

Supplementary Information

Fluorine- and rhenium-containing geldanamycin derivatives as leads
for the development of molecular probes for imaging Hsp90

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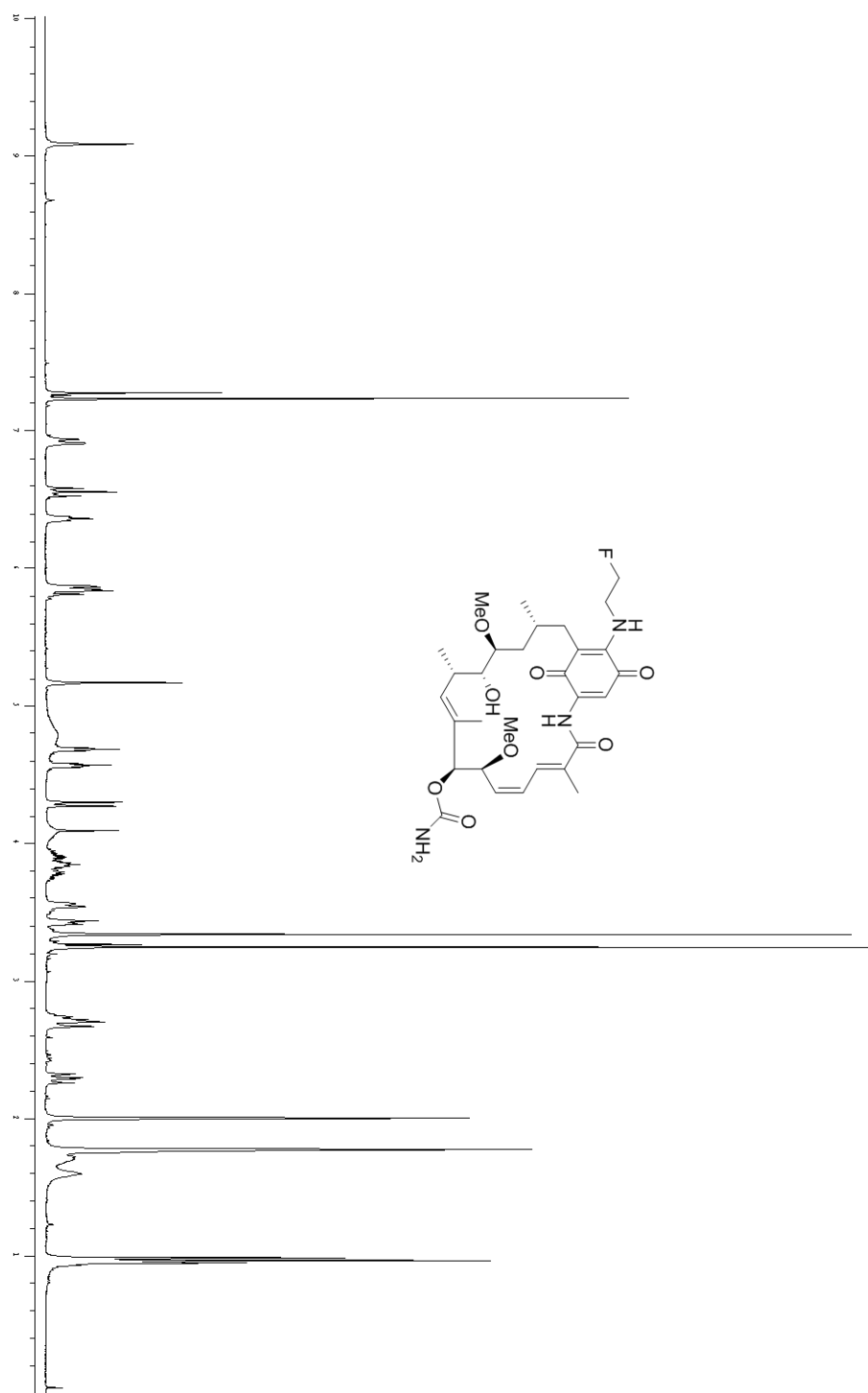
¹H-NMR spectra of compounds 1, 2, 3, 5, 7, and 15

¹⁹F-NMR spectra of compounds 1, 2, 3, 5 and 7

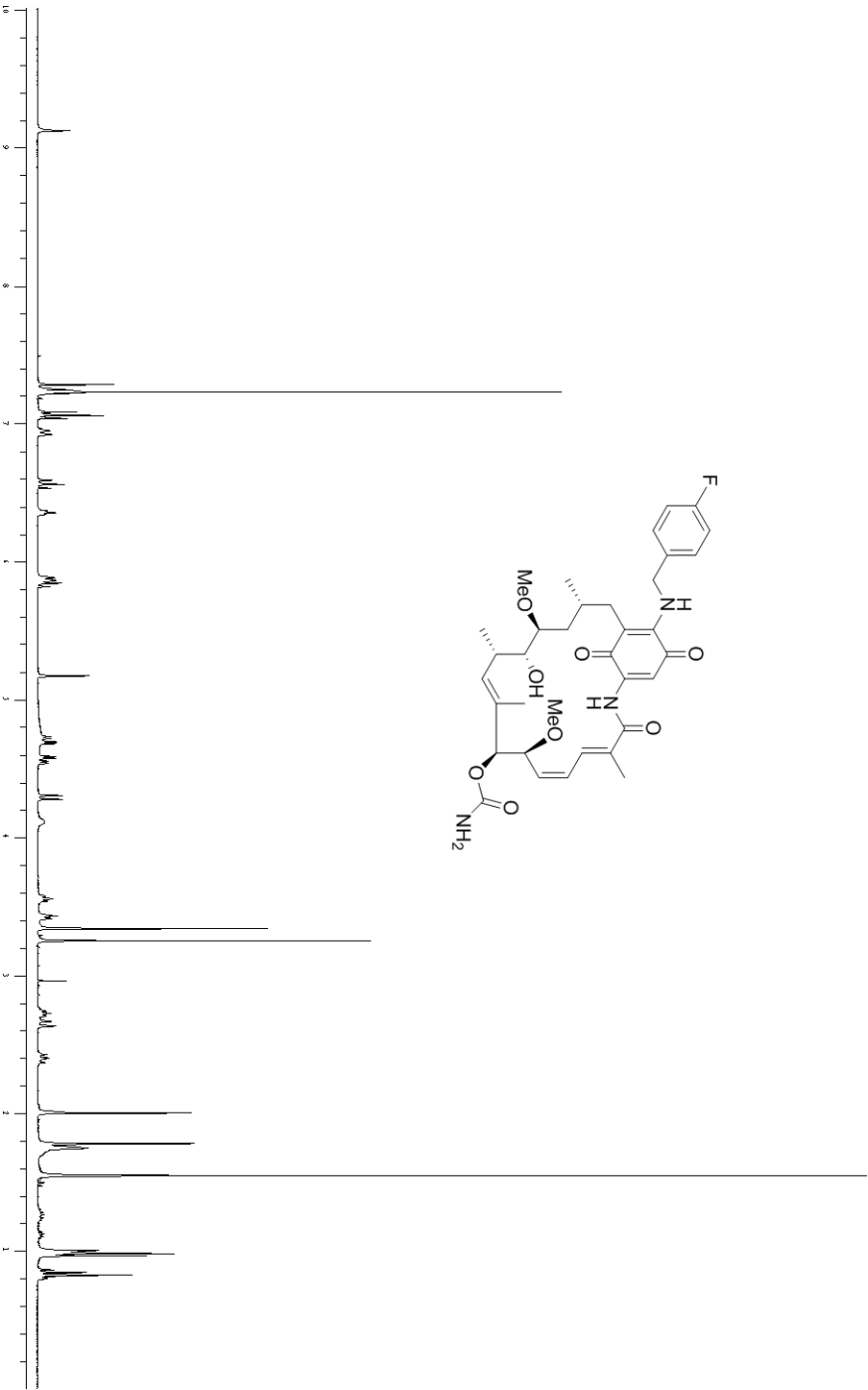
HPLC analyses of compounds 1, 2, 3, 5, 7, and 15

