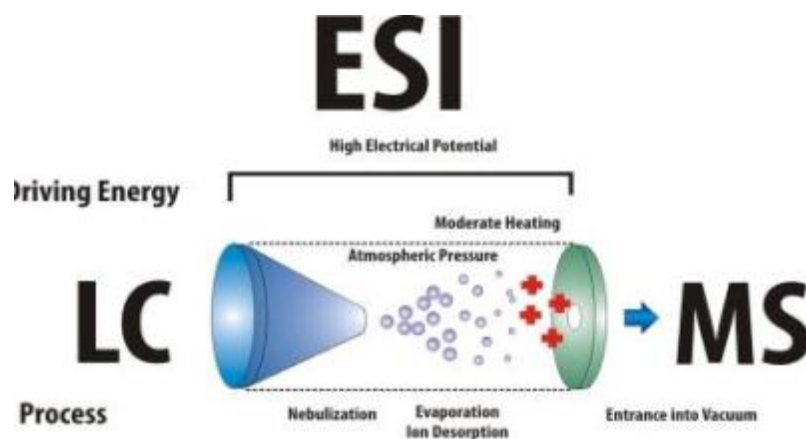


*Поисковая ЖХ-МС/МС библиотека для обзорного
анализа мочи (синтетические каннабимиметики и
иные дизайнерские наркотики)*



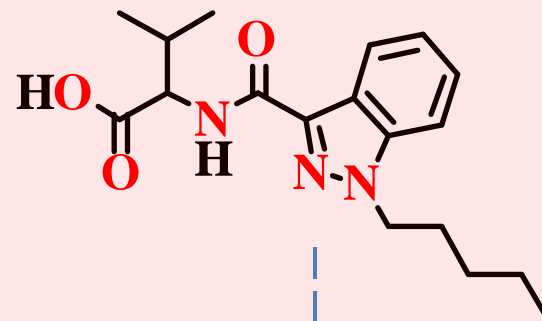
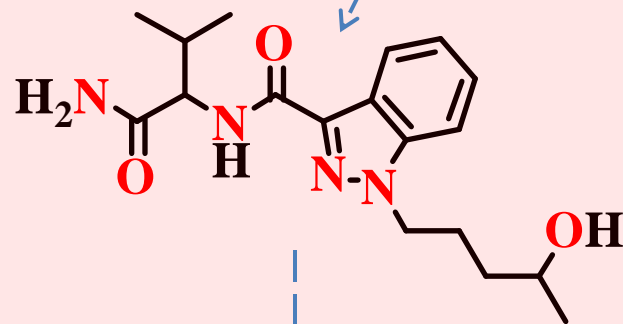
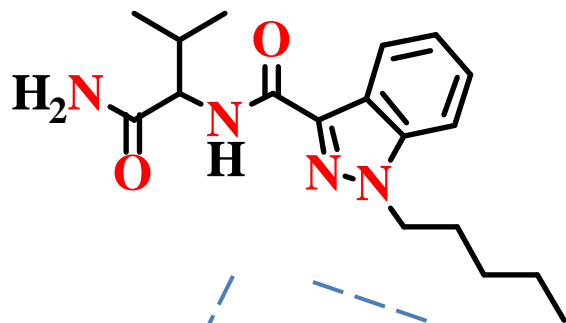
Заикина О.Л. (Ленинградский областной НД)

Григорьев А.М. (Московское областное БСМЭ)

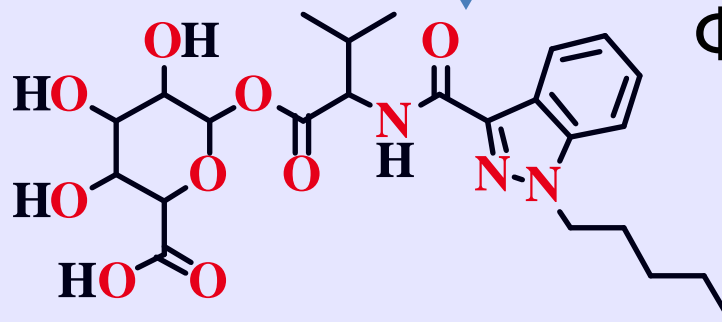
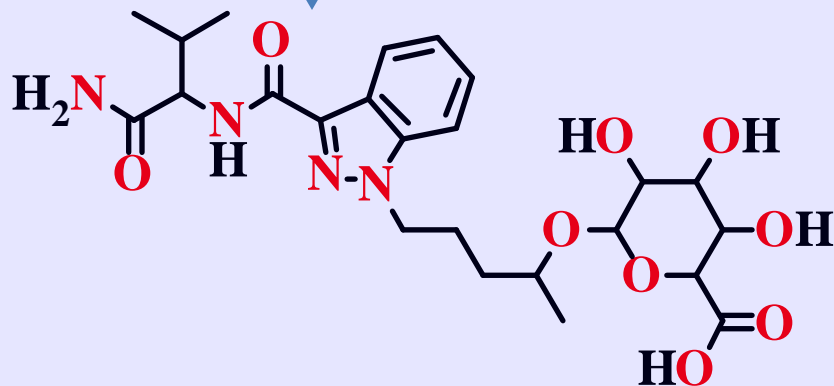
SHIMADZU LCMS-8040



Фазы биотрансформации.

