Supplementary Information (SI) for Analyst.

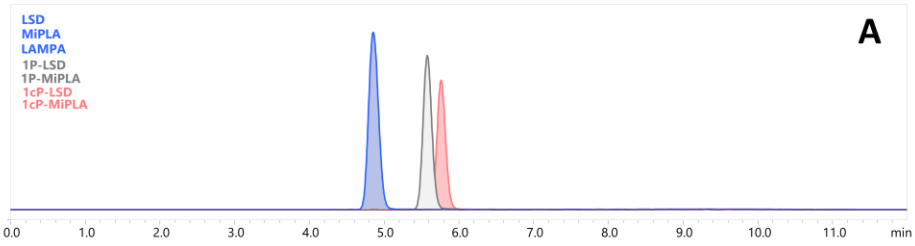
Table S1. Results of optimization of the sample preparation procedure with the use of liquid-liquid extraction (LLE) technique in different pH conditions.

	pH 7.4				pH 8				pH 9			
Substance	**Ethyl acetate**	**Hexane**	***Tert*-butyl methyl ether**	**Dichloro-methane**	**Ethyl acetate**	**Hexane**	***Tert*-butyl methyl ether**	**Dichloro-methane**	**Ethyl acetate**	**Hexane**	***Tert*-butyl methyl ether**	**Dichloro-methane**
ALD-52 (1A-LSD)	●●●●●	●●	●●●	●●●●●	●●●●	●●	●●●●	●●●●●	●●●●●	●●	●●	●●●●●
AL-LAD	●●●●●	●●	●●●●	●●●●●	●●●●●	●●	●●●●●	●●●●●	●●●●●	●●	●●●	●●●●●
LAMPA	●●●●●	●●	●●●	●●●●	●●●●	●●	●●●●●	●●●●●	●●●●●	●●	●●●	●●●●●
LSD	●●●●	●●	●●●	●●●●	●●●●	●●	●●●●	●●●●●	●●●●●	●●	●●●	●●●●●
LSM-775	●●●●	●●	●●●	●●●●	●●●●	●●	●●●	●●●●●	●●●●●	●●	●●●	●●●●●
LSZ	●●●●	●●	●●●	●●●●	●●●●	●●	●●●	●●●●●	●●●●●	●●	●●●	●●●●●
MiPLA	●●●●	●●	●●●	●●●●	●●●●	●●	●●●●	●●●●●	●●●●●	●●	●●●	●●●●●
1B-LSD	●●●	●●●●	●●●	●●●●●	●●●	●●●●	●●●●	●●●●●	●●●●●	●	●●●	●●●●●
1cP-LSD	●●●●	●●●	●●●●	●●●●●	●●●●	●●●●	●●●●●	●●●●●	●●●●●	●●●	●●●	●●●●●
1cP-MiPLA	●●●●	●●●	●●●	●●●●●	●●●●	●●●●	●●●●●	●●●●●	●●●●●	●●●	●●●	●●●●●
1P-LSD	●●●●●	●●●	●●●	●●●●●	●●●●	●●●	●●●●	●●●●●	●●●●●	●●●●	●●●	●●●●●
1P-MiPLA	●●●●	●●●	●●●	●●●●●	●●●●	●●●●	●●●●	●●●●●	●●●●●	●●●●	●●●	●●●●●
1V-LSD	●●●	●●●	●●●	●●●●●	●●●	●●●●	●●●	●●●●	●●●	●●●	●●	●●●●●
2-Bromo-LSD	●●●	●●	●●●	●●●●	●●●	●●	●●●●	●●●●	●●●●●	●●●	●●●	●●●●●
2-oxo-3-OH-LSD	●●●	●	●●	●●	●●●	●	●●	●●	●●●●●	●●	●●	●●●

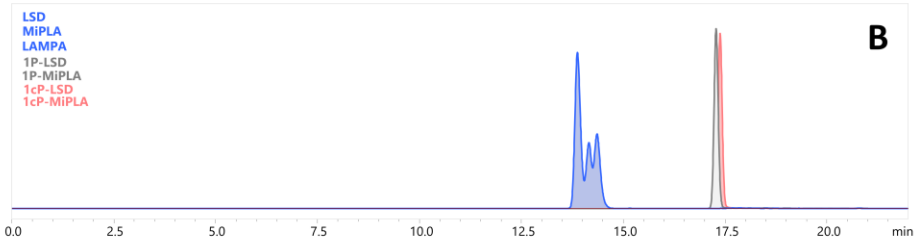
●●●●● The substance extracts the most effectively under given conditions; ●●●● The substance extracts very effectively under given conditions; ●●● The substance can be extracted under given conditions but the process is less efficient; ●● The substance extracts very poorly under given conditions; ● The substance practically cannot be extracted under given conditions

S2: Isomers separation

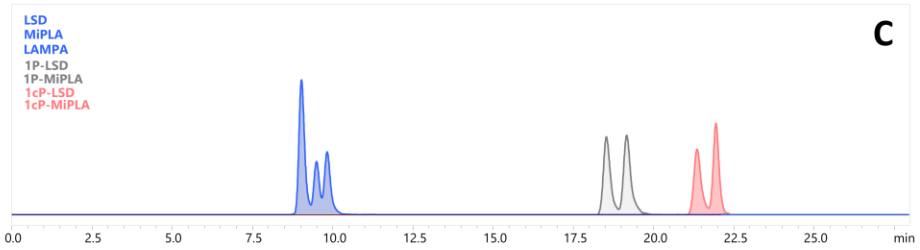
Fig. S2.1. Optimization of chromatographic conditions for separation of positional isomers



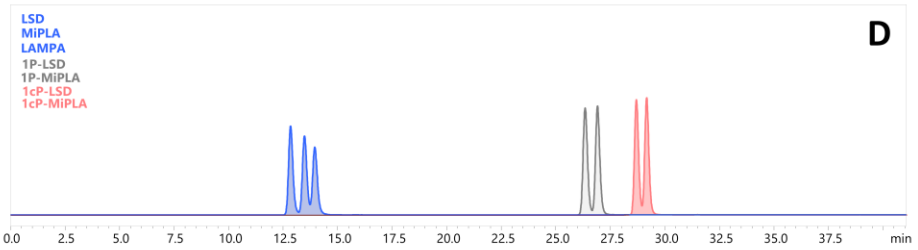
Time [min]	Flow [mL/min]	A [%]	B [%]
0.0	0.3	95.0	5.0
10.0		5.0	95.0
12.0		5.0	95.0
12.1		95.0	5.0
15.0		95.0	5.0



Time [min]	Flow [mL/min]	A [%]	B [%]
0.0	0.3	95.0	95.0
15.0		75.0	75.0
17.0		5.0	5.0
19.0		5.0	5.0
19.1		95.0	95.0
22.0		95.0	95.0

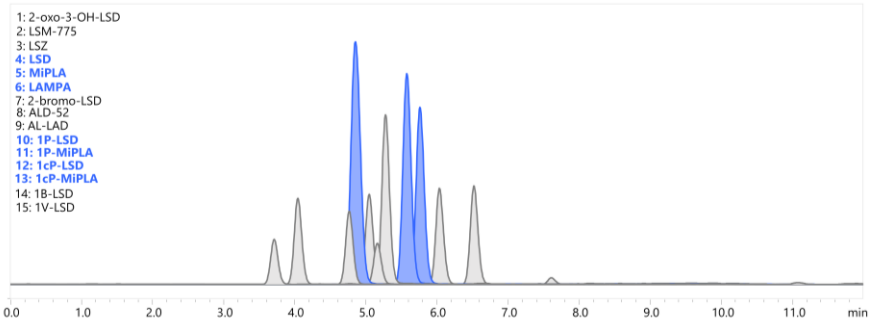


Time [min]	Flow [mL/min]	A [%]	B [%]
0.0	0.3	85.0	15.0
20.0		75.0	25.0
23.0		5.0	95.0
25.0		5.0	95.0
25.1		85.0	15.0
28.0		85.0	15.0

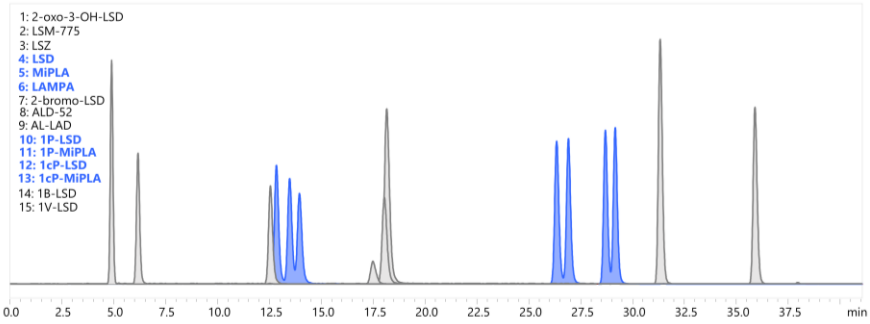


Time [min]	Flow [mL/min]	A [%]	B [%]
0.0	0.3	95.0	5.0
2.0		85.0	15.0
20.0		80.0	20.0
35.0		65.0	35.0
38.0		5.0	95.0
40.0		5.0	95.0
40.1		95.0	5.0
50.0		95.0	5.0

S3: Method development.



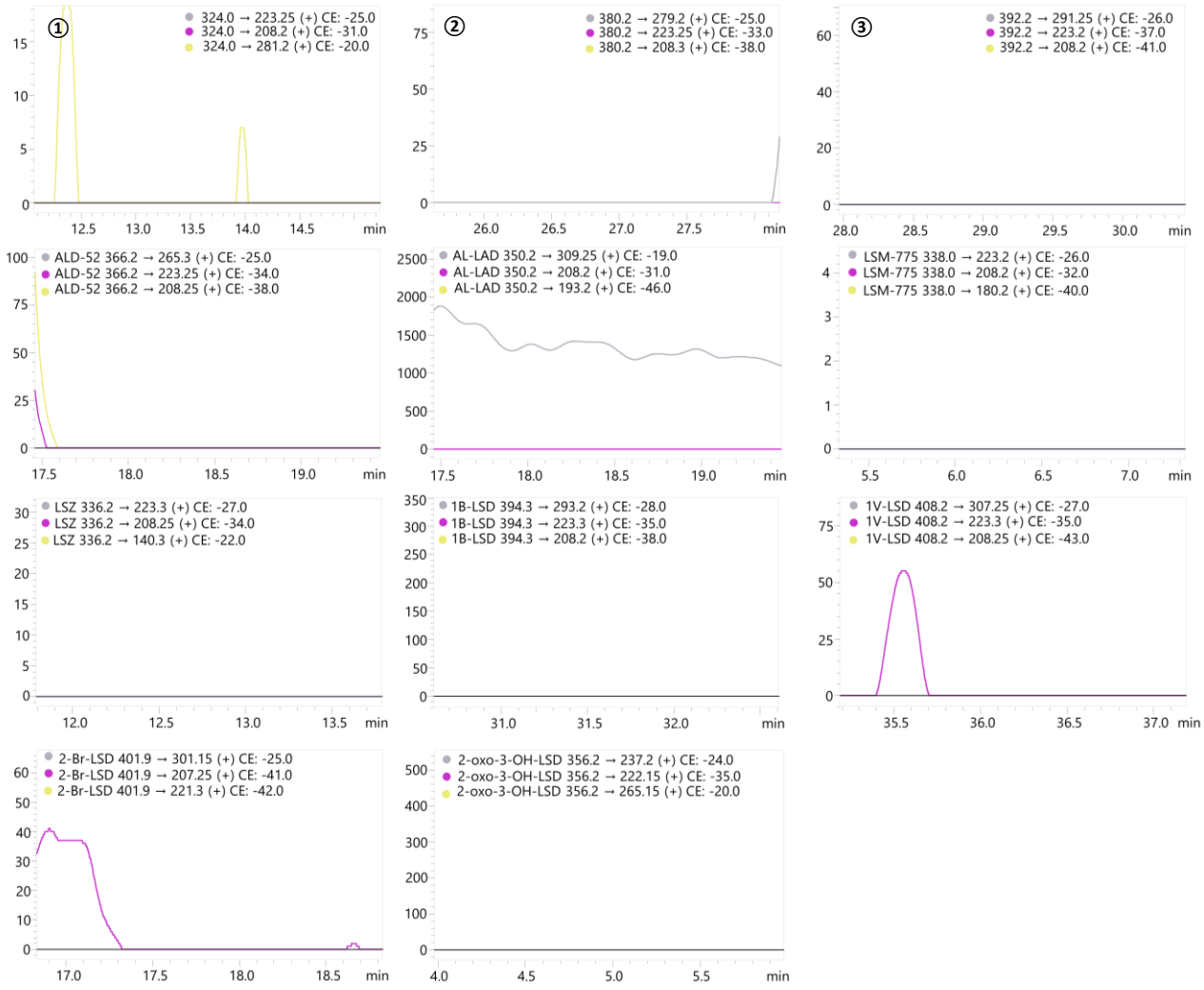
Time [min]	Flow [mL/min]	A [%]	B [%]
0.0		95.0	5.0
10.0		5.0	95.0
12.0	0.3	5.0	95.0
12.1		95.0	5.0
15.0		95.0	5.0



Time [min]	Flow [mL/min]	A [%]	B [%]
0.0		95.0	5.0
2.0		85.0	15.0
20.0		80.0	20.0
35.0	0.3	65.0	35.0
38.0		5.0	95.0
40.0		5.0	95.0
40.1		95.0	5.0
50.0		95.0	5.0

S4: Multiple reaction monitoring (MRM) chromatograms

Figure S4.1. Multiple reaction monitoring (MRM) chromatograms of BLANK samples (whole blood matrix)



① LSD, MiPLA and LAMPA; ② 1P-LSD and 1P-MiPLA; ③ 1cP-LSD and 1cP-MiPLA

Figure S4.2. Multiple reaction monitoring (MRM) chromatograms of samples in concentration of 1 ng/mL (whole blood matrix)

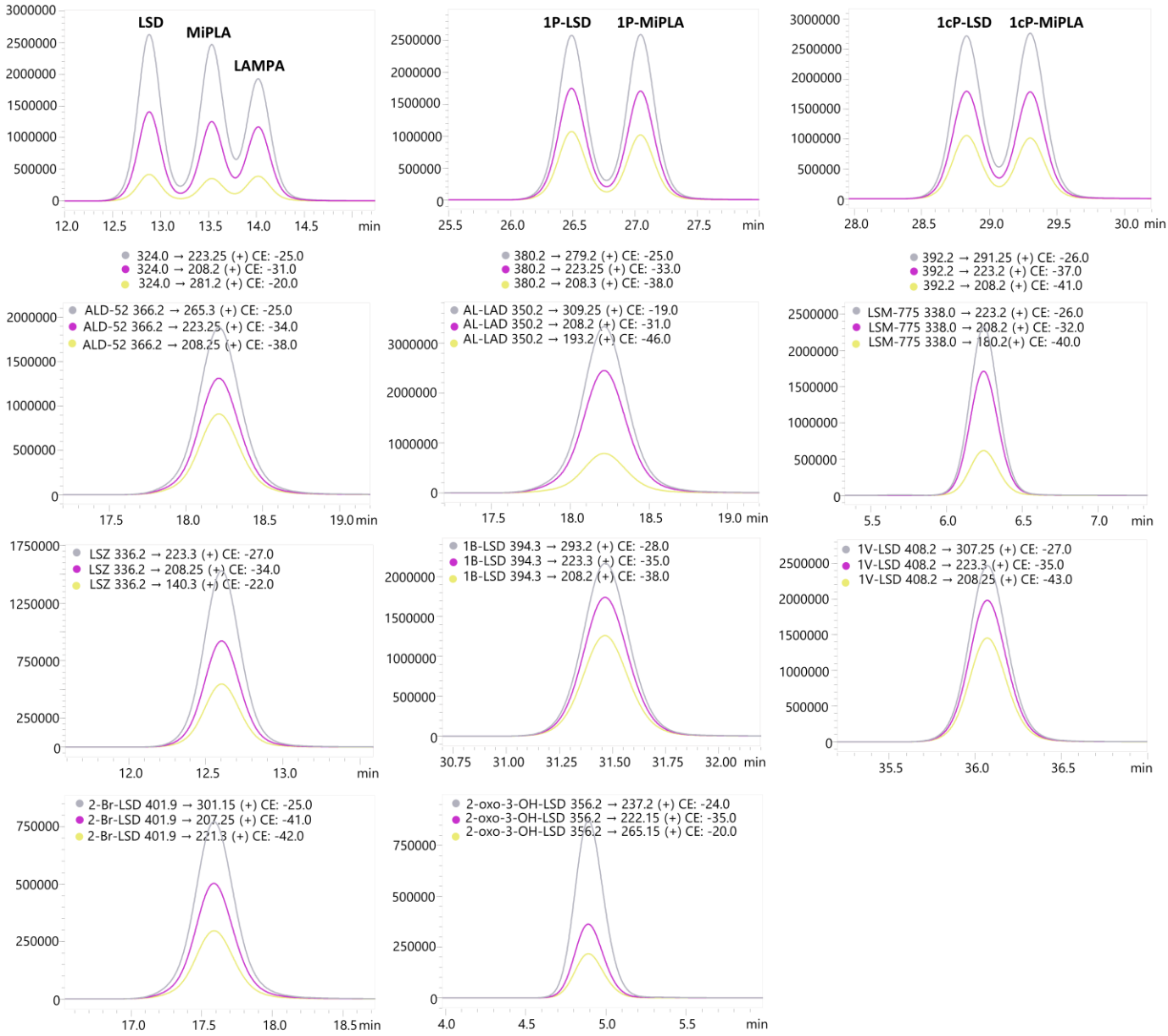


Table S5. Validation results.