Mass spectra of compounds 1, 2, 3, 5, 7, and 15

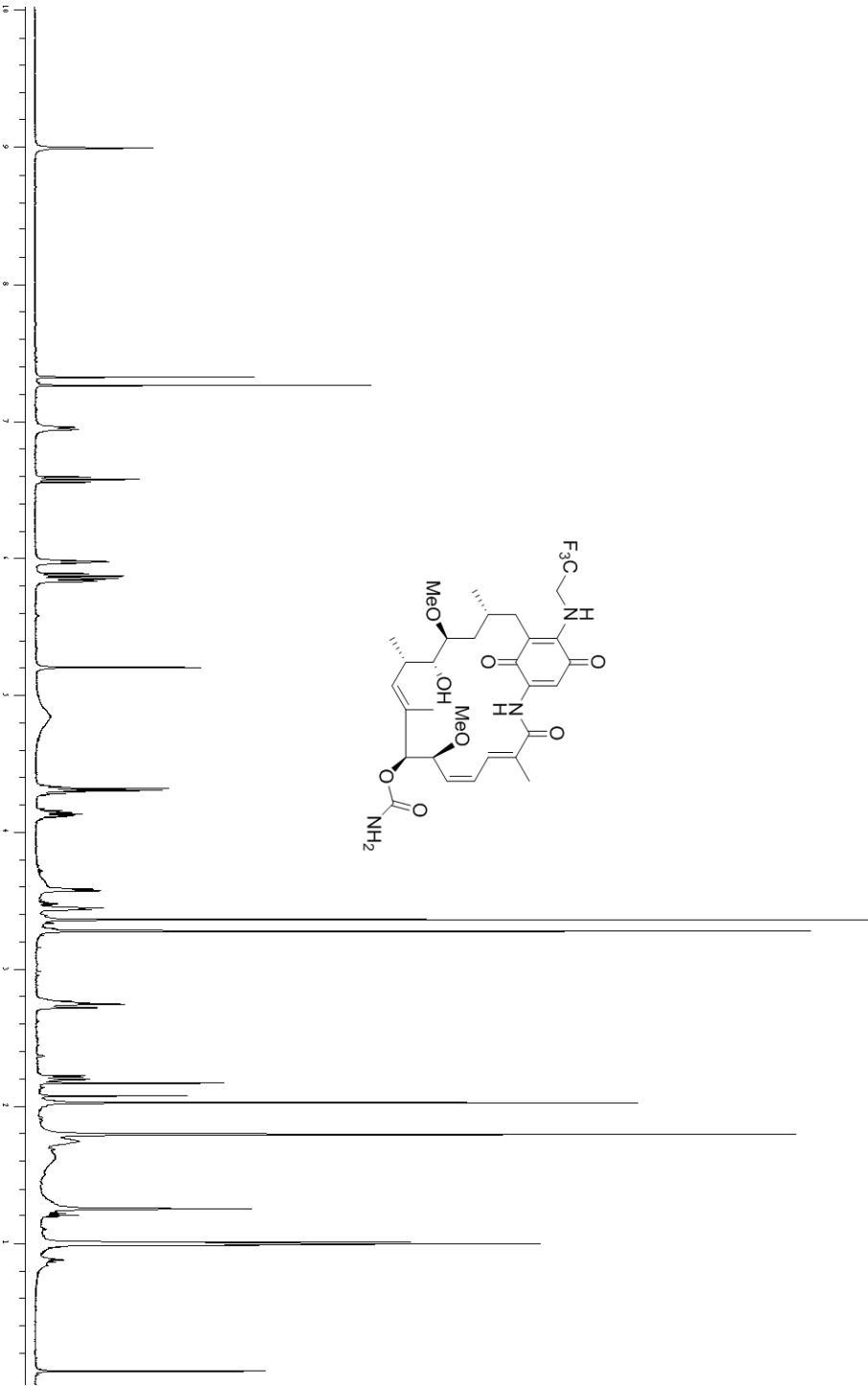
^1H -NMR: 17-(2-Fluoroethylamino)-17-demethoxy-geldanamycin 1