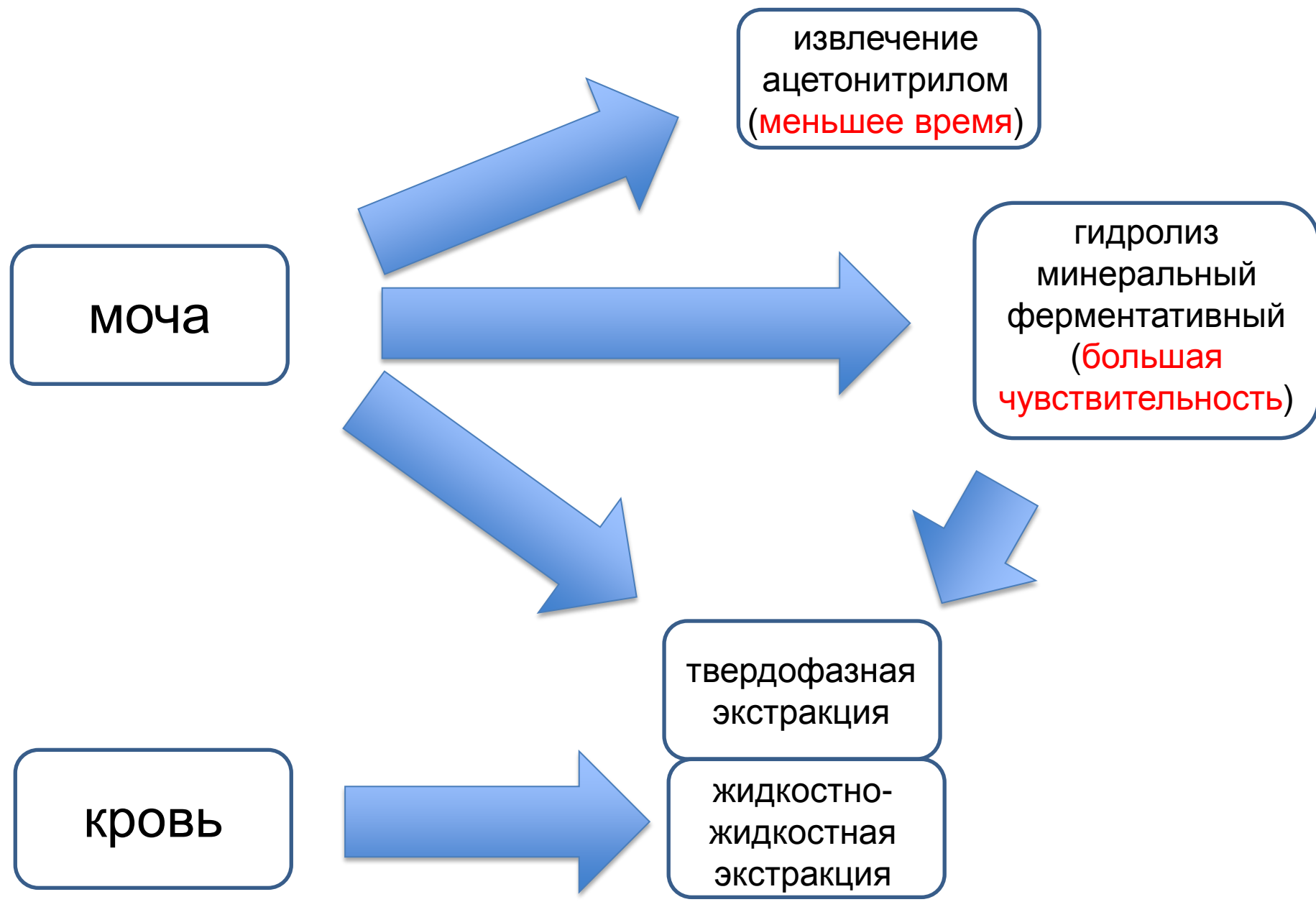


Фаза I

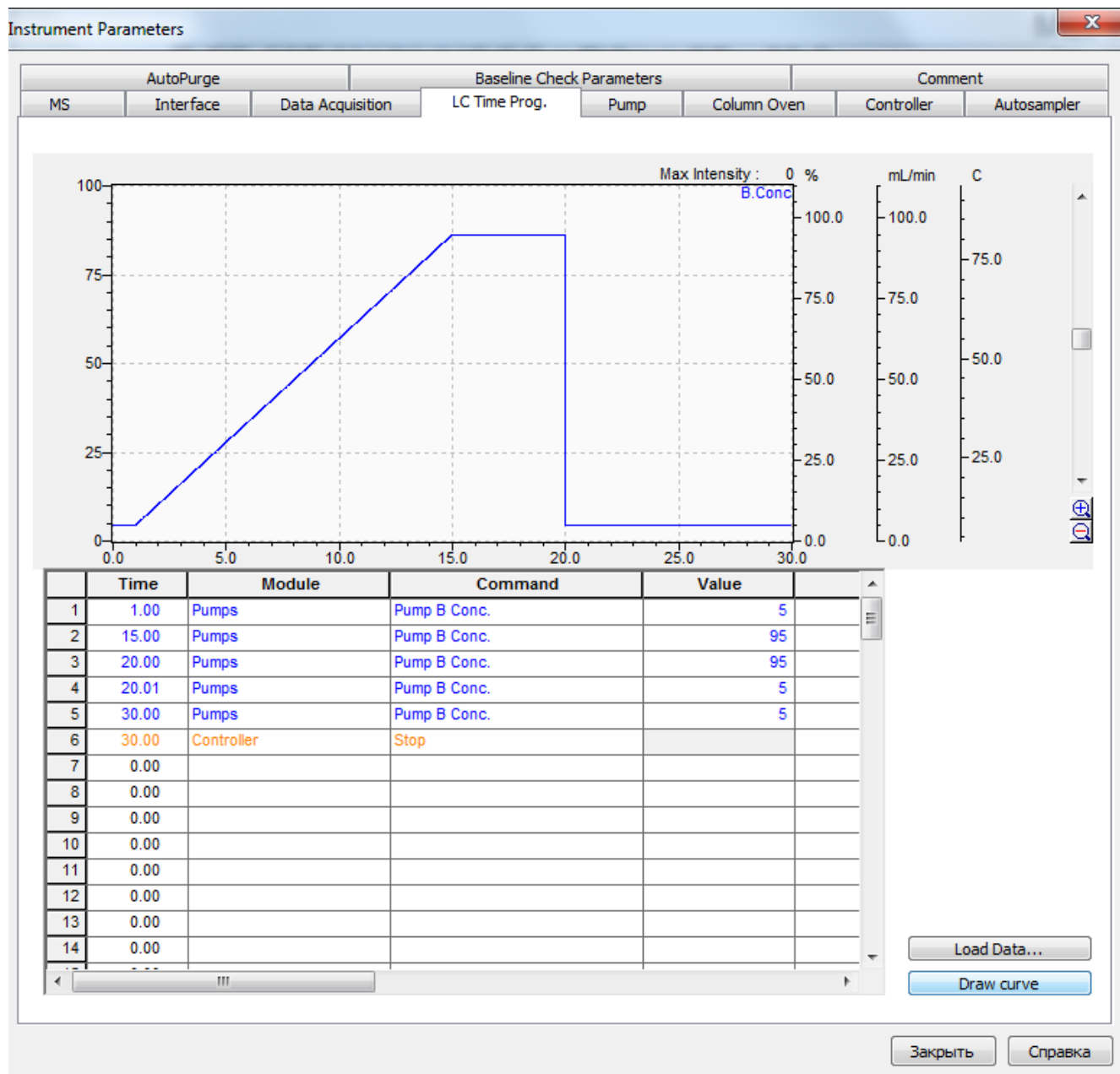


Фаза II

Подготовка проб.



Условия определения: LC Nexera XR (Shimadzu)



#A

5 mM HCOONH₄

0.17 об.% HCOOH

1 об.% CH₃CN

#B

CH₃CN

Условия определения: MS 8040 (QqQ, Shimadzu)

Режим регистрации:
Auto MS/MS

SCAN → Product Ion Spectra
MRM → Product Ion Spectra

Item	Setting	Units
Nebulizing Gas Flow	1.5	L/min
Drying Gas Flow	10	L/min
Interface Voltage	4.5	kV
DL Temperature	250	C
Heat Block Temperature	400	C
