
18 Nucleus 1H
19 Acquired Size 32768
20 Spectral Size 65536
1i
1.03 1.03 1.01 1.02 2.00 2.00 1.03 1.01 1.03 2.04 2.02 1.12 2.02 1.03 3.07 3.10 3.02
f1 (ppm)

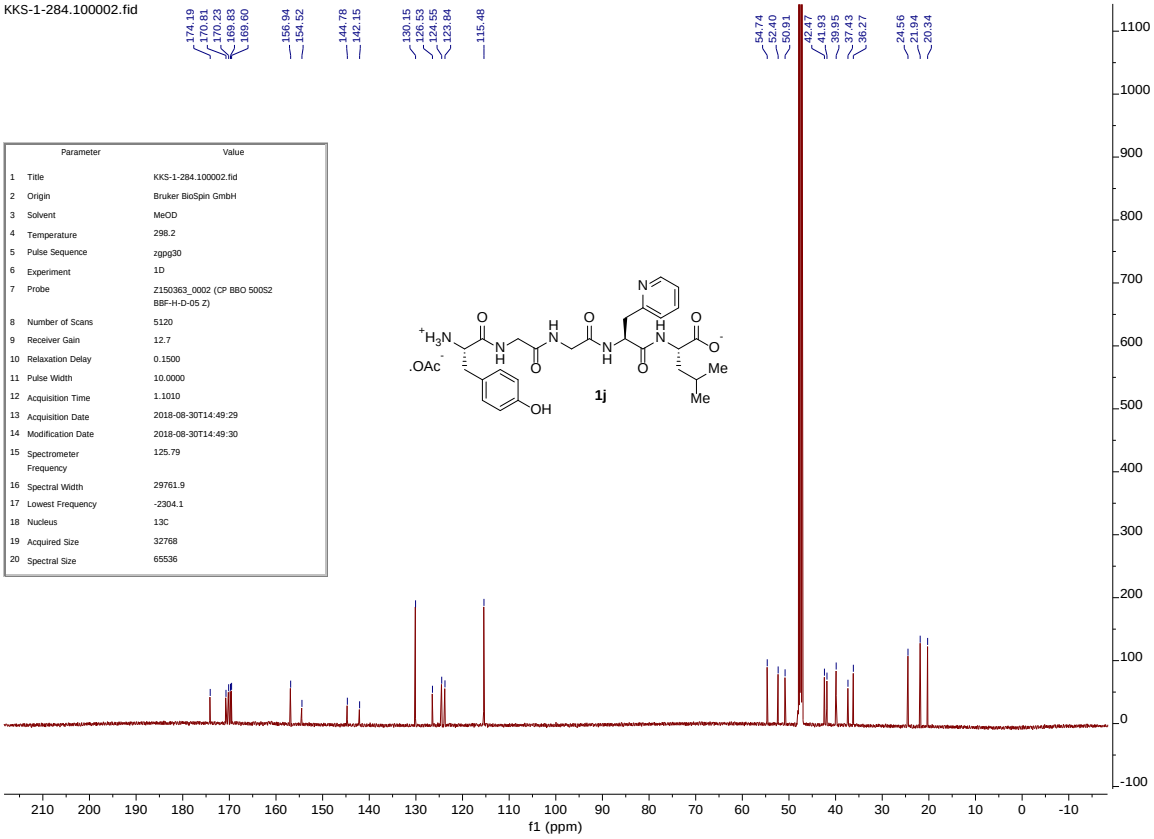

KKS-1-288.100002.fid
177.27 171.49 170.66 170.08 169.83 156.92 148.29 139.58 135.52 130.16 129.14 124.73 124.12 121.34 115.51
54.92 54.02 53.23 43.05 41.80 40.90 37.07 36.52 24.72 22.18 20.64
Parameter Value
1 Title KKS-1-288.100002.fid
2 Origin Bruker BioSpin GmbH
3 Solvent MeOD
4 Temperature 298.2
5 Pulse Sequence zgpg30
6 Experiment 1D
7 Probe Z150363_0002 (CP BBO 500S2 BBF-H-D-05 Z)
8 Number of Scans 5120
9 Receiver Gain 20.2
10 Relaxation Delay 0.1500
11 Pulse Width 9.1000
12 Acquisition Time 1.1010
13 Acquisition Date 2018-09-26T19:34:56
14 Modification Date 2018-09-26T19:34:56
15 Spectrometer Frequency 125.79
16 Spectral Width 29761.9
17 Lowest Frequency -2304.1
18 Nucleus 13C
19 Acquired Size 32768
20 Spectral Size 65536
1i
f1 (ppm)

