

## Supplementary Information

### Copper-free click chemistry with the short-lived positron emitter fluorine-18

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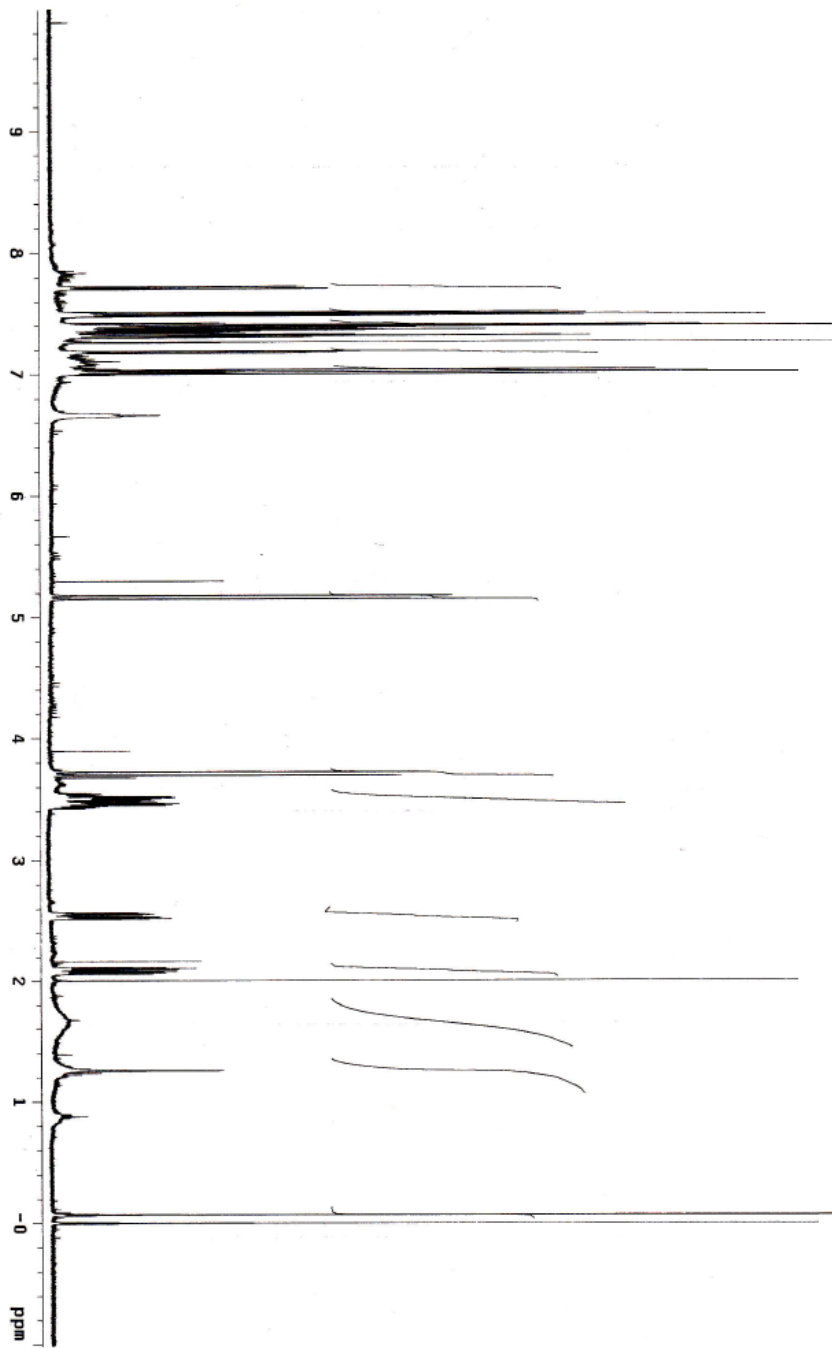
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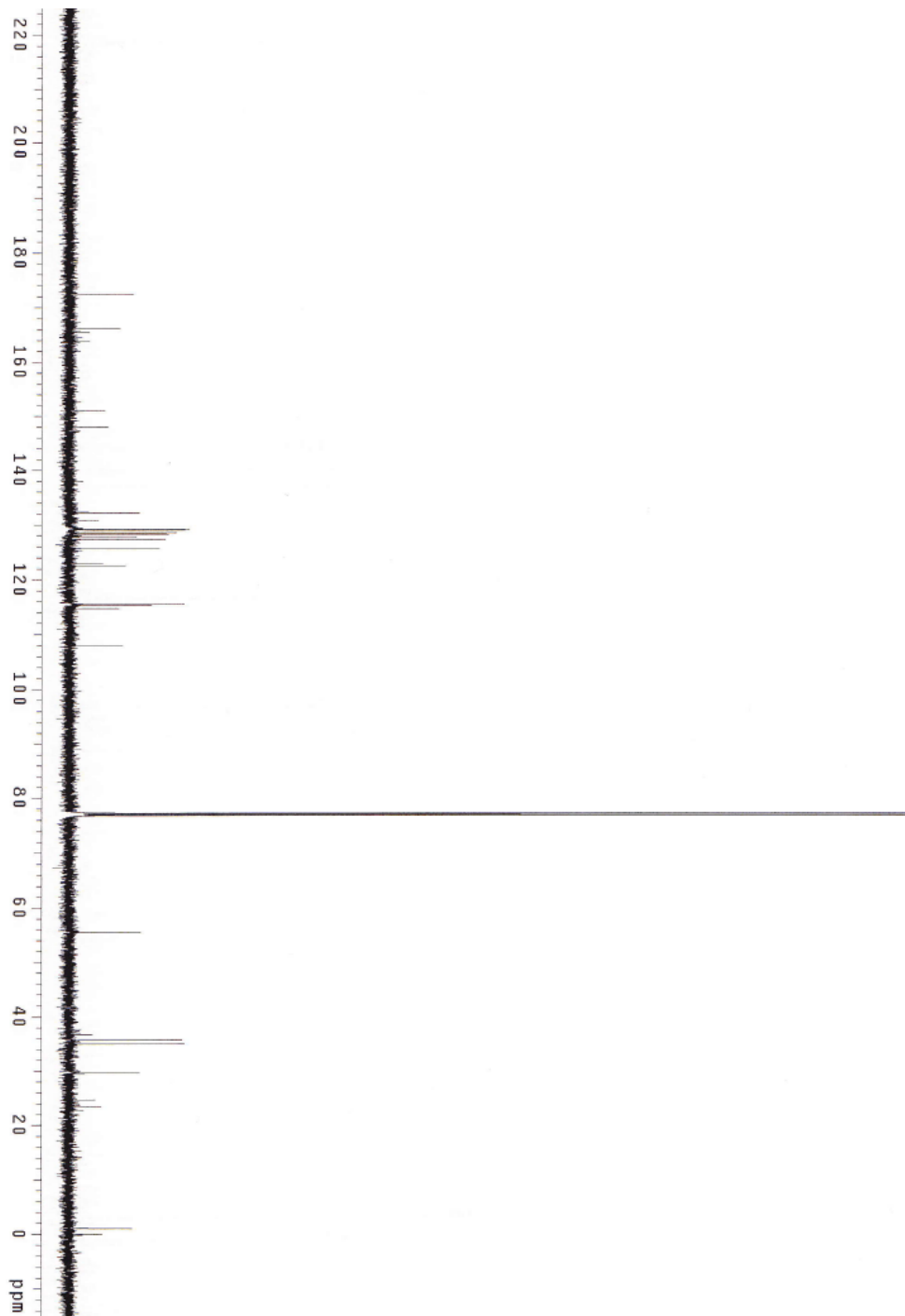
**Spectra (NMR and MS) and HPLC traces of all compounds**

**Radio-HPLC traces of all <sup>18</sup>F-labeled compounds**

**<sup>1</sup>H-NMR - 5,6-Dihydro-11,12-didehydrodibenzo-[b,f]azocino-3-oxoprop-yl-4-fluorobenzamide (FB-DBCO).**



**$^{13}\text{C}$ -NMR - 5,6-Dihydro-11,12-didehydrodibenzo-[*b,f*]azocino-3-oxoprop-yl-4-fluorobenzamide (FB-DBC0).**

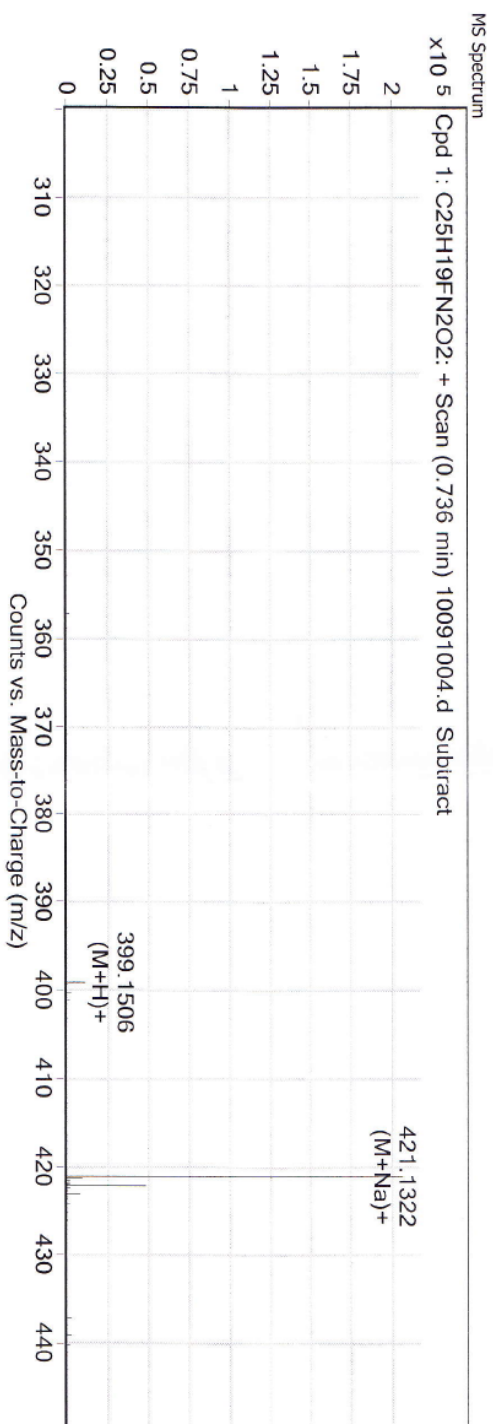


**MS - 5,6-Dihydro-11,12-didehydrodibenzo-[b,f]azocino-3-oxoprop-yl-4-fluorobenzamide (FB-DBCO).**

## Qualitative Compound Report

Comment V. Bouvet, Wuest, Oncology Sample Name vb 143  
Data File 10091004.d Instrument Name 6220 oaTOF  
Position -1 Operator ami  
Acq Method DA Method da ami low mass.m