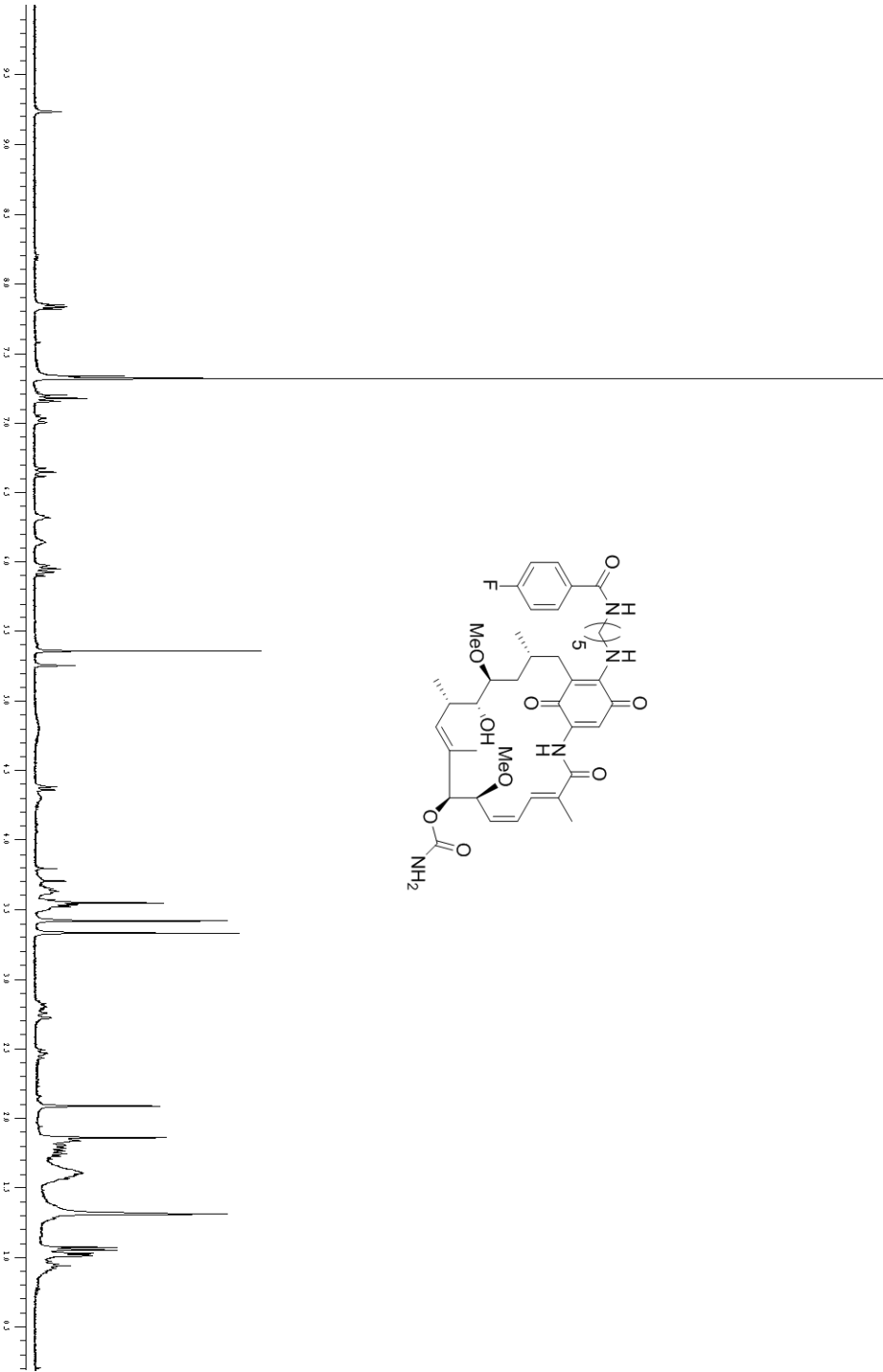
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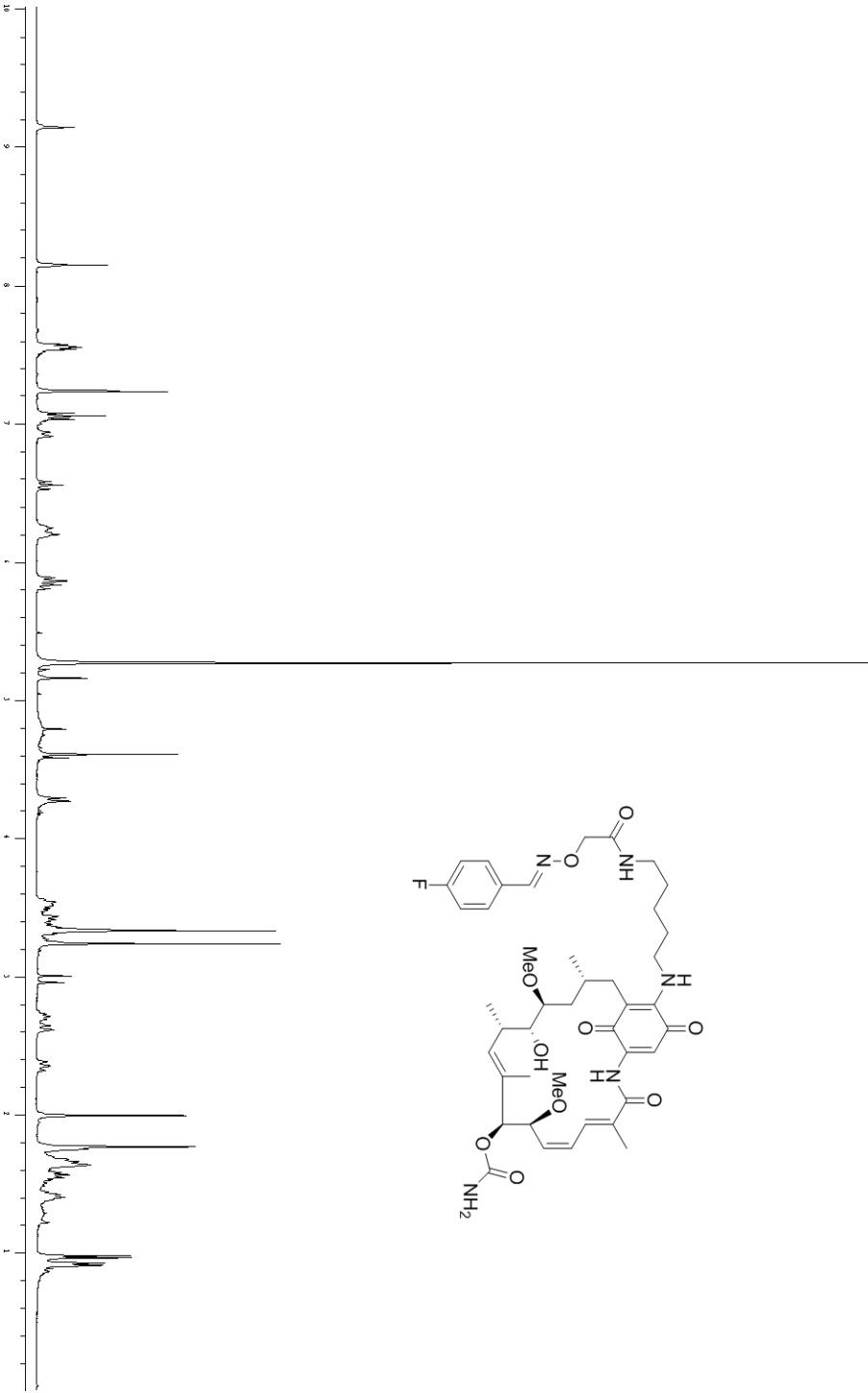
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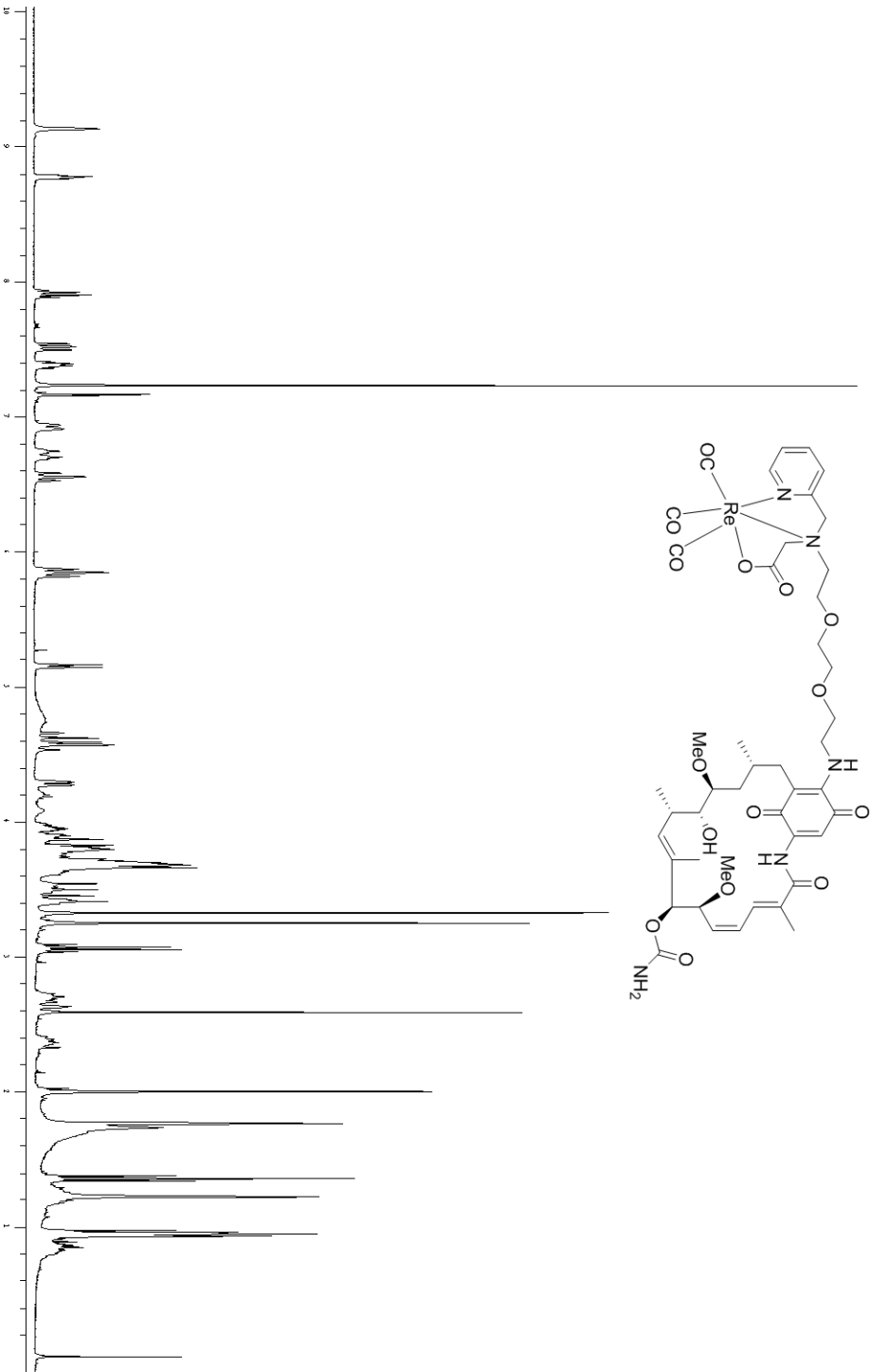
¹H-NMR: 17-(4-Fluorobenzamido)pentyl)amino)-17-demethoxy-
geldanamycin 5



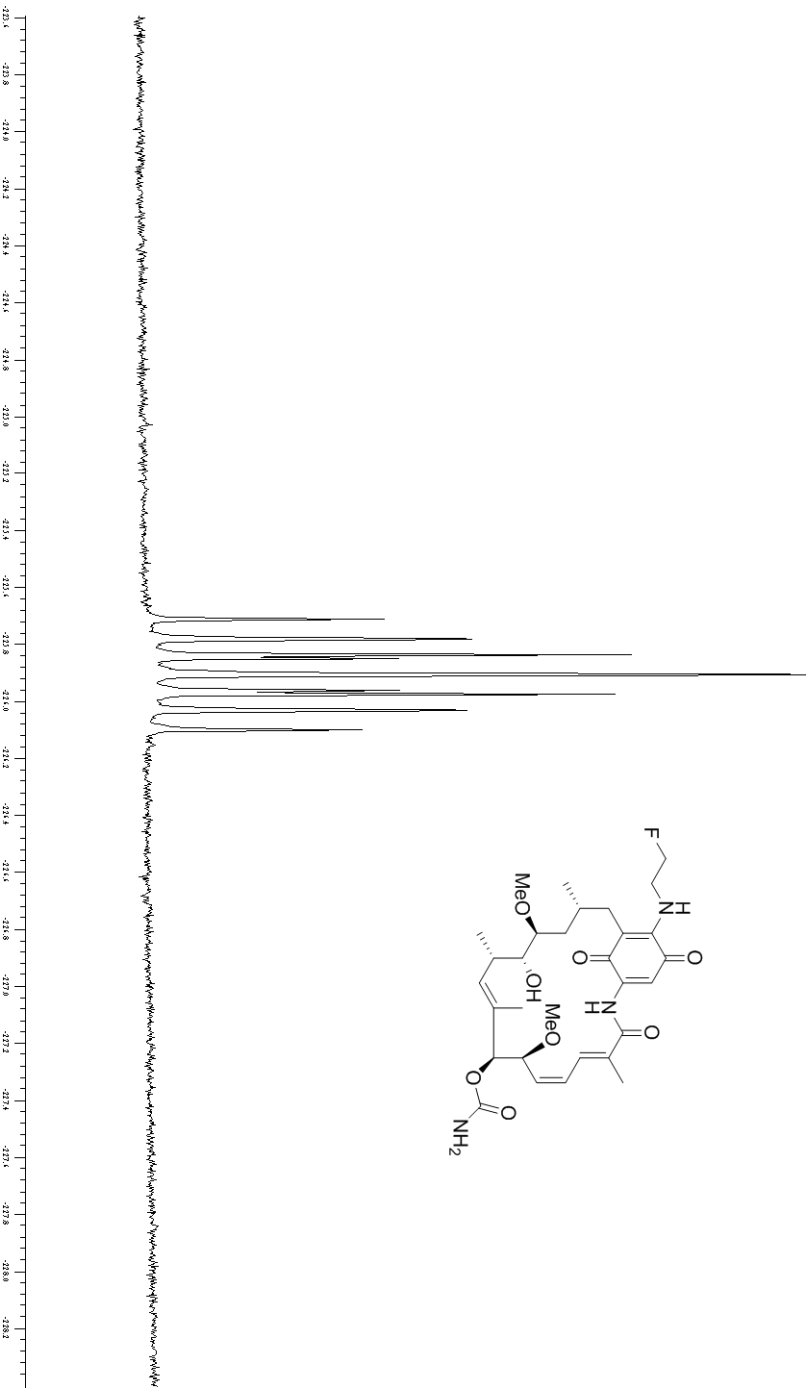
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17-demethoxy-geldanamycin 7**



