

Supplementary Information

Design, Synthesis and Biological Evaluation of a Novel PSMA-PI3K Small Molecule Drug Conjugate

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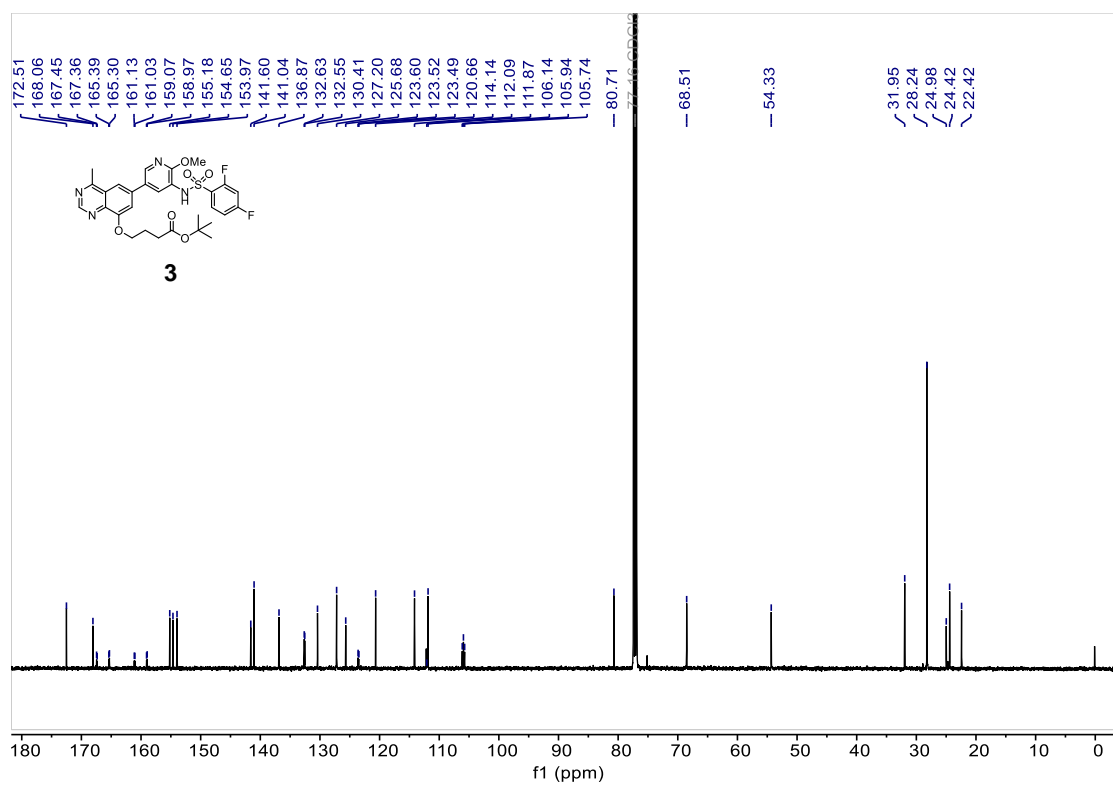
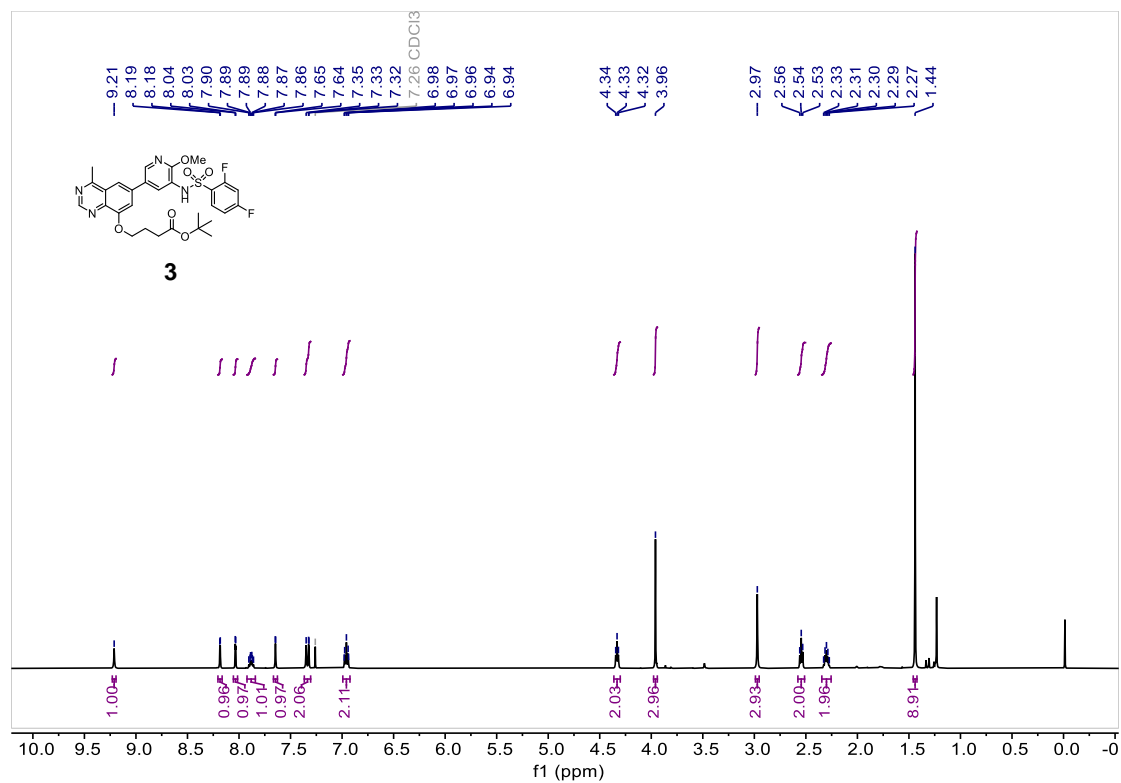
^c*CAMS Key Laboratory of Small Molecule Immuno-Oncology Drug Discovery, Chinese Academy of Medical Sciences, Beijing, 100050, China.*

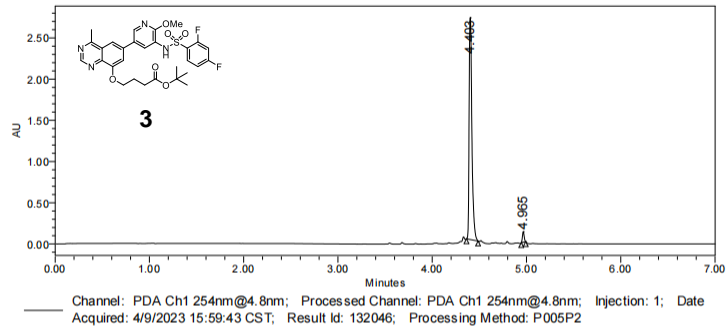
^d*Guang'anmen Hospital, China Academy of Chinese Medical Sciences, Beijing, 100053, China*