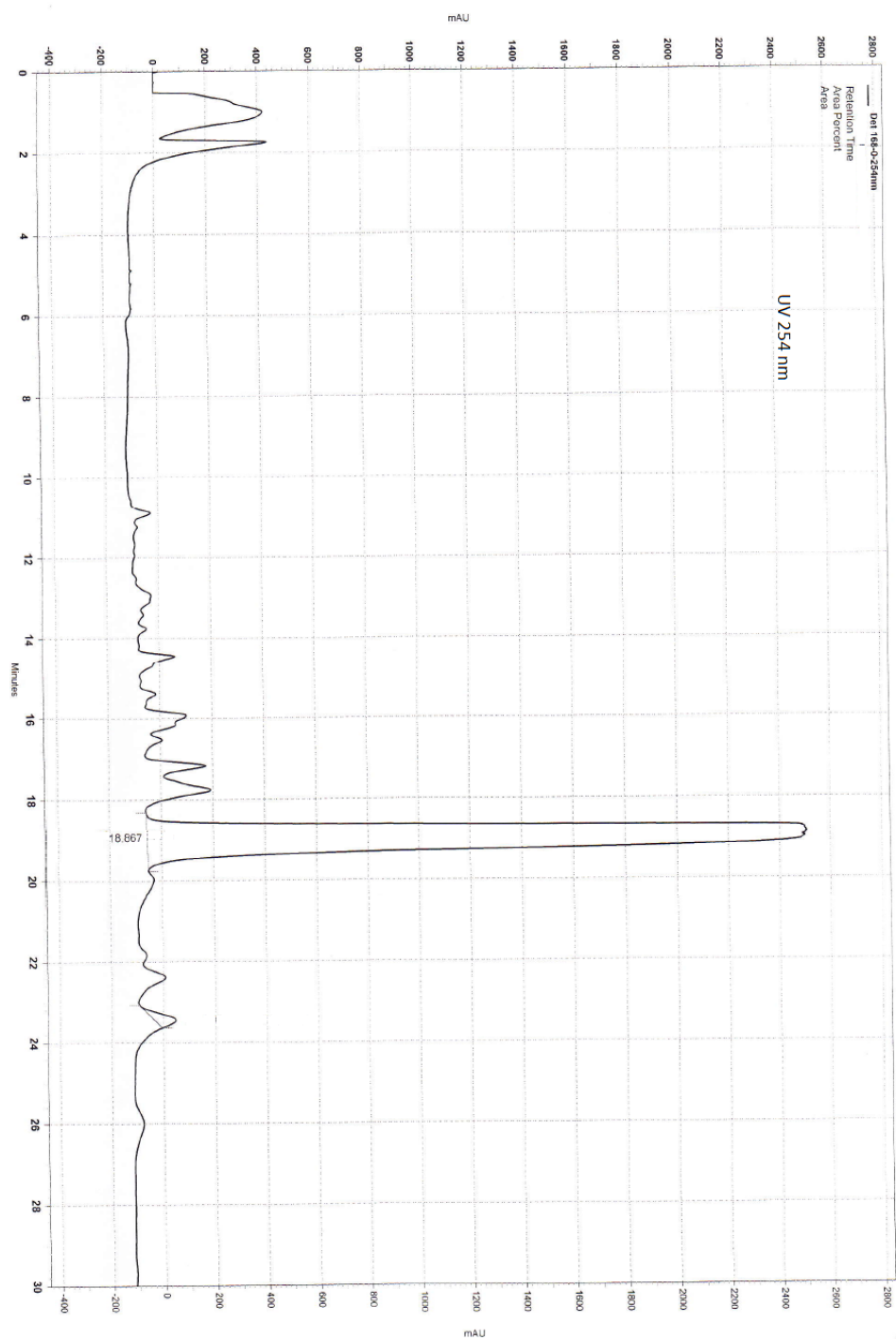
### Compound Table



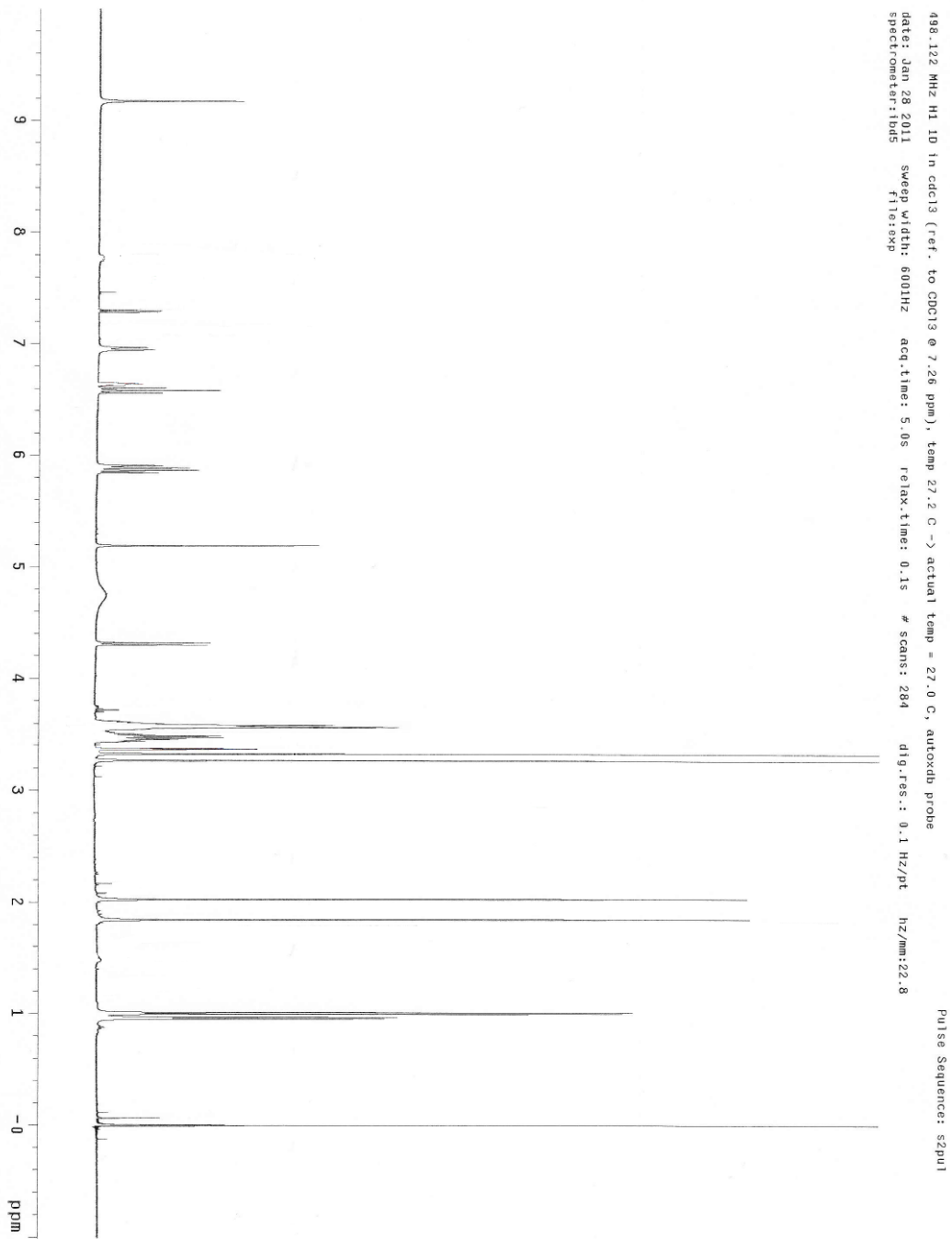
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
399.1506	399.1503	0.64	1	11273	C25 H20 F N2 O2	(M+H)+
421.1322	421.1323	-0.17		207434	C25 H19 F N2 Na O2	(M+Na)+