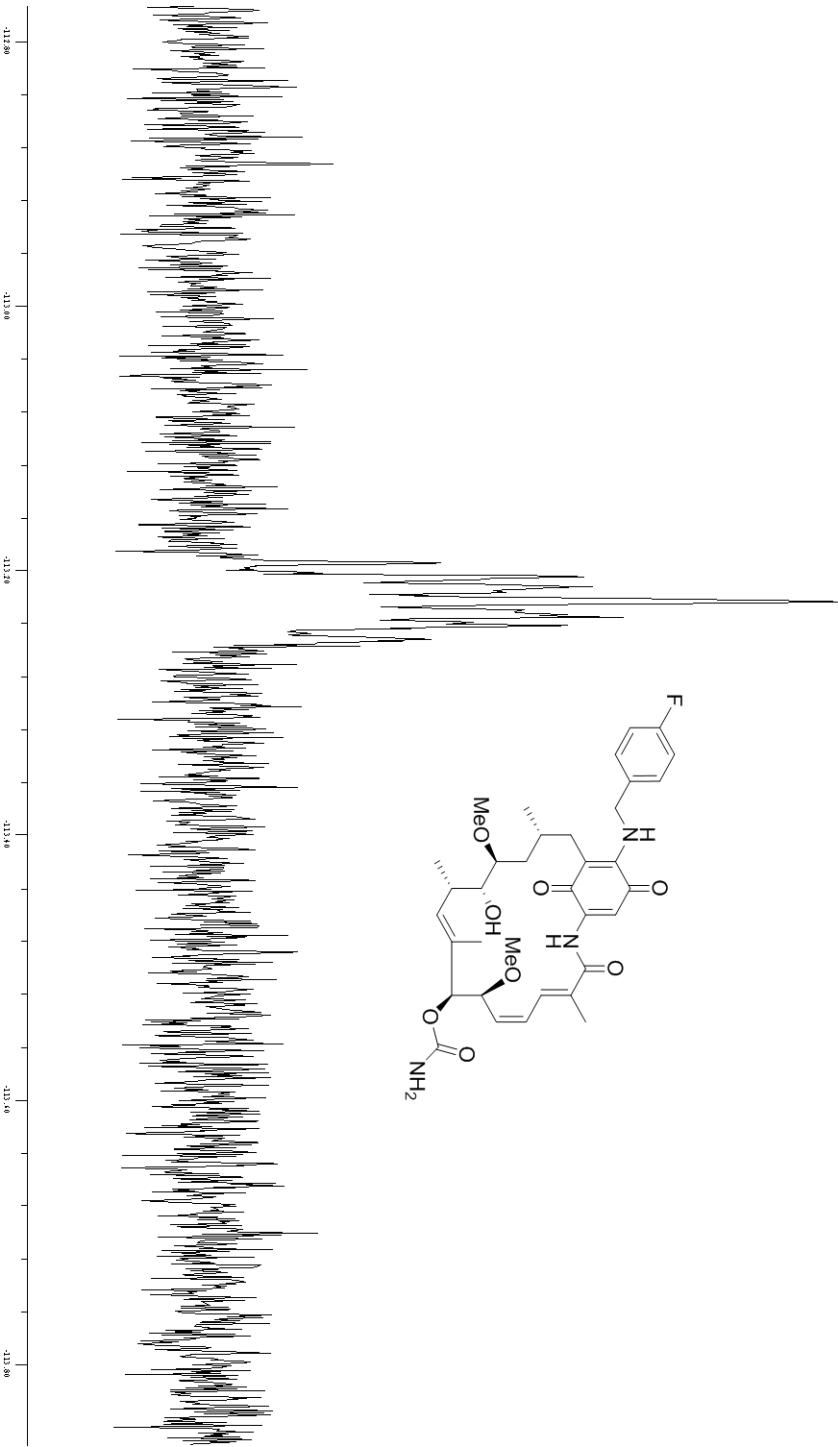
¹H-NMR: Tricarbonyl-{17-({2-[2-(2-Amino-ethoxy)-ethoxy]-ethyl}-pyridin-2-yl-methyl-amino)-acetic acid-17-demethoxy-geld-anamycin}rhenium(I) 15