KKS-1-284.1.fid

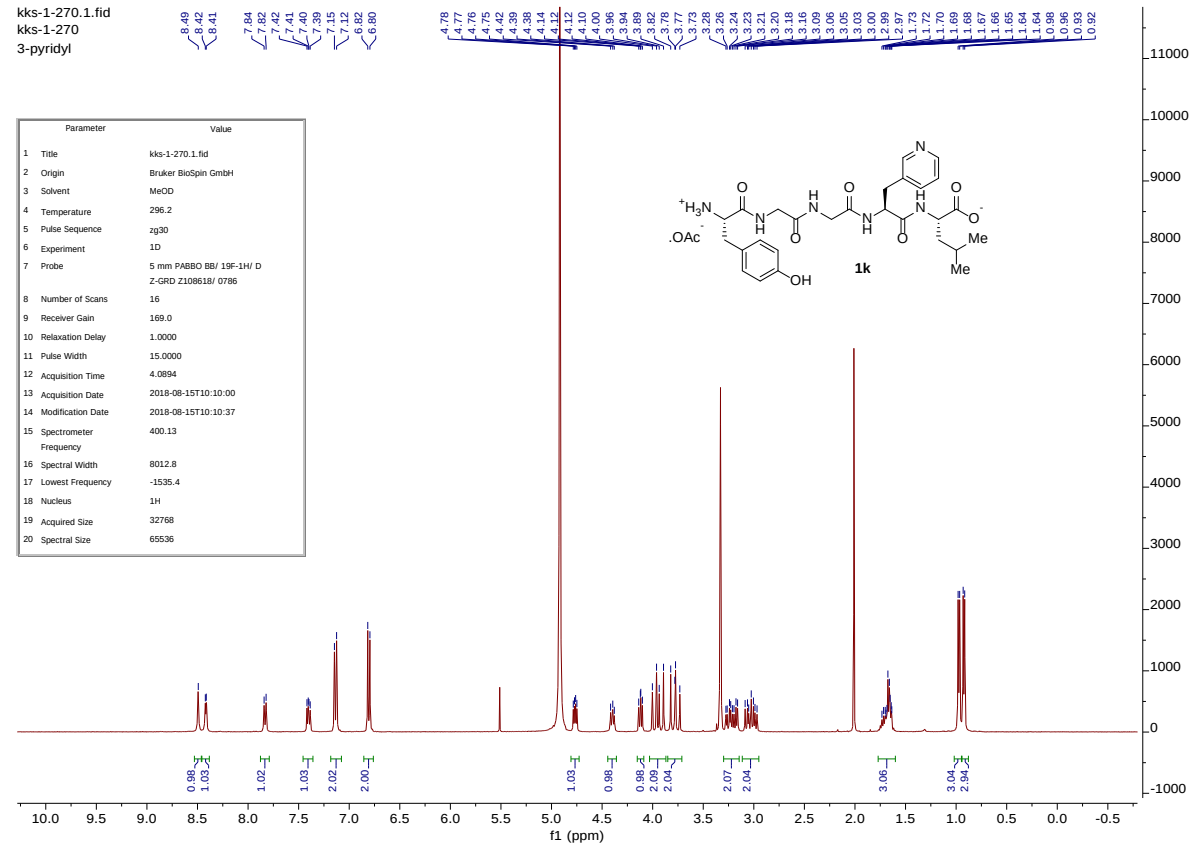


	Parameter	Value
1	Title	KKS-1-284.1.fid
2	Origin	Bruker BioSpin GmbH
3	Solvent	MeOD
4	Temperature	298.2
5	Pulse Sequence	zg30
6	Experiment	1D
7	Probe	Z150363_0002 (CP BBO 500S2 BBF-H-D-05 Z)
8	Number of Scans	16
9	Receiver Gain	8.0
10	Relaxation Delay	1.0000
11	Pulse Width	12.0000
12	Acquisition Time	3.2768
13	Acquisition Date	2018-08-30T12:55:23
14	Modification Date	2018-08-30T12:55:23
15	Spectrometer Frequency	500.19
16	Spectral Width	10000.0
17	Lowest Frequency	-1911.3
18	Nucleus	1H
19	Acquired Size	32768
20	Spectral Size	65536