--- End Of Report ---

**HPLC trace (254 nm) - 5,6-Dihydro-11,12-didehydrodibenzo-[b,f]azocino-3-oxoprop-yl-4-fluorobenzamide (FB-DBCO).**



**<sup>1</sup>H-NMR - 17-[11-Azido-3,6,9-trioxaundane-1-amino]-17-desmethoxy geldanamycin (6)**

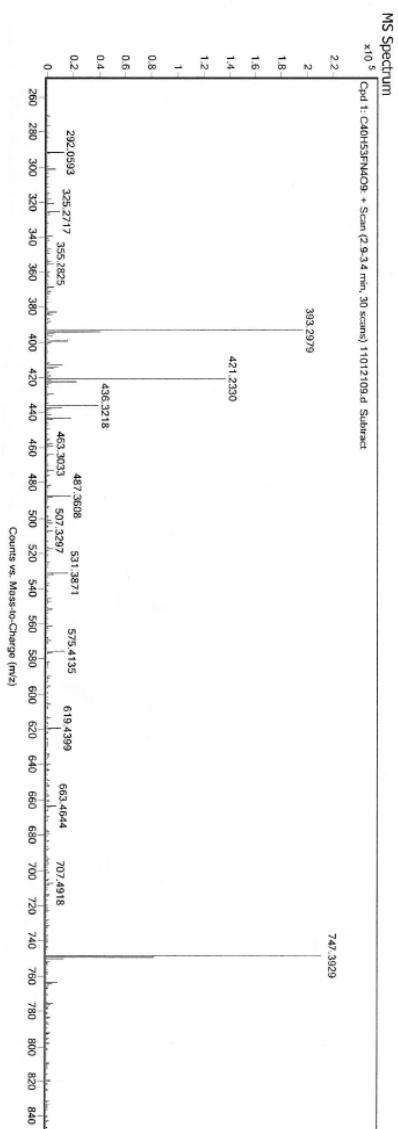


### MS - 17-[11-Azido-3,6,9-trioxaundane-1-amino]-17-desmethoxy geldanamycin (6)

## Qualitative Compound Report

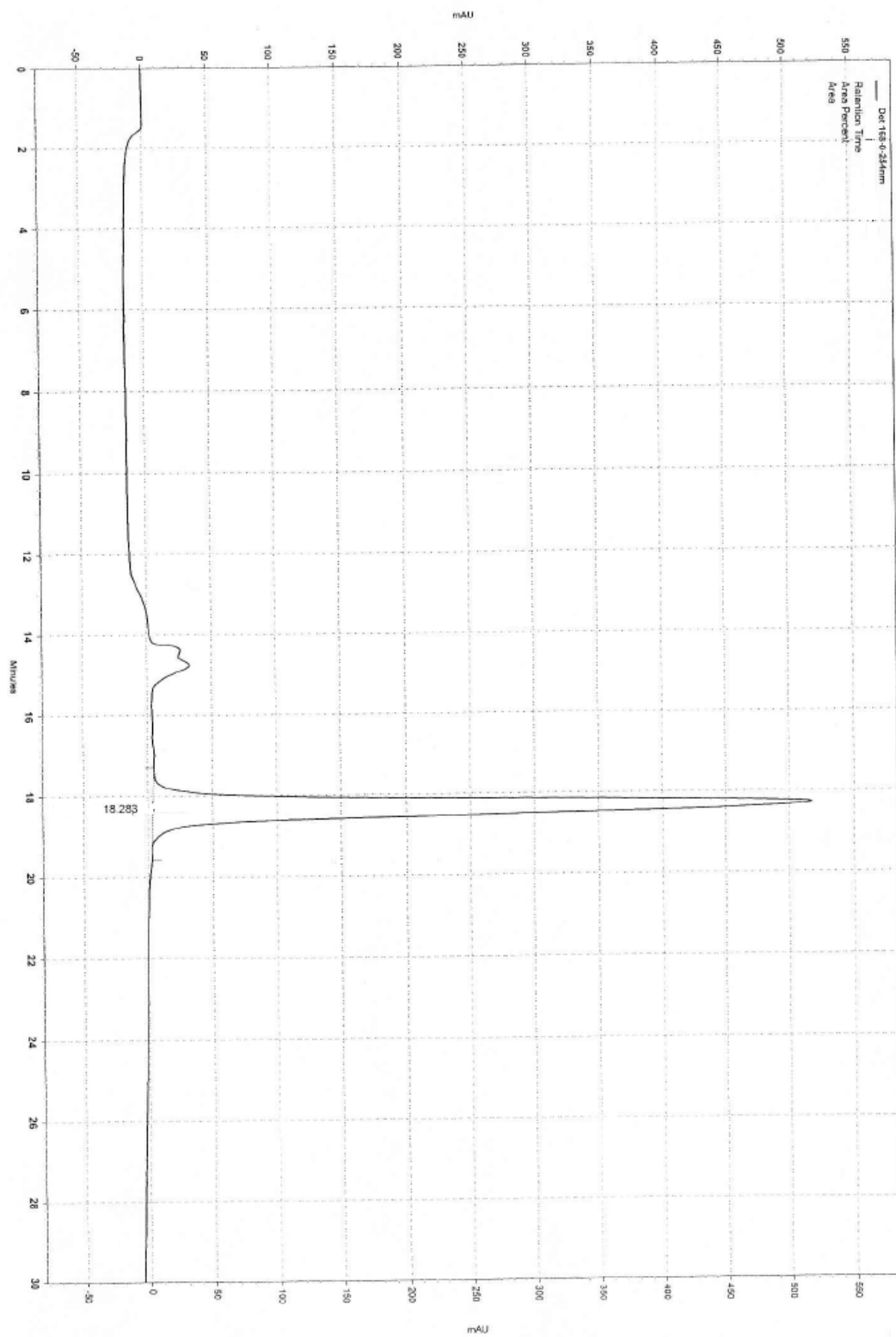
Comment	V. Bouvet, Wuest, Oncology	Sample Name	Wb_193
Data File	11012109.D	Instrument Name	6220 03TOF
Position	-1	Operator	amh
Acq Method		DA Method	da_ami_low_mass.m

#### Compound Table



--- End Of Report ---

HPLC trace (254 nm) - 17-[11-Azido-3,6,9-trioxaudane-1-amino]-17-desmethoxy geldanamycin (6)



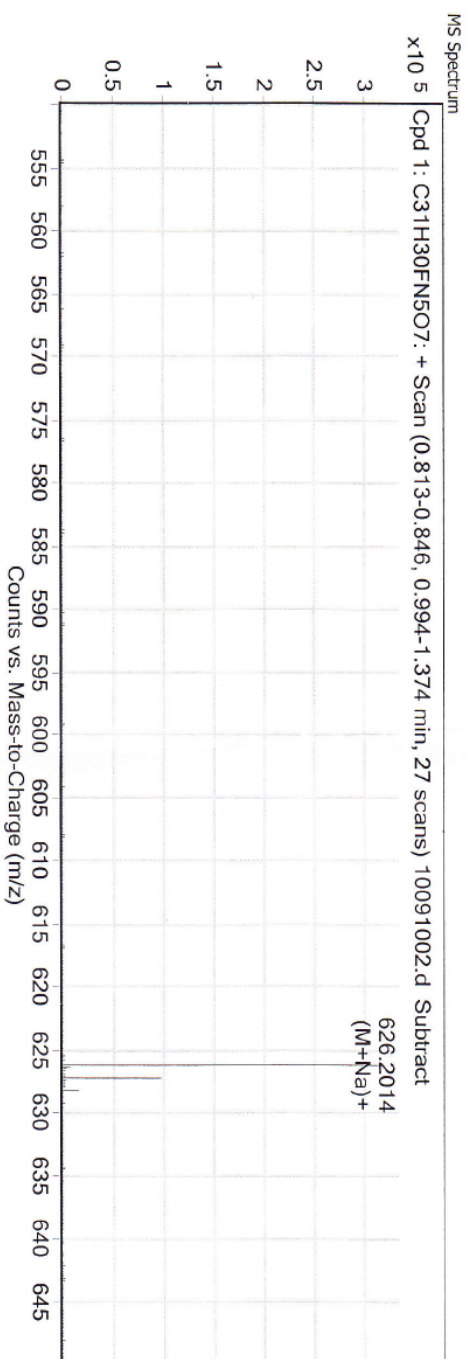


## MS regioisomer 1 – 6-FB-DBCO-coupled triazole (7)

### Qualitative Compound Report

Comment V. Bouvet, Wuest, Oncology Sample Name vb 145a  
Data File 10091002.d Instrument Name 6220 oaTOF  
Position -1 Operator ami  
Acq Method DA Method da anni low mass.m

#### Compound Table



#### MS Spectrum Peak List

m/z	Calc m/z	Diff (ppm)	Abund	Formula	Ion
626.2014	626.2021	-1.16	316653	C31 H30 F N5 Na O7	(M+Na)+

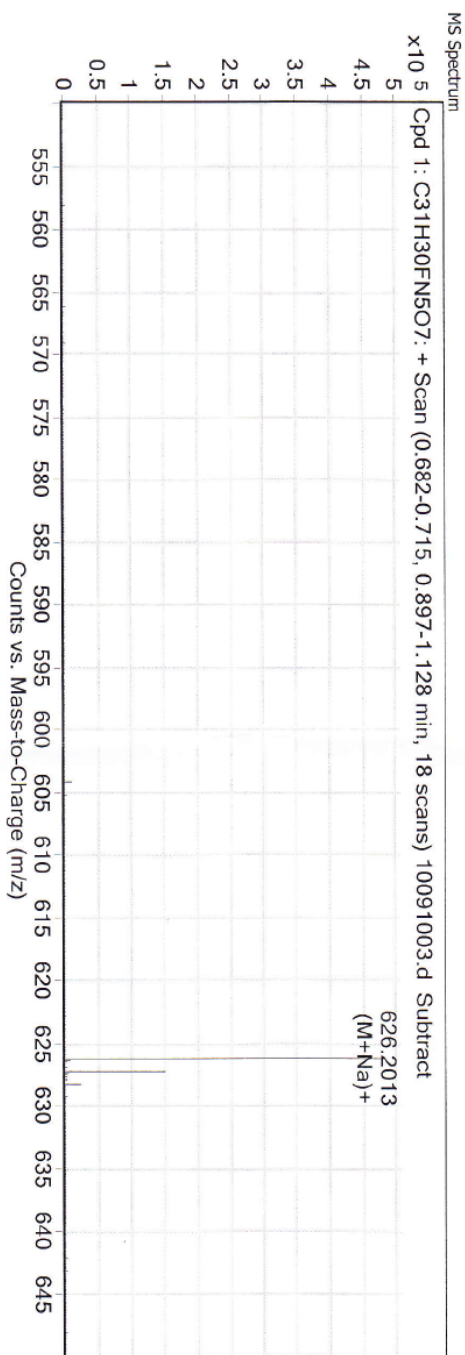
--- End Of Report ---

## MS regioisomer 2 – 6-FB-DBCO-coupled triazole (7)

### Qualitative Compound Report

Comment V. Bouvet, Wuest, Oncology Sample Name vb 145b  
Data File 10091003.d Instrument Name 6220 oaTOF  
Position -1 Operator ami  
Acq Method DA Method da anil low mass.m