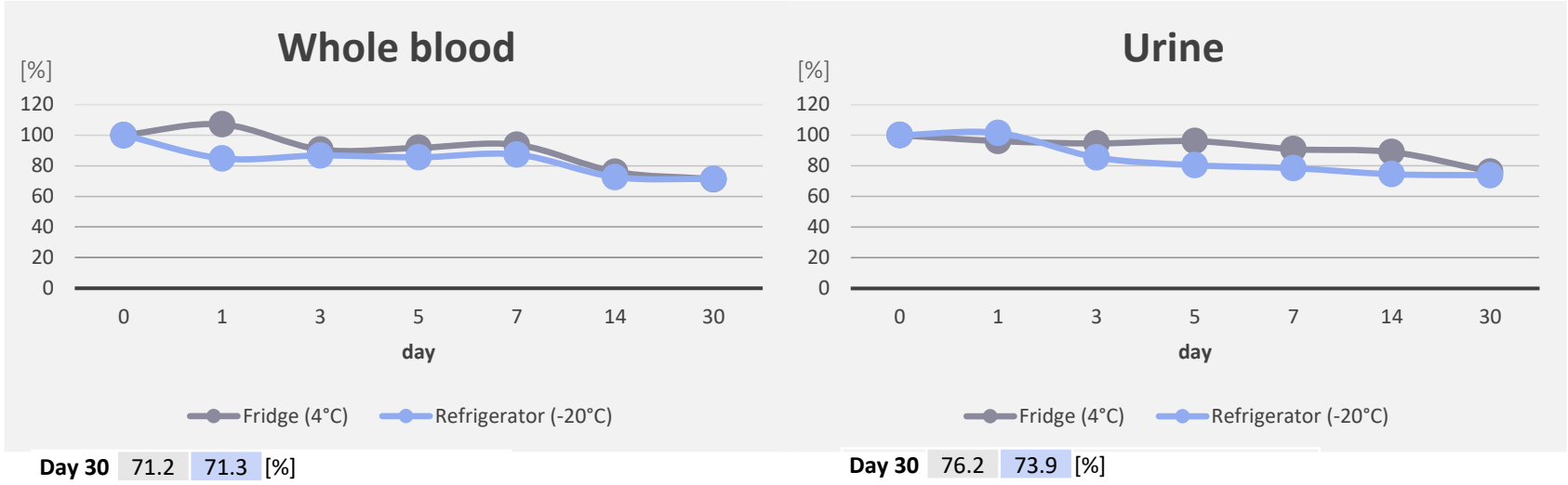
Substance	The coefficient of determination (R^2)	Concentration level [pg/mL]	Intraday		Interday		Recovery [%]*	Matrix effect [%]*	Process efficiency [%] *
			Precision [%]*	Accuracy [%]*	Precision [%]*	Accuracy [%]*			
ALD-52	0.9999	5	4.0	8.5	6.8	-3.1	96.5	-3.5	76.8
		500	8.3	9.0	12.2	-5.6	110.3	10.3	86.8
		1000	6.9	9.3	7.3	-0.5	113.4	13.4	88.2
AL-LAD	0.9999	5	6.3	-5.8	1.4	-9.1	87.4	-12.6	62.6
		500	7.2	-13.3	5.5	-5.2	105.2	5.2	67.9
		1000	9.7	-10.9	11.4	-9.7	88.4	11.6	71.1
LAMPA	0.9998	5	0.3	7.5	0.7	7.3	101.8	1.8	77.5
		500	6.9	8.5	8.5	7.4	109.8	9.8	89.4
		1000	1.1	-0.3	1.6	0.0	109.2	9.2	92.2
LSD	0.9995	5	5.5	6.1	9.2	-4.2	104.4	4.4	82.6
		500	7.6	13.2	7.8	5.5	109.9	9.9	90.2
		1000	6.6	2.2	5.9	1.7	108.4	8.4	93.2
MiPLA	0.9997	5	4.9	6.8	2.3	1.5	103.2	3.2	85.0
		500	5.8	2.6	4.8	3.2	104.7	4.7	90.2
		1000	9.6	2.5	7.6	-4.3	102.4	2.4	91.0
LSM-775	0.9999	5	5.4	12.0	10.5	8.2	98.4	-1.6	86.7
		500	9.1	6.0	15.6	1.6	116.6	16.6	96.5
		1000	15.8	9.1	2.0	-1.8	107.2	7.2	87.0
LSZ	0.9999	5	12.2	10.3	7.8	13.6	94.8	-5.2	75.9
		500	8.2	9.4	12.1	6.6	118.6	18.6	88.7
		1000	3.6	0.0	1.2	-7.3	107.5	7.5	84.6
1B-LSD	0.9998	5	5.5	7.5	5.9	-1.1	89.5	-10.5	72.2
		500	6.3	7.7	8.2	-3.6	111.3	11.3	89.0
		1000	7.2	8.1	6.3	0.5	109.4	9.4	85.4
1V-LSD	0.9998	5	7.8	3.8	5.8	-3.2	91.5	-8.5	80.0
		500	4.1	7.6	3.4	5.7	102.3	2.3	76.8
		1000	5.5	4.8	1.6	9.3	109.1	9.1	97.3
1cP-LSD	0.9986	5	7.2	8.0	15.3	-7.5	110.1	10.1	73.0
		500	6.8	-9.5	10.5	-11.8	115.4	15.4	84.1
		1000	8.5	-2.8	1.9	4.5	113.2	13.2	98.1
1cP-MiPLA	0.9987	5	6.8	6.8	3.8	-1.0	102.9	2.9	84.0
		500	5.8	8.6	0.4	3.8	97.2	-2.8	84.8
		1000	6.0	3.8	2.6	10.2	105.5	5.5	101.9
1P-LSD	0.9996	5	3.8	-0.5	1.3	3.1	109.1	9.1	74.4
		500	9.2	0.8	8.0	-0.1	117.1	17.1	70.4
		1000	3.3	8.0	3.7	2.8	111.4	11.4	93.0
1P-MiPLA	0.9999	5	8.7	-7.2	2.6	-14.4	114.5	14.5	75.2
		500	7.2	-1.8	12.9	-5.5	106.8	6.8	80.1
		1000	9.7	-5.1	12.0	-3.3	110.0	10.0	97.1
2-Bromo-LSD	0.9999	5	7.6	4.5	9.2	-4.2	80.6	-19.4	60.3
		500	4.5	8.3	7.8	5.5	103.0	3.0	70.1
		1000	9.9	13.4	5.9	1.7	111.9	11.9	83.7
2-oxo-3-OH-LSD	0.9993	5	7.8	6.3	5.8	7.2	82.1	-17.9	69.3
		500	9.5	8.9	9.4	8.1	89.9	-10.1	78.9
		1000	10.1	5.8	4.6	10.4	92.5	-7.5	89.5

* n=5;

Limit of quantification (LOQ) for all substances was 0.5 pg/mL

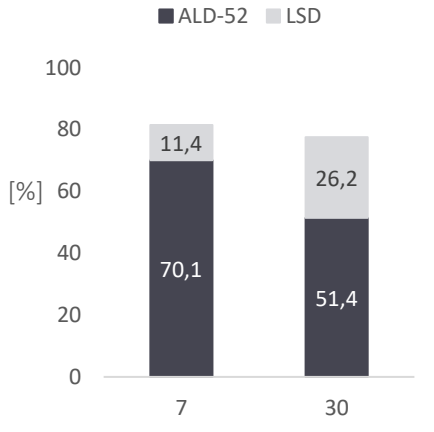
S6. Results of stability study

Figure S6.1. Results of stability experiments (a) and (b) for **ALD-52**

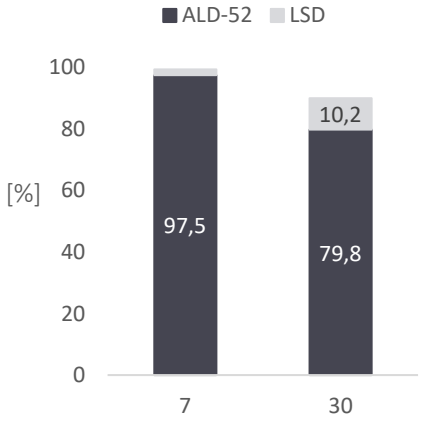


Day 30 71.2 71.3 [%]

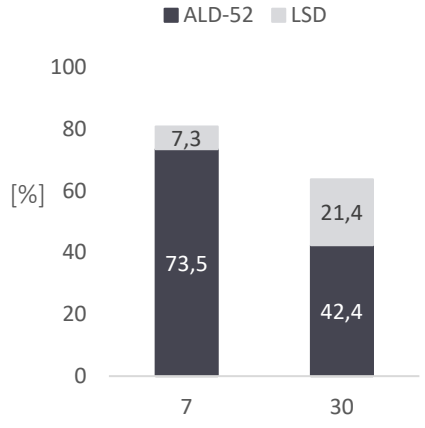
Day 30 76.2 73.9 [%]



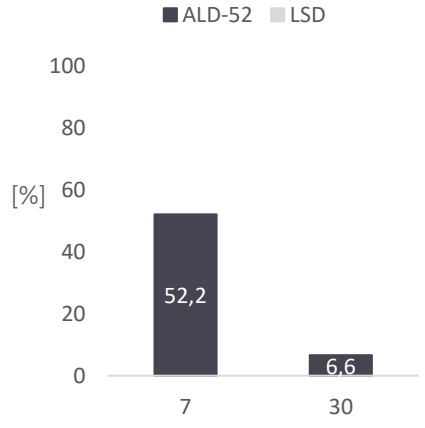
Plasma		
	ALD-52 [%]	LSD [%]
Day 0	100.0	0.0
Day 7	70.1	11.4
Day 30	51.4	26.2



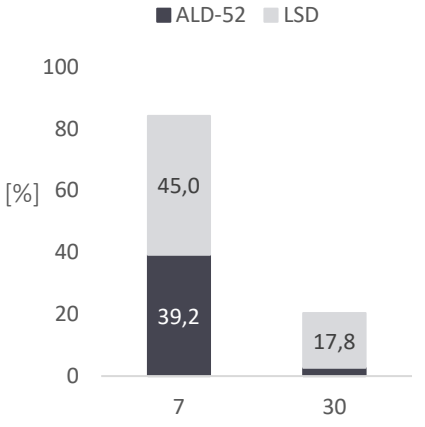
Whole blood / NaF		
	ALD-52 [%]	LSD [%]
Day 0	100.0	0.0
Day 7	97.5	1.8
Day 30	79.8	10.2



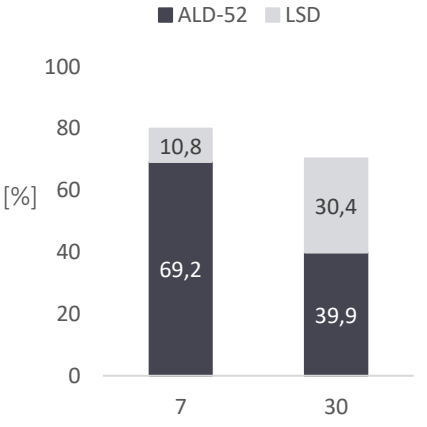
Whole blood / Citrate		
	ALD-52 [%]	LSD [%]
Day 0	100.0	0.0
Day 7	73.5	7.3
Day 30	42.4	21.4



Urine / NaF		
	ALD-52 [%]	LSD [%]
Day 0	100.0	0.0
Day 7	52.2	0.0
Day 30	6.6	0.0

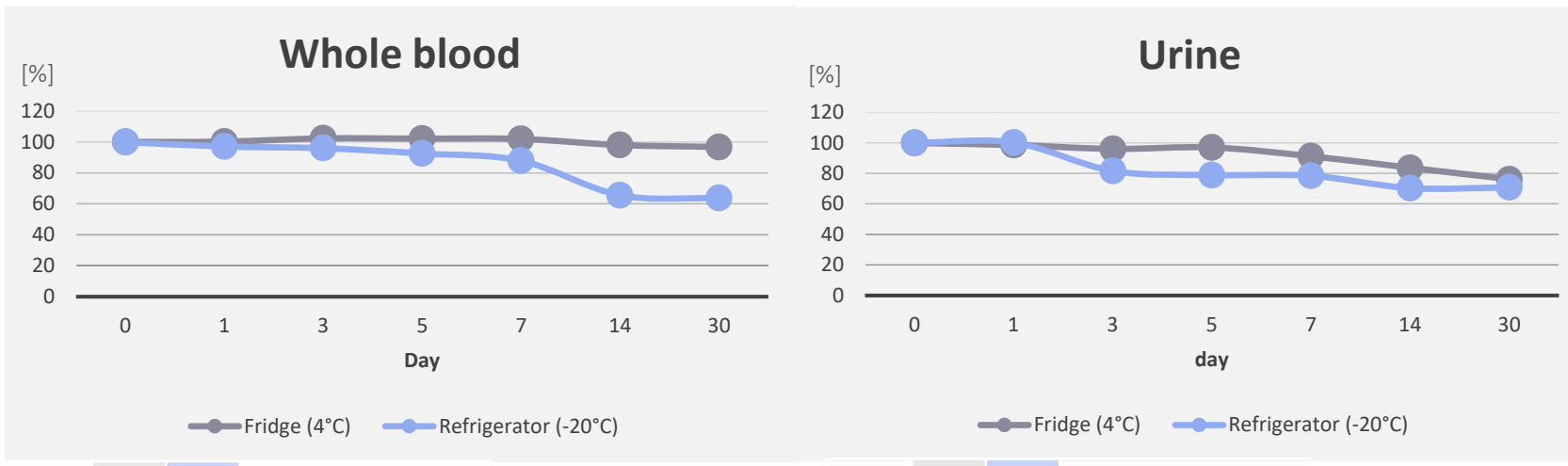


Urine / borax		
	ALD-52 [%]	LSD [%]
Day 0	100.0	0.0
Day 7	39.2	45.0
Day 30	2.6	17.8



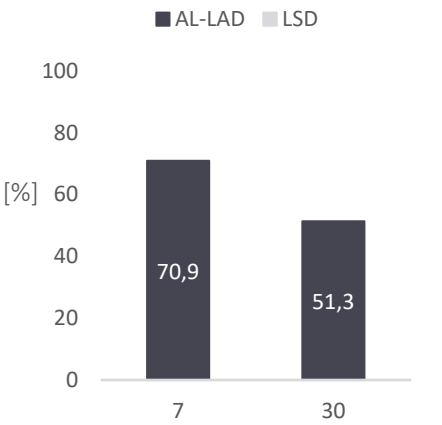
Serum		
	ALD-52 [%]	LSD [%]
Day 0	100.0	0.0
Day 7	69.2	10.8
Day 30	39.9	30.4