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$^1\text{H}/^{13}\text{C}$ NMR, LCMS and HRMS Spectra of Key Compounds

Compound 3

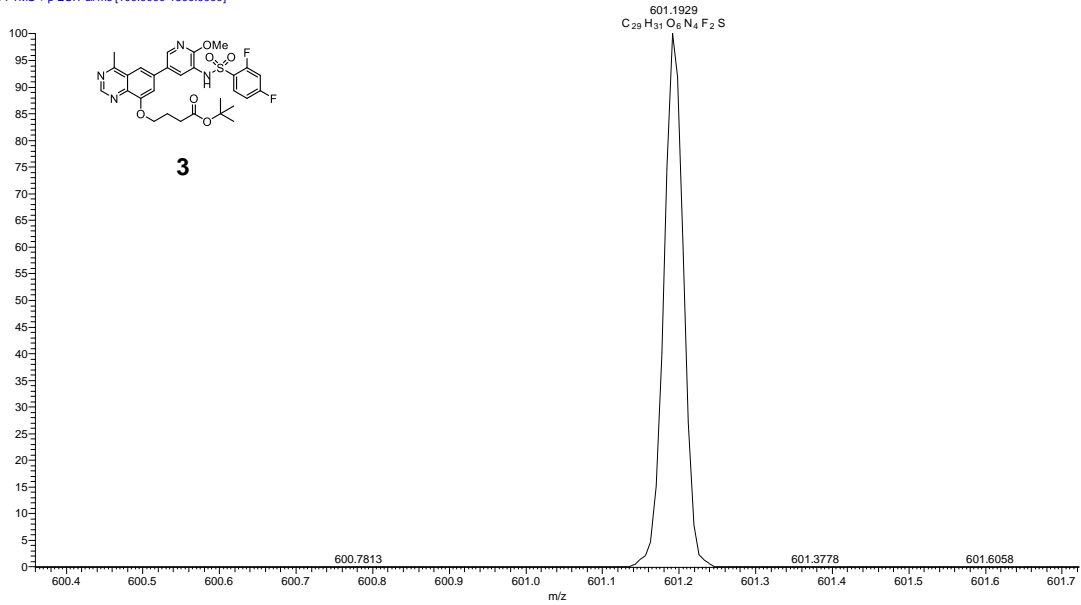




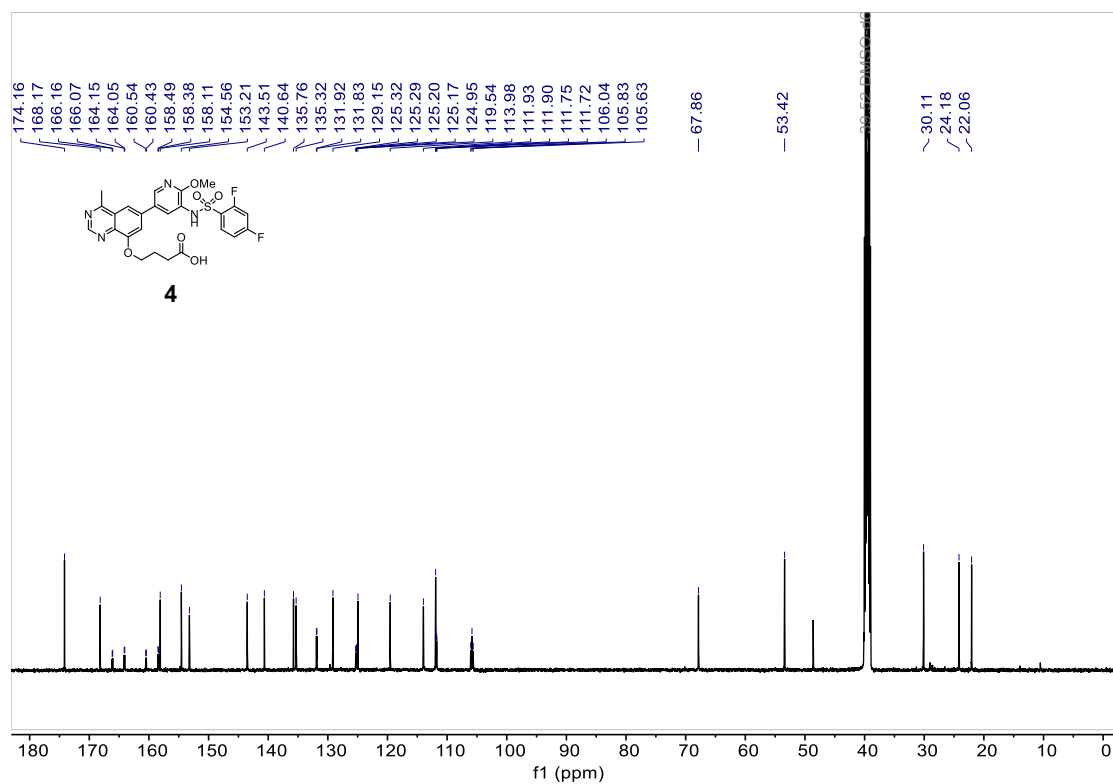
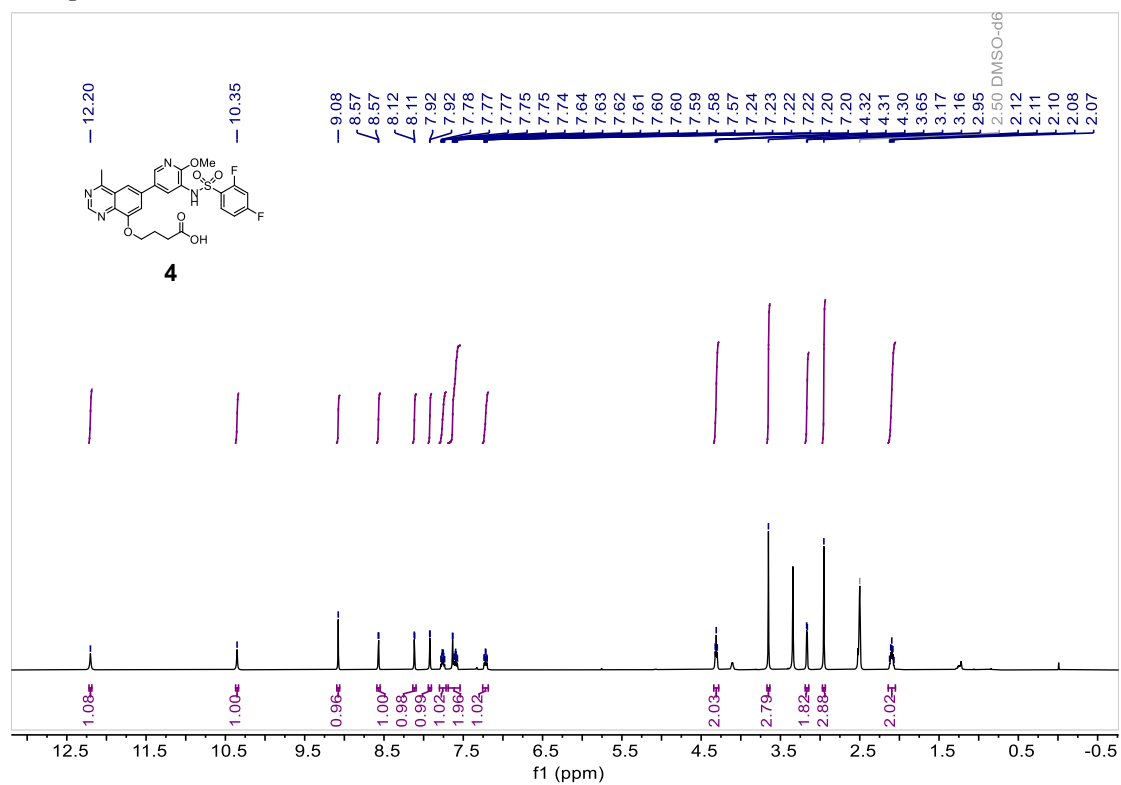
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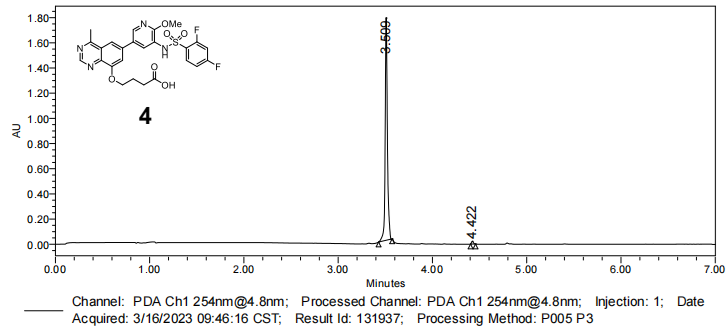
	Injection	RT	Area	% Area
1	1	4.965	164428	2.89
2	1	4.403	5516323	97.11
Mean		4.684		
Std. Dev.		0.398		
% RSD		8.49		