#### Compound Table

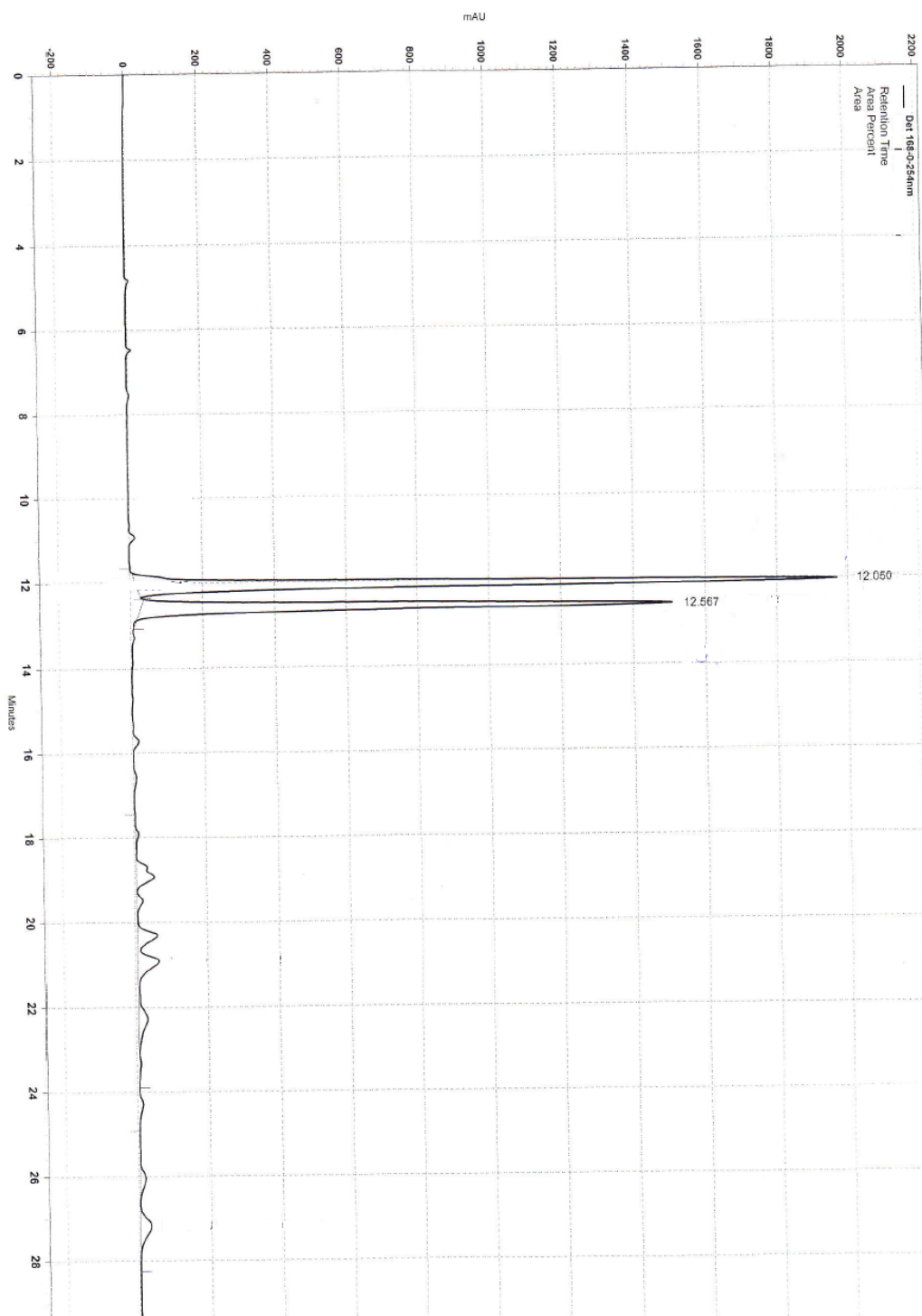


#### MS Spectrum Peak List

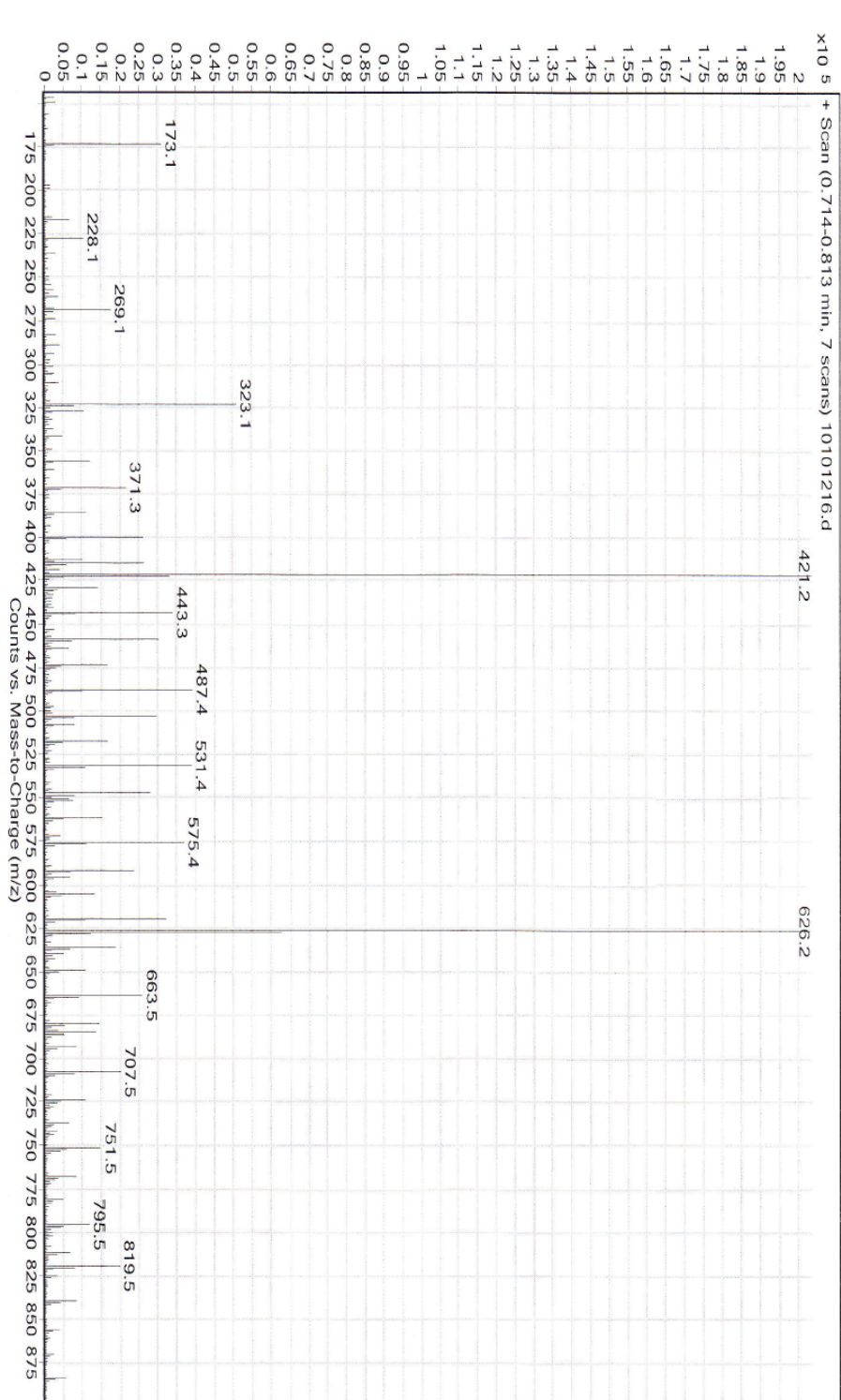
m/z	Calc m/z	Diff(ppm)	Abund	Formula	Ion
626.2013	626.2021	-1.4	482245	C31 H30 F N5 Na O7	(M+Na)+

--- End Of Report ---

### HPLC trace (254 nm) – 6-FB-DBCO-coupled triazole (7)

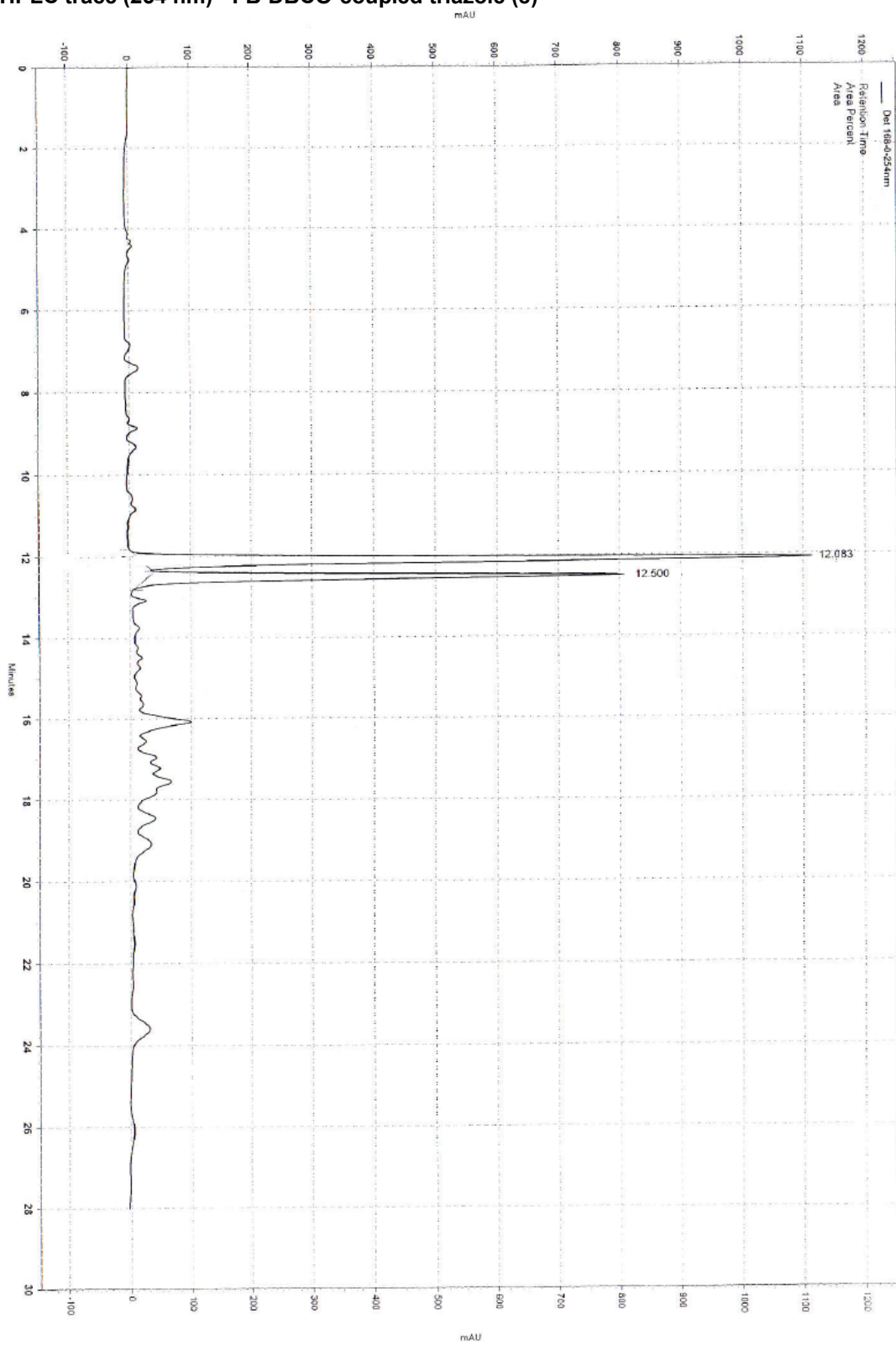


### MS - FB-DBCO-coupled triazole (8)

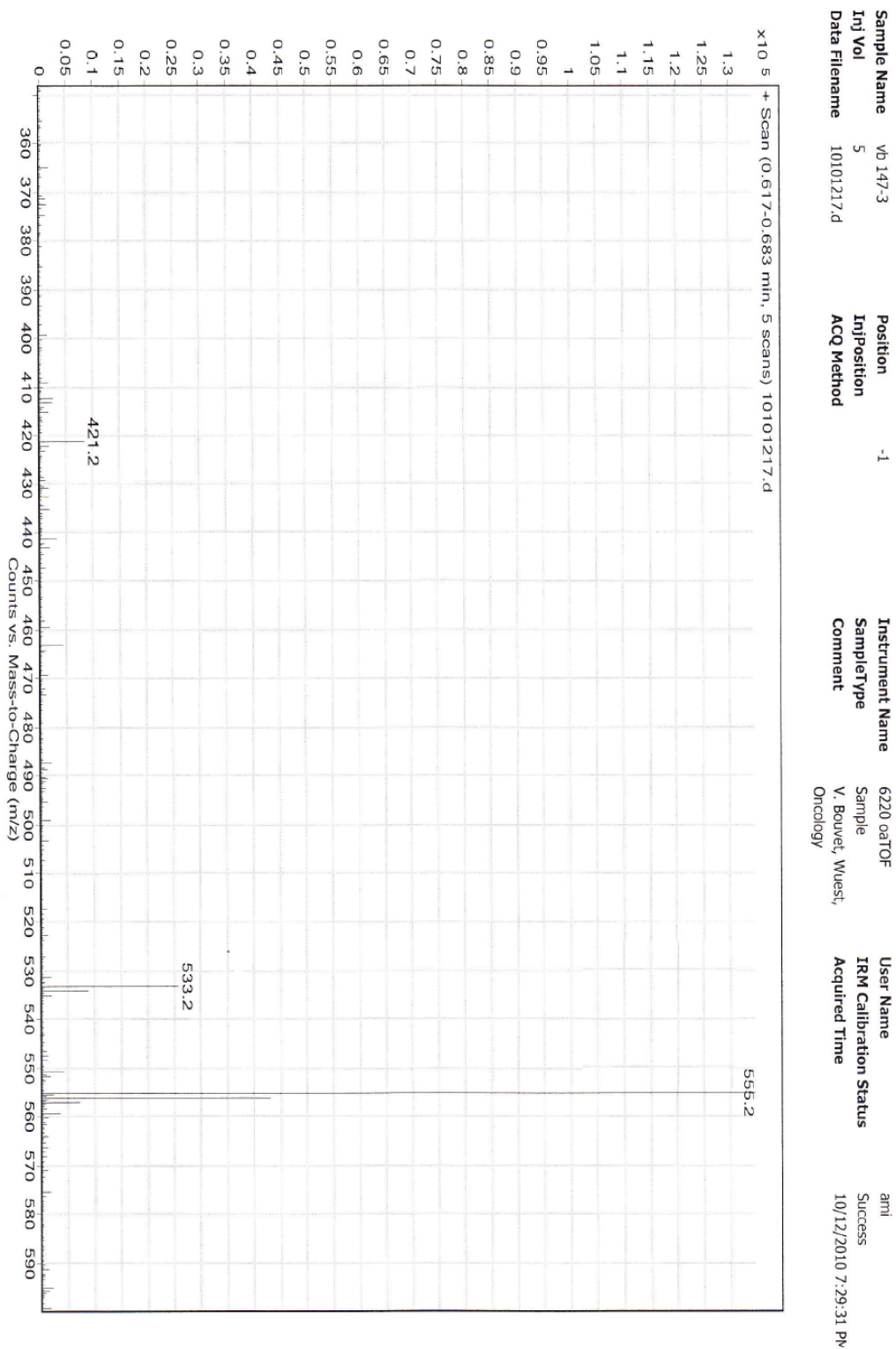


Sample Name	vb 147-1	Position	-1	Instrument Name	6220 oaTOF	User Name	anti
Inj Vol	5	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	10101216.d	ACQ Method		Comment	V. Bouvet, Wuest, Oncology	Acquired Time	10/12/2010 7:16:15 PM