Figure S6.2. Results of stability experiments (a) and (b) for **AL-LAD**

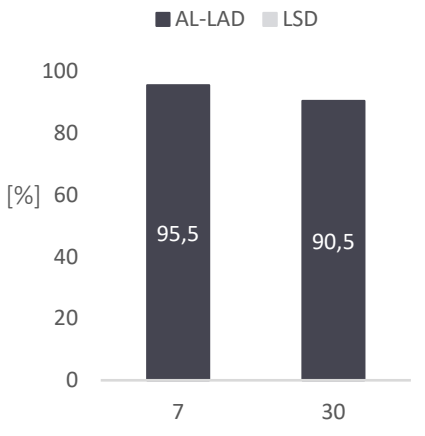


Day 30 96.8 63.7 [%]

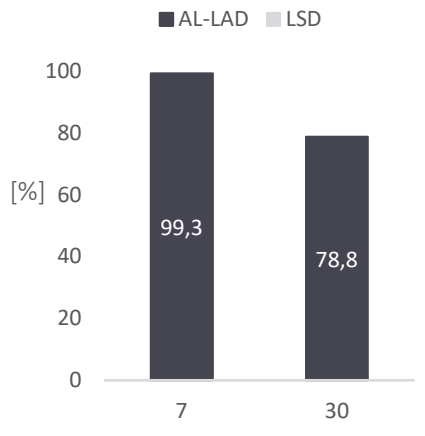
Day 30 76.1 70.9 [%]



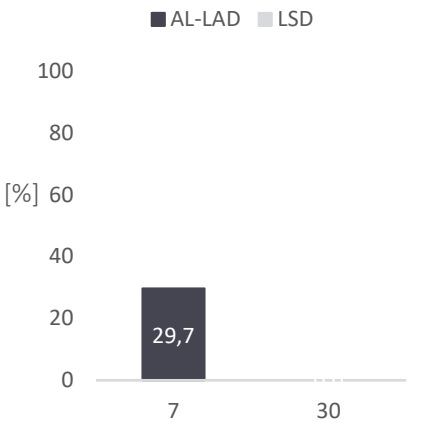
Plasma		
	AL-LAD [%]	LSD [%]
Day 0	100.0	0.0
Day 7	70.9	0.0
Day 30	51.3	0.0



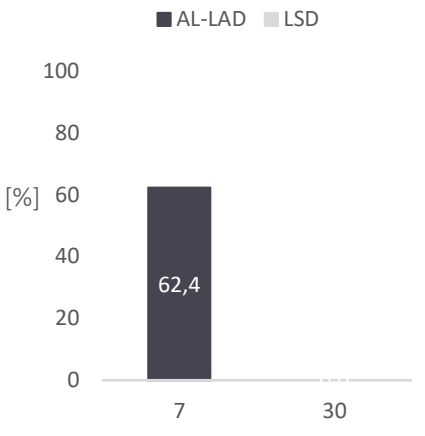
Whole blood / NaF		
	AL-LAD [%]	LSD [%]
Day 0	100.0	0.0
Day 7	95.5	0.0
Day 30	90.5	0.0



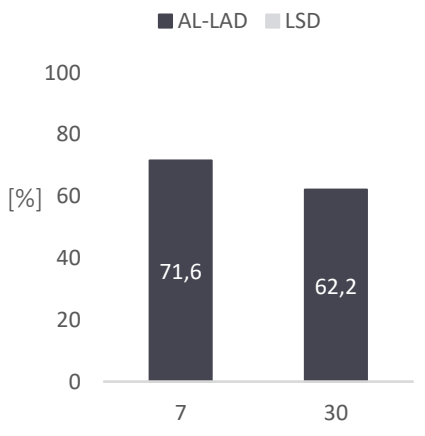
Whole blood / Citrate		
	AL-LAD [%]	LSD [%]
Day 0	100.0	0.0
Day 7	99.3	0.0
Day 30	78.8	0.0



Urine / NaF		
	AL-LAD [%]	LSD [%]
Day 0	100.0	0.0
Day 7	29.7	0.0
Day 30	0.0	0.0

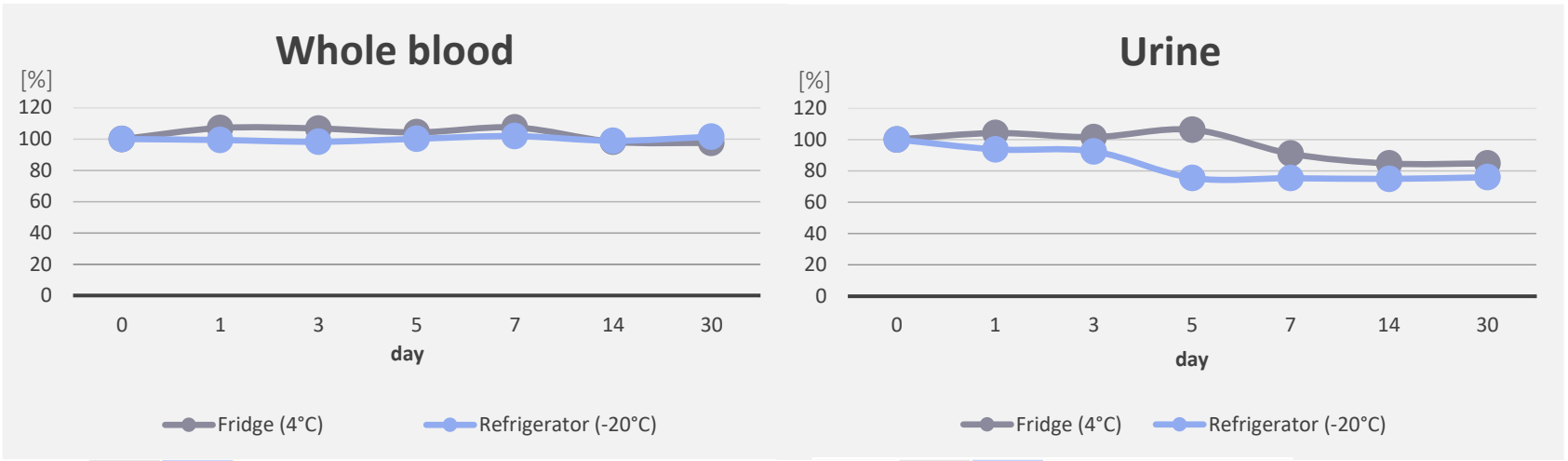


Urine / borax		
	AL-LAD [%]	LSD [%]
Day 0	100.0	0.0
Day 7	62.4	0.0
Day 30	0.0	0.0



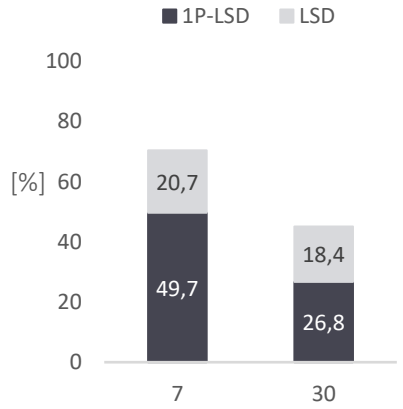
Serum		
	AL-LAD [%]	LSD [%]
Day 0	100.0	0.0
Day 7	71.6	0.0
Day 30	62.2	0.0

Figure S6.3. Results of stability experiments (a) and (b) for **1P-LSD**

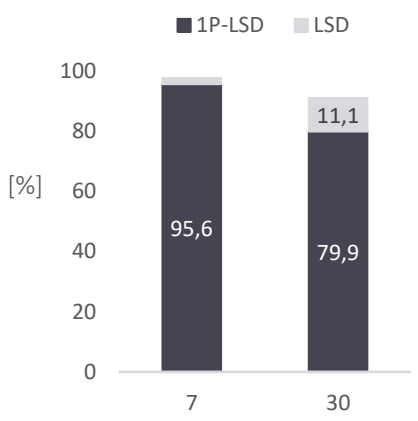


Day 30 97.5 101.5 [%]

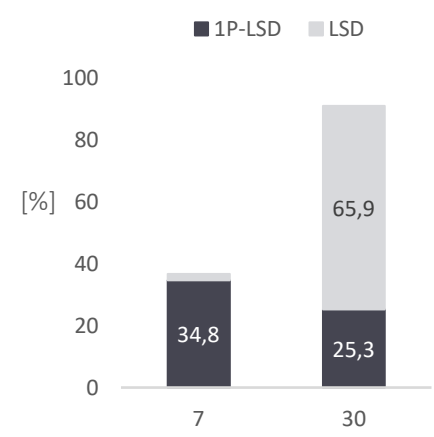
Day 30 84.7 75.9 [%]



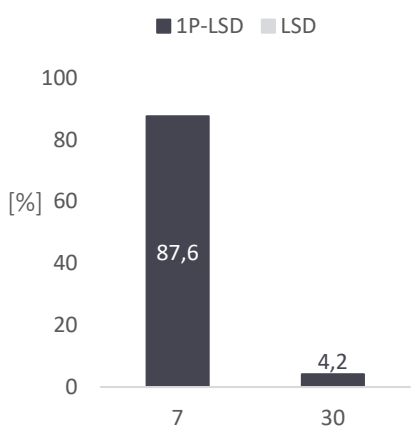
Plasma		
	1P-LSD [%]	LSD [%]
Day 0	100.0	0.0
Day 7	49.7	20.7
Day 30	26.8	18.4



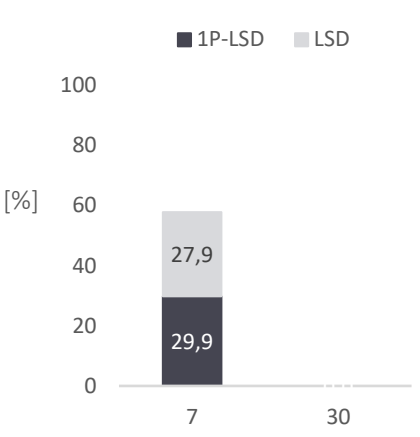
Whole blood / NaF		
	1P-LSD [%]	LSD [%]
Day 0	100.0	0.0
Day 7	95.6	2.0
Day 30	79.9	11.1



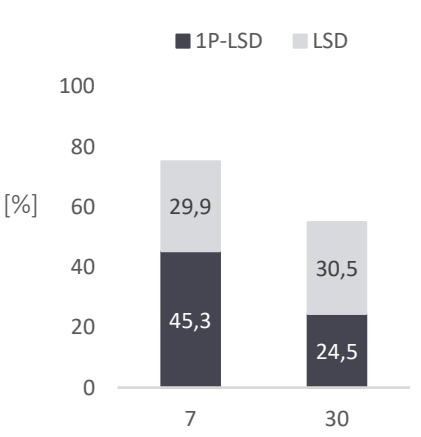
Whole blood / Citrate		
	1P-LSD [%]	LSD [%]
Day 0	100.0	0.0
Day 7	34.8	25.3
Day 30	2.0	65.9



Urine / NaF		
	1P-LSD [%]	LSD [%]
Day 0	100.0	0.0
Day 7	87.6	0.0
Day 30	4.2	0.0

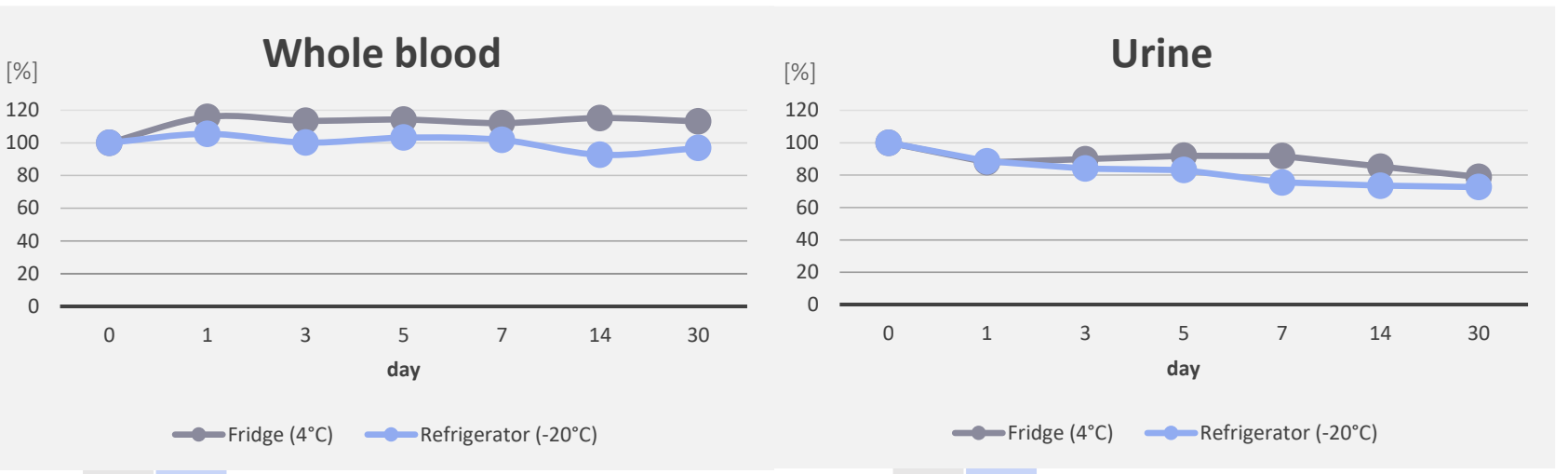


Urine / borax		
	1P-LSD [%]	LSD [%]
Day 0	100.0	0.0
Day 7	29.9	27.9
Day 30	0.0	0.0



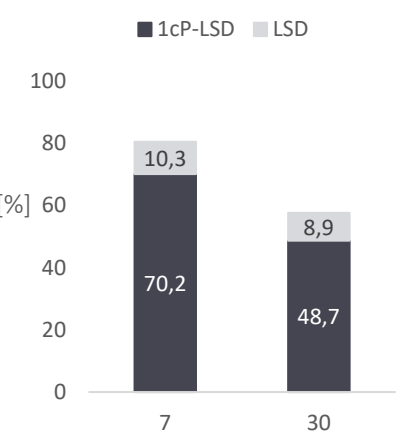
Serum		
	1P-LSD [%]	LSD [%]
Day 0	100.0	0.0
Day 7	45.3	29.9
Day 30	24.5	30.5

Figure S6.4. Results of stability experiments (a) and (b) for **1cP-LSD**

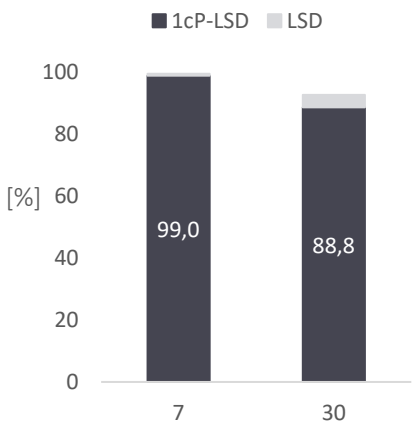


Day 30 113.0 96.8 [%]

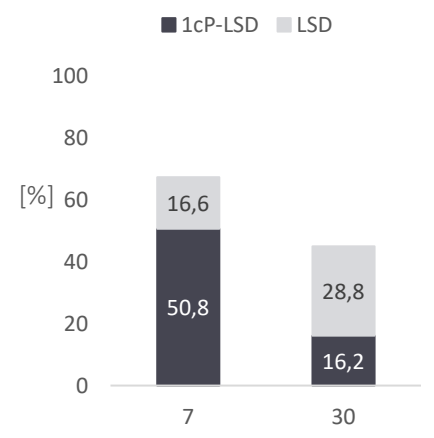
Day 30 78.9 72.7 [%]



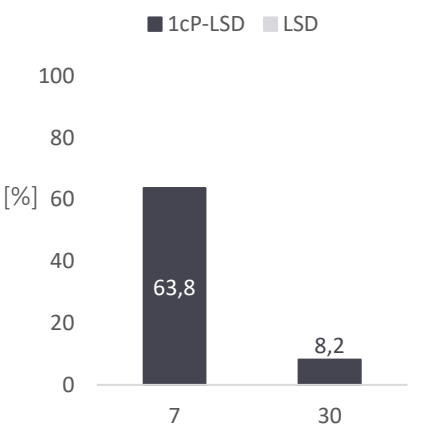
Plasma		
	1cP-LSD [%]	LSD [%]
Day 0	100.0	0.0
Day 7	70.2	10.3
Day 30	48.7	8.9