P05-1 #1450-1603 RT: 4.82-5.32 AV: 154 NL: 1.71E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



Compound 4

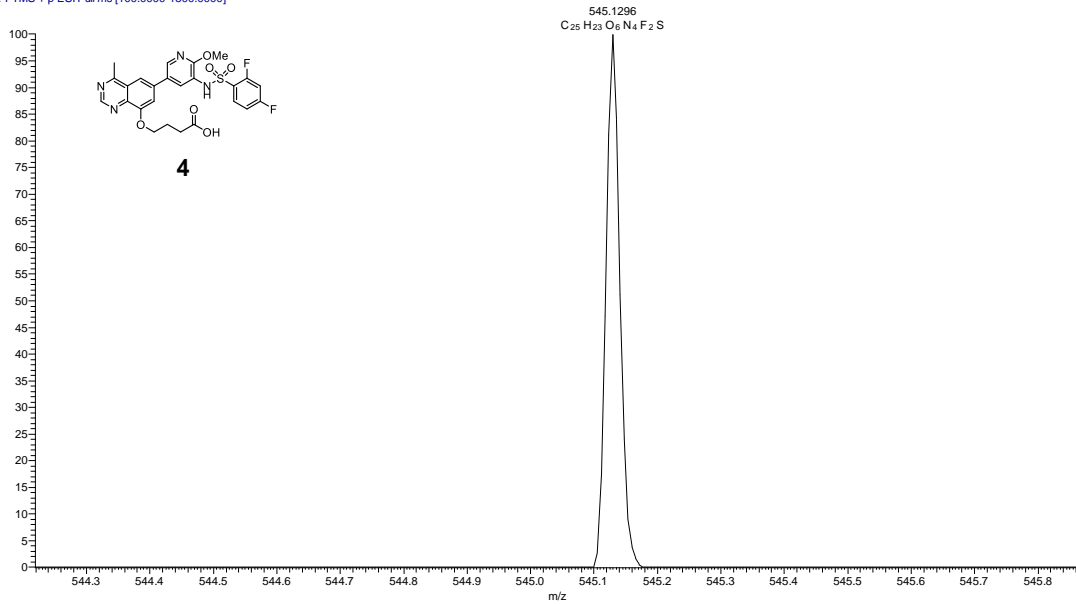


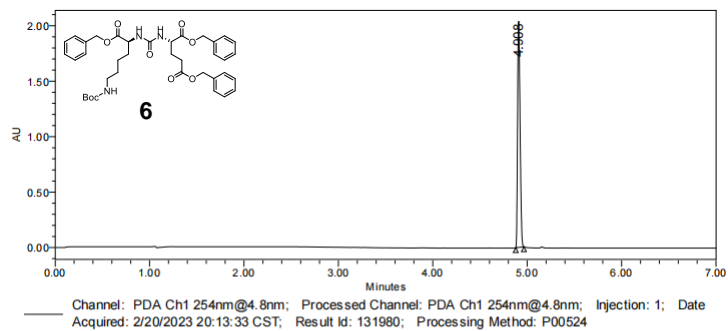


Peak Name:

	Injection	RT	Area	% Area
1	1	4.422	29497	1.00
2	1	3.509	2906558	99.00
Mean		3.966		
Std. Dev.		0.646		
% RSD		16.29		

P05-1 #1754-1774 RT: 5.91-6.00 AV: 21 NL: 2.21E5
T: FTMS + p ESI Full ms [100.0000-1500.0000]