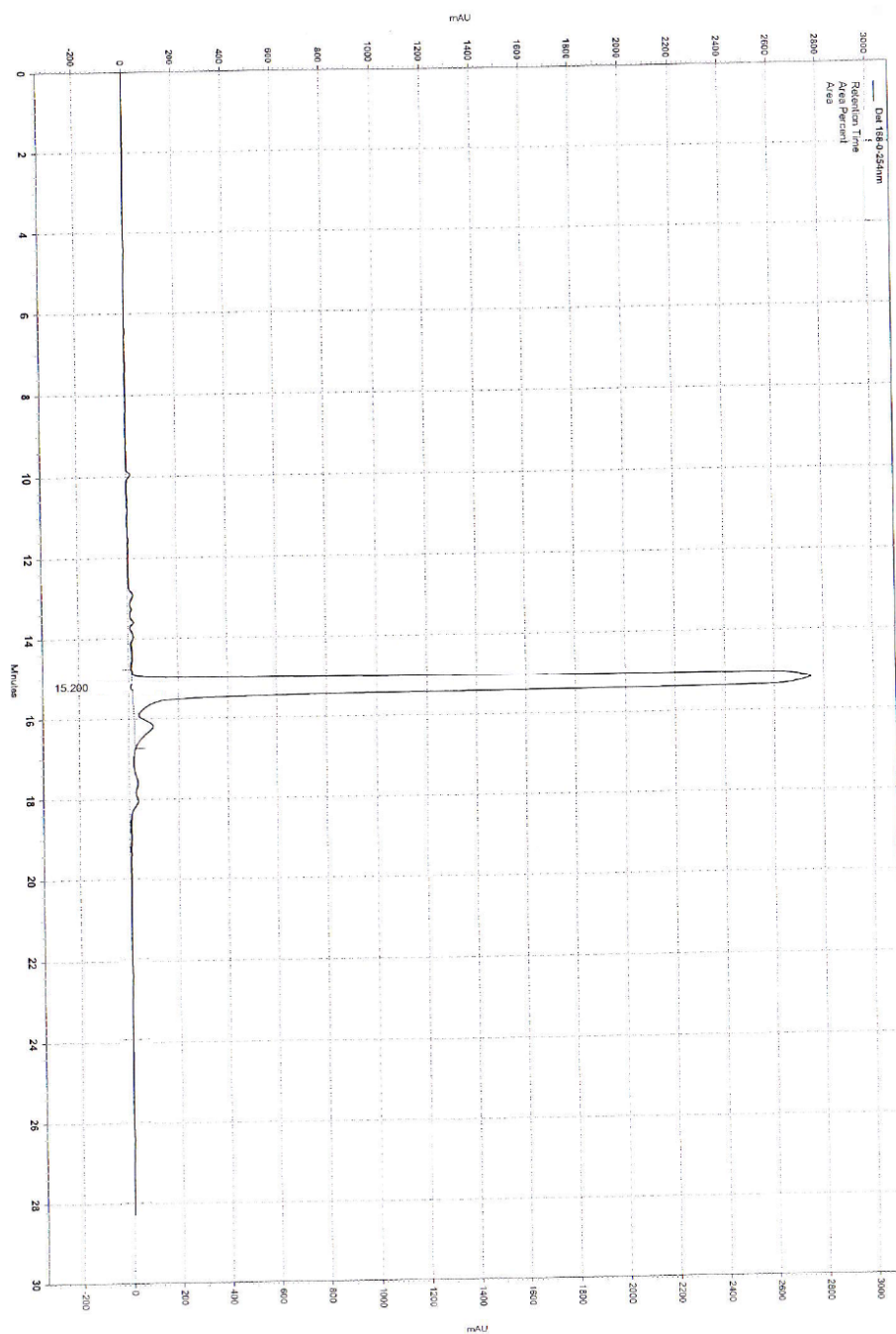
### HPLC trace (254 nm) - FB-DBCO-coupled triazole (8)



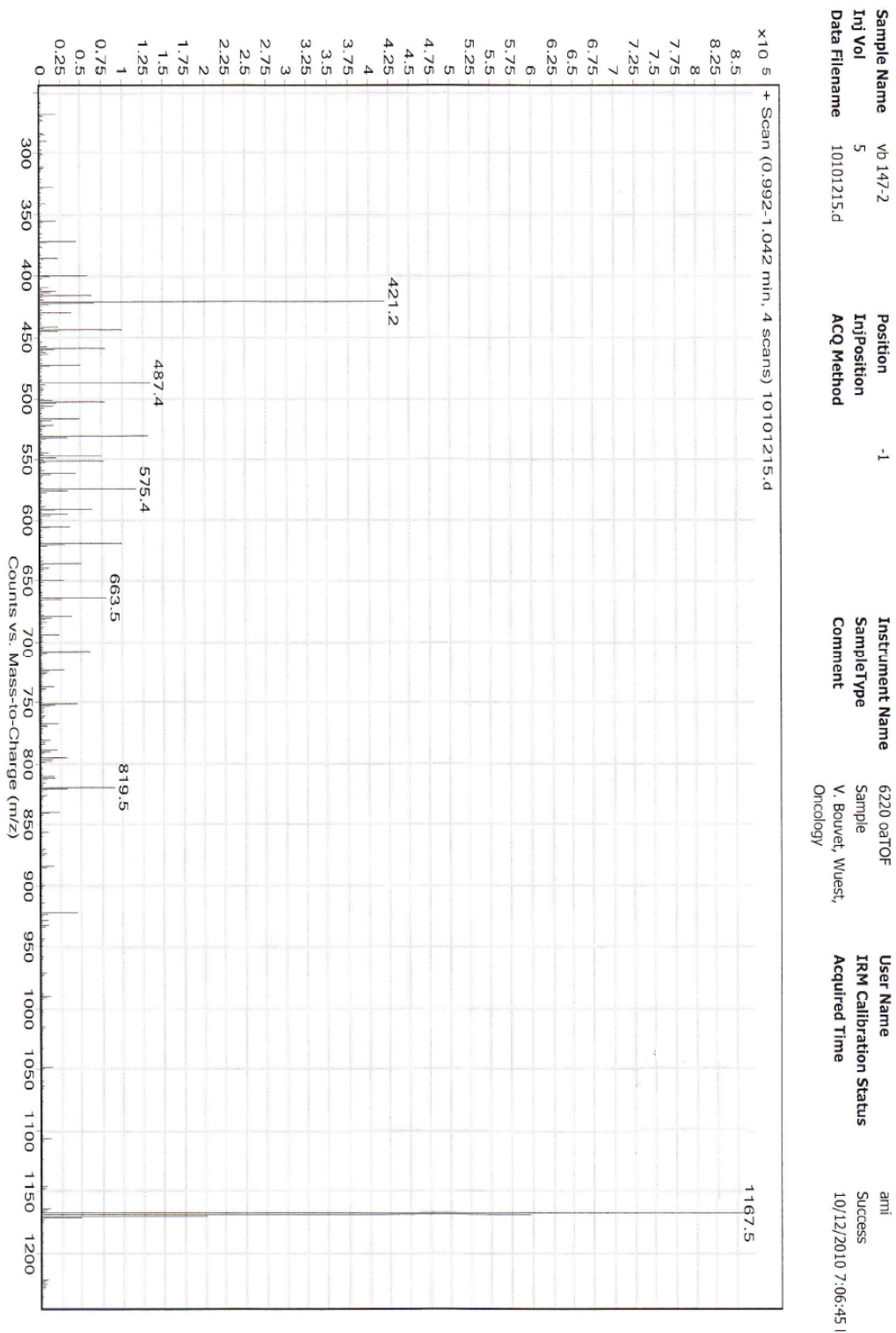
### MS - FB-DBCO-coupled triazole (9)