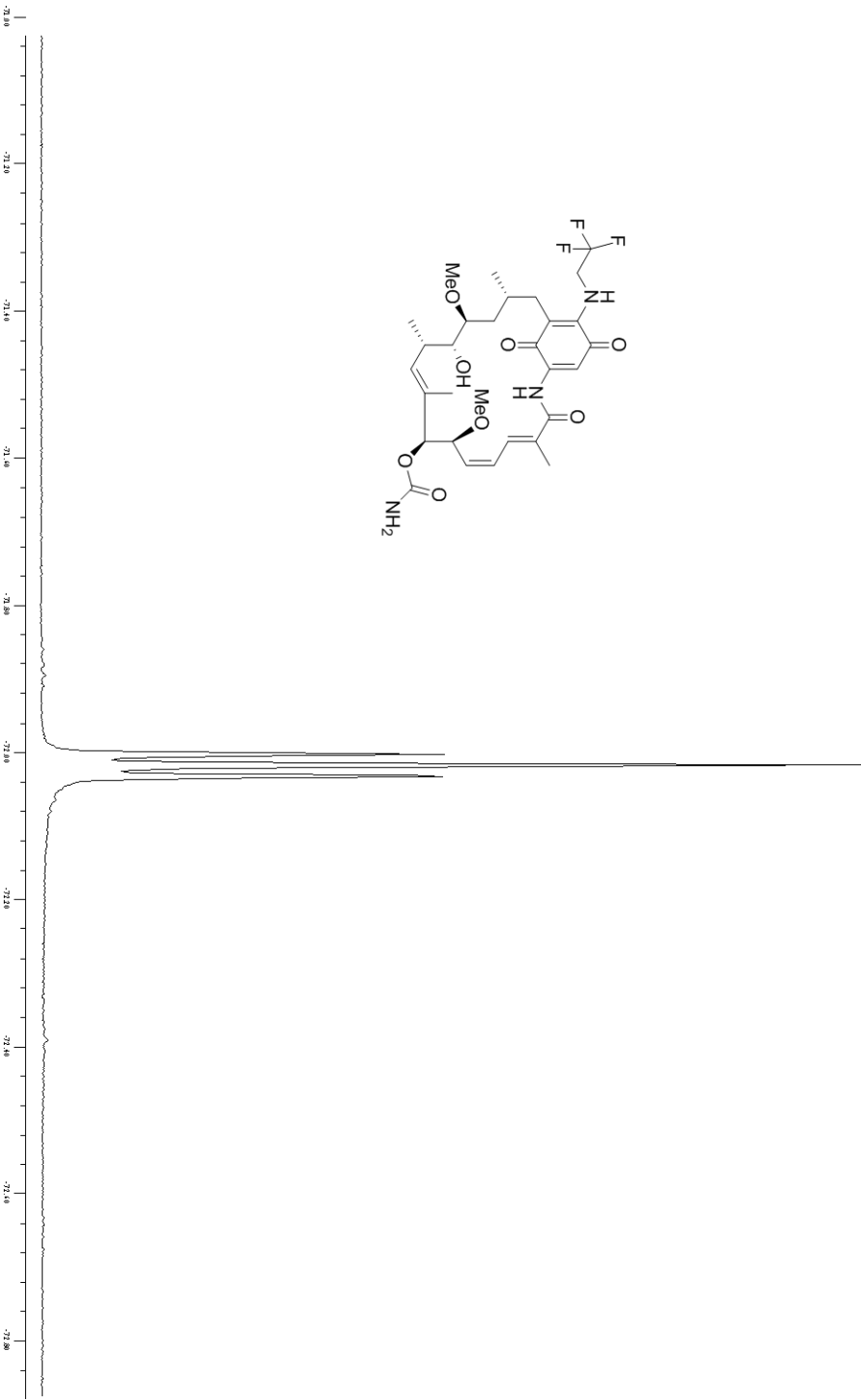
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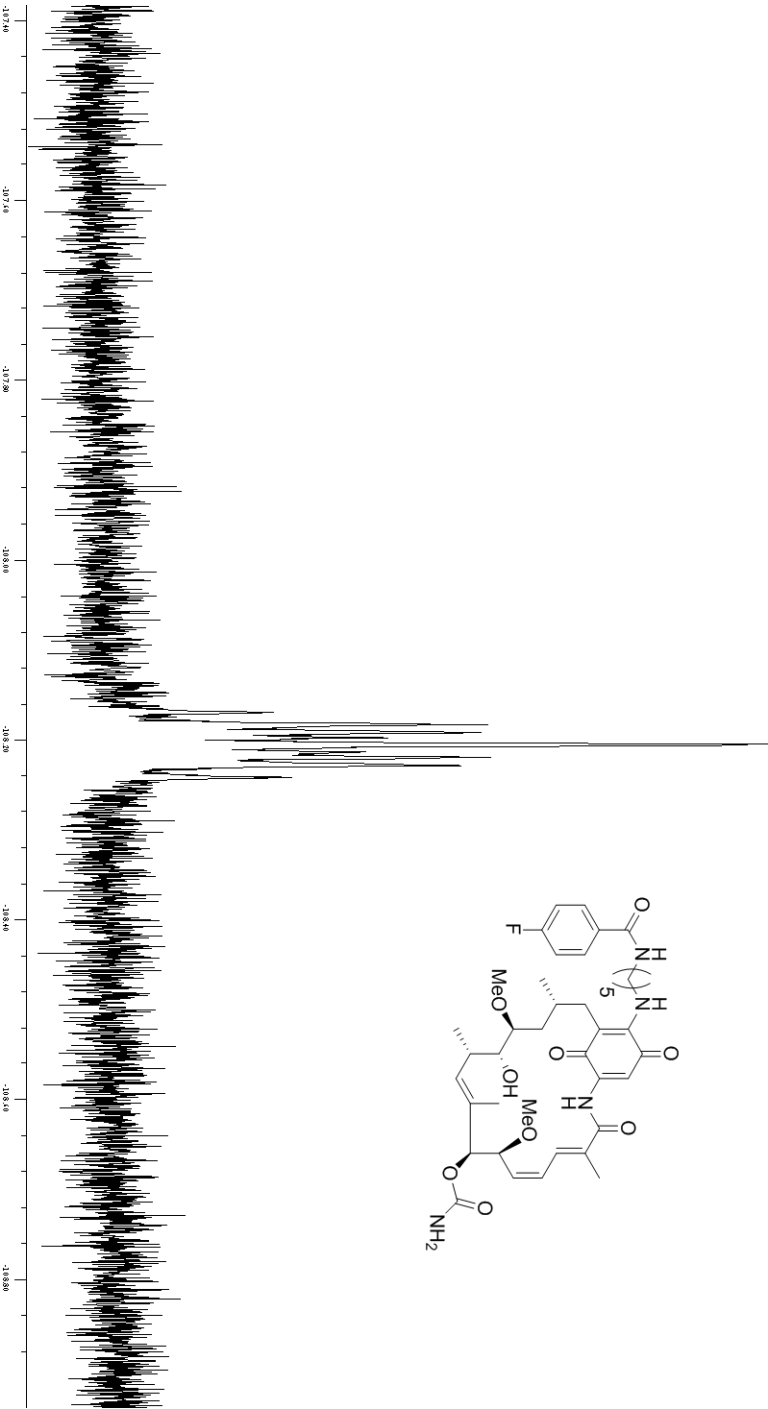
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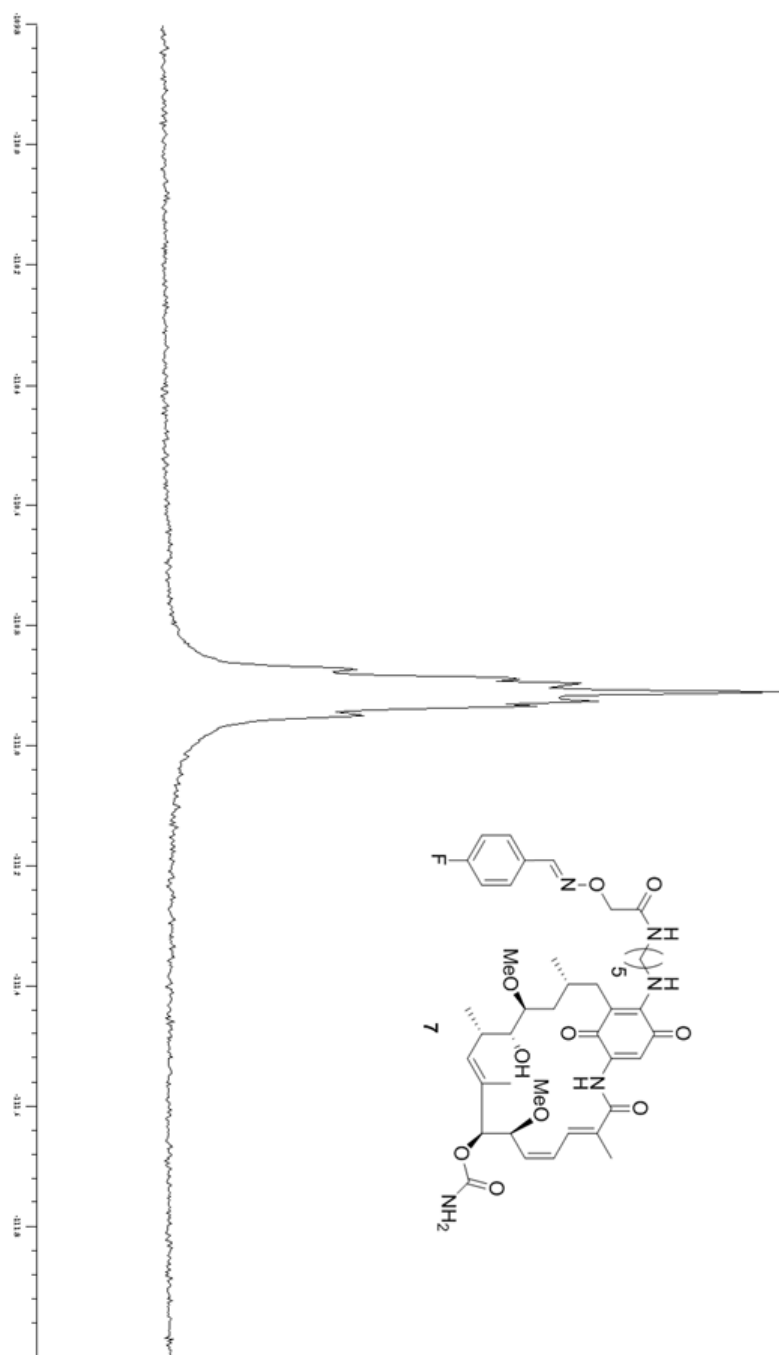
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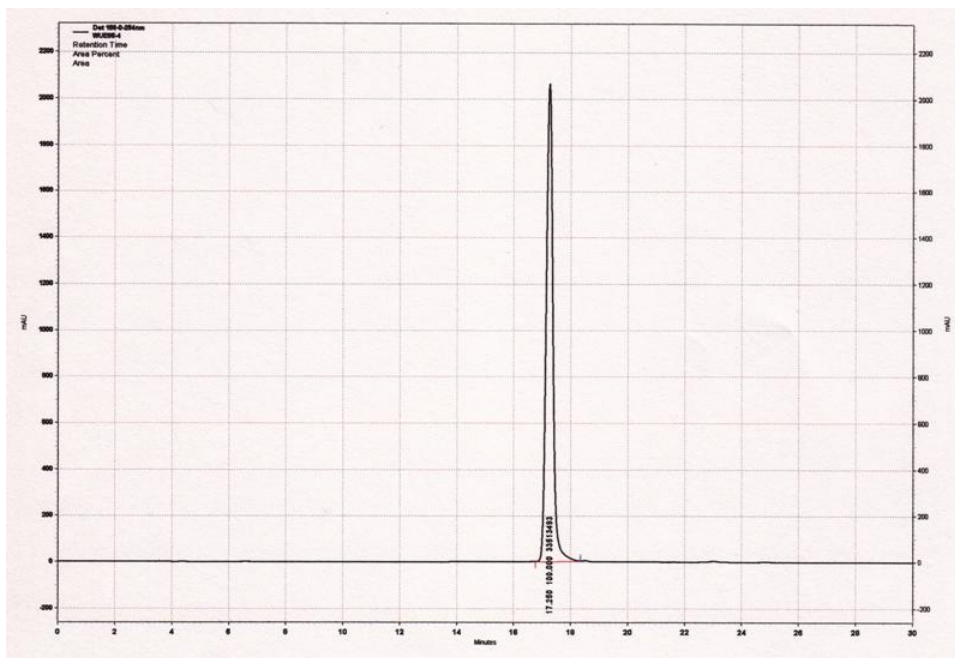
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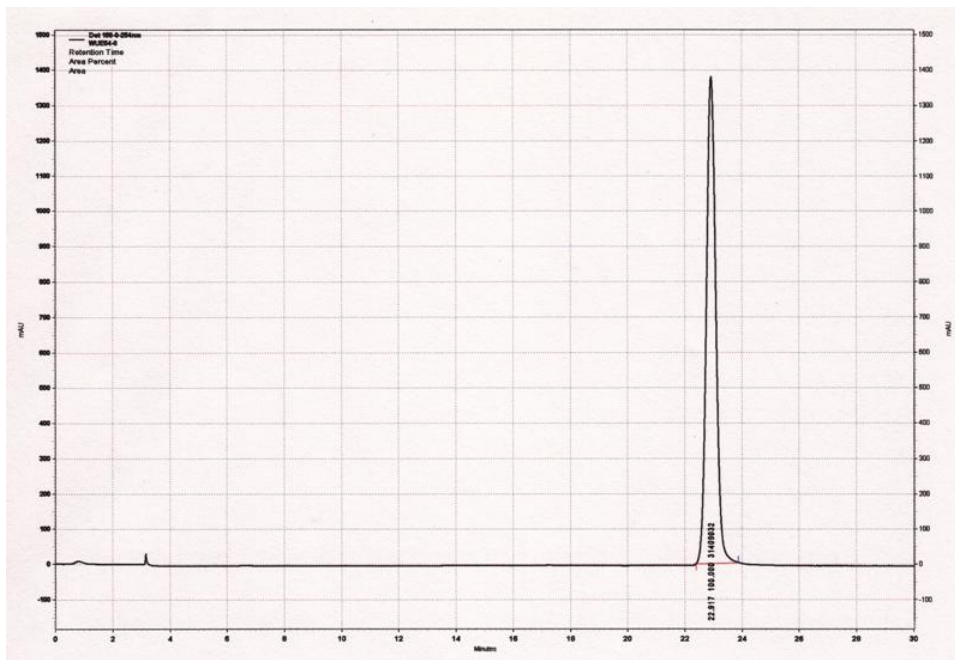
**¹⁹F-NMR: 17-(2-(((4-fluorobenzylidene)amino)oxy)acetamido)pentyl)-amino)-
17-demethoxy-geldanamycin 7**