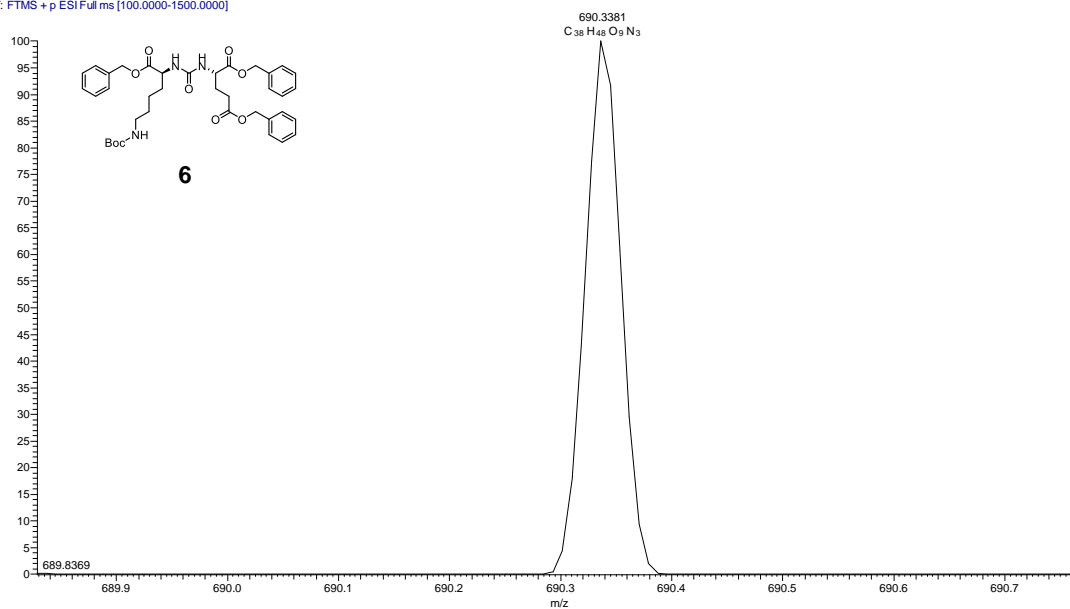




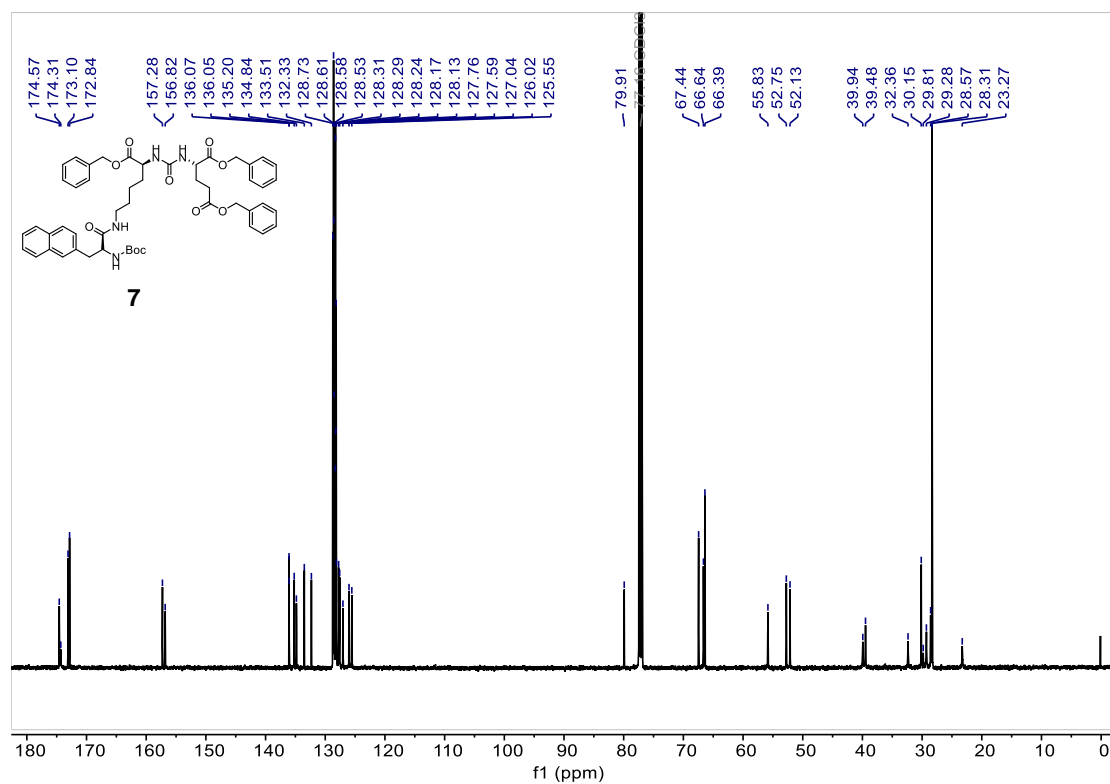
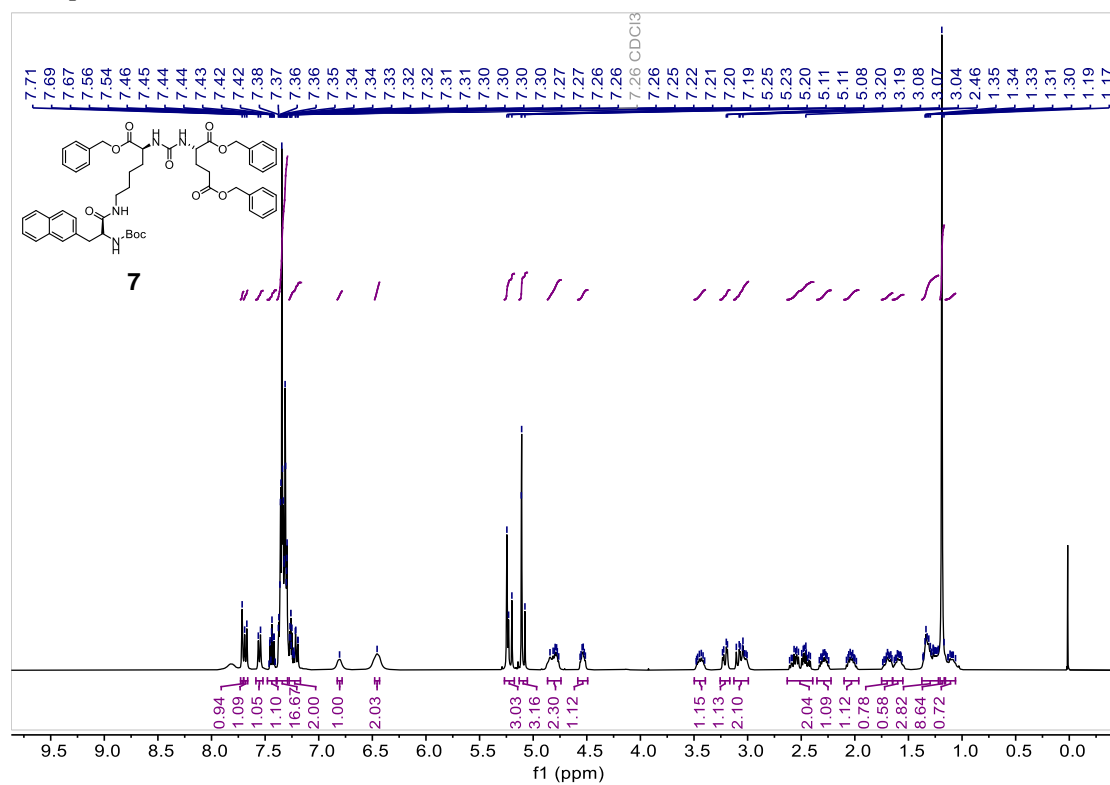
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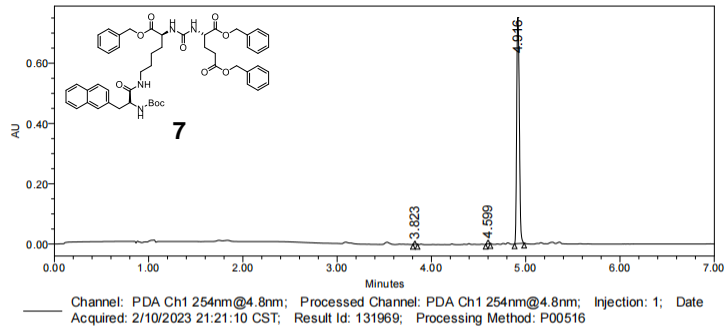
	Injection	RT	Area	% Area
	1	4.908	3729426	100.00
Mean		4.908		
Std. Dev.				
% RSD				