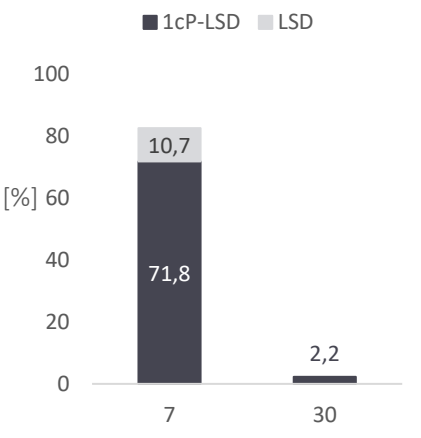
Whole blood / NaF		
	1cP-LSD [%]	LSD [%]
Day 0	100.0	0.0
Day 7	99.0	0.7
Day 30	88.8	4.0



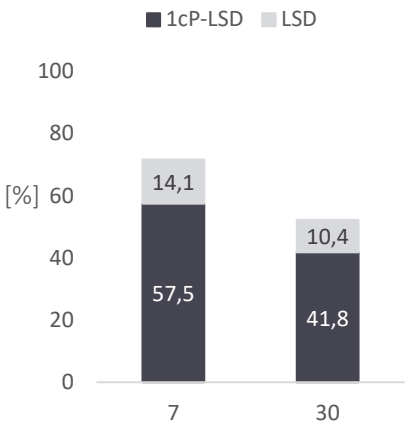
Whole blood / Citrate		
	1cP-LSD [%]	LSD [%]
Day 0	100.0	0.0
Day 7	50.8	16.6
Day 30	16.2	28.8



Urine / NaF		
	1cP-LSD [%]	LSD [%]
Day 0	100.0	0.0
Day 7	63.8	0.0
Day 30	8.2	0.0

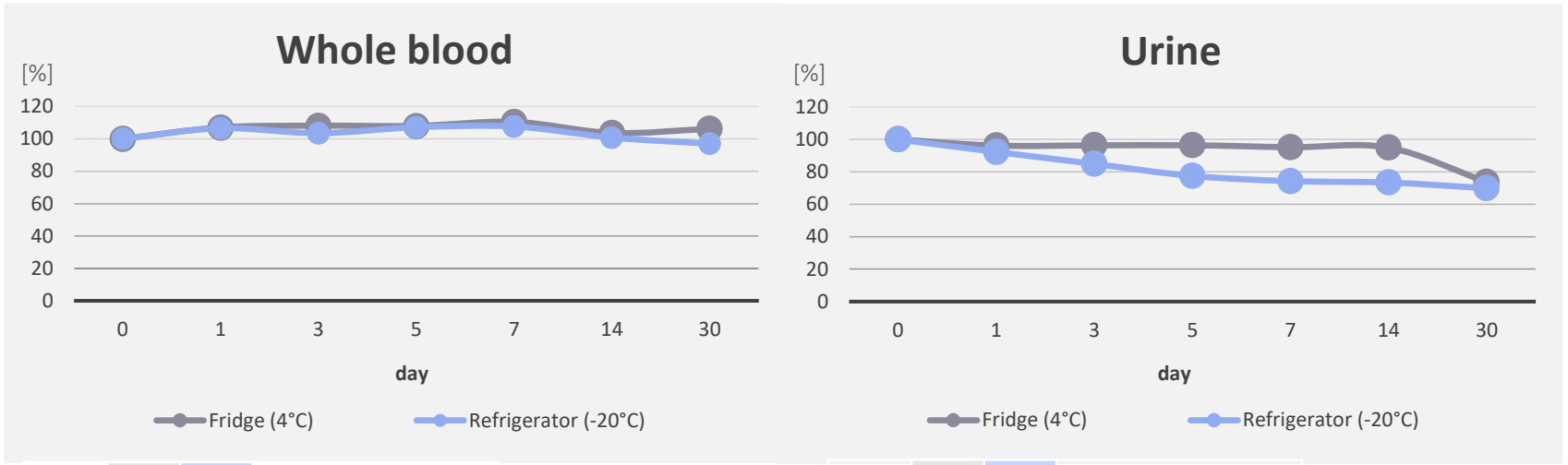


Urine / borax		
	1cP-LSD [%]	LSD [%]
Day 0	100.0	0.0
Day 7	71.8	10.7
Day 30	2.2	0.0



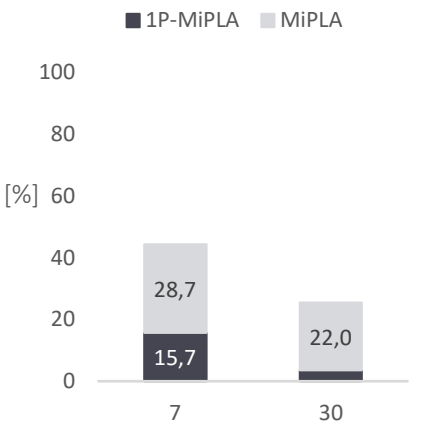
Serum		
	1cP-LSD [%]	LSD [%]
Day 0	100.0	0.0
Day 7	57.5	14.1
Day 30	41.8	10.4

Figure S6.5. Results of stability experiments (a) and (b) for **1P-MiPLA**

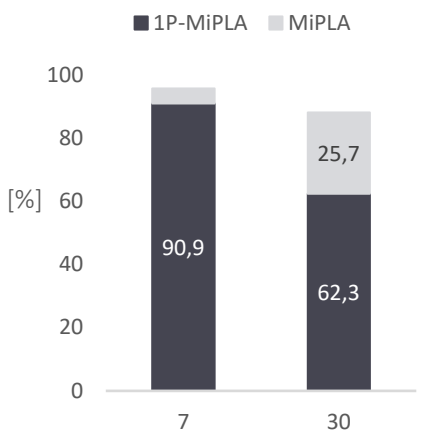


Day 30 106.1 97.0 [%]

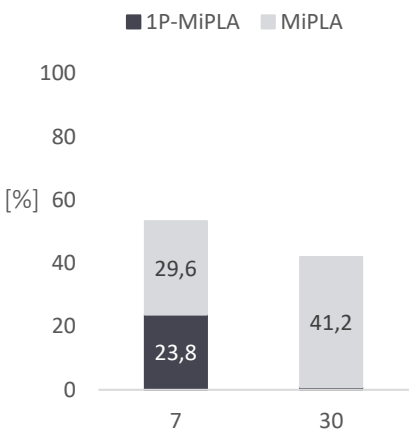
Day 30 73.6 69.9 [%]



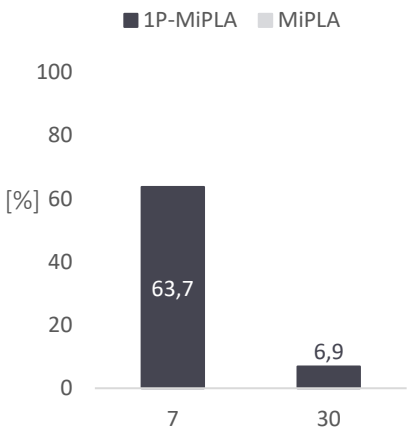
Plasma		
	1P-MiPLA [%]	MiPLA [%]
Day 0	100.0	0.0
Day 7	15.7	28.7
Day 30	3.6	22.0



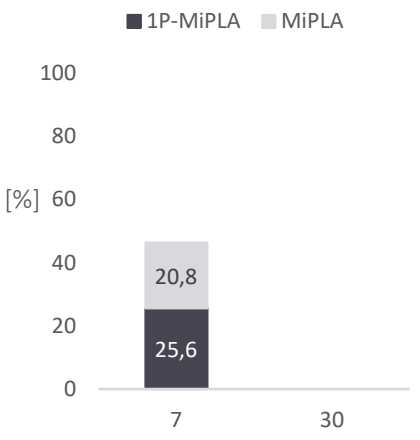
Whole blood / NaF		
	1P-MiPLA [%]	MiPLA [%]
Day 0	100.0	0.0
Day 7	90.9	4.8
Day 30	62.3	25.7



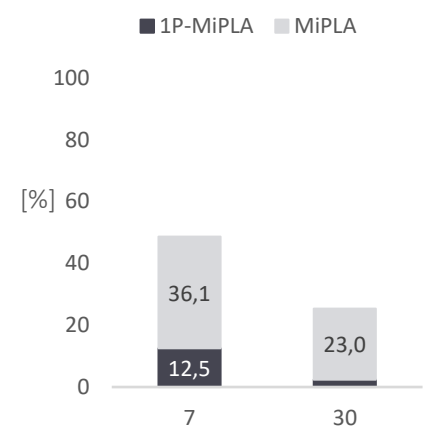
Whole blood / Citrate		
	1P-MiPLA [%]	MiPLA [%]
Day 0	100.0	0.0
Day 7	23.8	29.6
Day 30	0.8	41.2



Urine / NaF		
	1P-MiPLA [%]	MiPLA [%]
Day 0	100.0	0.0
Day 7	63.7	0.0
Day 30	6.9	0.0

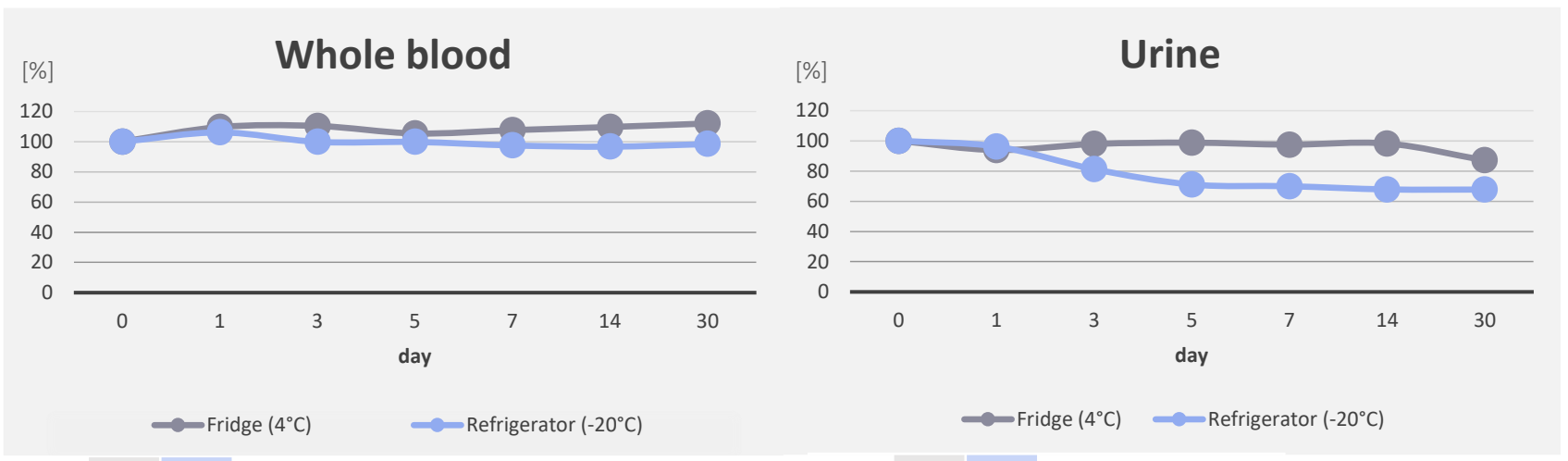


Urine / borax		
	1P-MiPLA [%]	MiPLA [%]
Day 0	100.0	0.0
Day 7	25.6	20.8
Day 30	0.0	0.0



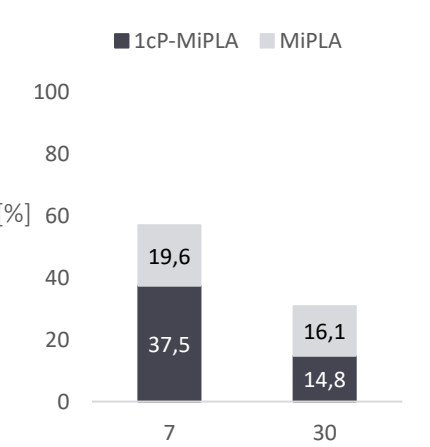
Serum		
	1P-MiPLA [%]	MiPLA [%]
Day 0	100.0	0.0
Day 7	12.5	36.1
Day 30	2.3	23.0

Figure S6.6. Results of stability experiments (a) and (b) for **1cP-MiPLA**

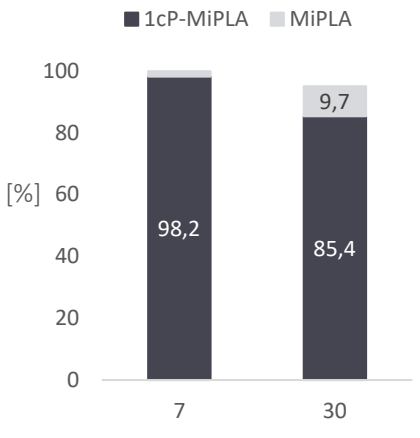


Day 30 112.1 98.5 [%]

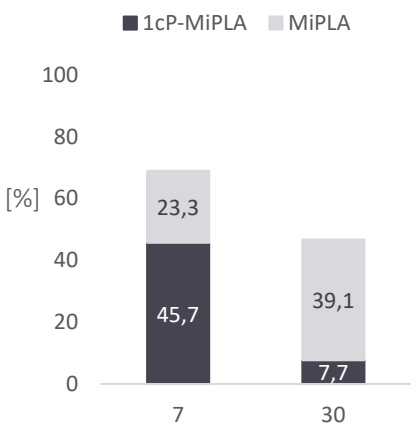
Day 30 87.2 67.7 [%]



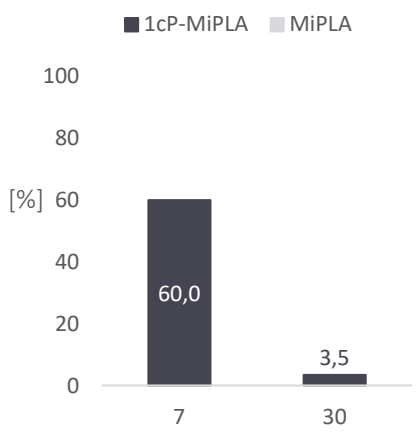
Plasma		
	1cP-MiPLA [%]	MiPLA [%]
Day 0	100.0	0.0
Day 7	37.5	19.6
Day 30	14.8	16.1



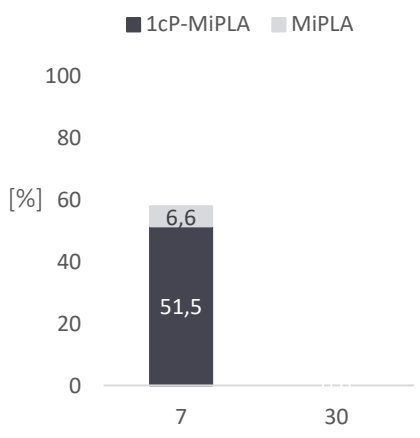
Whole blood / NaF		
	1cP-MiPLA [%]	MiPLA [%]
Day 0	100.0	0.0
Day 7	98.2	1.7
Day 30	85.4	9.7



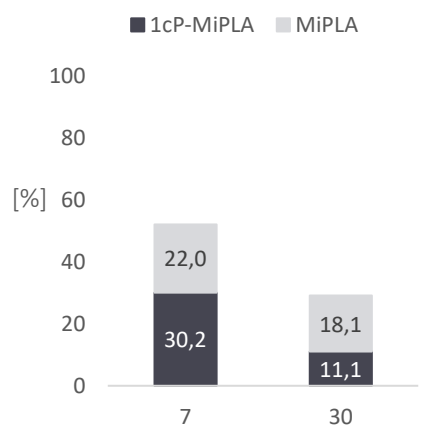
Whole blood / Citrate		
	1cP-MiPLA [%]	MiPLA [%]
Day 0	100.0	0.0
Day 7	45.7	23.3
Day 30	7.7	39.1



Urine / NaF		
	1cP-MiPLA [%]	MiPLA [%]
Day 0	100.0	0.0
Day 7	60.0	0.0
Day 30	3.5	0.0