### HPLC trace (254 nm) - FB-DBCO-coupled triazole (9)

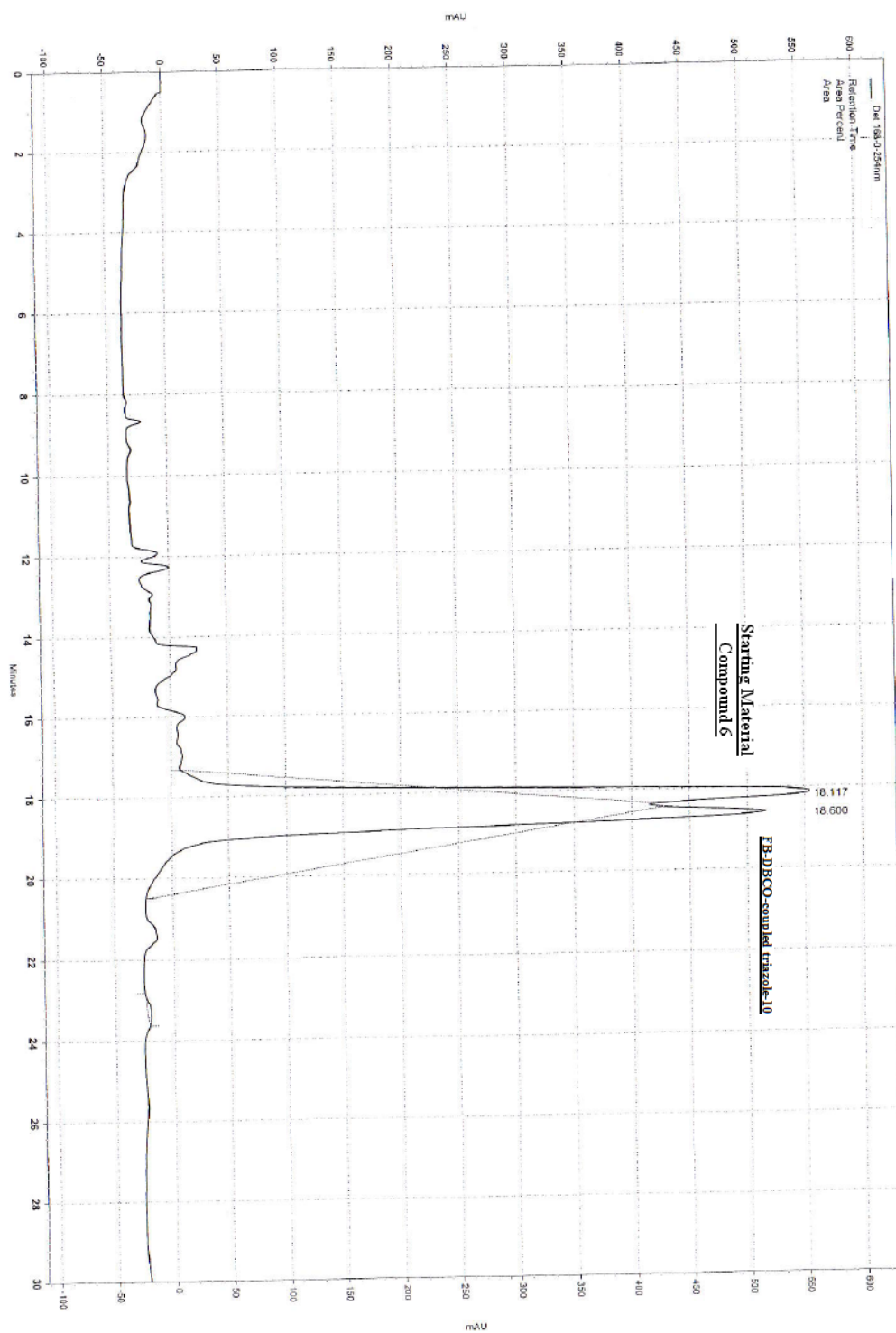


### MS - FB-DBCO-coupled triazole (10)

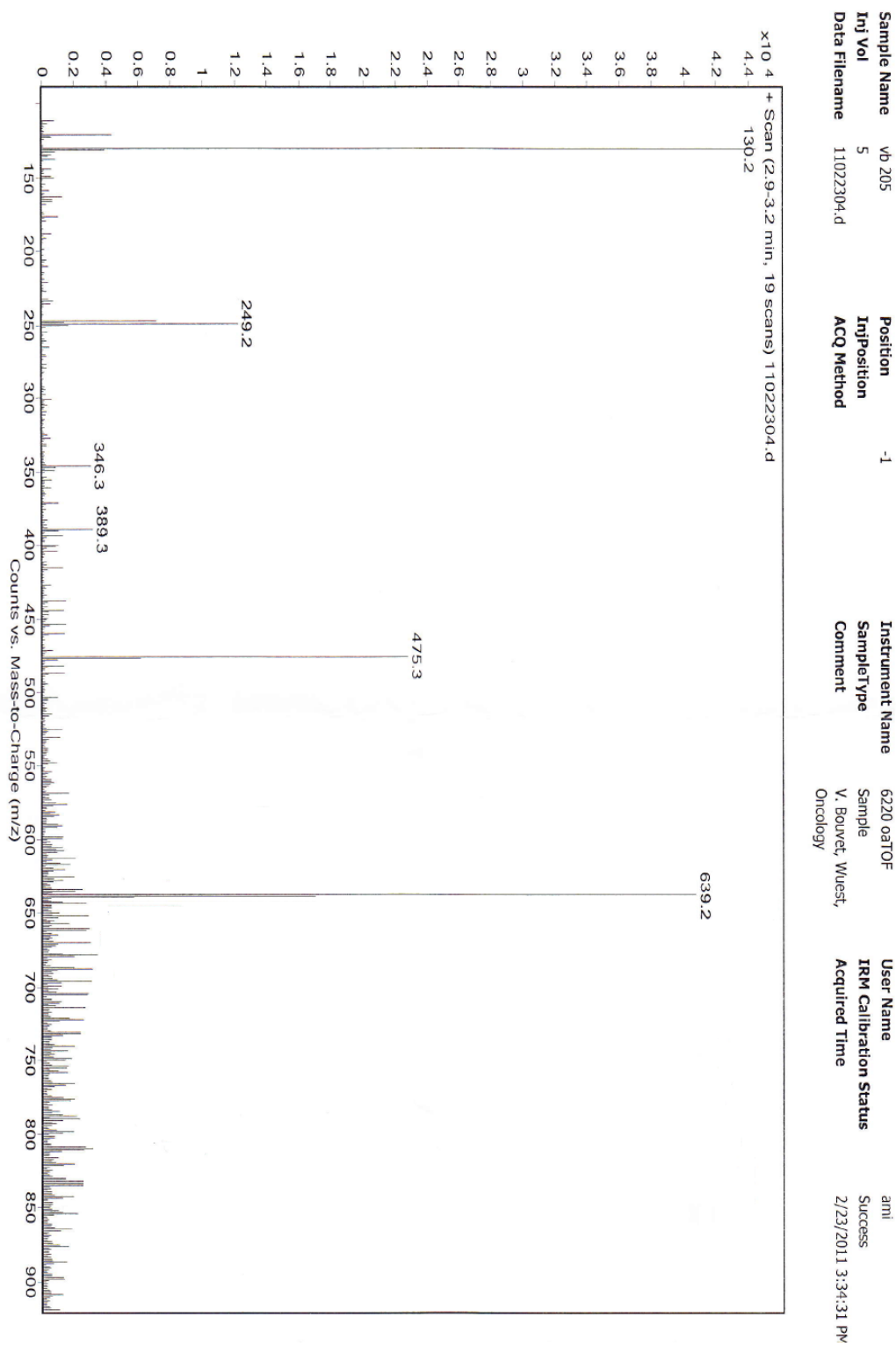




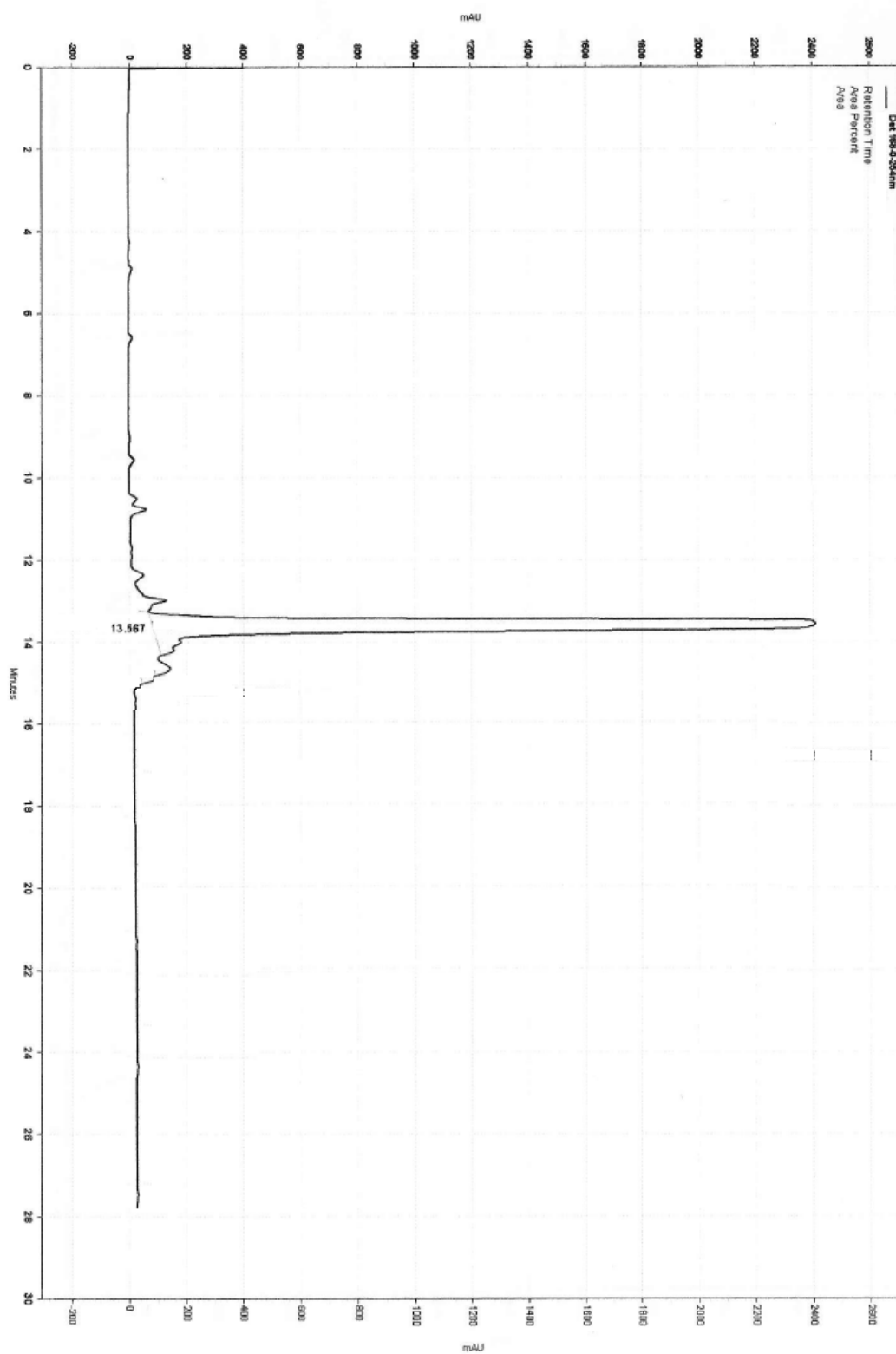
### HPLC trace (254 nm) - FB-DBCO-coupled triazole (10)