Conversion Dynode	6.0	kV
Detector Voltage	1.76	kV

☐ Instrument Parameters View Normal Advanced End Time : 30.00 min

MS Interface Data Acquisition LC Time Prog. Pump Column Oven Controller Autosampler AutoPurge

☒ Positive ☐ Negative End Time: 17.680 min ☐ MS Program Edit Valve and MS Program...

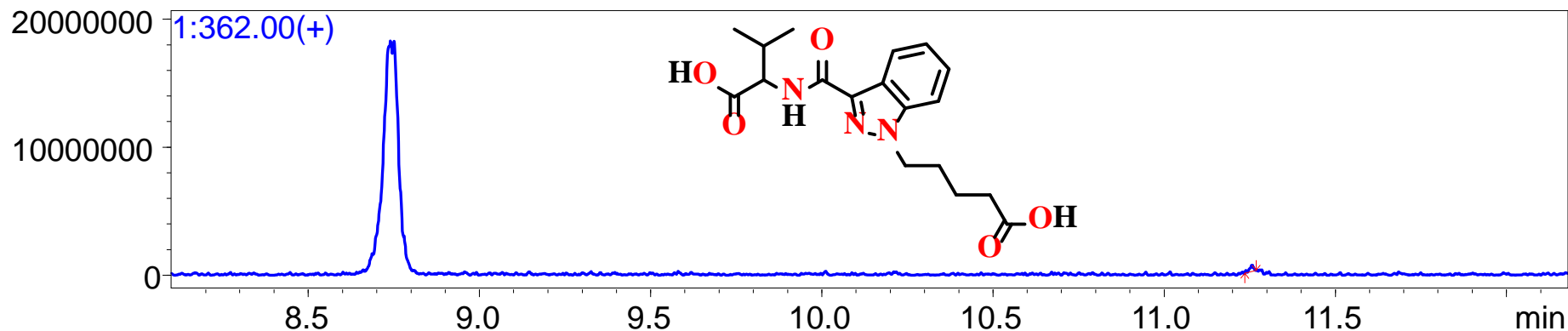
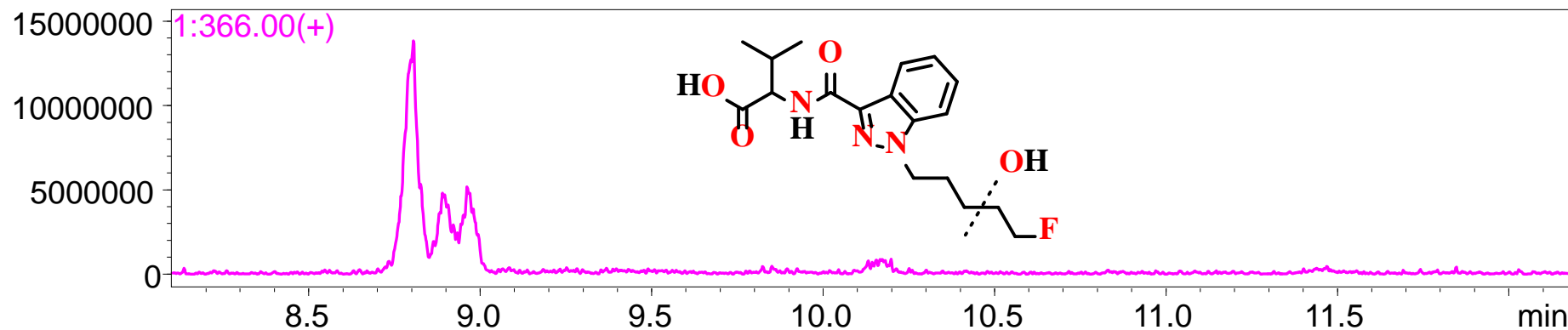
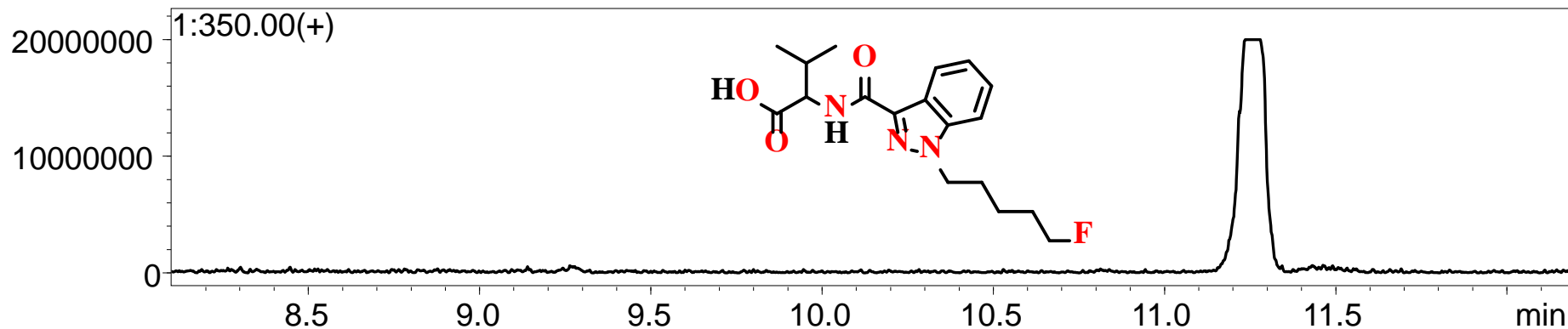
MRM(+) Product Ion Scan(+) Precursor Ion Scan(+) Neutral Loss Scan(+) SIM(+) Scan(+)