P05-2 #1206-1258 RT: 5.99-6.32 AV: 53 NL: 5.24E5
T: FTMS + p ESI Full ms [100.0000-1500.0000]



Compound 7

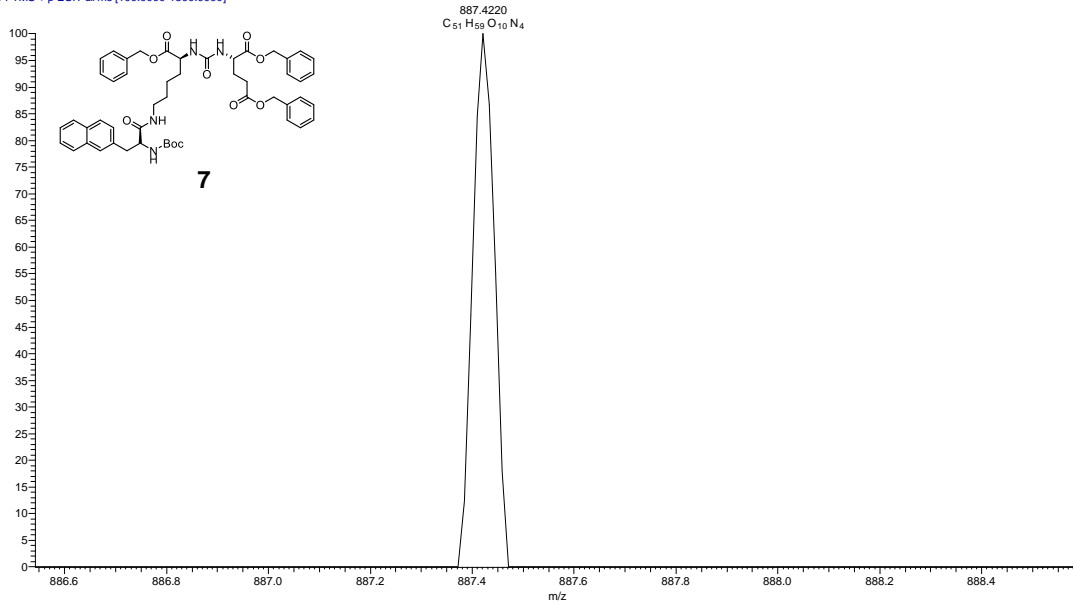




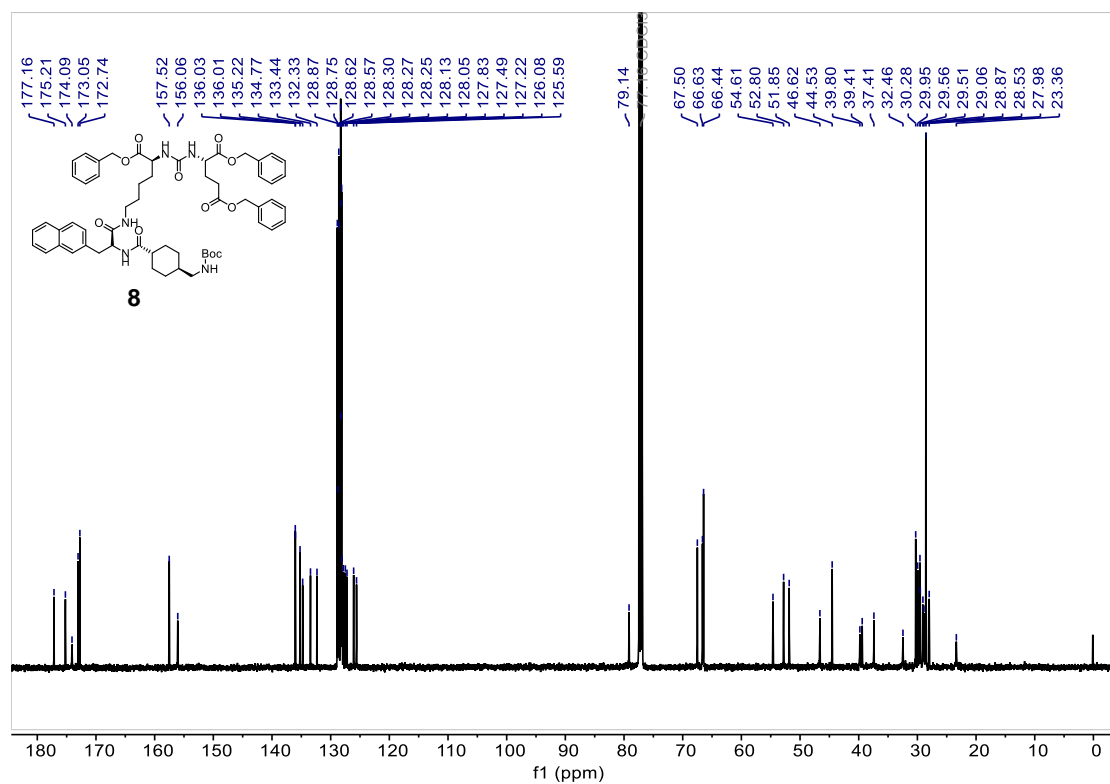
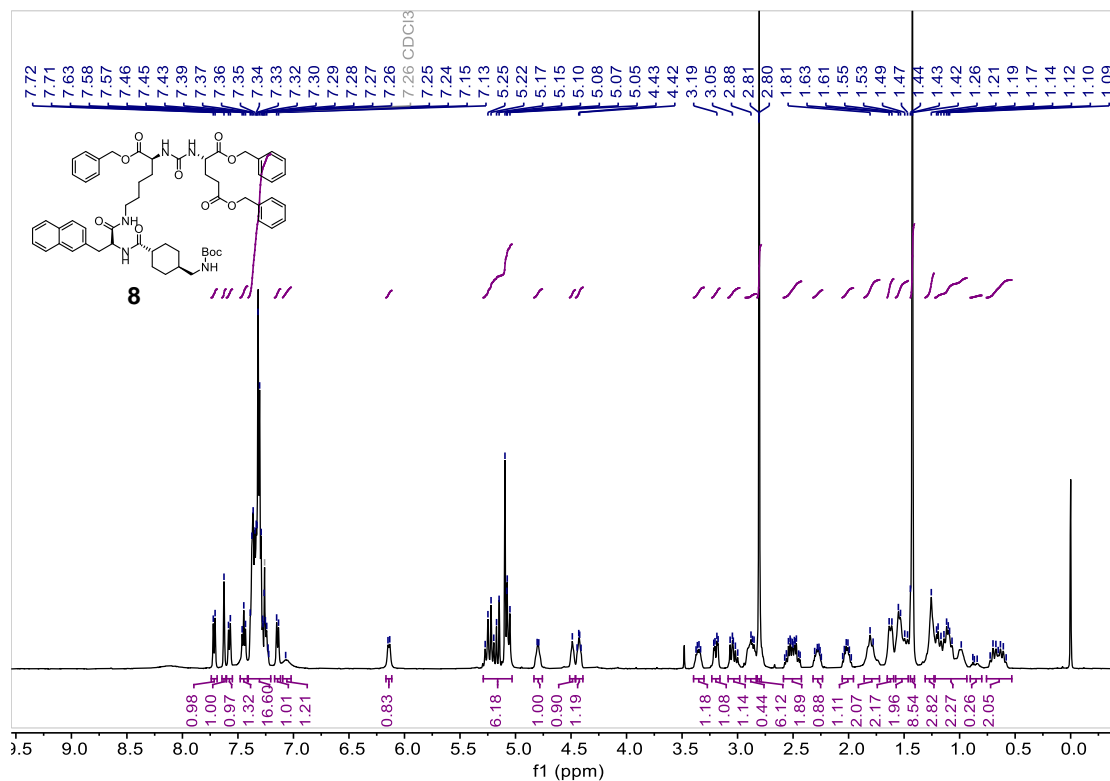
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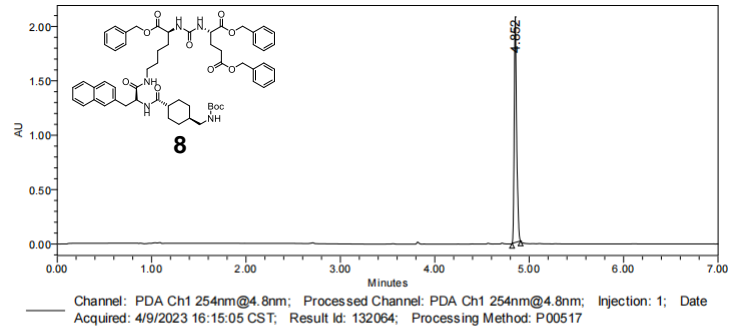
	Injection	RT	Area	% Area
1	1	3.823	12817	0.85
2	1	4.916	1476769	98.03
3	1	4.599	16807	1.12
Mean		4.446		
Std. Dev.		0.562		
% RSD		12.65		