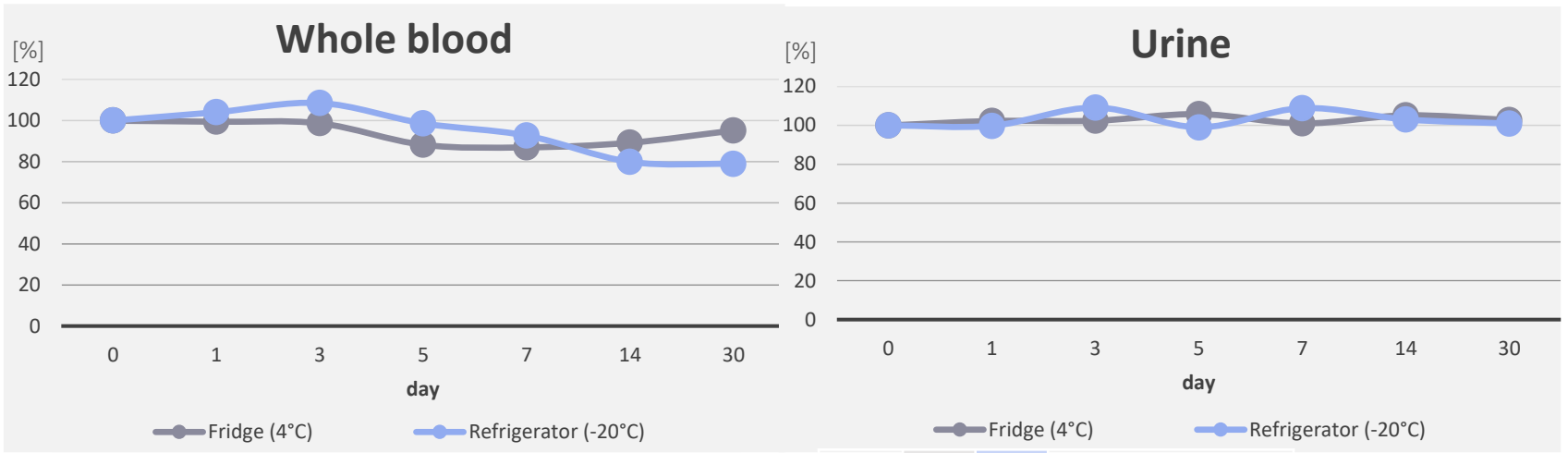


Urine / borax		
	1cP-MiPLA [%]	MiPLA [%]
Day 0	100.0	0.0
Day 7	51.5	6.6
Day 30	0.0	0.0



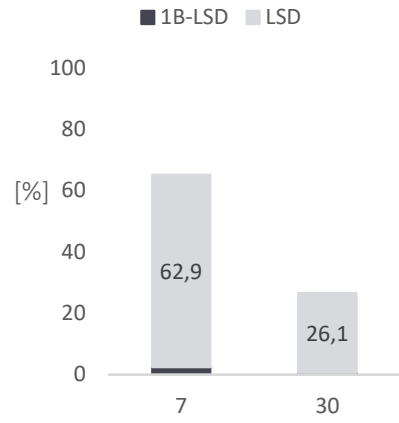
Serum		
	1cP-MiPLA [%]	MiPLA [%]
Day 0	100.0	0.0
Day 7	30.2	22.0
Day 30	11.1	18.1

Figure S6.7. Results of stability experiments (a) and (b) for **1B-LSD**

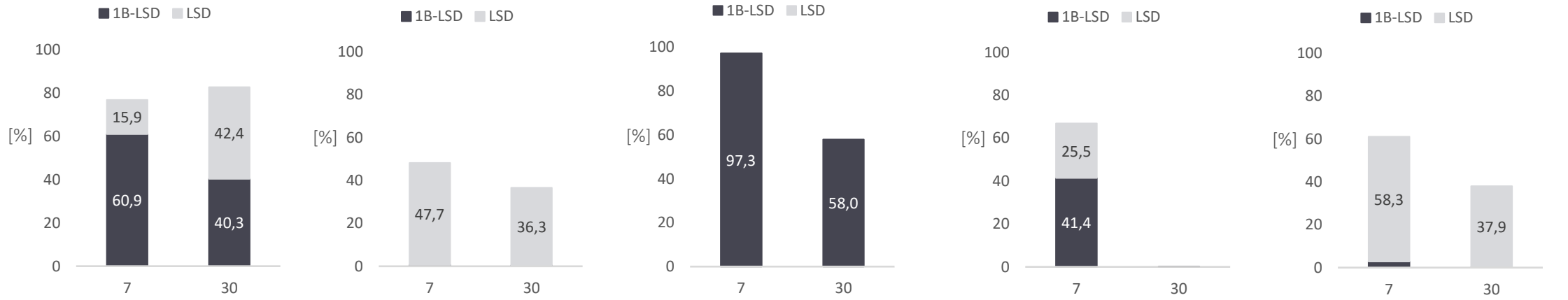


Day 30 95.2 78.9 [%]

Day 30 102.8 101.0 [%]



Plasma		
	1B-LSD [%]	LSD [%]
Day 0	100.0	0.0
Day 7	2.3	62.9
Day 30	0.6	26.1



Whole blood / NaF		
	1B-LSD	LSD
0	100.0	0.0
7	60.9	15.9
30	40.3	42.4

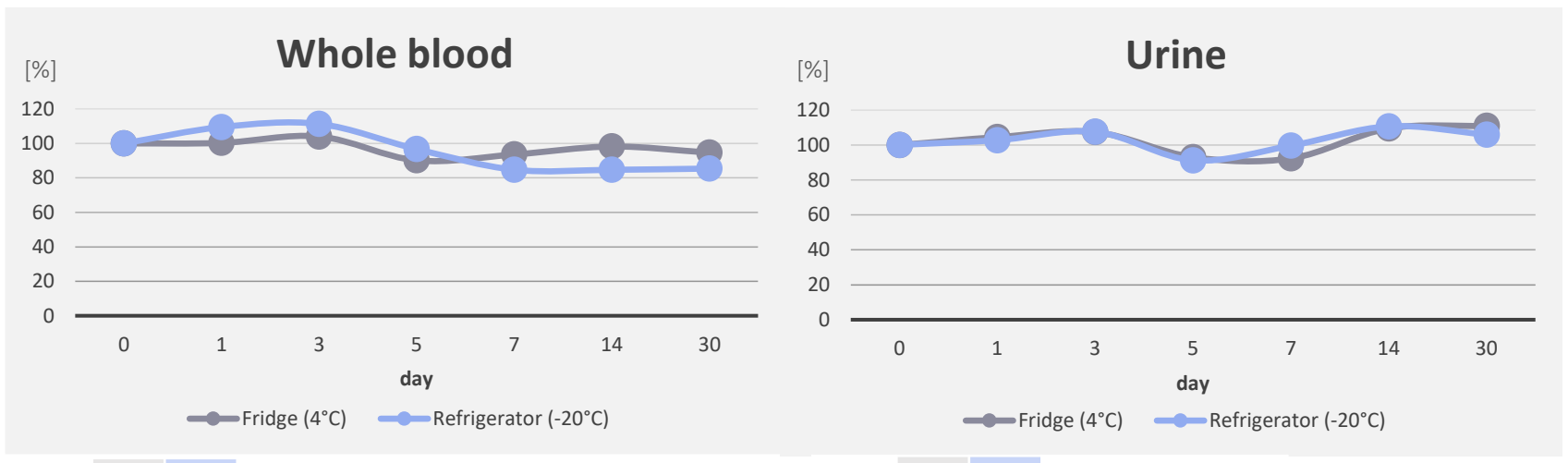
Whole blood / Citrate		
	1B-LSD [%]	LSD [%]
Day 0	100.0	0.0
Day 7	0.5	47.7
Day 30	0.3	36.3

Urine / NaF		
	1B-LSD [%]	LSD [%]
Day 0	100.0	0.0
Day 7	97.3	0.0
Day 30	58.0	0.0

Urine / borax		
	1B-LSD [%]	LSD [%]
Day 0	100.0	0.0
Day 7	41.4	25.5
Day 30	0.2	0.0

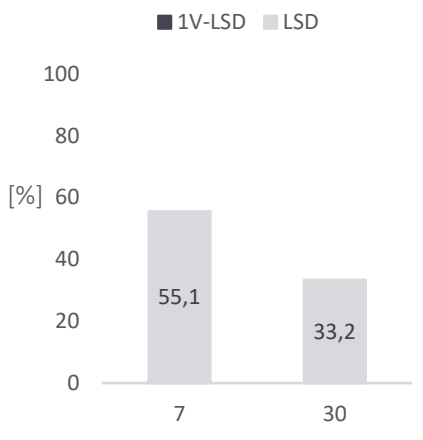
Serum		
	1B-LSD [%]	LSD [%]
Day 0	100.0	0.0
Day 7	2.9	58.3
Day 30	0.2	37.9

Figure S6.8. Results of stability experiments (a) and (b) for **1V-LSD**

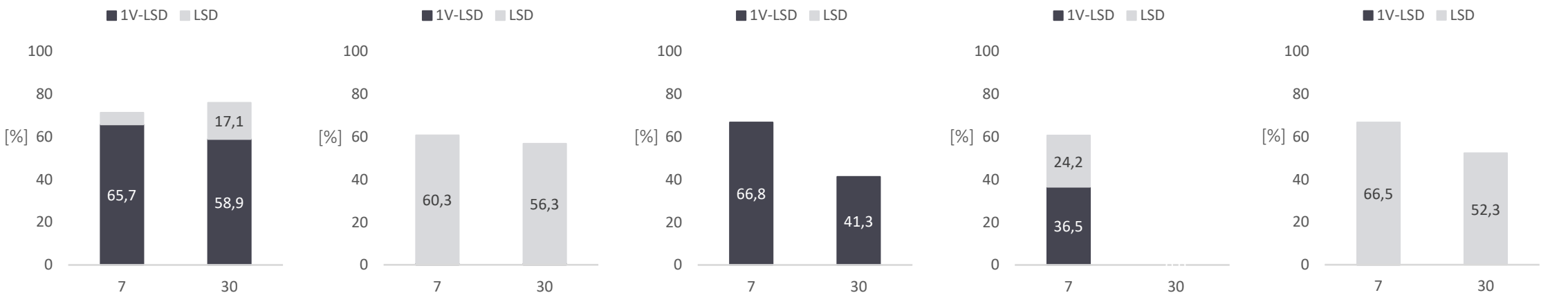


Day 30 94.7 85.4 [%]

Day 30 111.0 105.9 [%]



Plasma		
	1V-LSD [%]	LSD [%]
0	100.0	0.0
7	0.5	55.1
30	0.2	33.2



Whole blood / NaF		
	1V-LSD [%]	LSD [%]
Day 0	100.0	0.0
Day 7	65.7	5.6
Day 30	58.9	17.1

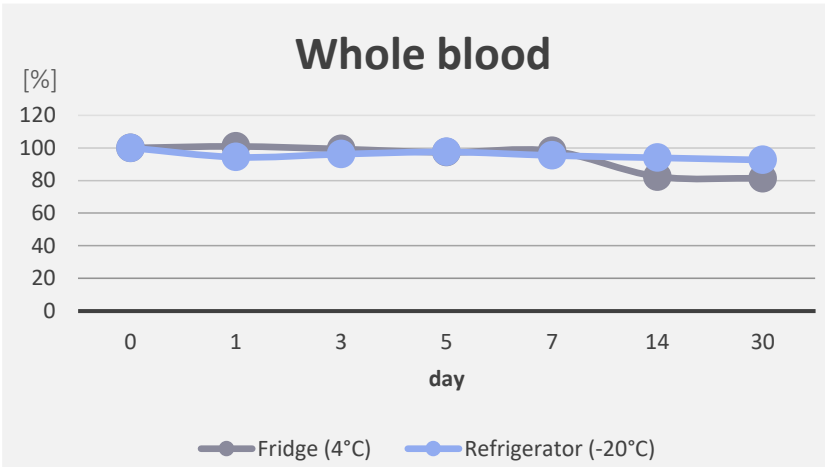
Whole blood / Citrate		
	1V-LSD [%]	LSD [%]
Day 0	100.0	0.0
Day 7	0.5	60.3
Day 30	0.5	56.3

Urine / NaF		
	1V-LSD [%]	LSD [%]
Day 0	100.0	0.0
Day 7	66.8	0.0
Day 30	41.3	0.0

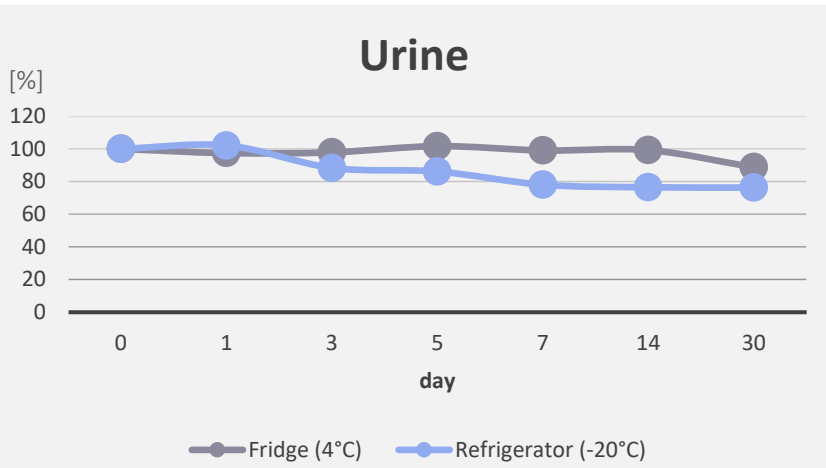
Urine / borax		
	1V-LSD [%]	LSD [%]
Day 0	100.0	0.0
Day 7	36.5	24.2
Day 30	0.0	0.0

Serum		
	1V-LSD [%]	LSD [%]
Day 0	100.0	0.0
Day 7	0.2	66.5
Day 30	0.0	52.3

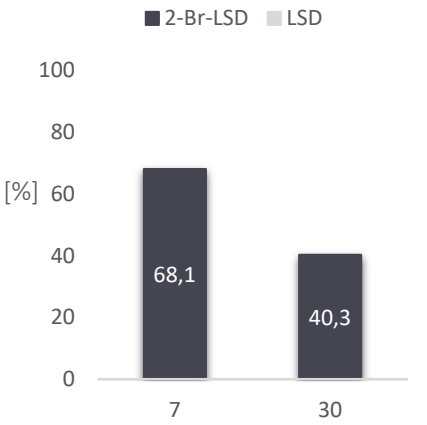
Figure S6.9. Results of stability experiments (a) and (b) for **2-Bromo-LSD**



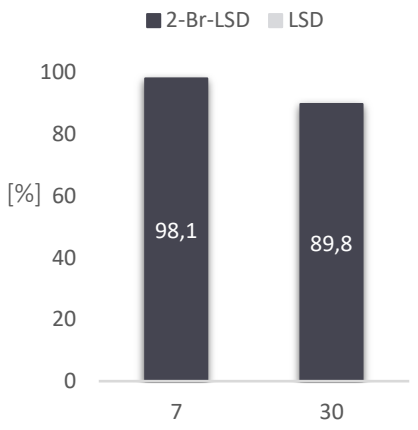
Day 30 81.3 92.7 [%]



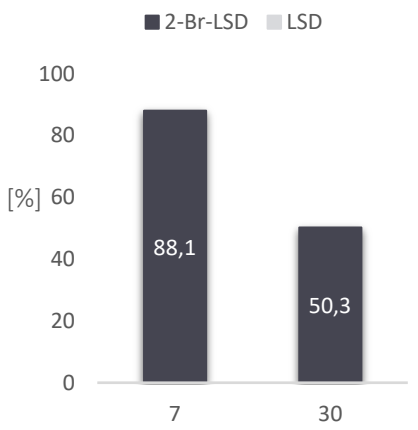
Day 30 88.9 76.4 [%]



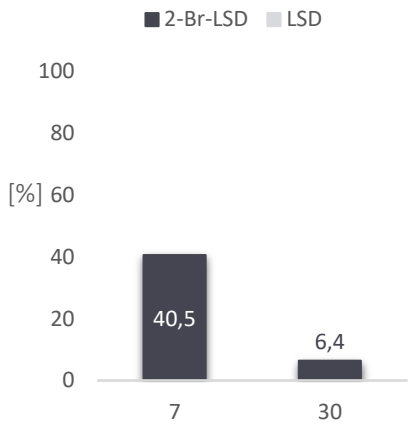
Plasma		
	2-Br-LSD [%]	LSD [%]
Day 0	100.0	0.0
Day 7	68.1	0.0
Day 30	40.3	0.0