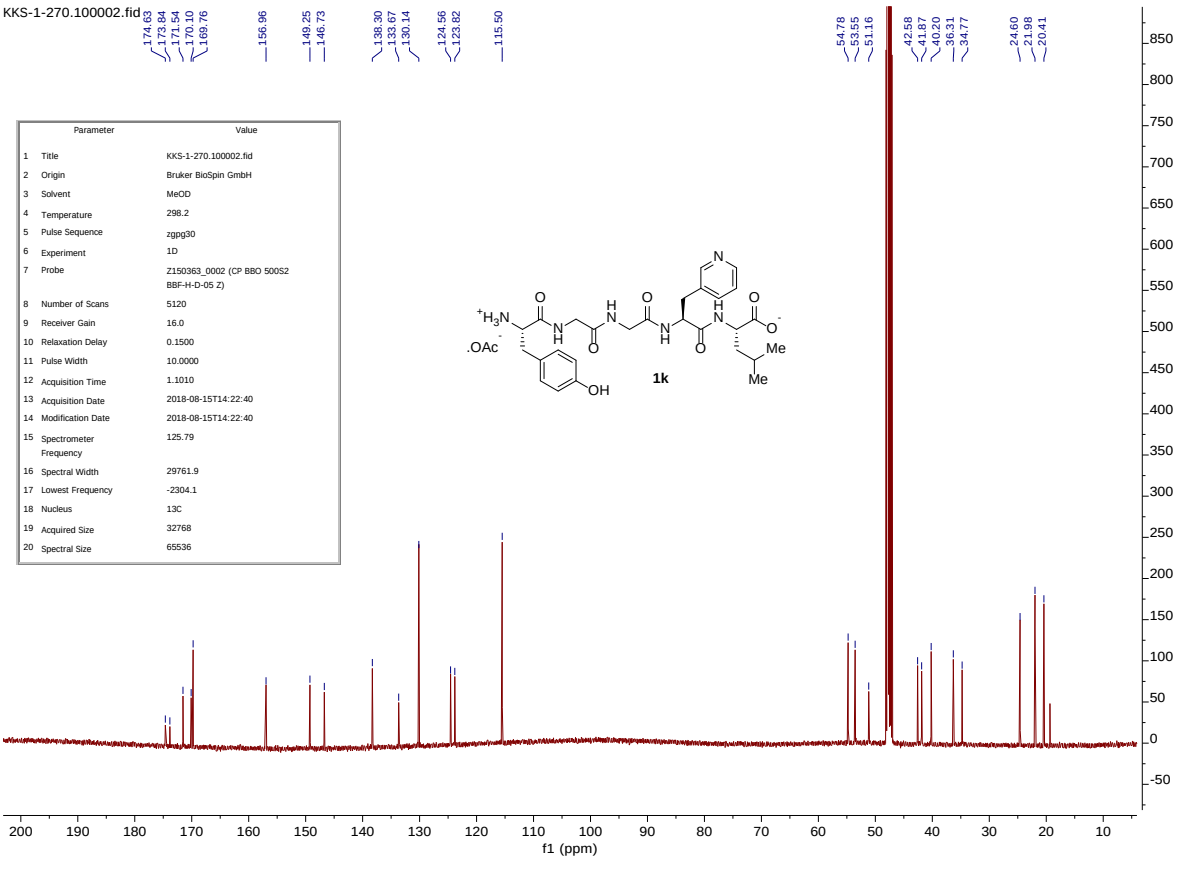
KKS-1-284.100002.fid



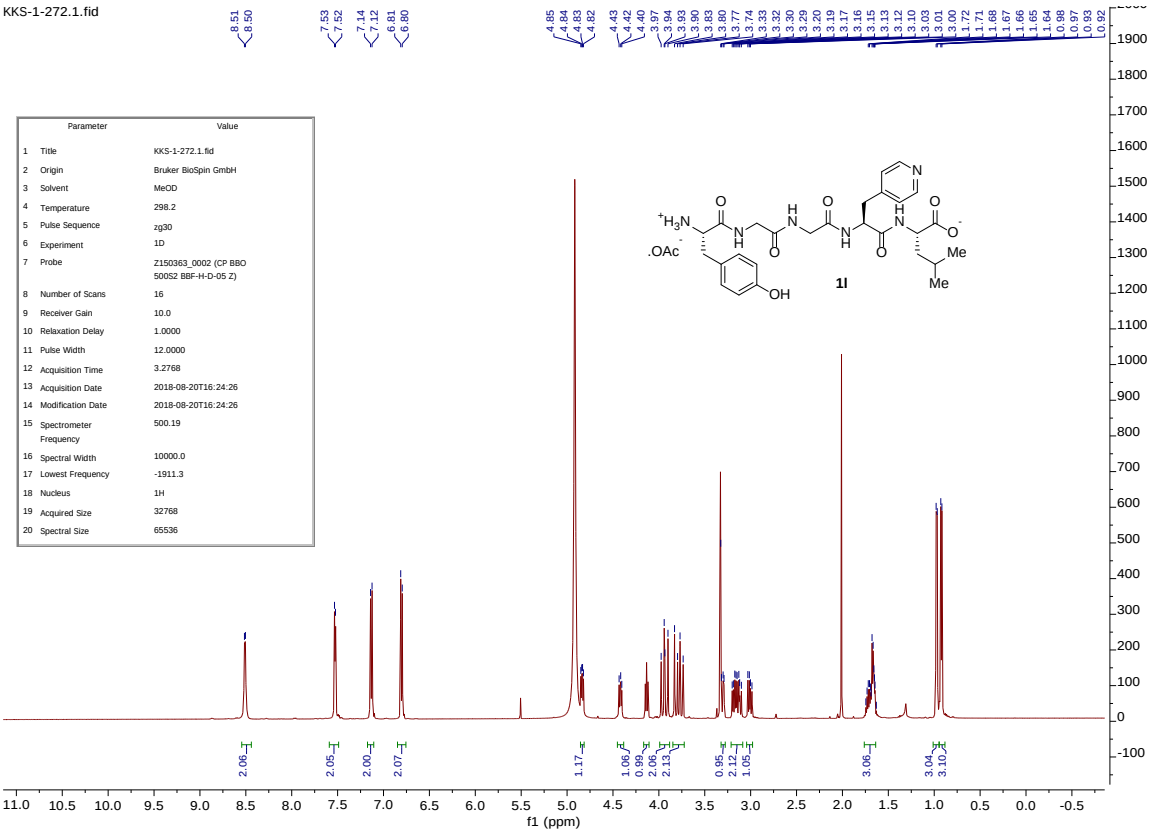
	Parameter	Value
1	Title	KKS-1-284.100002.fid
2	Origin	Bruker BioSpin GmbH
3	Solvent	MeOD
4	Temperature	298.2
5	Pulse Sequence	zgpg30
6	Experiment	1D
7	Probe	Z150363_0002 (CP BBO 500S2 BBF-H-D-05 Z)
8	Number of Scans	5120
9	Receiver Gain	12.7
10	Relaxation Delay	0.1500
11	Pulse Width	10.0000
12	Acquisition Time	1.1010
13	Acquisition Date	2018-08-30T14:49:29
14	Modification Date	2018-08-30T14:49:30
15	Spectrometer Frequency	125.79
16	Spectral Width	29761.9
17	Lowest Frequency	-2304.1
18	Nucleus	13C
19	Acquired Size	32768
20	Spectral Size	65536