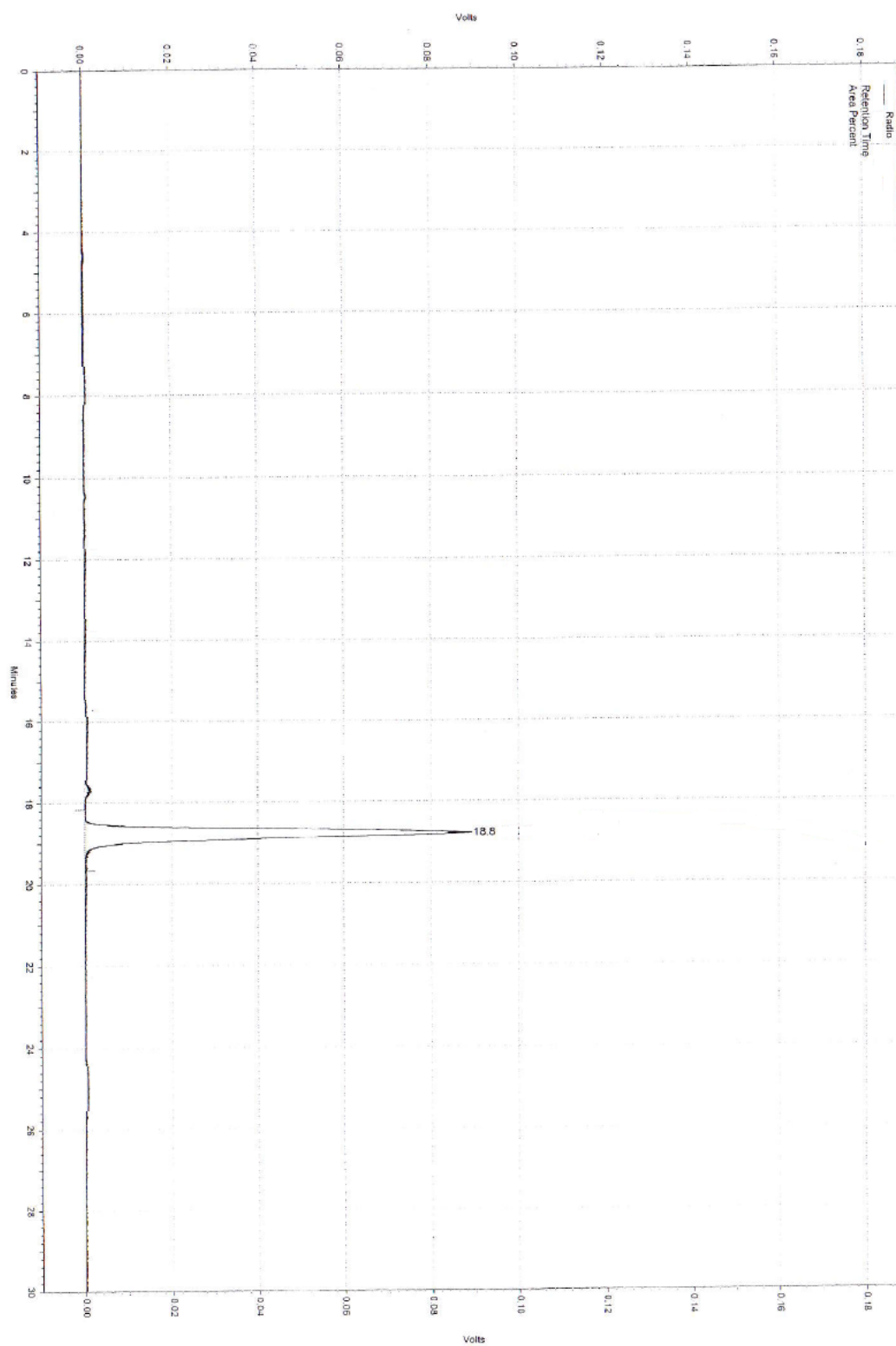
### MS -FB-DBCO-coupled triazole (11)



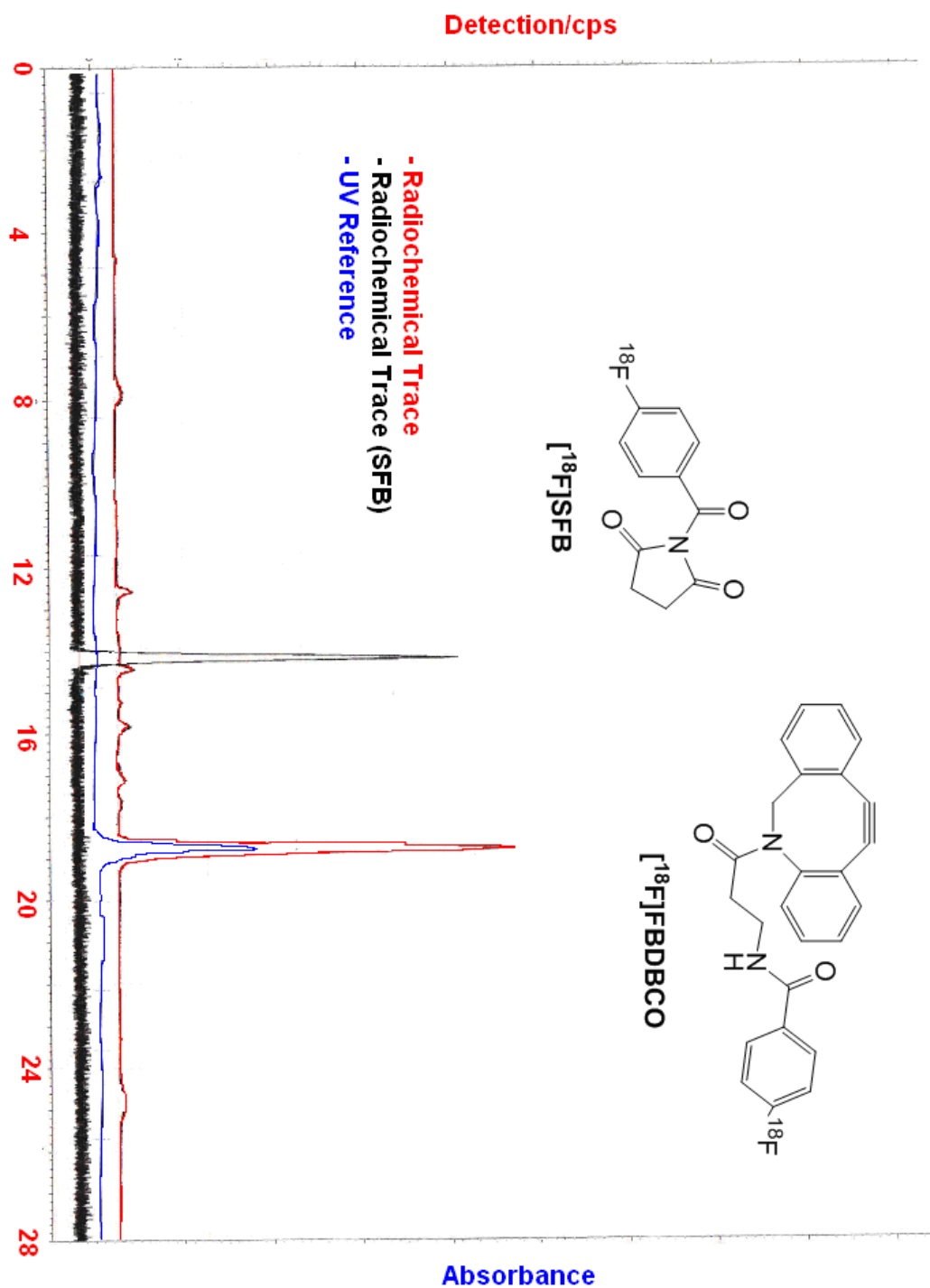
### HPLC trace (254 nm) -FB-DBCO-coupled triazole (11)



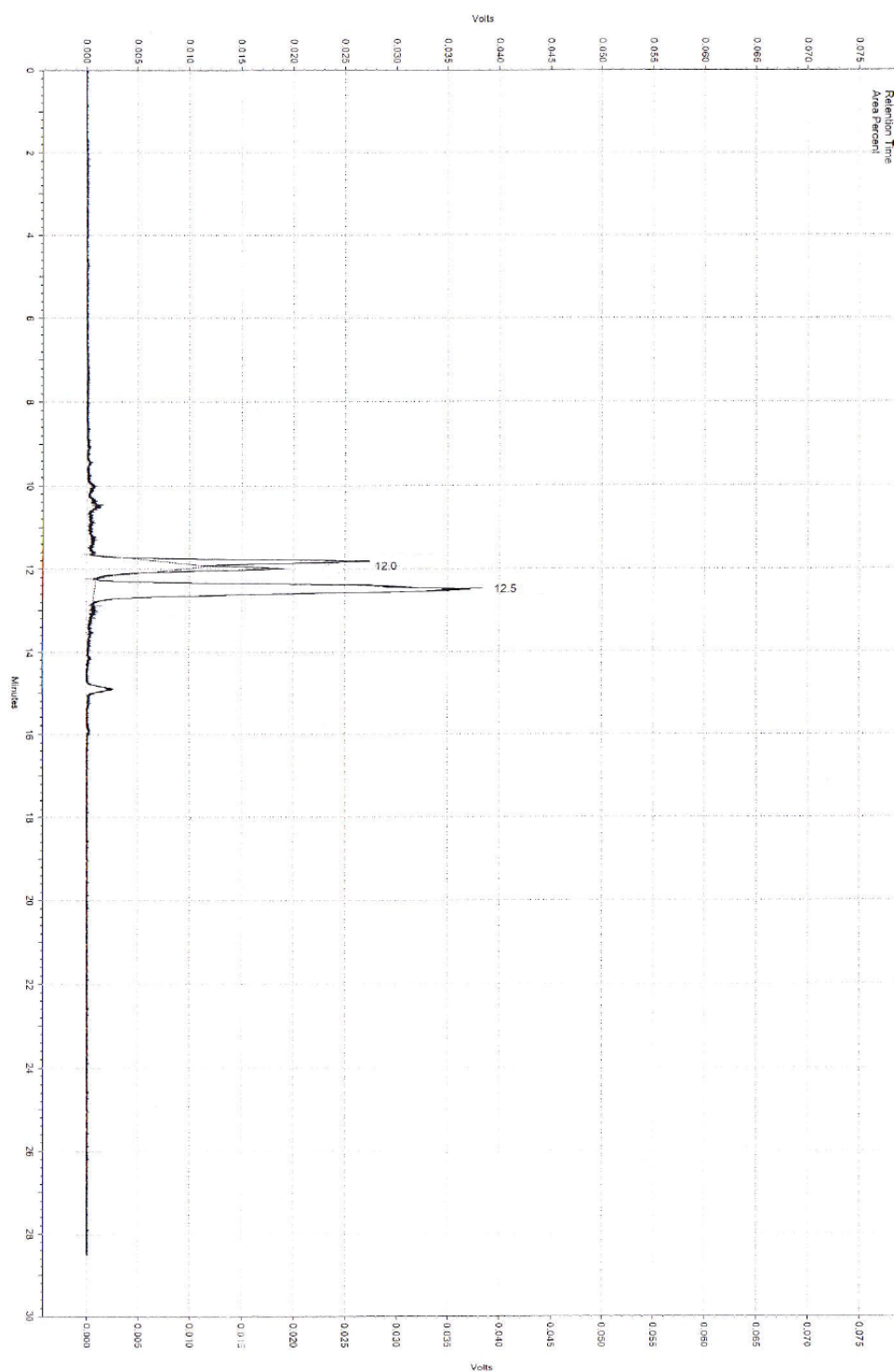
### Radio-HPLC trace [<sup>18</sup>F]FB-DBCO