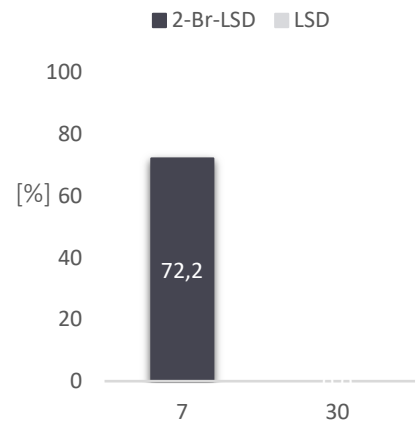
Whole blood / NaF		
	2-Br-LSD [%]	LSD [%]
Day 0	100.0	0.0
Day 7	98.1	0.0
Day 30	89.8	0.0



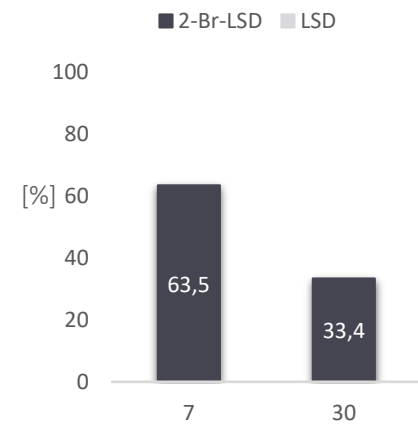
Whole blood / Citrate		
	2-Br-LSD [%]	LSD [%]
Day 0	100.0	0.0
Day 7	88.1	0.0
Day 30	50.3	0.0



Urine / NaF		
	2-Br-LSD [%]	LSD [%]
Day 0	100.0	0.0
Day 7	40.5	0.0
Day 30	6.4	0.0

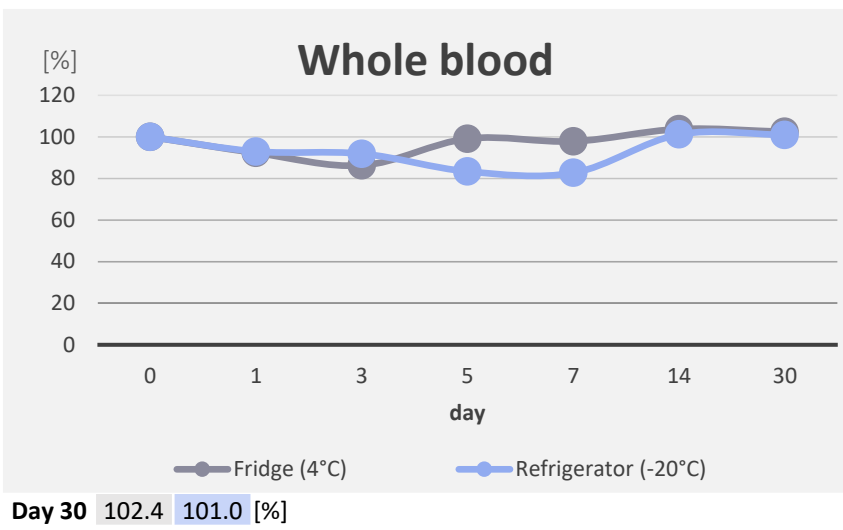


Urine / borax		
	2-Br-LSD [%]	LSD [%]
Day 0	100.0	0.0
Day 7	72.2	0.0
Day 30	0.0	0.0

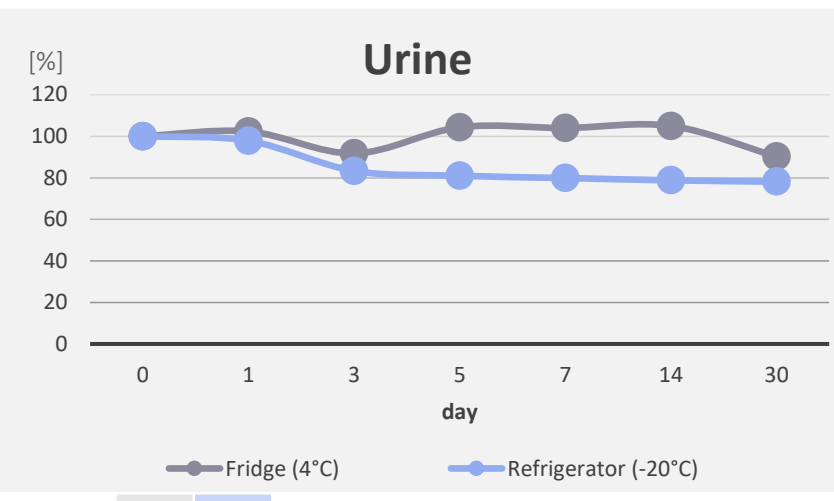


Serum		
	2-Br-LSD [%]	LSD [%]
Day 0	100.0	0.0
Day 7	63.5	0.0
Day 30	33.4	0.0

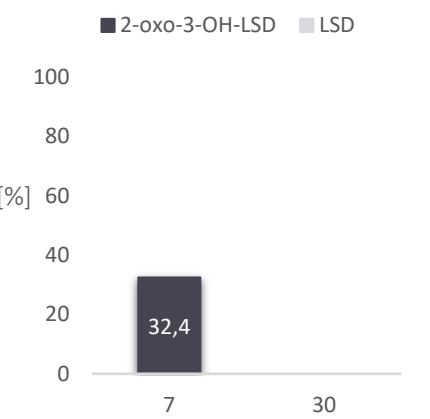
Figure S6.10. Results of stability experiments (a) and (b) for **2-oxo-3-OH-LSD**



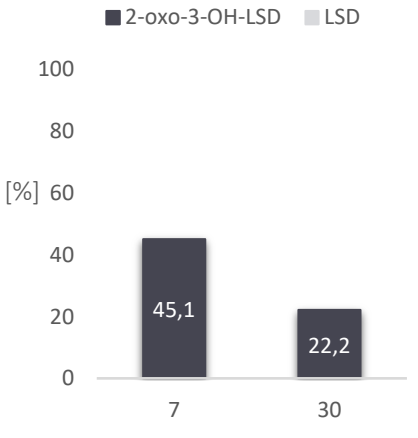
Day 30 102.4 101.0 [%]



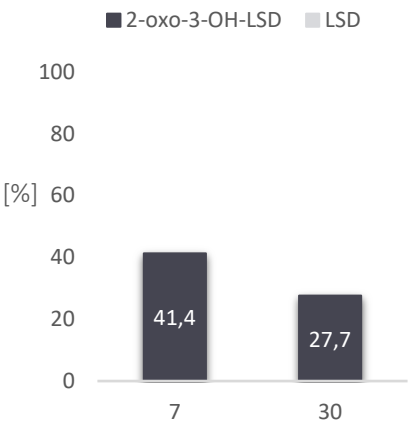
Day 30 90.3 78.2 [%]



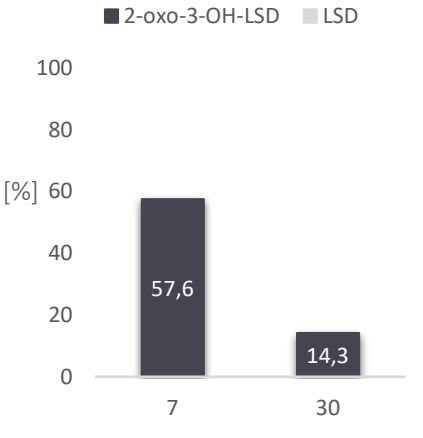
Plasma		
	Metabolite [%]	LSD [%]
Day 0	100.0	0.0
Day 7	32.4	0.0
Day 30	0.0	0.0



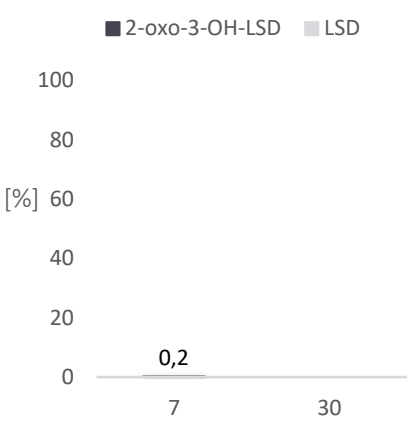
Whole blood / NaF		
	Metabolite [%]	LSD [%]
Day 0	100.0	0.0
Day 7	45.1	0.0
Day 30	22.2	0.0



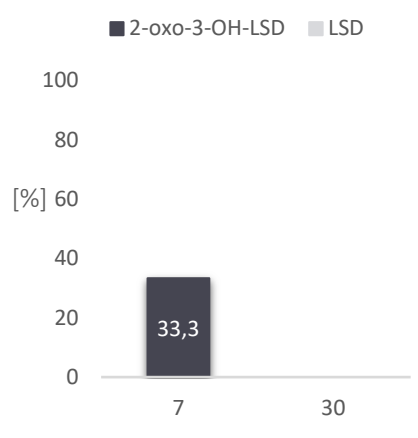
Whole blood / Citrate		
	Metabolite [%]	LSD [%]
Day 0	100.0	0.0
Day 7	41.4	0.0
Day 30	27.7	0.0



Urine / NaF		
	Metabolite [%]	LSD [%]
Day 0	100.0	0.0
Day 7	57.6	0.0
Day 30	14.3	0.0

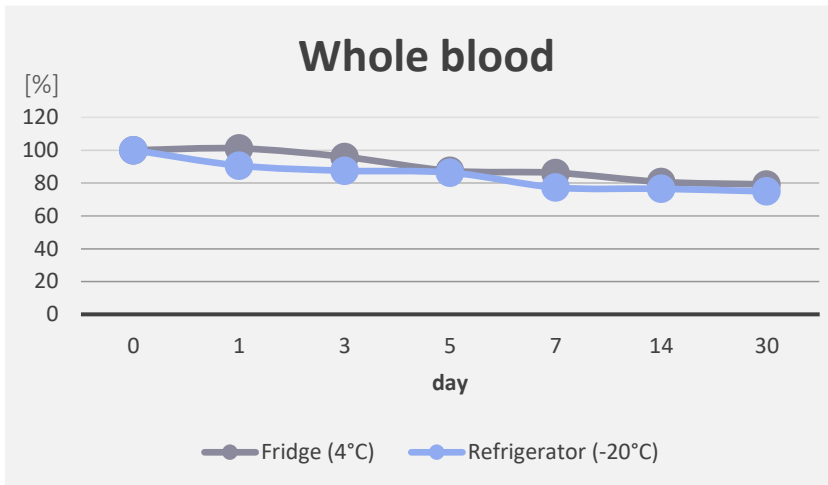


Urine / borax		
	Metabolite [%]	LSD [%]
Day 0	100.0	0.0
Day 7	0.2	0.0
Day 30	0.0	0.0

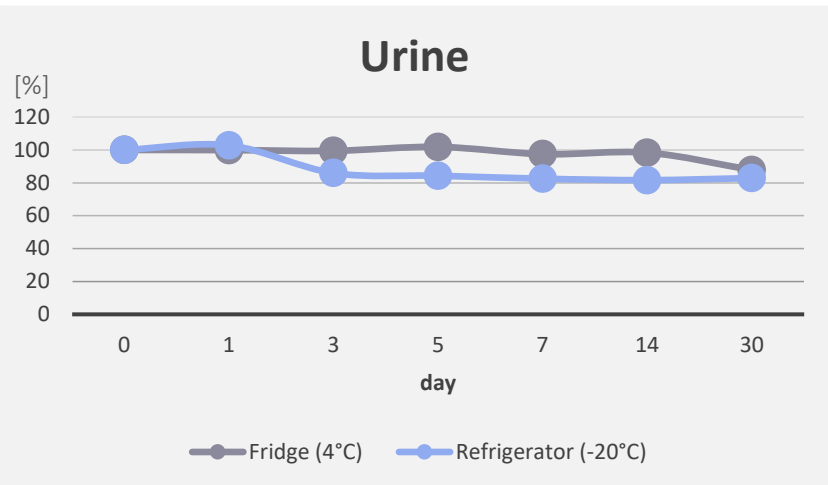


Serum		
	Metabolite [%]	LSD [%]
Day 0	100.0	0.0
Day 7	33.3	0.0
Day 30	0.0	0.0

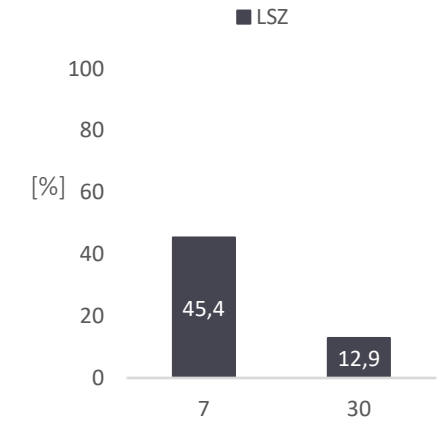
Figure S6.11. Results of stability experiments (a) and (b) for **LSZ**



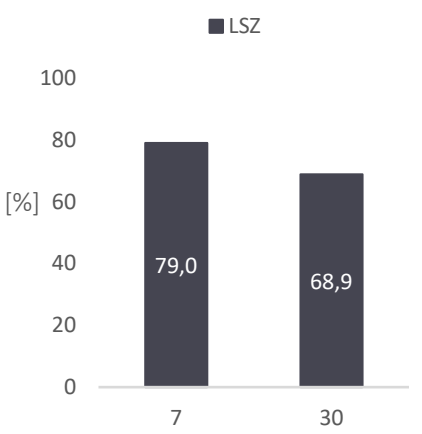
Day 30 79.1 75.0 [%]



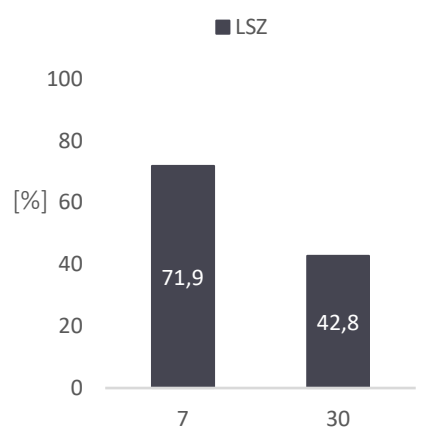
Day 30 87.8 82.8 [%]



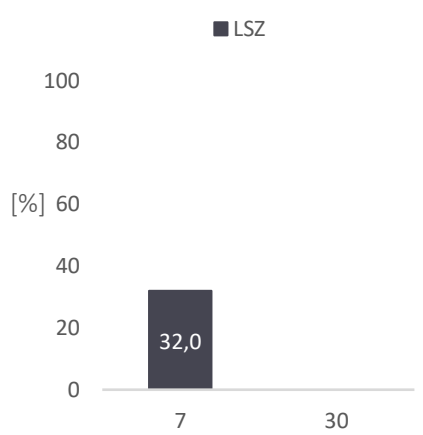
Plasma	
	LSZ [%]
Day 0	100.0
Day 7	45.4
Day 30	12.9



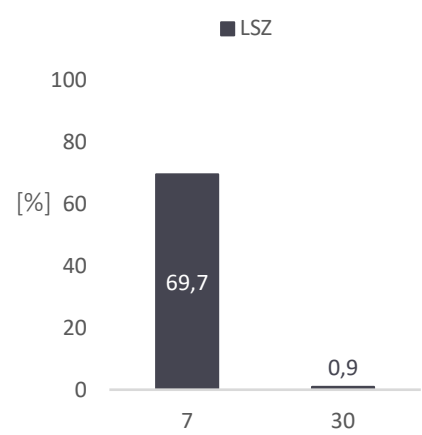
Whole blood / NaF	
	LSZ [%]
Day 0	100.0
Day 7	79.0
Day 30	68.9



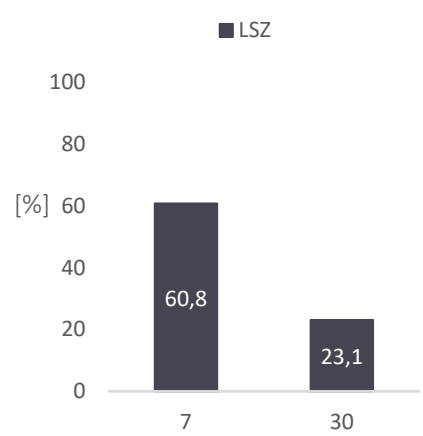
Whole blood / Citrate	
	LSZ [%]
Day 0	100.0
Day 7	71.9
Day 30	42.8