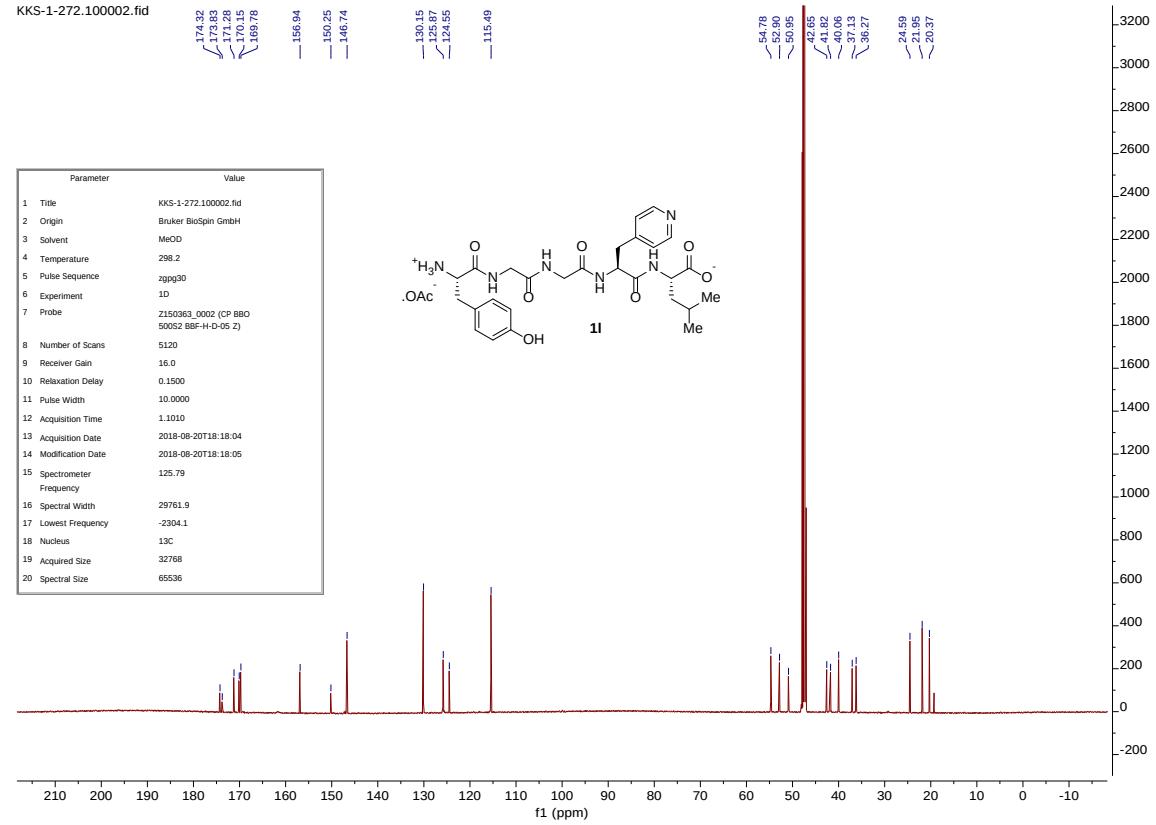


	Parameter	Value
1	Title	kks-1-270.1.fid
2	Origin	Bruker BioSpin GmbH
3	Solvent	MeOD
4	Temperature	296.2
5	Pulse Sequence	zg30
6	Experiment	1D
7	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0786
8	Number of Scans	16
9	Receiver Gain	169.0
10	Relaxation Delay	1.0000
11	Pulse Width	15.0000
12	Acquisition Time	4.0894
13	Acquisition Date	2018-08-15T10:10:00
14	Modification Date	2018-08-15T10:10:37
15	Spectrometer Frequency	400.13
16	Spectral Width	8012.8
17	Lowest Frequency	-1535.4
18	Nucleus	1H
19	Acquired Size	32768
20	Spectral Size	65536

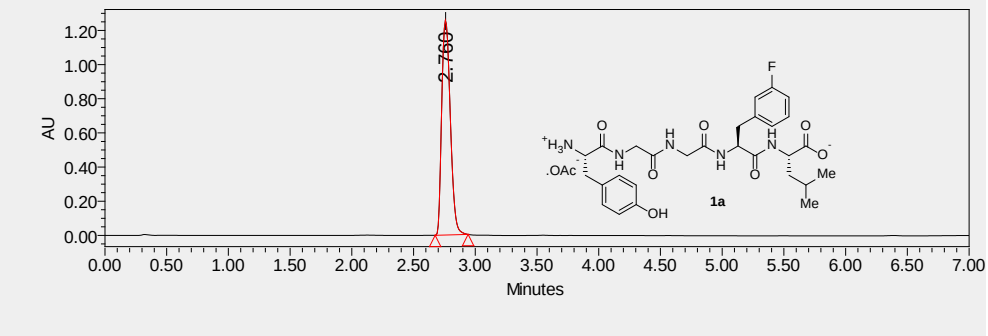


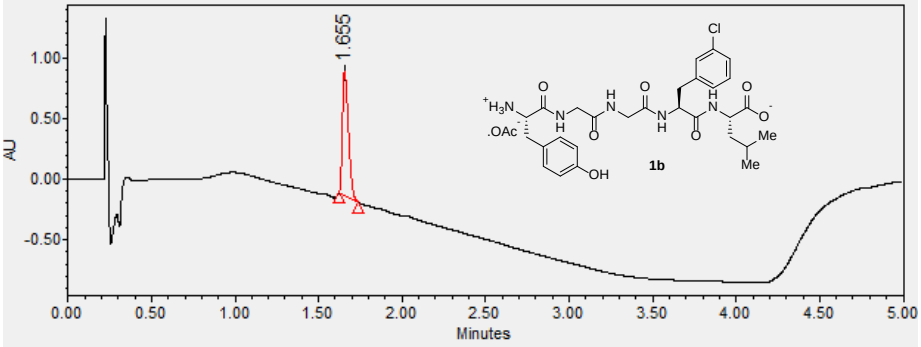
	Parameter	Value
1	Title	KKS-1-270.100002.fid
2	Origin	Bruker BioSpin GmbH
3	Solvent	MeOD
4	Temperature	298.2
5	Pulse Sequence	zgpg30
6	Experiment	1D
7	Probe	Z150363_0002 (CP BBO 500S2 BBF-H-D-05 Z)
8	Number of Scans	5120
9	Receiver Gain	16.0
10	Relaxation Delay	0.1500
11	Pulse Width	10.0000
12	Acquisition Time	1.1010
13	Acquisition Date	2018-08-15T14:22:40
14	Modification Date	2018-08-15T14:22:40
15	Spectrometer Frequency	125.79
16	Spectral Width	29761.9
17	Lowest Frequency	-2304.1
18	Nucleus	13C
19	Acquired Size	32768
20	Spectral Size	65536