☒ CID Gas CID Gas... Attenuation... Loop Time...

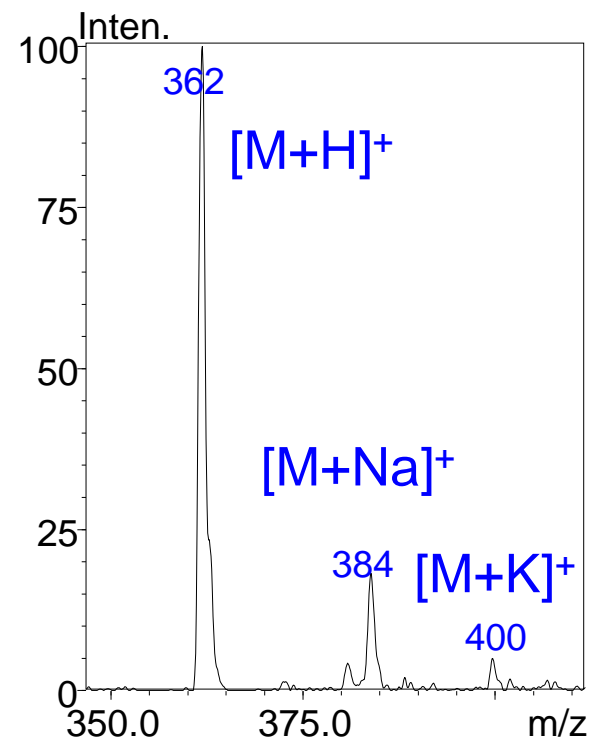
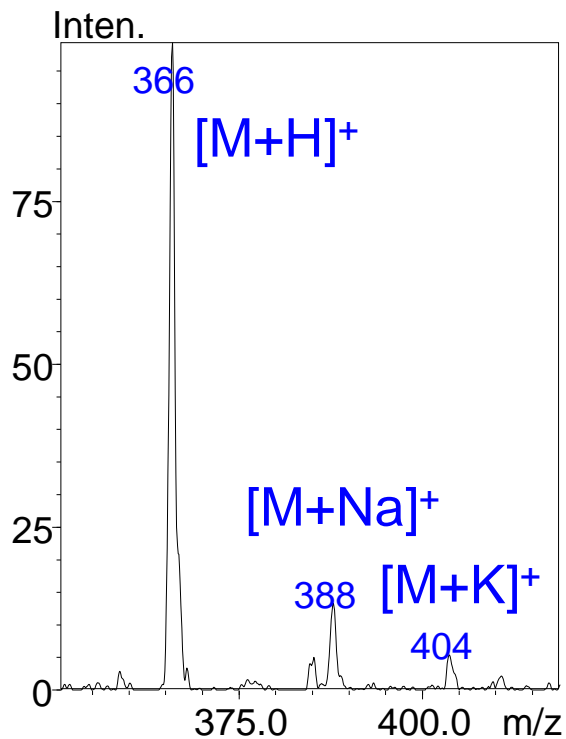
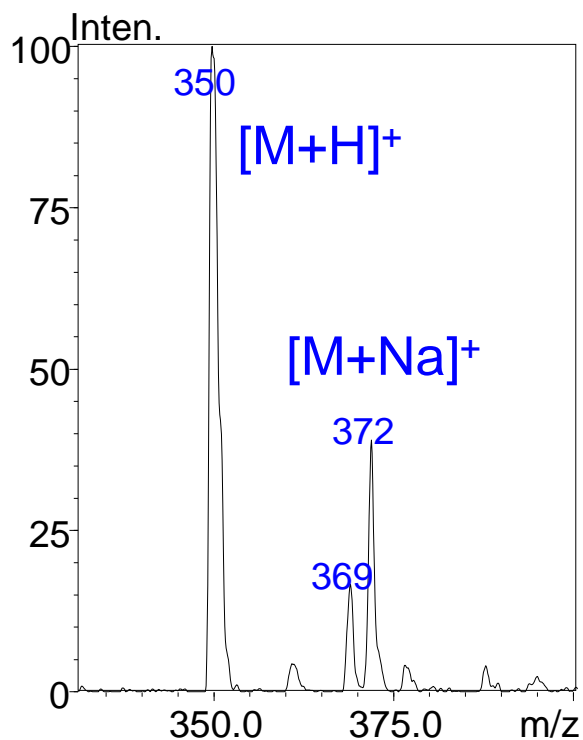
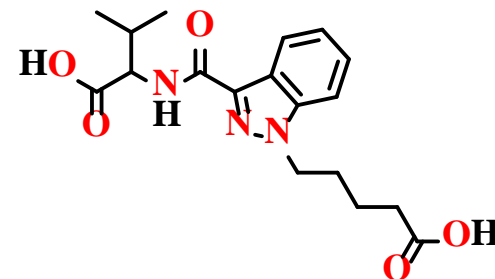
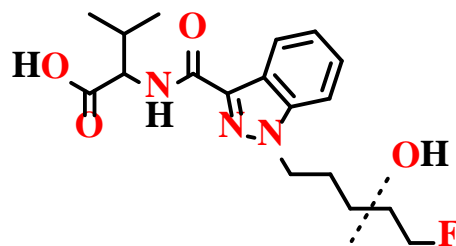
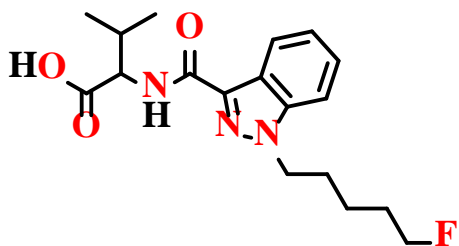
Type ^	Event#	+/-	Compound Name m/z	Time (0.000 min - 17.680 min)
MRM	122	+	AB-CHMINACA-M (HOOC-) 358.00>241.00	
- Product Ion Scan	123	+	> 50.00:368.00	
MRM	62	+	AB-CHMINACA-M (HOOC-HO-) 374.00>257.00	
- Product Ion Scan	63	+	> 50.00:384.00	