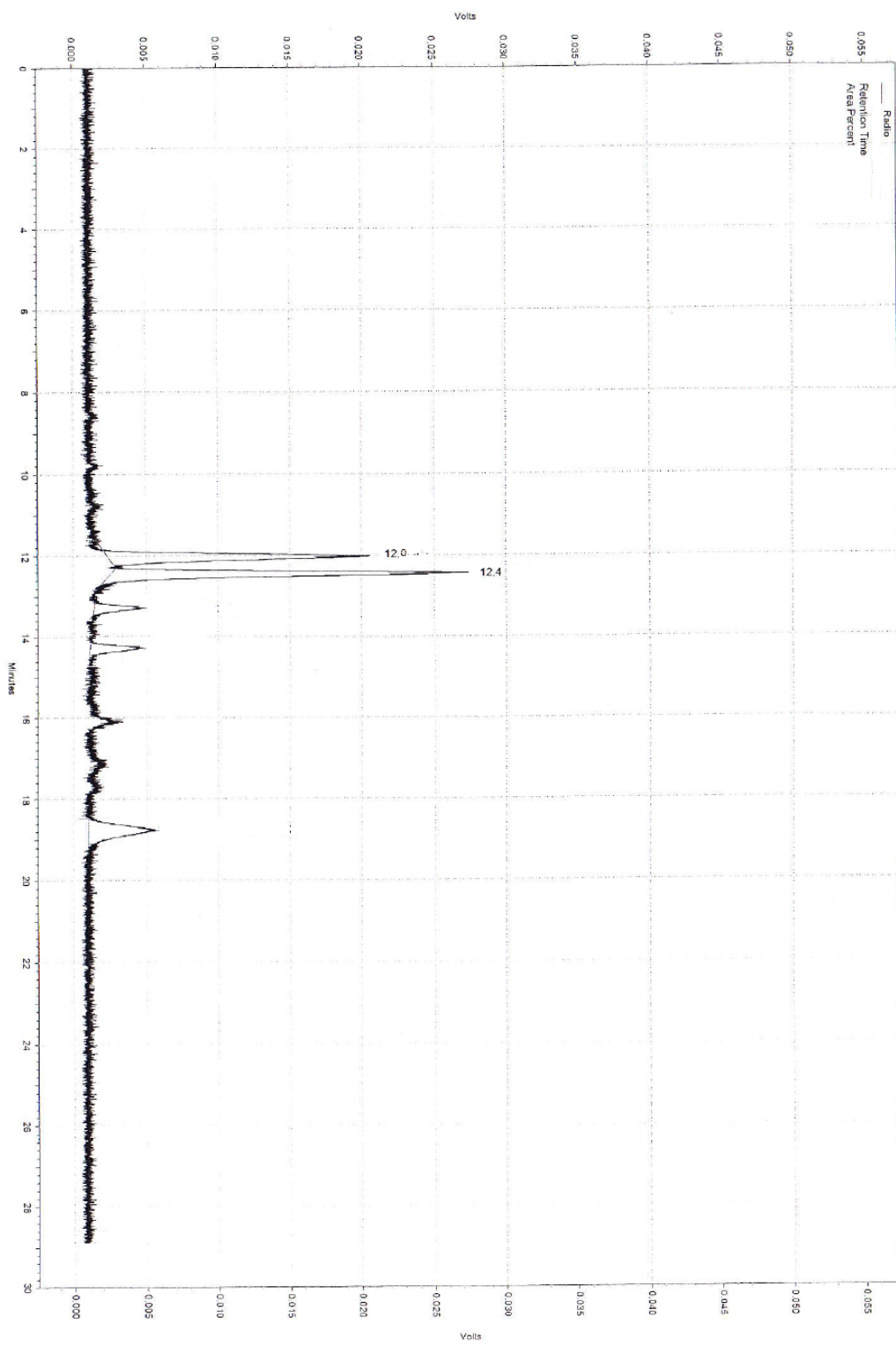
Radio-HPLC trace of [ $^{18}\text{F}$ ]FB-DBCO (with co-injection of reference compounds FB-DBCO)



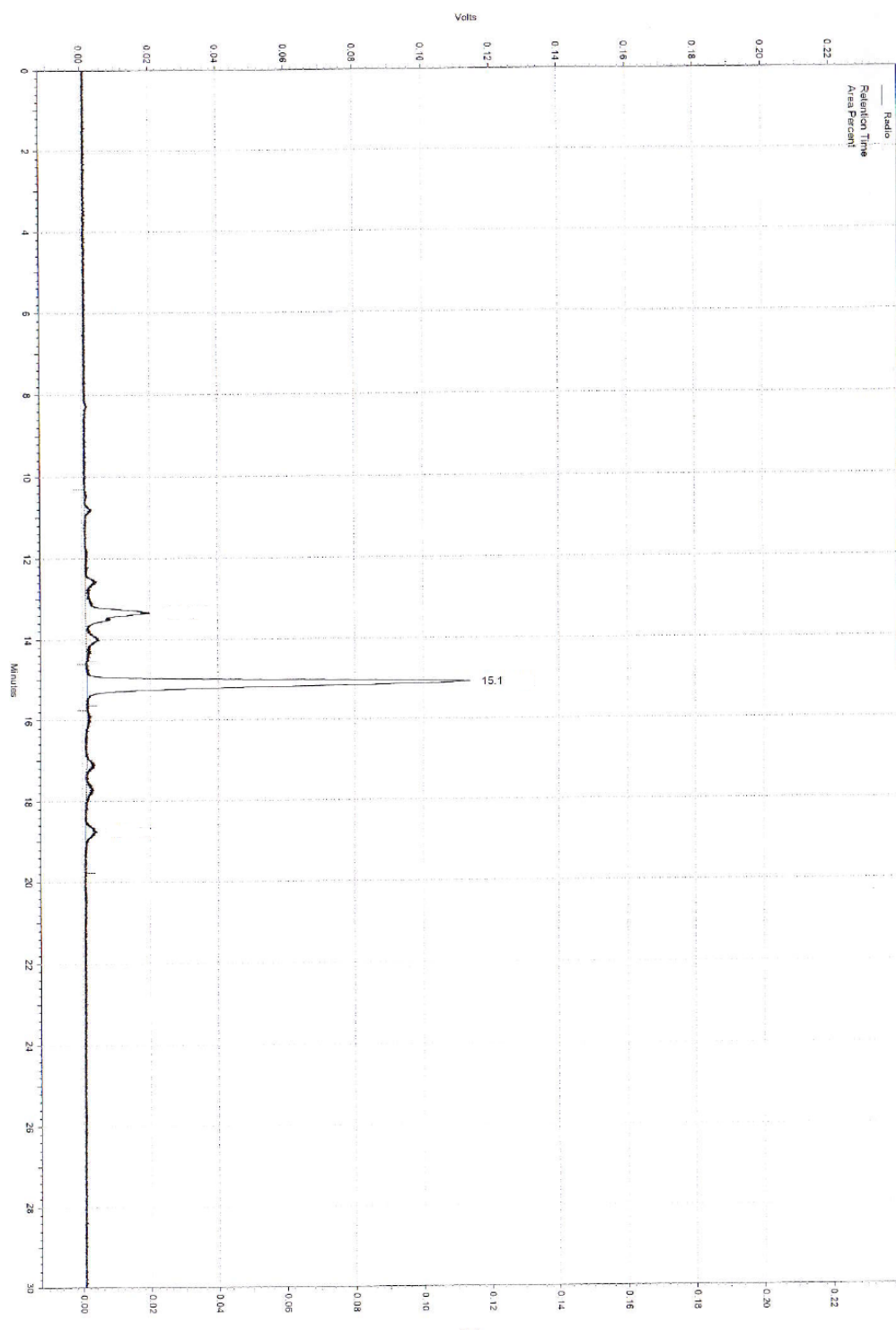
### Radio-HPLC trace of [<sup>18</sup>F]FB-DBCO-coupled triazole ([<sup>18</sup>F]7)



### Radio-HPLC trace of [ $^{18}\text{F}$ ]FB-DBCO-coupled triazole ([ $^{18}\text{F}$ ]8)

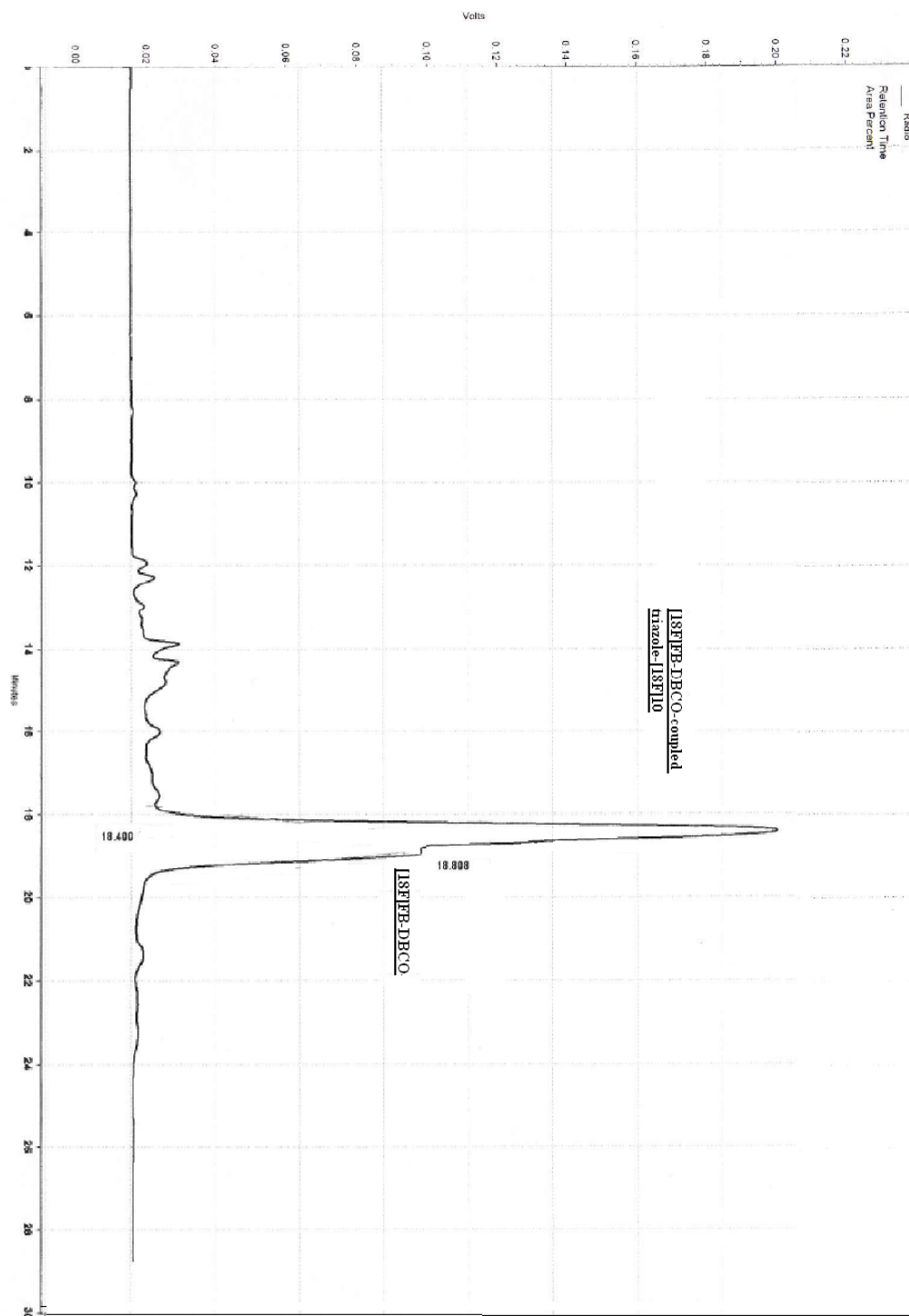


### Radio-HPLC trace of [ $^{18}\text{F}$ ]FB-DBCO-coupled triazole ( $[^{18}\text{F}]\mathbf{9}$ )





### Radio-HPLC trace of [ $^{18}\text{F}$ ]FB-DBCO-coupled triazole ([ $^{18}\text{F}$ ]10)



### Radio-HPLC trace of [ $^{18}\text{F}$ ]FB-DBCO-coupled triazole ([ $^{18}\text{F}$ ]11)