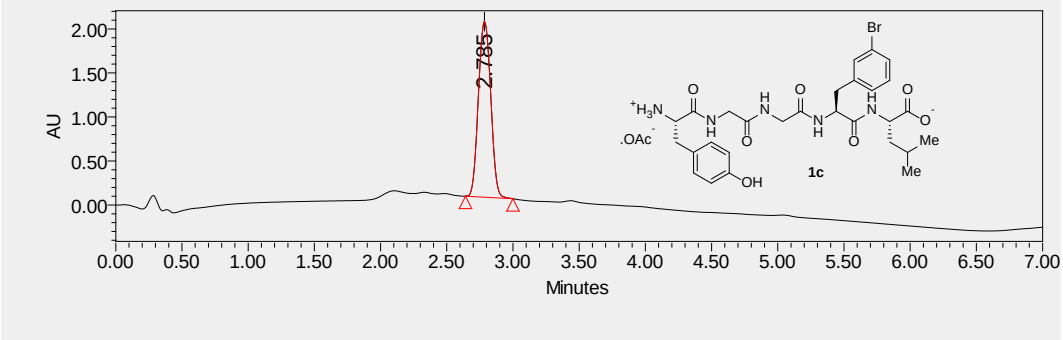

KKS-1-272.1.fid
8.51
8.50
7.53
7.52
7.14
7.12
6.81
6.80
4.85
4.84
4.83
4.82
4.43
4.42
4.40
3.97
3.94
3.93
3.90
3.83
3.80
3.77
3.74
3.33
3.32
3.30
3.29
3.20
3.19
3.17
3.16
3.15
3.13
3.12
3.10
3.03
3.01
3.00
1.72
1.71
1.68
1.67
1.66
1.65
1.64
0.98
0.97
0.93
0.92
Parameter Value
1 Title KKS-1-272.1.fid
2 Origin Bruker BioSpin GmbH
3 Solvent MeOD
4 Temperature 298.2
5 Pulse Sequence zg30
6 Experiment 1D
7 Probe Z150363_0002 (CP BBO 500S2 BBF-H-D-05 Z)
8 Number of Scans 16
9 Receiver Gain 10.0
10 Relaxation Delay 1.0000
11 Pulse Width 12.0000
12 Acquisition Time 3.2768
13 Acquisition Date 2018-08-20T16:24:26
14 Modification Date 2018-08-20T16:24:26
15 Spectrometer Frequency 500.19
16 Spectral Width 10000.0
17 Lowest Frequency -1911.3
18 Nucleus 1H
19 Acquired Size 32768
20 Spectral Size 65536
1l
2.06
2.05
2.00
2.07
1.17
1.06
0.99
2.06
2.13
0.95
2.12
1.05
3.06
3.04
3.10
f1 (ppm)

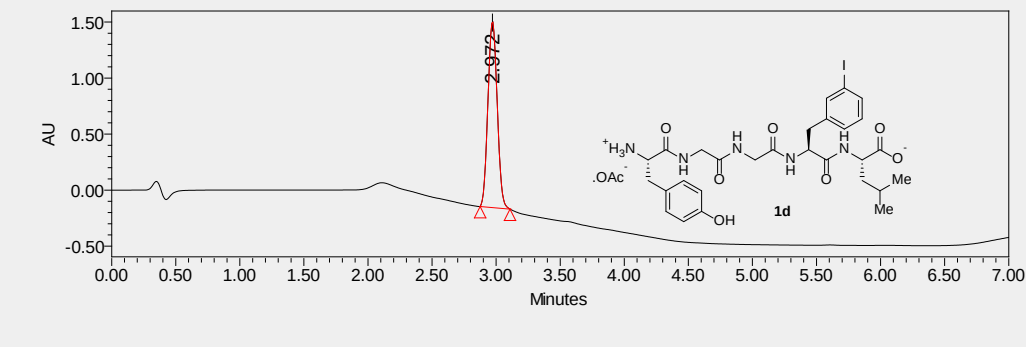

KKS-1-272.100002.fid
174.32
173.83
171.28
170.15
169.78
156.94
150.25
146.74
130.15
125.87
124.55
115.49
54.78
52.90
50.95
42.65
41.82
40.06
37.13
36.27
24.59
21.95
20.37
Parameter Value
1 Title KKS-1-272.100002.fid
2 Origin Bruker BioSpin GmbH
3 Solvent MeOD
4 Temperature 298.2
5 Pulse Sequence zgpg30
6 Experiment 1D
7 Probe Z150363_0002 (CP BBO 500S2 BBF-H-D-05 Z)
8 Number of Scans 5120
9 Receiver Gain 16.0
10 Relaxation Delay 0.1500
11 Pulse Width 10.0000
12 Acquisition Time 1.1010
13 Acquisition Date 2018-08-20T18:18:04
14 Modification Date 2018-08-20T18:18:05
15 Spectrometer Frequency 125.79
16 Spectral Width 29761.9
17 Lowest Frequency -2304.1
18 Nucleus 13C
19 Acquired Size 32768
20 Spectral Size 65536
1l
f1 (ppm)