Метаболиты фазы I АВ-FPINACA в моче

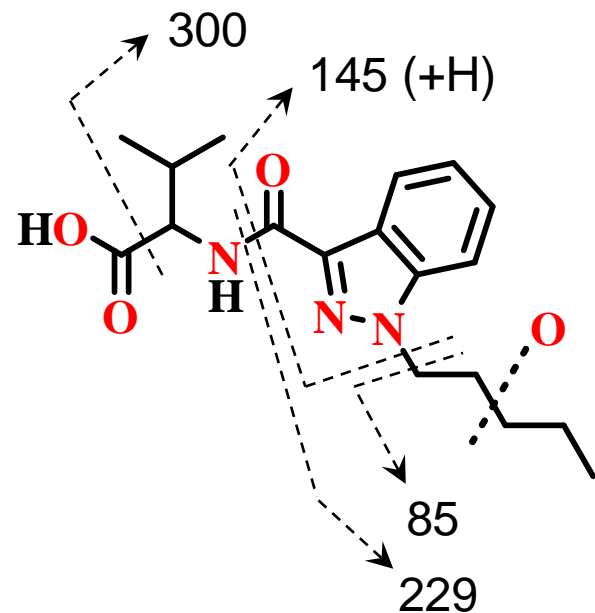
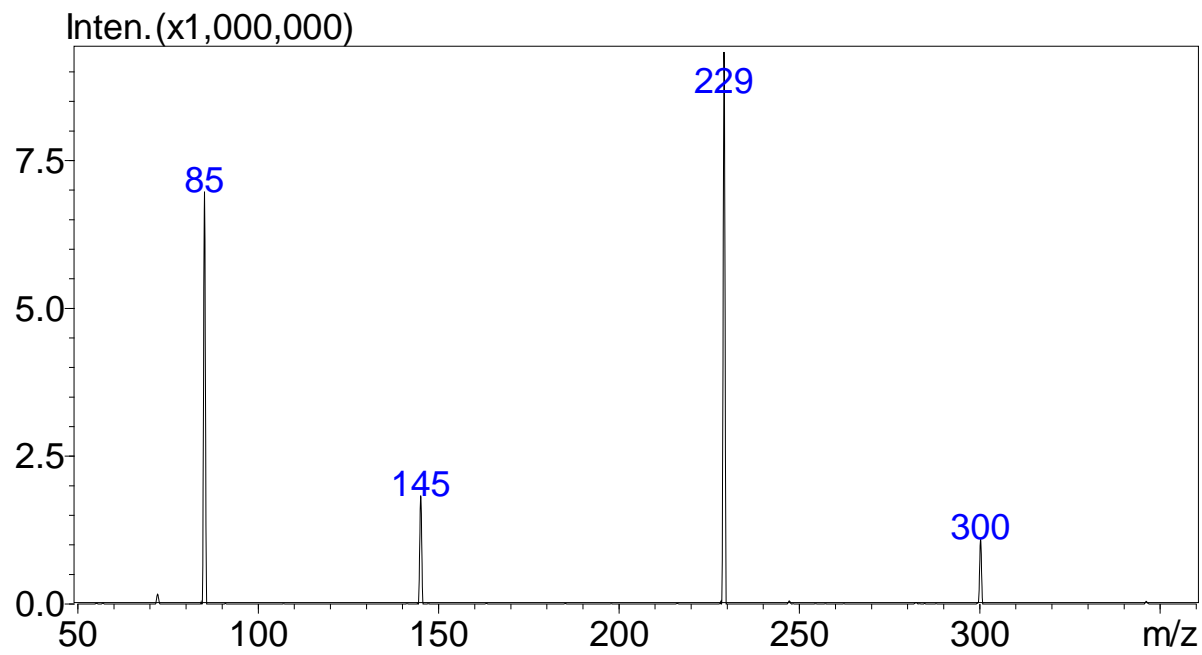
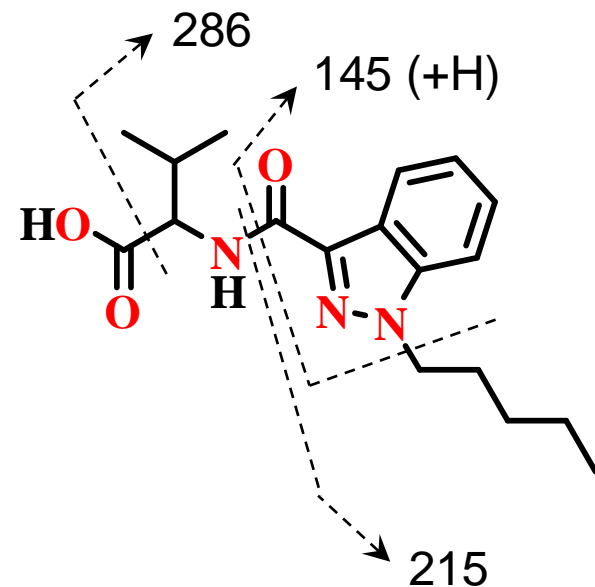
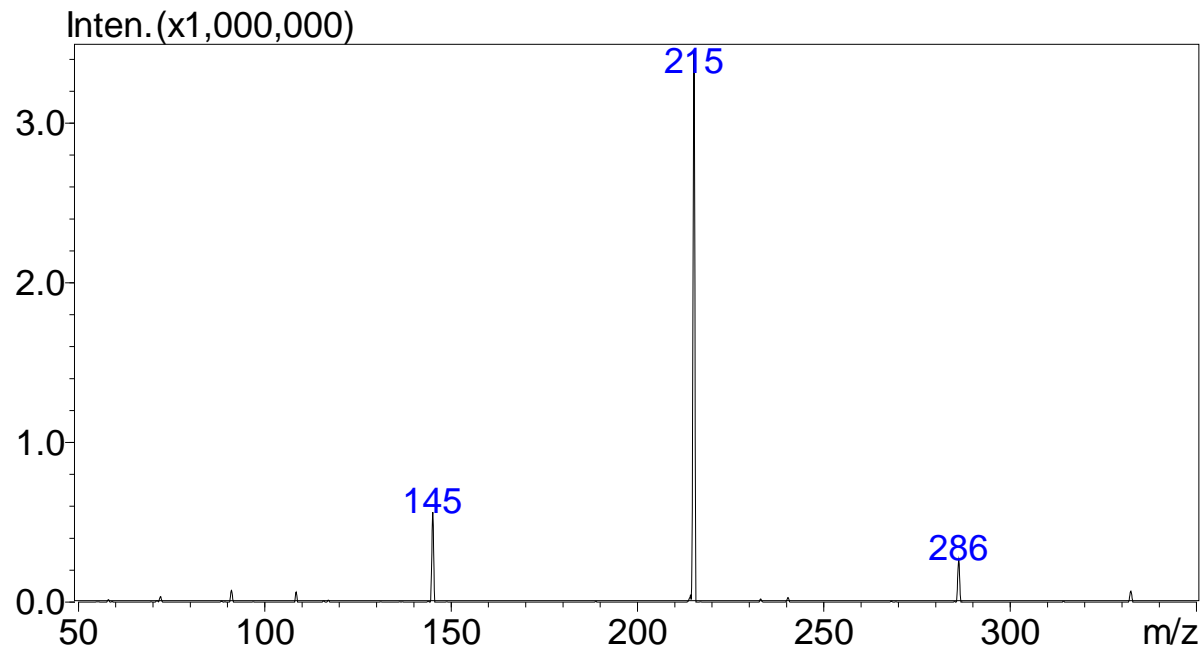
(EIC, MS1)