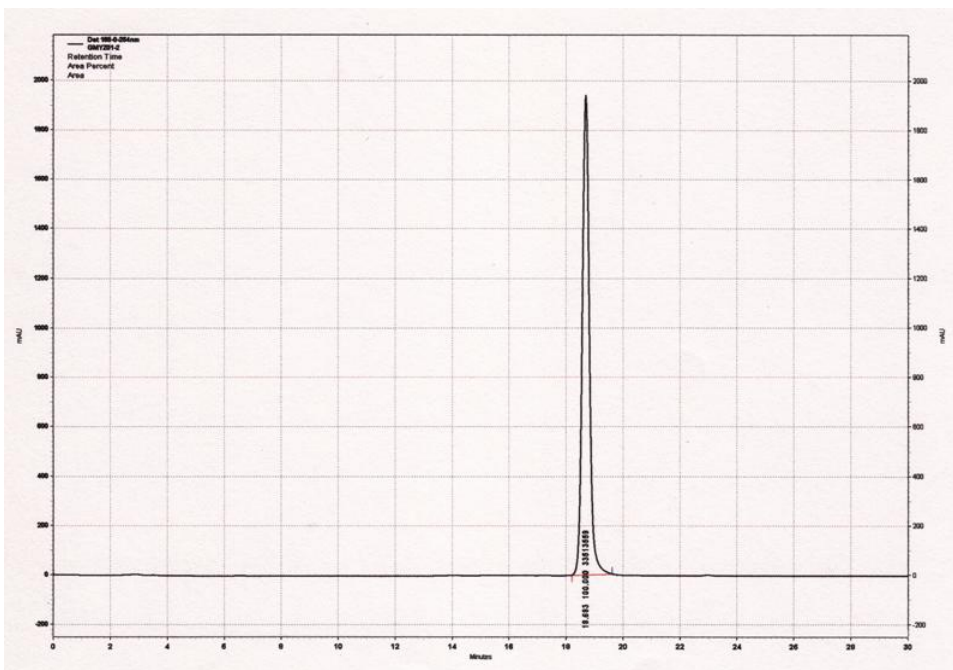
HPLC: 17-(2-Fluoroethylamino)-17-demethoxy-geldanamycin 1



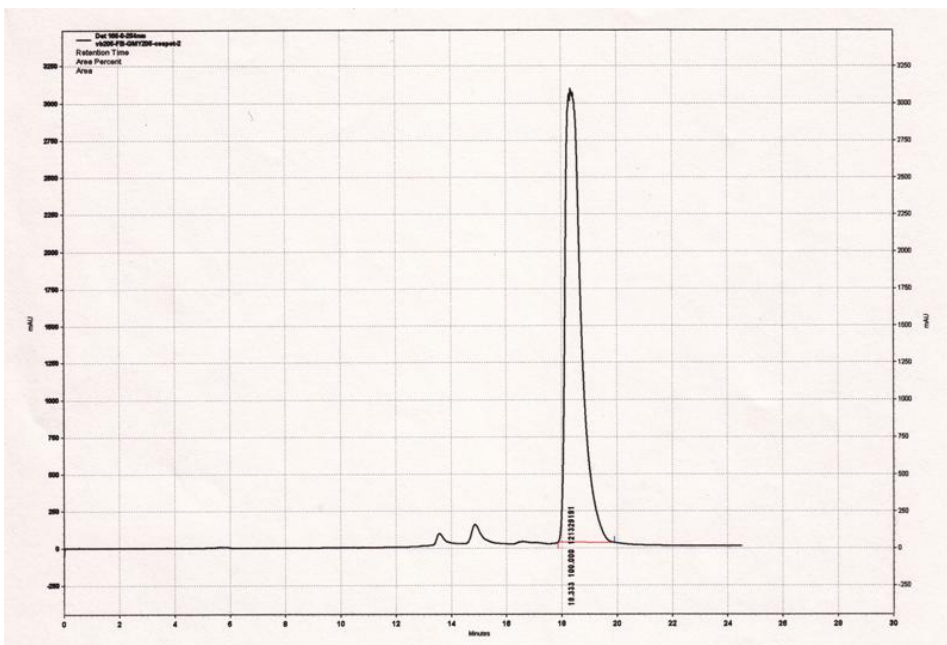
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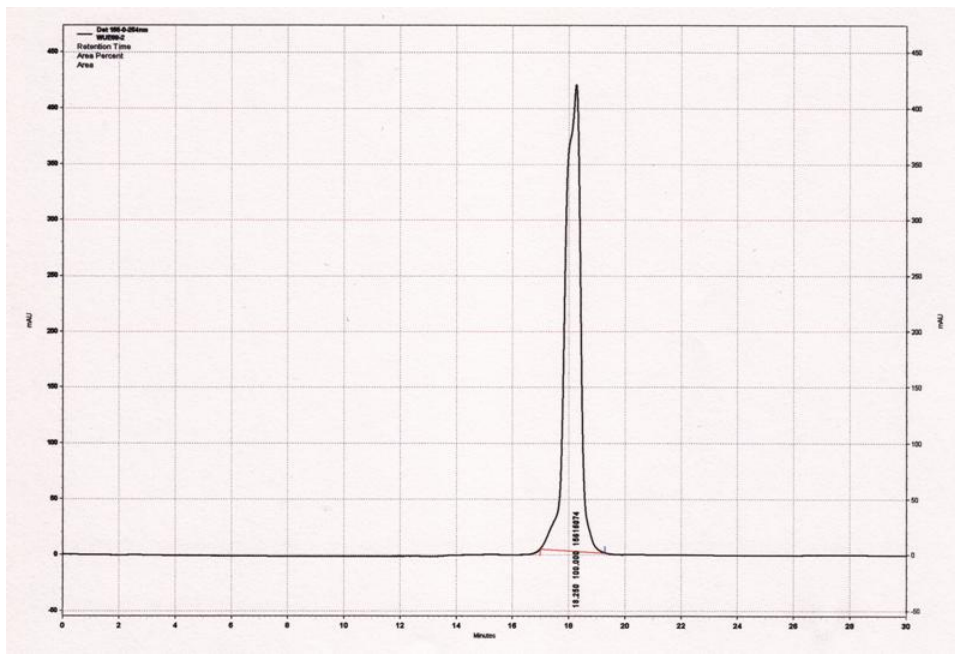
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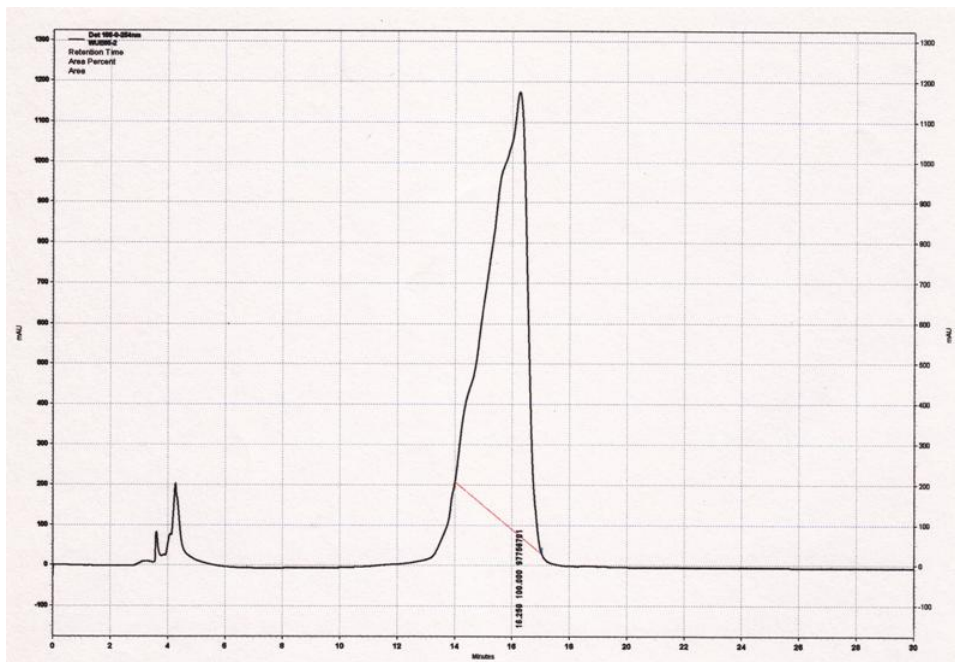
HPLC: 17-(4-Fluorobenzamido)pentyl)amino)-17-demethoxy-geldanamycin 5