P05-3 #1284-1330 RT: 6.78-7.08 AV: 47 NL: 1.56E2
T: FTMS + p ESI Full ms [100.0000-1500.0000]



Compound 8

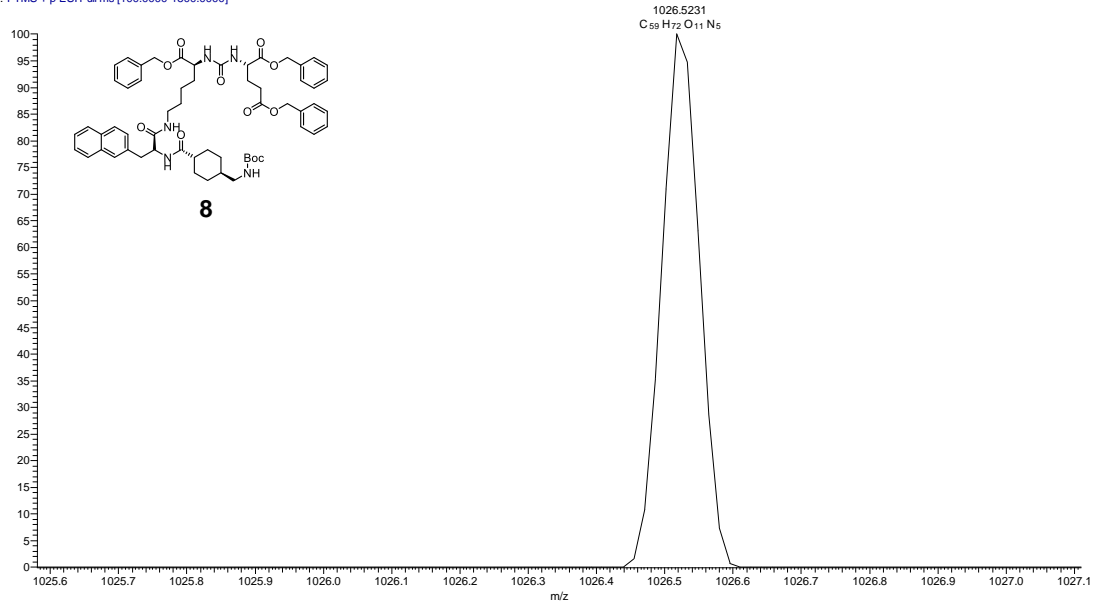




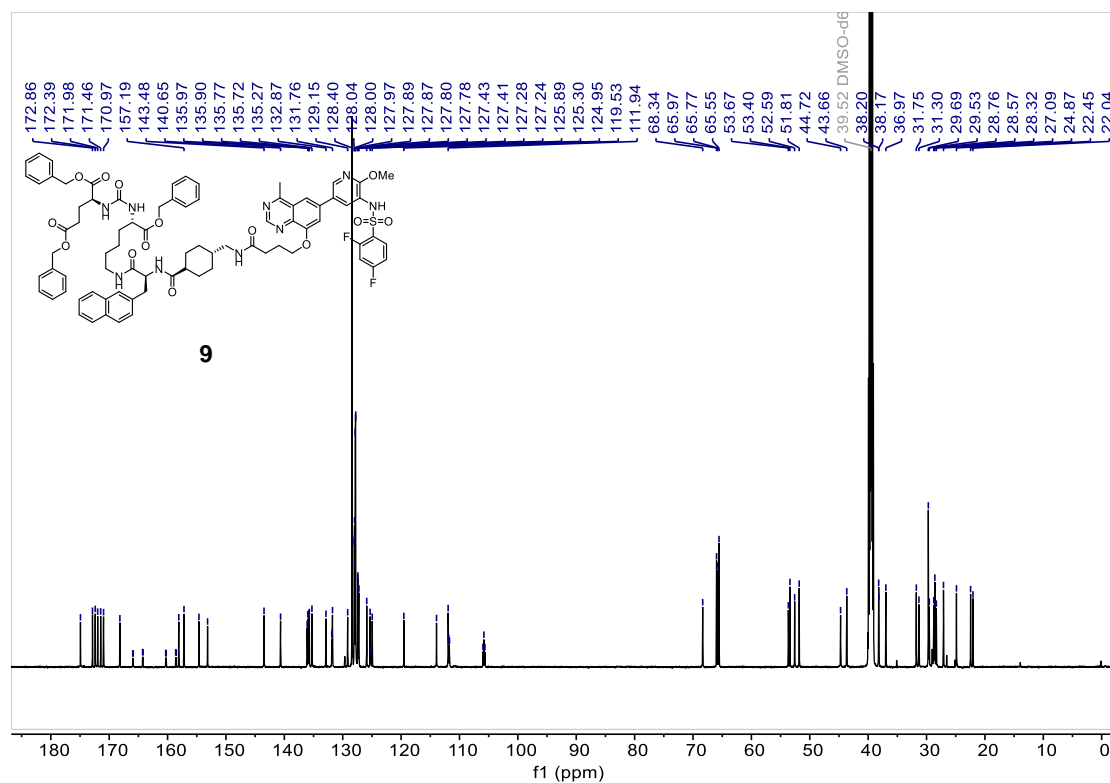
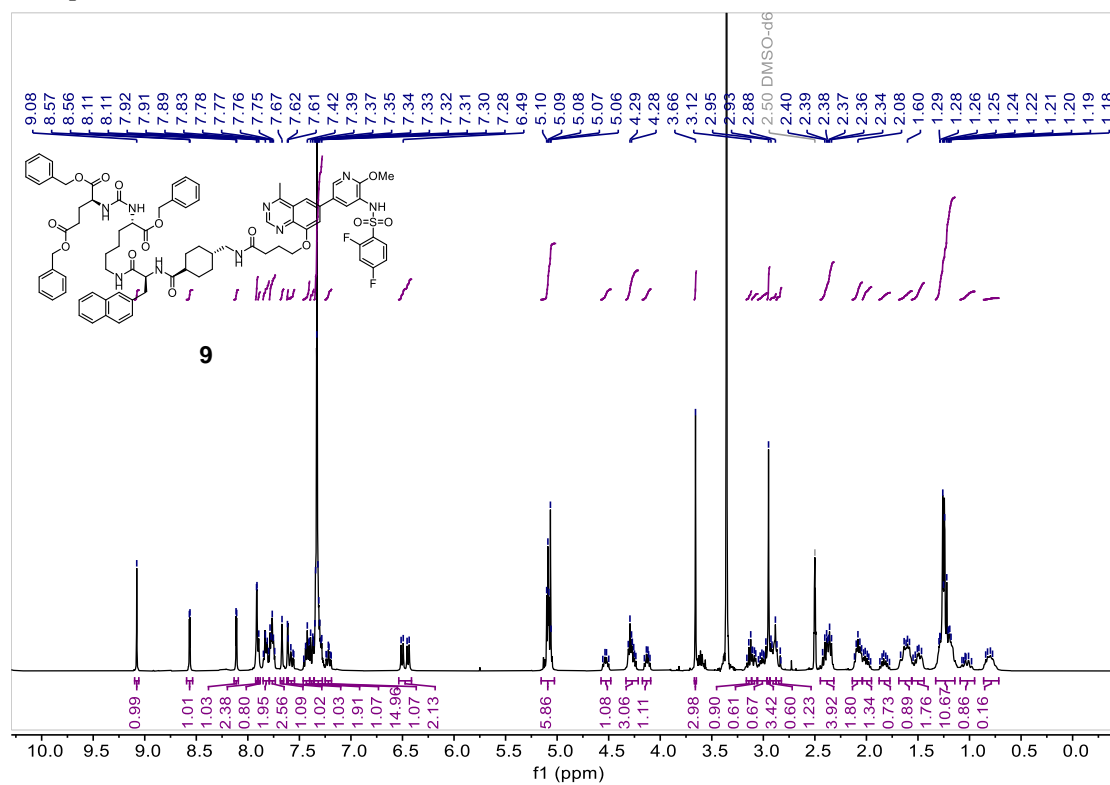
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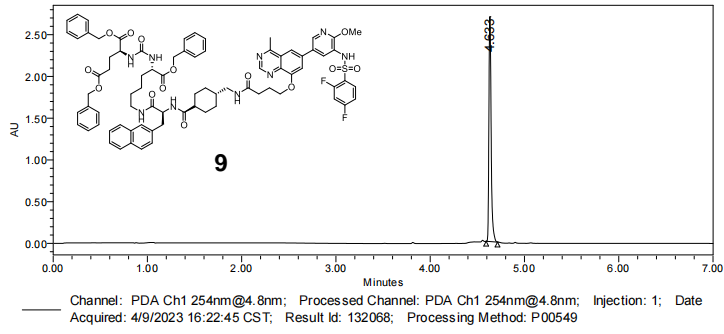
Injection	RT	Area	% Area
1	4.852	3678820	100.00
Mean	4.852		
Std. Dev.			
% RSD			

P005-17 #915-922 RT: 5.91-5.96 AV: 8 NL: 1.72E3
T: FTMS + p ESI Full ms [100.0000-1500.0000]