Urine / NaF	
	LSZ [%]
Day 0	100.0
Day 7	32.0
Day 30	0.0

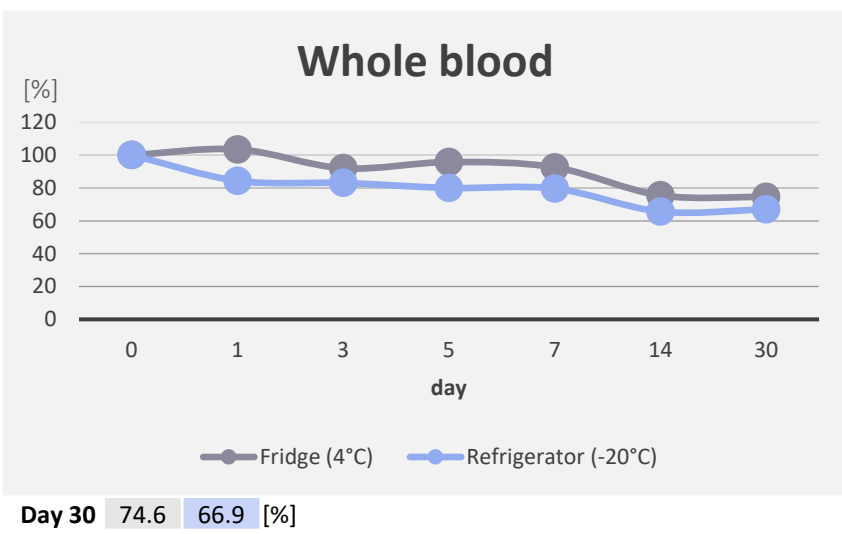


Urine / borax	
	LSZ [%]
Day 0	100.0
Day 7	69.7
Day 30	0.9

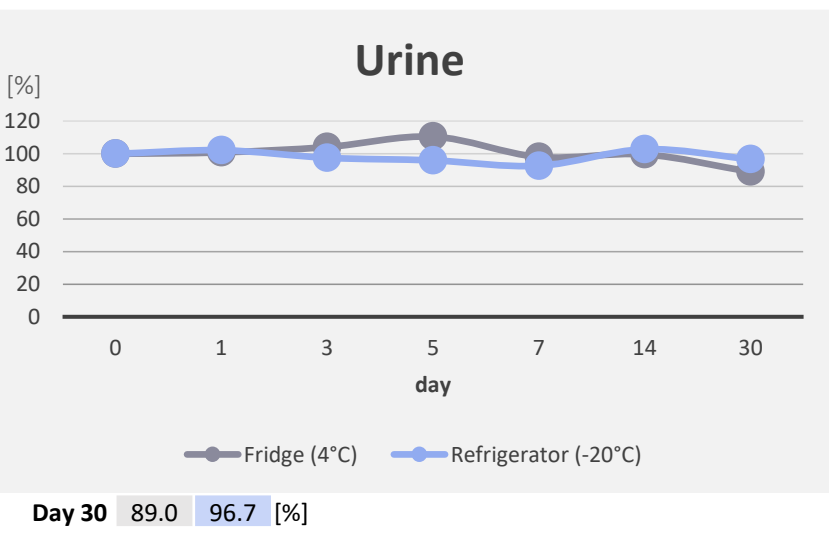


Serum	
	LSZ [%]
Day 0	100.0
Day 7	60.8
Day 30	23.1

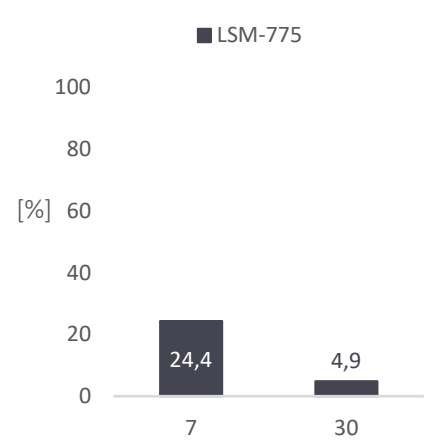
Figure S6.12. Results of stability experiments (a) and (b) for **LSM-775**



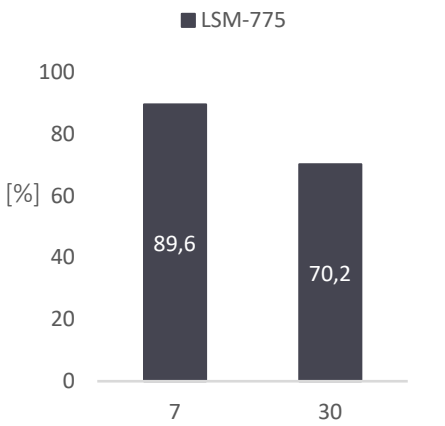
Day 30 74.6 66.9 [%]



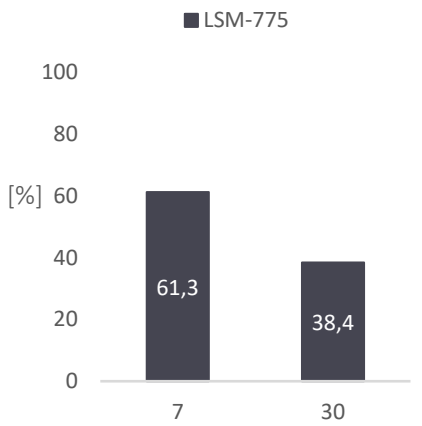
Day 30 89.0 96.7 [%]



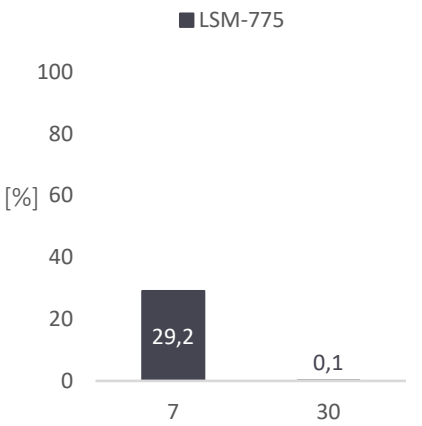
Plasma	
	LSM-775 [%]
Day 0	100.0
Day 7	24.4
Day 30	4.9



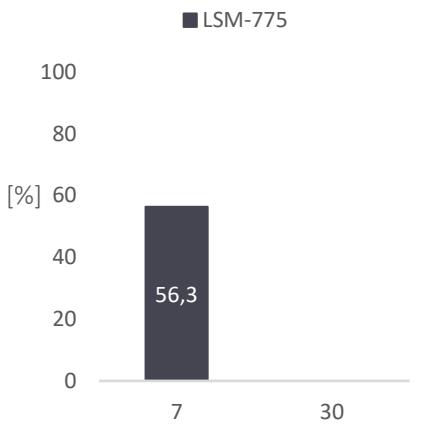
Whole blood / NaF	
	LSM-775 [%]
Day 0	100.0
Day 7	89.6
Day 30	70.2



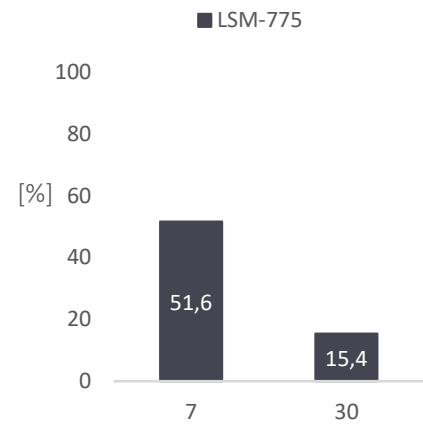
Whole blood / Citrate	
	LSM-775 [%]
Day 0	100.0
Day 7	61.3
Day 30	38.4



Urine / NaF	
	LSM-775 [%]
Day 0	100.0
Day 7	29.2
Day 30	0.1

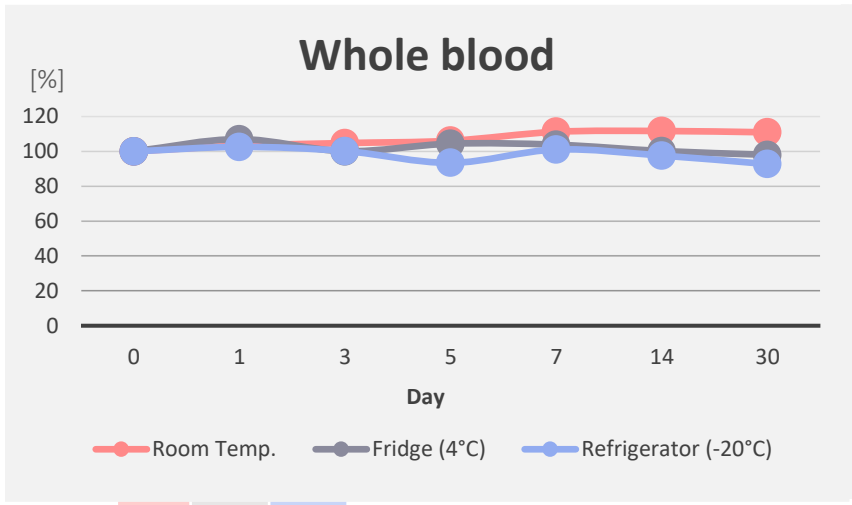


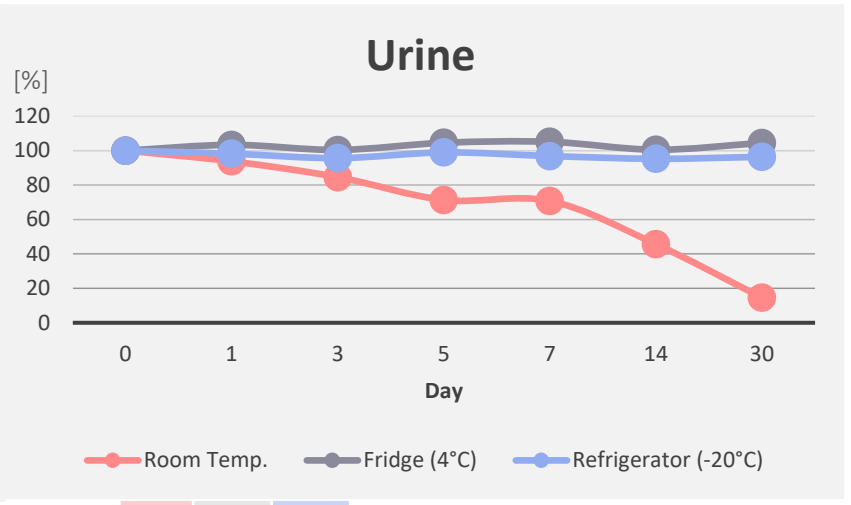
Urine / borax	
	LSM-775 [%]
Day 0	100.0
Day 7	56.3
Day 30	0.0



Serum	
	LSM-775 [%]
Day 0	100.0
Day 7	51.6
Day 30	15.4

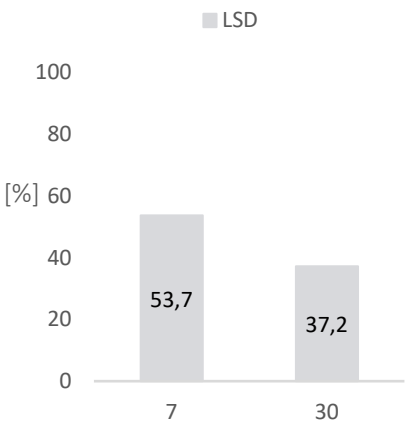
Figure S6.13. Results of stability experiment (a) for **LSD**

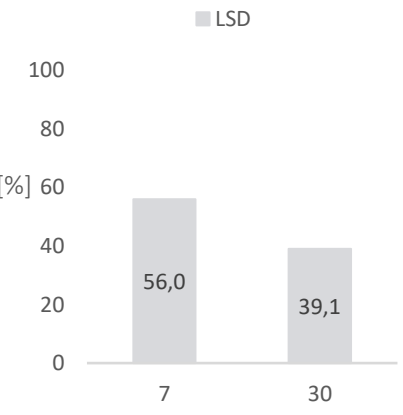


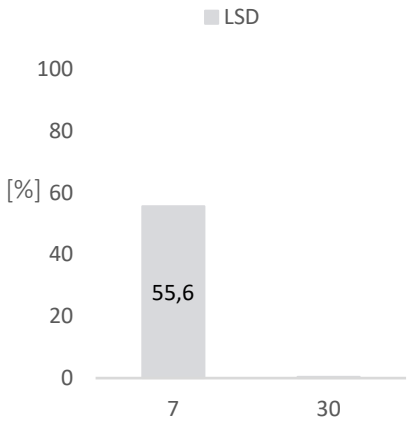


Day 30 111.0 98.0 92.8 [%]

Day 30 14.5 104.4 96.4 [%]





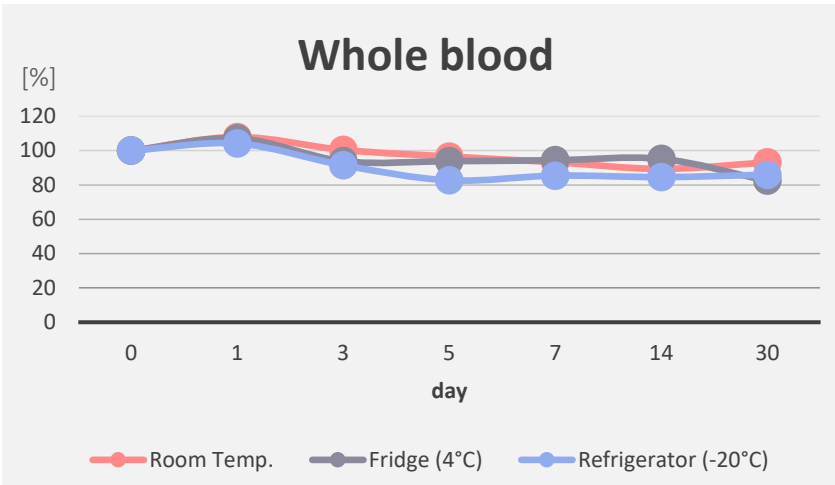


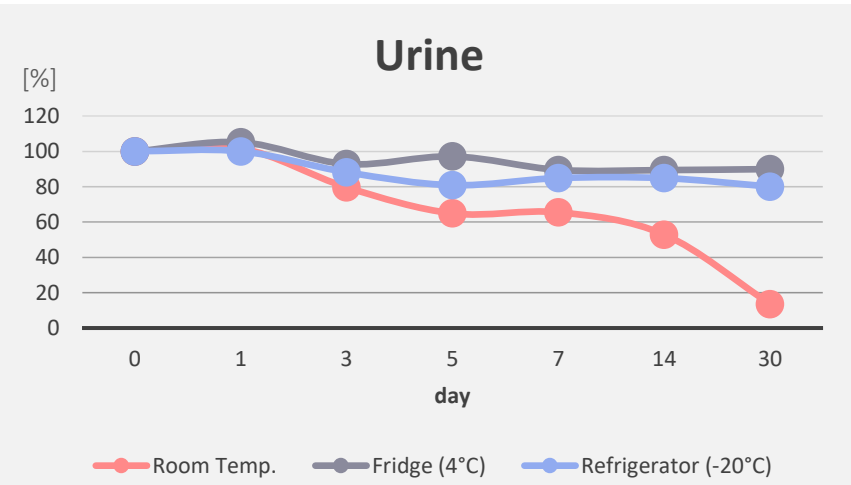
Serum	
	LSD [%]
Day 0	100.0
Day 7	53.7
Day 30	37.2

Plasma	
	LSD [%]
Day 0	100.0
Day 7	56.0
Day 30	39.1

Urine / borax	
	LSD [%]
Day 0	100.0
Day 7	55.6
Day 30	0.4

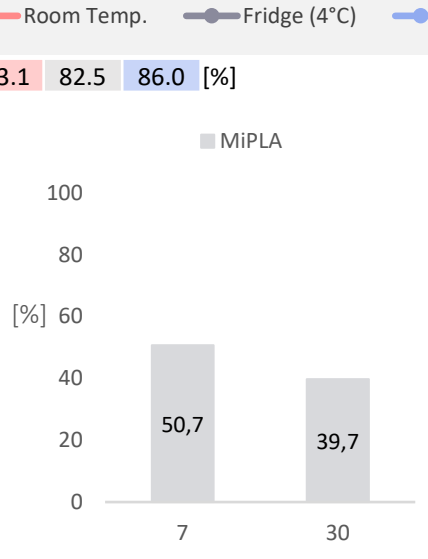
Figure S6.14. Results of stability experiment (a) for **MiPLA**