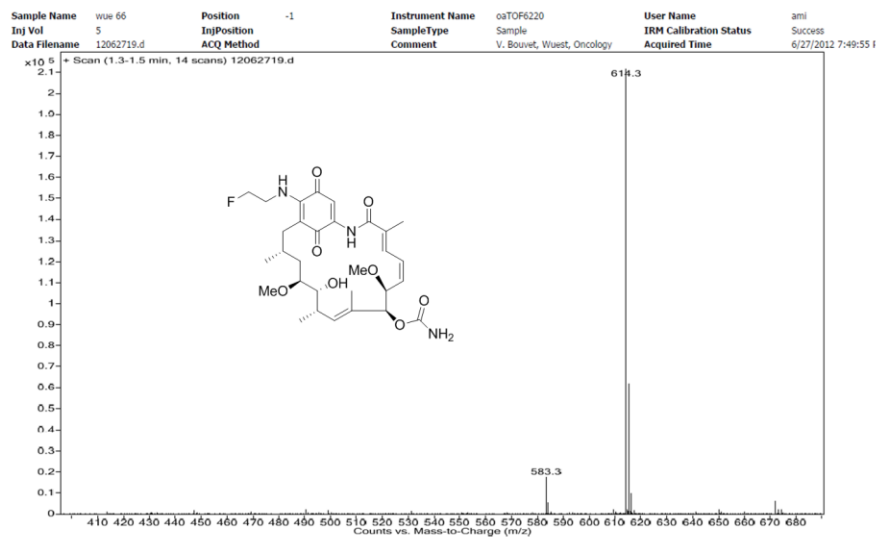
HPLC: 17-(2-(((4-fluorobenzylidene)amino)oxy)acetamido)pentyl)-amino)-17-demethoxy-geldanamycin 7



HPLC: Tricarbonyl-{17-({2-[2-(2-amino-ethoxy)-ethoxy]-ethyl}-pyridine-2-yl-methyl-amino)-acetic acid-17-demethoxy-geld-anamycin}rhenium(I) 15



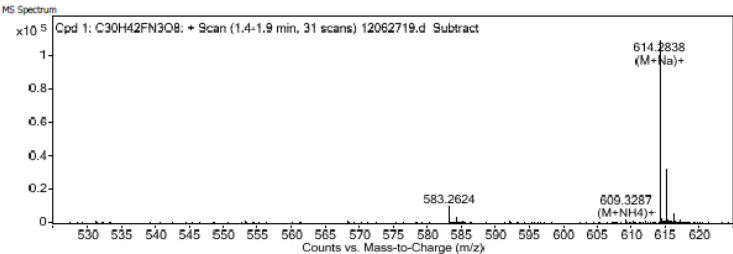
MS: 17-(2-Fluoroethylamino)-17-demethoxy-geldanamycin 1



Qualitative Compound Report

Comment: V. Bouvet, Wuest, Oncology Sample Name: wue 66
Data File: 12062719.d Instrument Name: oaTOF6220
Position: -1 Operator: ami
Acq Method: DA Method: da ami low mass.m

Compound Table

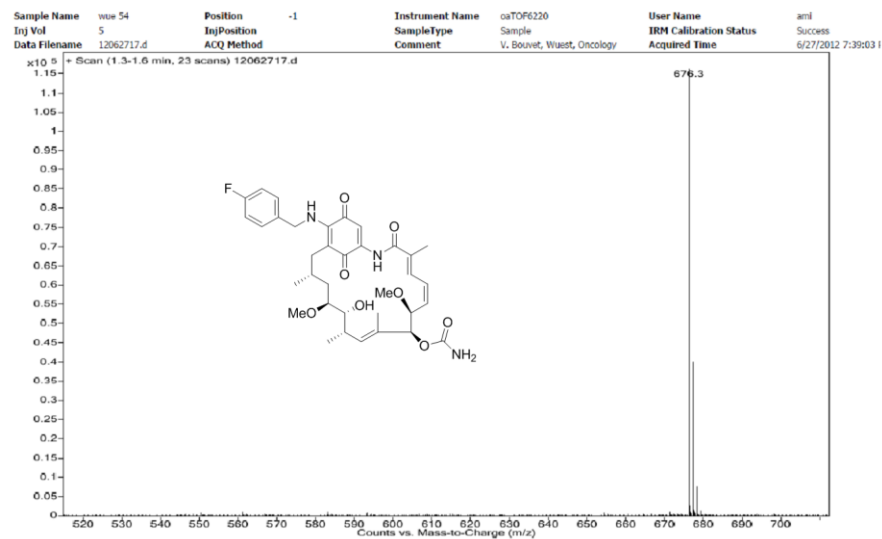


MS Spectrum Peak List

m/z	Calc m/z	Diff (ppm)	z	Abund	Formula	Ion
609.3287	609.3294	-1.22	1	1080	C30 H46 F N4 O8	(M+NH4)+
614.2838	614.2848	-1.73	1	108903	C30 H42 F N3 Na O8	(M+Na)+

— End Of Report —

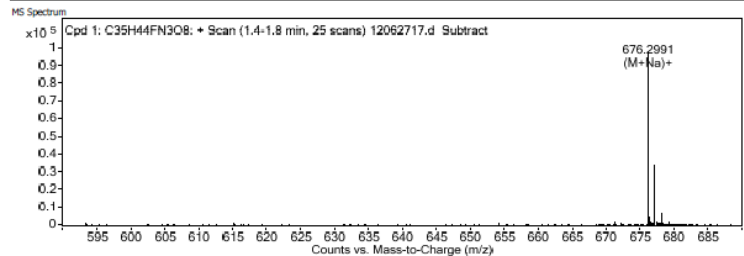
MS: 17-(4-Fluorobenzylamino)-17-demethoxy-geldanamycin 2



Qualitative Compound Report

Comment V. Bouvet, Wuest, Oncology Sample Name wue 54
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Acq Method DA Method da aml low mass.m

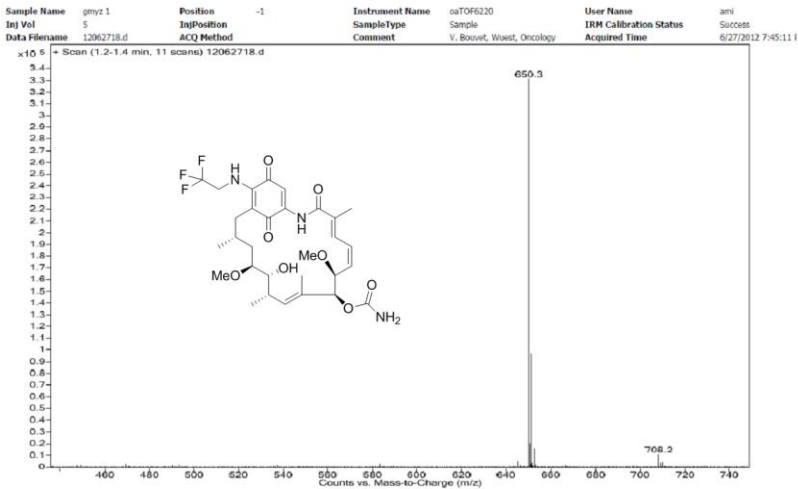
Compound Table



MS Spectrum Peak List				
m/z	Calc m/z	Diff(ppm)	Abund	Formula
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— End Of Report —