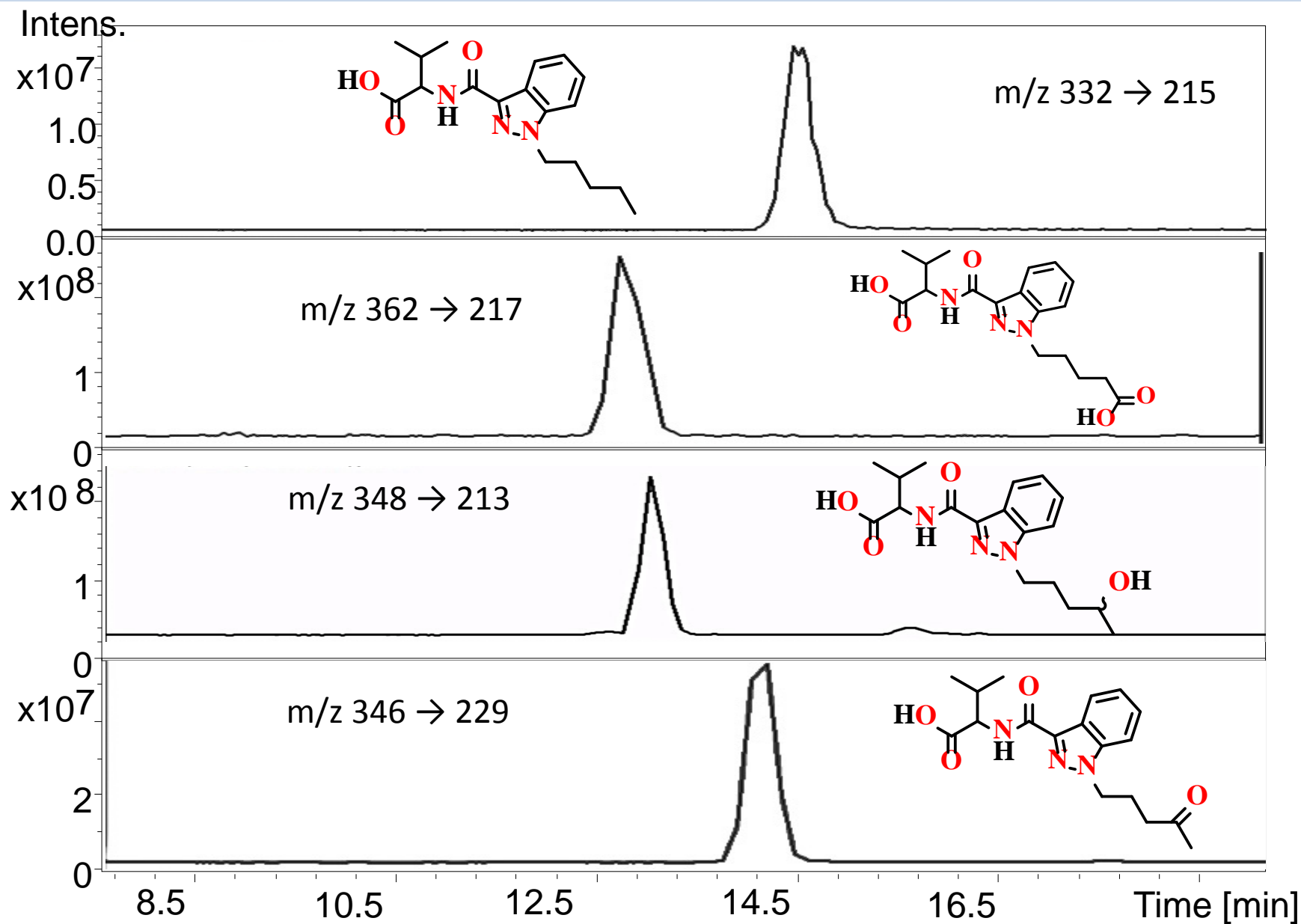
Масс-спектры метаболитов фазы I



Спектры MS2: метаболиты АВ-PINACA



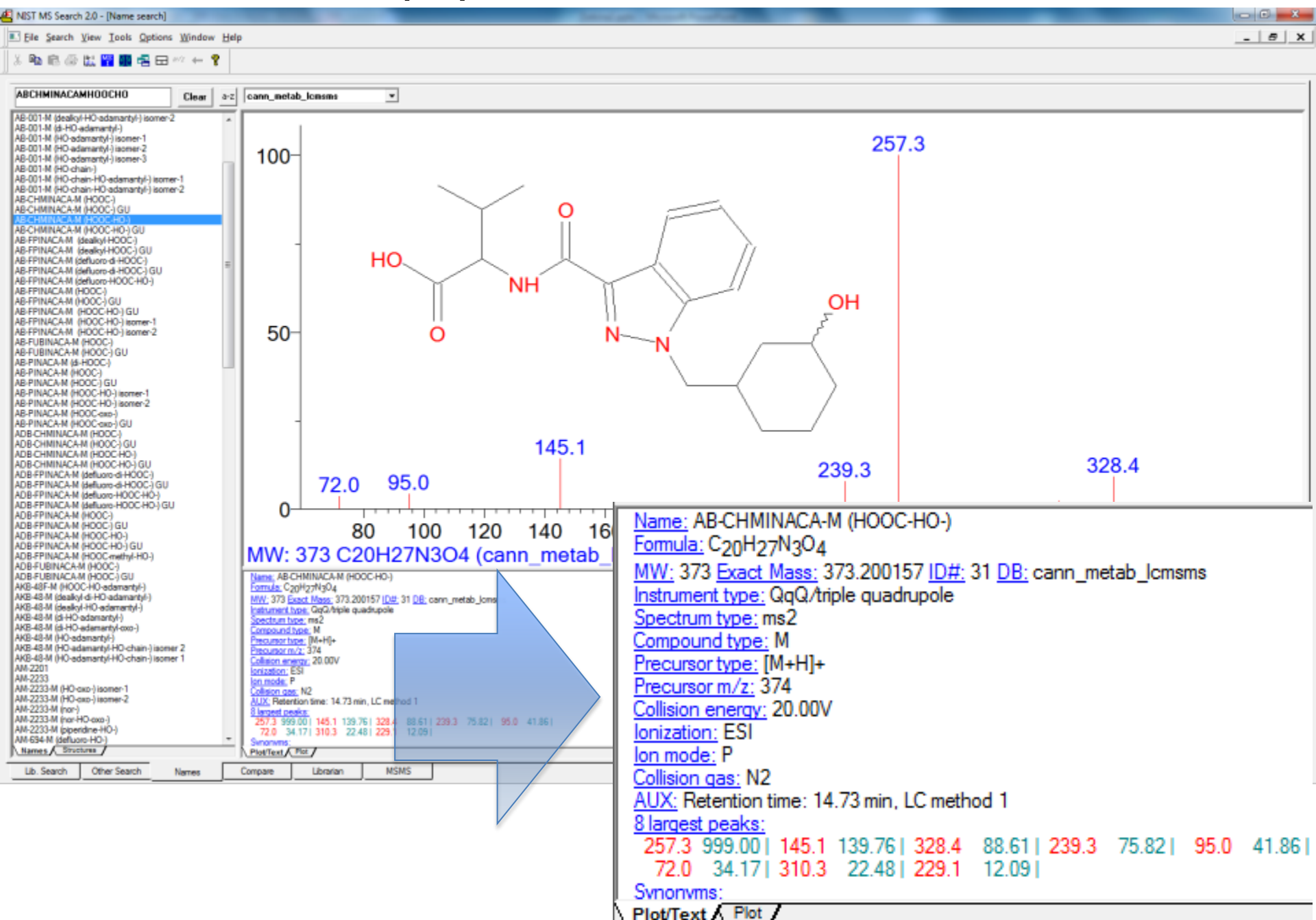
AB-PINACA. Метаболиты фазы I



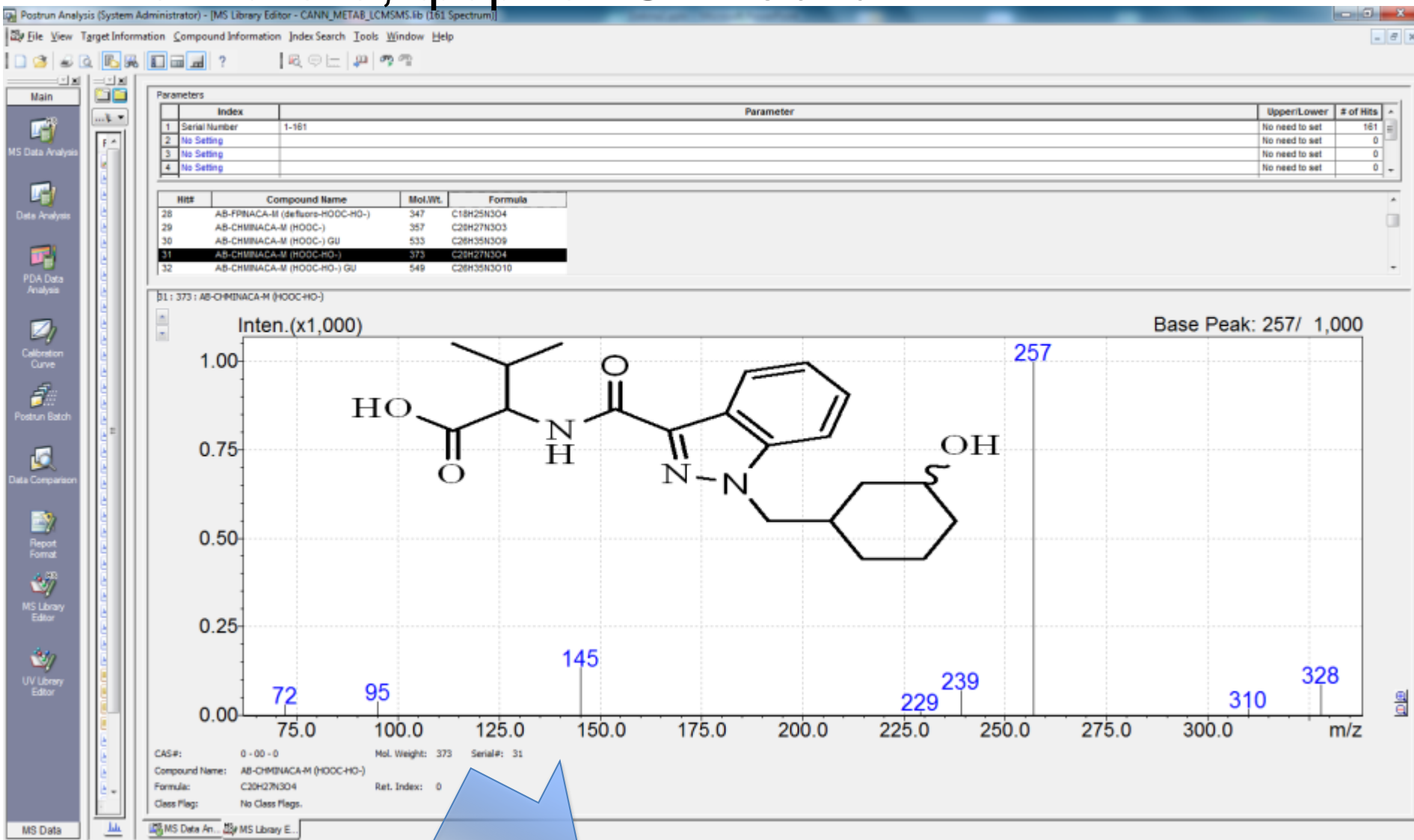
Состав библиотеки

- около 200 метаболитов фаз I и II, образованных от > 30 синтетических каннабимиметиков;
- 105 психоактивных веществ
- 70 снотворных препаратов

Библиотека; формат NIST



Библиотека; формат Shimadzu



CAS#: 0 - 00 - 0 Mol. Weight: 373 Serial#: 31

Compound Name: AB-CHMINACA-M (HOOC-HO-)

Formula: C20H27N3O4 Ret. Index: 0

Class Flag: Drugs

СПАСИБО ЗА ВНИМАНИЕ !!!

8 No Setting

Hit#	Compound Name	Mol.Wt.	Formula
3	AB-PINACA-M (HOOC-)	331	C18H25N3O3
4	AB-PINACA-M (HOOC-) GU	507	C24H33N3O9
5	AB-PINACA-M (HOOC-HO-) isomer-1	347	C18H25N3O4