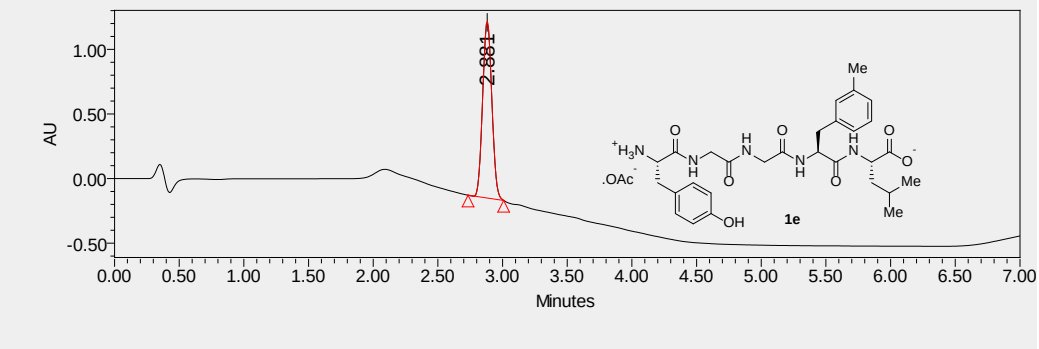
HPLC Chromatograms of Peptides

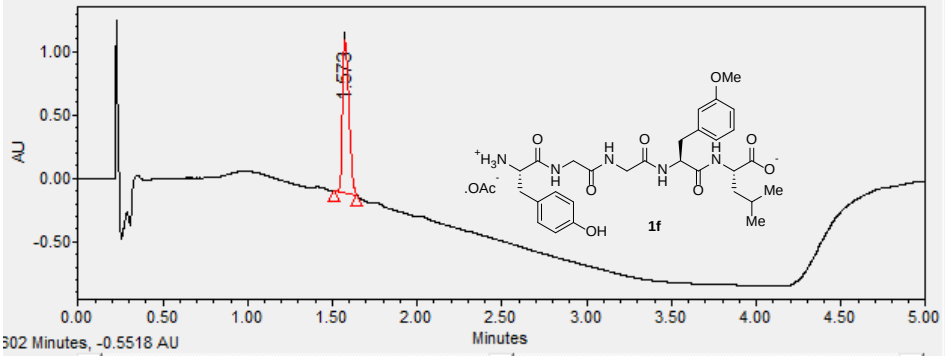


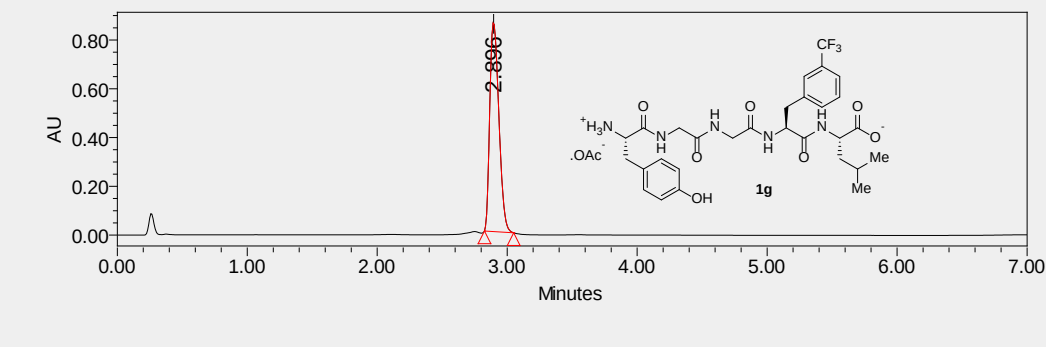


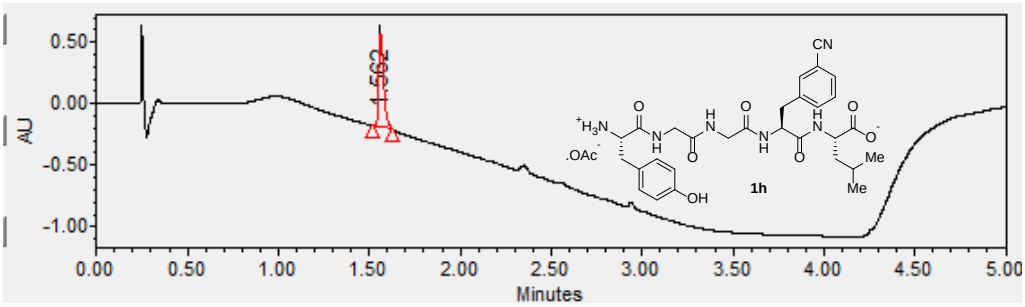


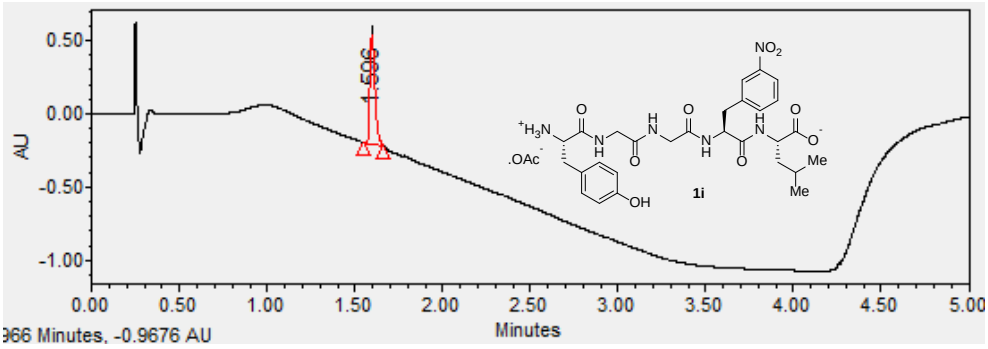

AU
Minutes
2.972
1d

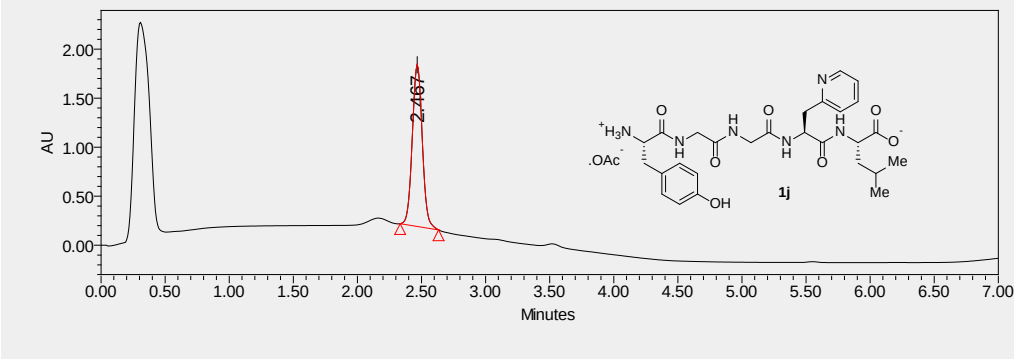

AU
Minutes
2.881
1e

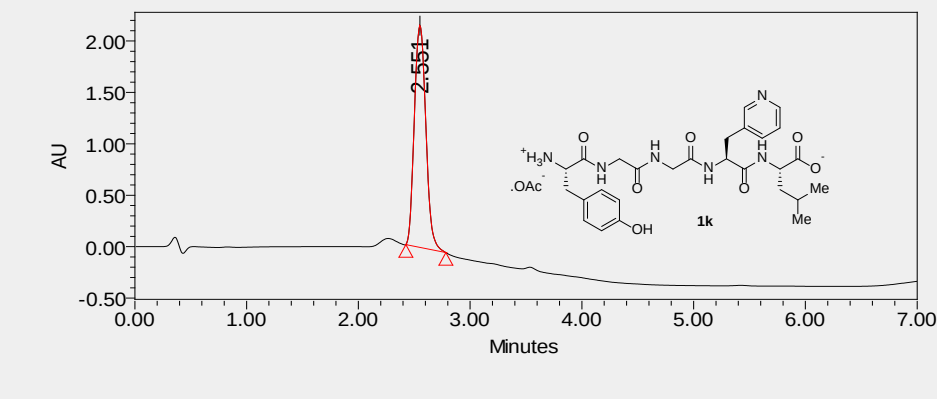

AU
Minutes
1.573
1f

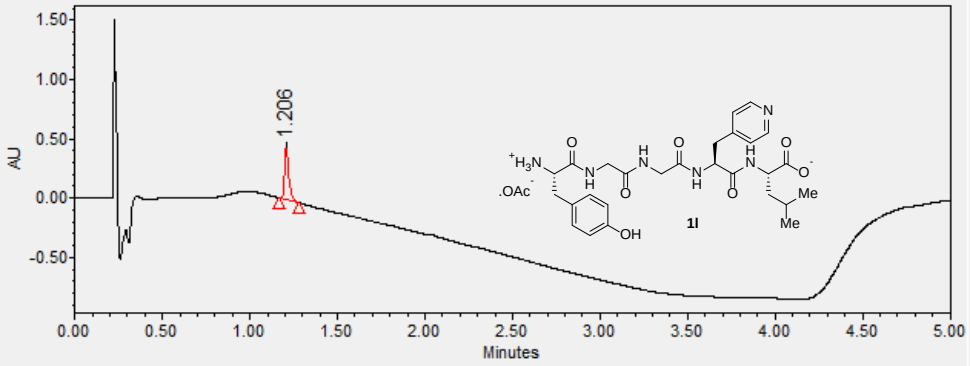

AU
0.80
0.60
0.40
0.20
0.00
2.896
0.00
1.00
2.00
3.00
4.00
5.00
6.00
7.00
Minutes
CF3
.OAc
OH
Me
Me
1g


AU
0.50
0.00
-0.50
-1.00
1.562
0.00
0.50
1.00
1.50
2.00
2.50
3.00
3.50
4.00
4.50
5.00
Minutes
CN
.OAc
OH
Me
Me
1h


AU
0.50
0.00
-0.50
-1.00
1.506
0.00
0.50
1.00
1.50
2.00
2.50
3.00
3.50
4.00
4.50
5.00
Minutes
966 Minutes, -0.9676 AU
NO2
.OAc
OH
Me
Me
1i


AU
Minutes
2.167
1j


AU
Minutes
2.551
1k


AU
Minutes
1.206
1l