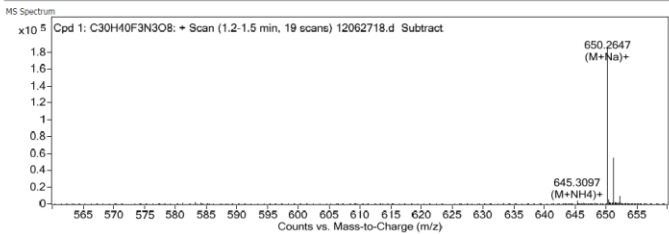
MS: 17-(2,2,2-Trifluoroethylamino)-17-demethoxy-geldanamycin 3



Qualitative Compound Report

Comment V. Bouvet, Wuest, Oncology Sample Name gmyz 1
Data File 12062718.d Instrument Name oaTOF6220
Position -1 Operator ami
Acq Method DA Method da ami low mass.m

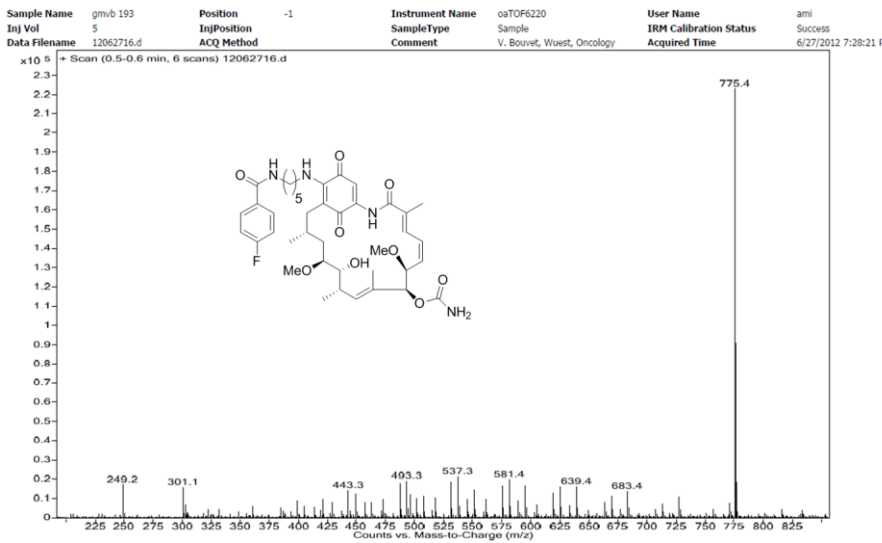
Compound Table



m/z	Calc m/z	Diff(ppm)	Abund	Formula	Ion
645.3097	645.3106	-1.35	2539	C30 H44 F3 N4 O8	(M+NH4)+
650.2647	650.266	-2.01	185935	C30 H40 F3 N3 Na O8	(M+Na)+

--- End Of Report ---

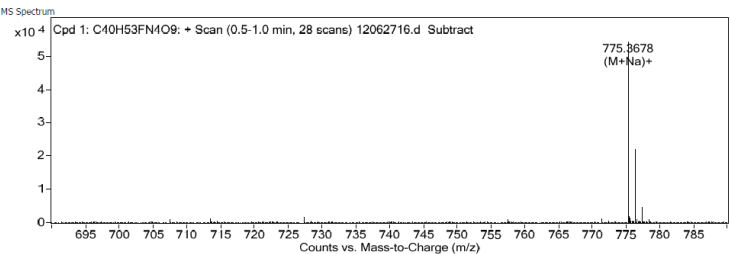
MS: 17-(4-Fluorobenzamido)pentyl)-17-demethoxy-geldanamycin 5



Qualitative Compound Report

Comment V. Bouvet, Wuest, Oncology Sample Name gmbv 193
Data File 12062716.d Instrument Name oaTOF6220
Position -1 Operator ami
Acq Method DA Method da ami low mass.m

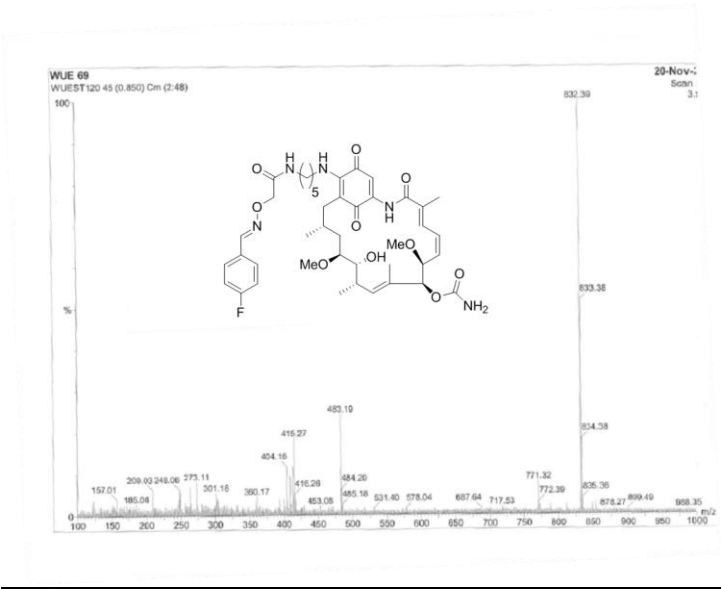
Compound Table



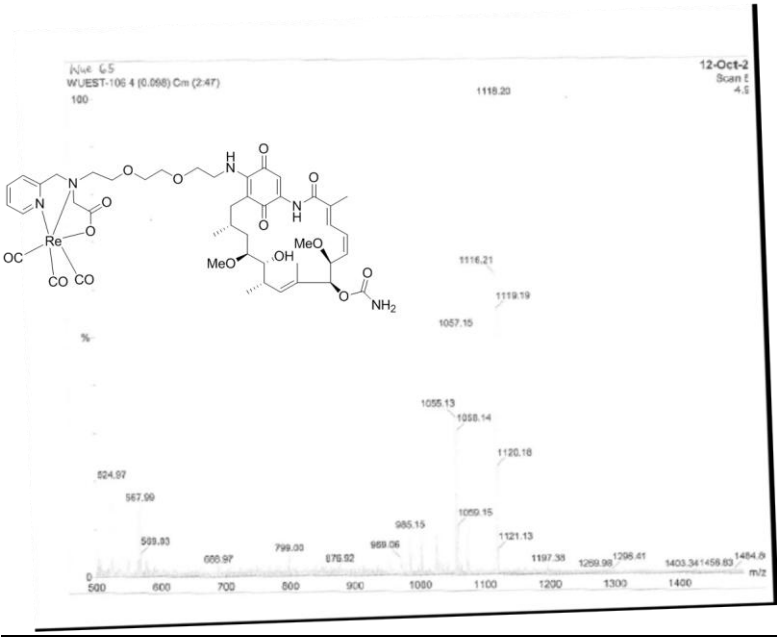
MS Spectrum Peak List					
m/z	Calc m/z	Diff(ppm)	Abund	Formula	Ion
775.3678	775.3689	-1.43	54276	C40 H53 F N4 Na O9	(M+Na)+

--- End Of Report ---

MS: 17-((4-fluorobenzylidene)amino)oxy)acetamido)pentyl)-amino)-17-demethoxy-geldanamycin 7



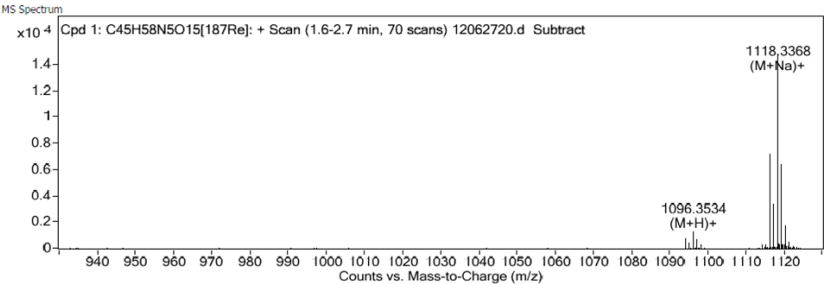
MS: Tricarbonyl-{17-({2-[2-(2-Amino-ethoxy)-ethoxy]-ethyl}-pyridin-2-yl-methyl-amino)-acetic acid-17-demethoxy-geld-anamycin}rhenium(I) 15



Qualitative Compound Report

Comment V. Bouvet, Wuest, Oncology
Data File 12062720.d
Position -1
Acq Method
Sample Name wue 65
Instrument Name caTOF6220
Operator ami
DA Method da ami low mass.m

Compound Table



m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
1096.3534	1096.356	-2.35	1	1250	C45 H59 N5 O15 [187Re]	(M+H)+
1118.3368	1118.3379	-0.98	1	14808	C45 H58 N5 Na O15 [187Re]	(M+Na)+

--- End Of Report ---