6	AB-PINACA-M (HOOC-HO-) isomer-2	347	C18H25N3O4
7	AB-PINACA-M (HOOC-oxo-)	345	C18H23N3O4
8	AB-PINACA-M (HOOC-oxo-) GU	521	C24H31N3O10
9	AB-PINACA-M (di-HOOC-)	361	C18H23N3O5
10	ADB-FPINACA-M (HOOC-) GU	539	C25H34FN3O9
11	ADB-FPINACA-M (HOOC-)	363	C19H26FN3O3
12	ADB-FPINACA-M (defluoro-di-HOOC-)	375	C19H25N3O5
13	ADB-FPINACA-M (defluoro-di-HOOC-) GU	551	C25H33N3O11
14	ADB-FPINACA-M (defluoro-HOOC-HO-)	361	C19H27N3O4
15	ADB-FPINACA-M (defluoro-HOOC-HO-) GU	537	C25H35N3O10
16	ADB-FPINACA-M (HOOC-HO-)	379	C19H26FN3O4
17	ADB-FPINACA-M (HOOC-methyl-HO-)	379	C19H26FN3O4
18	ADB-FPINACA-M (HOOC-HO-) GU	555	C25H34FN3O10
19	AB-FPINACA-M (HOOC-)	349	C18H24FN3O3
20	AB-FPINACA-M (HOOC-) GU	525	C24H32FN3O9
21	AB-FPINACA-M (defluoro-di-HOOC-)	361	C18H23N3O5

Edit Compound Information

CAS#: 0 - 0 - 0 ☐ Ignore in Search Results

Compound Name: AB-PINACA-M (HOOC-)

Formula: C18H25N3O3 Mol. 331

Class Flag:

- Steroids
- Alkaloids
- Drugs
- Derivatives
- Amino Acids
- Metals
- Carbohydrates
- Miscellaneous Natural Products

 Ret. Index: 0

OK Cancel Help

3 : 331 : AB-PINACA-M (HOOC-)

Inten.(x1,000)

242.9980 242.9983 242.9985 242.9988 242.9990 242.9992 242.9995 242.9998 243.0000 243.0002 243.0005 243.0008 243.0

Inten.(x1,000)

242.9980 242.9983 242.9985 242.9988 242.9990 242.9992 242.9995 242.9998 243.0000 243.0002 243.0005 243.0008 243.0

CAS#: 0 - 00 - 0 Mol. Weight: 331 Serial#: 3

Compound Name: AB-PINACA-M (HOOC-)

Formula: C18H25N3O3 Ret. Index: 0

Class Flag: No Class Flags.

MS Data An... MS Library E... UV Library ...