Compound 9

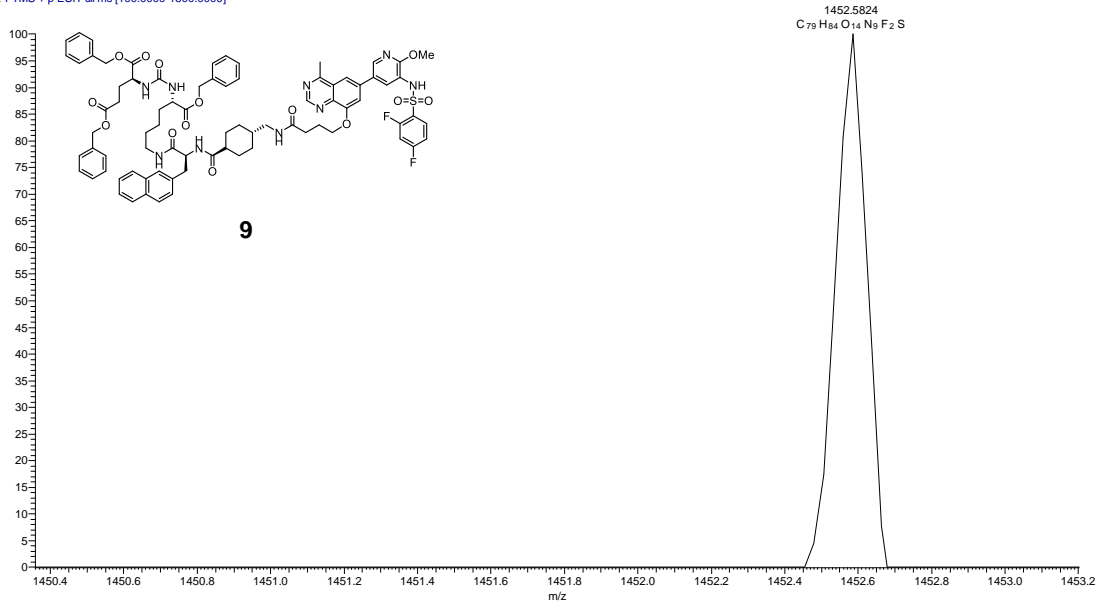




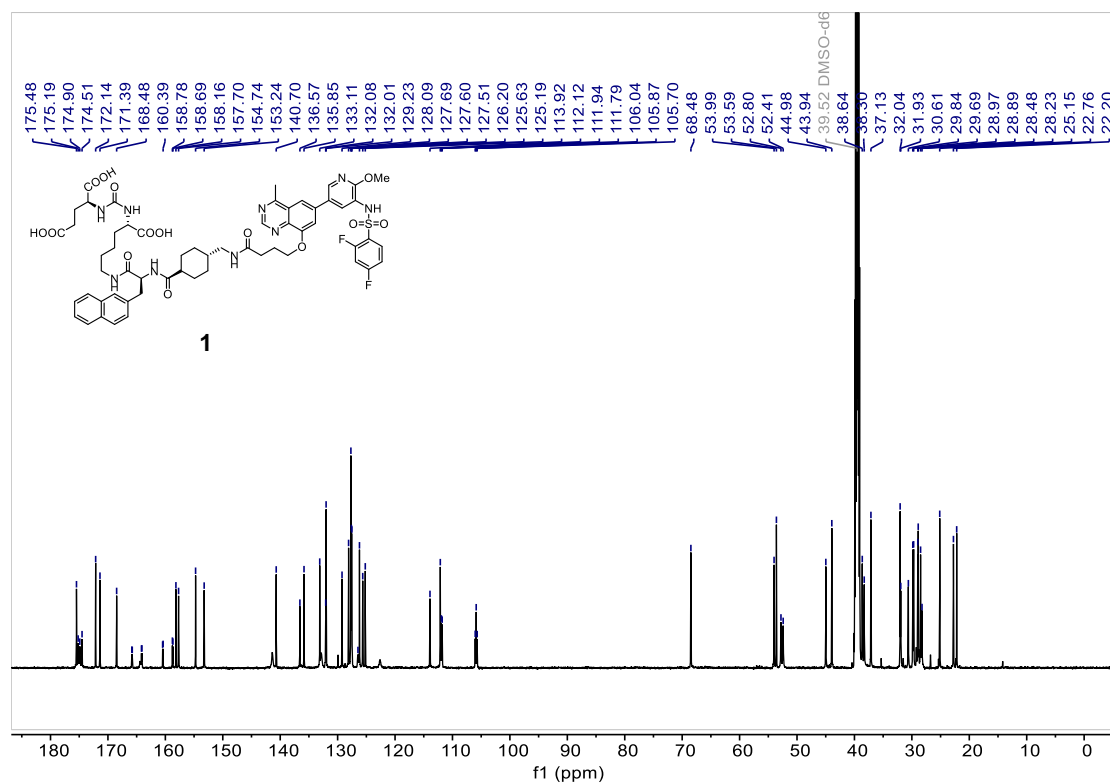
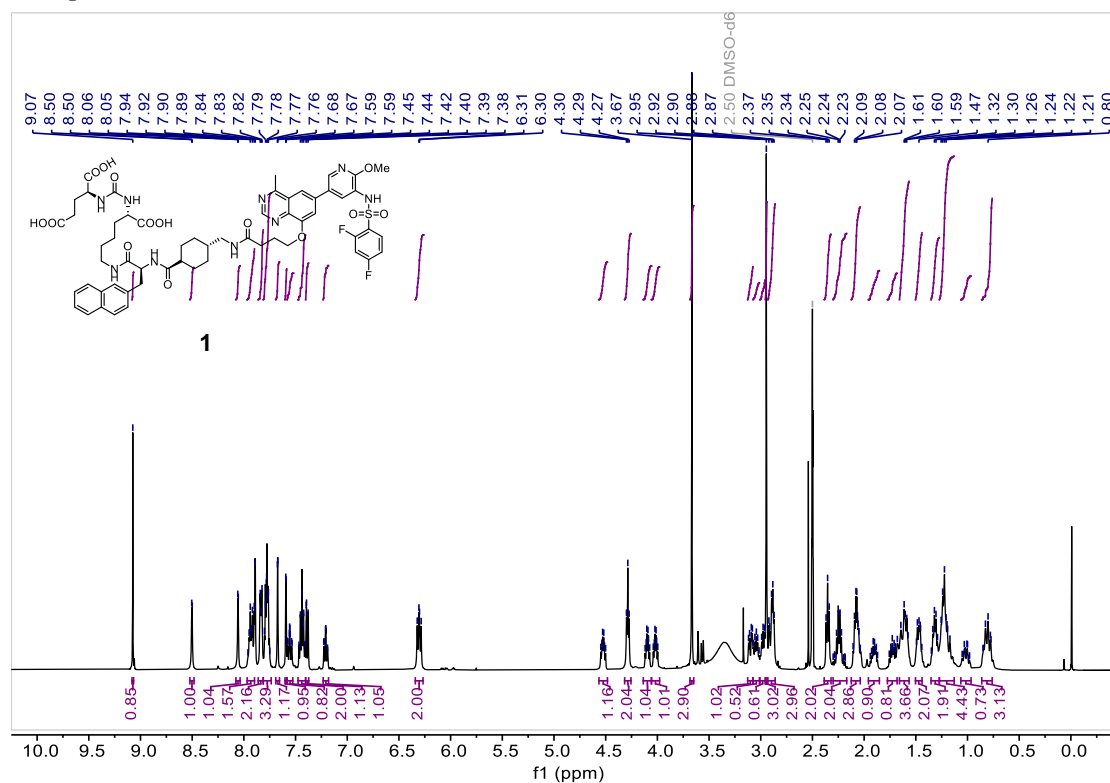
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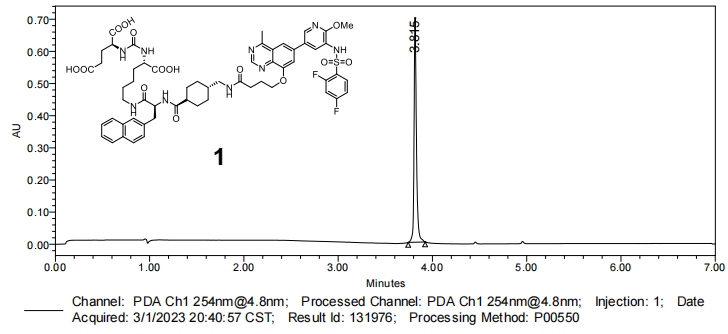
	Injection	RT	Area	% Area
1	1	4.633	4464941	100.00
Mean		4.633		
Std. Dev.				
% RSD				

P05-4 #1221 RT: 5.79 AV: 1 NL: 4.06E3
T: FTMS + p ESI Full ms [100.0000-1500.0000]



Compound 1





Peak Name:

	Injection	RT	Area	% Area
1	1	3.815	1217154	100.00
Mean		3.815		
Std. Dev.				
% RSD				

P05-4 #1026-1054 RT: 4.53-4.71 AV: 29 NL: 1.92E4
T: FTMS + p ESI Full ms [100.0000-1500.0000]