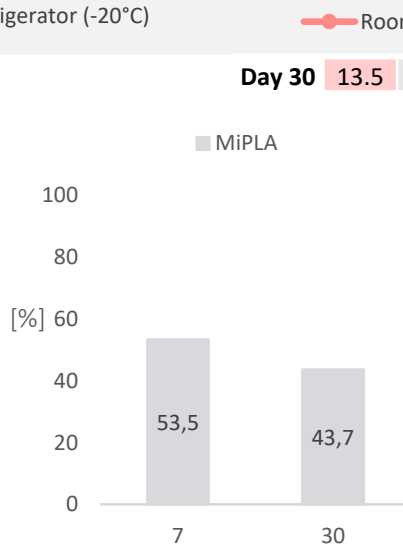


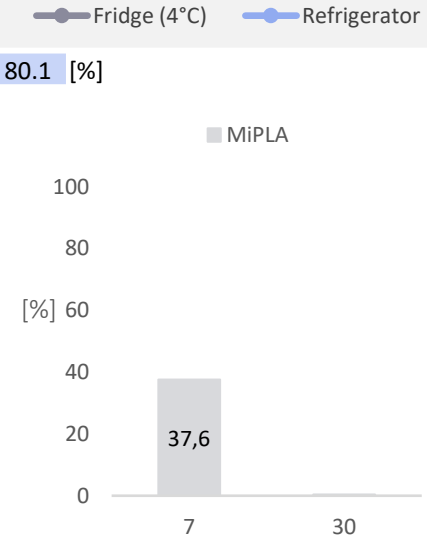


Day 30 93.1 82.5 86.0 [%]

Day 30 13.5 90.0 80.1 [%]





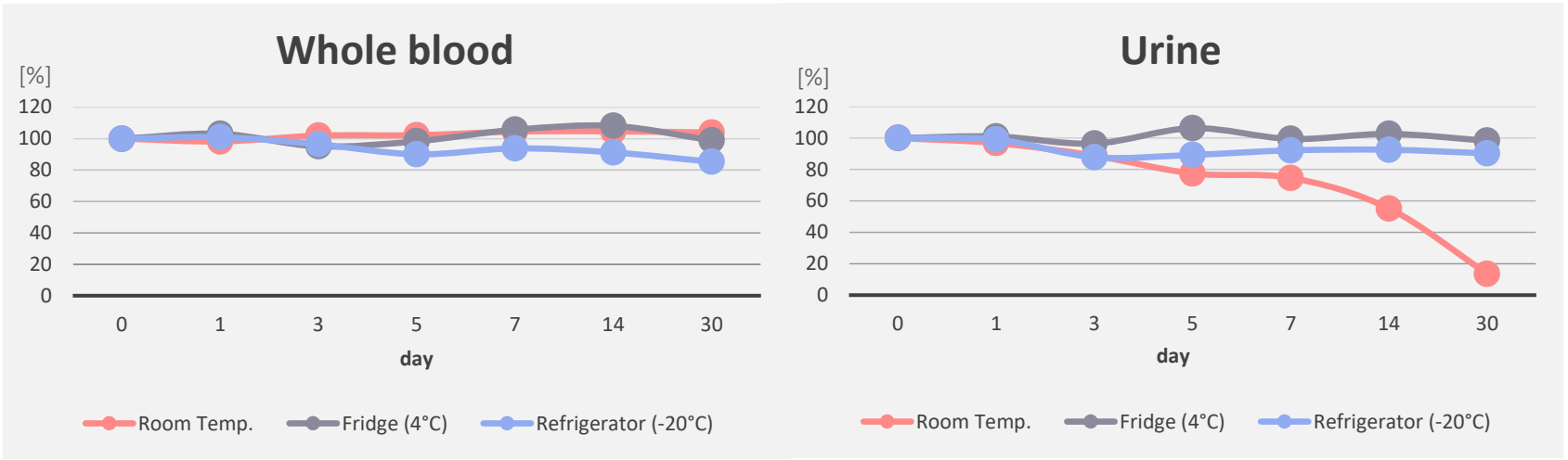


Serum	
	MiPLA [%]
Day 0	100.0
Day 7	50.7
Day 30	39.7

Plasma	
	MiPLA [%]
Day 0	100.0
Day 7	53.5
Day 30	43.7

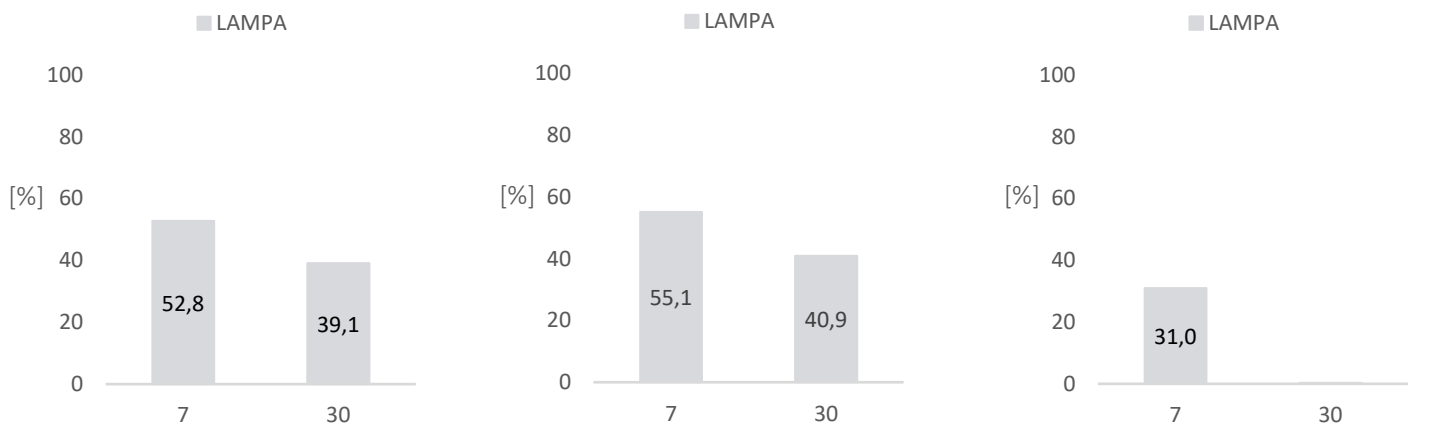
Urine / borax	
	MiPLA [%]
Day 0	100.0
Day 7	37.6
Day 30	0.4

Figure S6.15. Results of stability experiment (a) for **LAMPA**



Day 30 103.9 99.0 85.3 [%]

Day 30 13.6 98.3 90.3 [%]



Serum	
	LAMPA [%]
Day 0	100.0
Day 7	52.8
Day 30	39.1

Plasma	
	LAMPA [%]
Day 0	100.0
Day 7	55.1
Day 30	40.9

Urine / borax	
	LAMPA [%]
Day 0	100.0
Day 7	31.0
Day 30	0.3

Figure S6.16. Stability of LSD formed from other analogs in various biological matrices

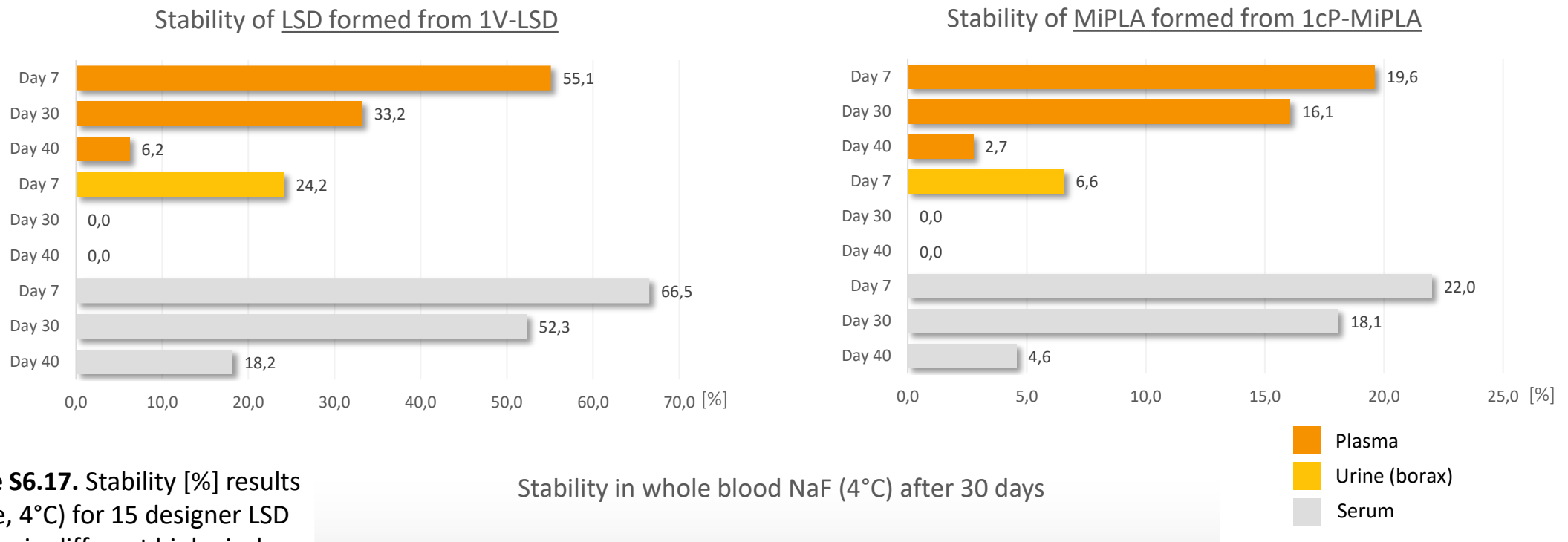
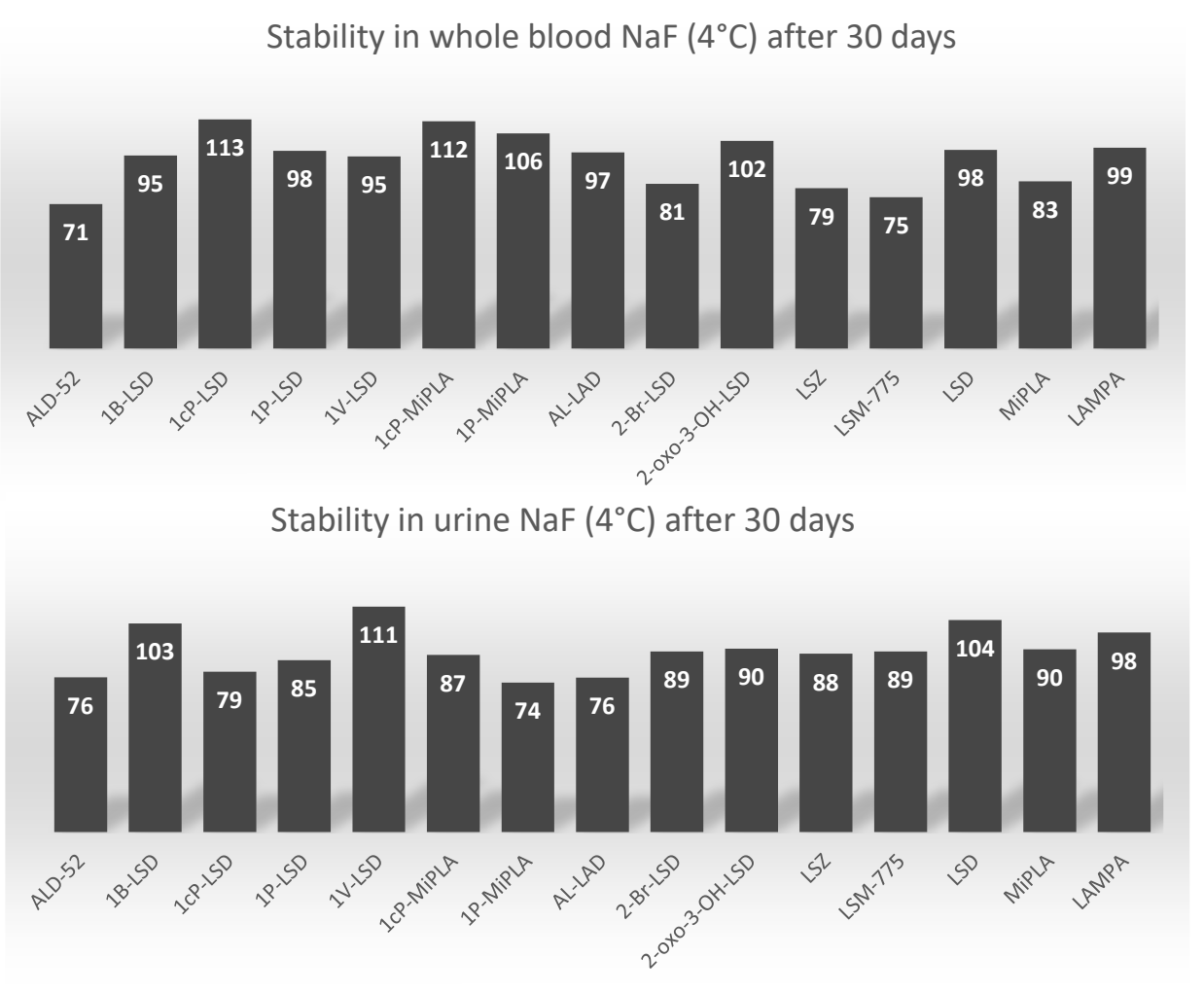


Figure S6.17. Stability [%] results (fridge, 4°C) for 15 designer LSD analogs in different biological matrices after 30 days



S7: Summarization of modern analytical methods for determination of LSD in biological samples

Table S7.1. Summarization of modern liquid chromatographic methods coupled with mass spectrometry for determination of LSD in biological samples.

No	Biological sample	Determined substances [a]	Internal standard	Sample preparation	Method	Mode	LOQ [pg/mL] [b]	Year	Reference
L1	Urine (5 mL) Blood (1 mL)	LSD 2-oxo-3-OH-LSD	OH-LAMPA	LLE combined with SPE (in case of blood)	LC-MS (SIM)	ESI	100	2000	Sklerov et al.
L2	Urine Plasma Blood (1 mL)	LSD Iso-LSD Nor-LSD 2-oxo-3-OH-LSD	LSD-d_3	LLE	HPLC-MS/MS (MRM)	ESI	20	2001	Canezin et al.
L3	Urine (2 mL)	LSD Nor-LSD	LSD-d_3	LLE	HPLC-MS (SIM)	ESI	50	1997	Hoja et al.
L4	Oral fluid (900 µL)	LSD	LSD-d_3	Microextraction by packed sorbent C18 (MEPS)	HPLC-MS/MS (MRM)	ESI	2470	2023	Lesne et al.
L5	Urine (100 µL)	LSD 2-oxo-3-OH-LSD	LSD-d_3	LLE	UPLC-QTRAP -MS/MS (MRM)	ESI	25	2015	Jang et al.
L6	Blood Urine (1 mL)	LSD *iso*-LSD 2-oxo-3-OH-LSD	LSD-d_3	LLE	HPLC-MS/MS (MRM)	ESI	10	2005	Johansen et al.
L7	Blood Urine (1 mL)	LSD Iso-LSD Nor-LSD O-H-LSD	LSD-d_3	LLE	UPLC-MS/MS (MRM)	ESI	20	2009	Chung et al.
L8	Blood (200 µL)	LSD 2-oxo-3-OH-LSD	LSD-d_3	Precipitation with ACN / LLE	HPLC-MS/MS (MRM)	ESI	12.5	2023	Dimitrova et al.
L9	Serum Plasma (1 mL) Urine (0.5 mL)	LSD Iso-LSD Nor-LSD OH-LSD	LSD-d_3	Hydrolysis with β-glucuronidase (in case of urine samples); SPE	LC-MS/MS (MRM)	ESI	12	2013	Martin et al.

[a] LSD analogs, [b] the lowest limit of quantification in the group of determined LSD analogs; LOQ – limit of quantification, LLE – liquid liquid extraction, LC – liquid chromatography, HPLC – high-performance liquid chromatography, UPLC – ultra-performance liquid chromatography, MS/MS – tandem mass spectrometry, ACN – acetonitrile, MRM – multiple reaction monitoring, ESI – electrospray ionsource, APCI – atmospheric pressure ionization, QTRAP – quadrupole-ion-trap mass spectrometer, SIM – single ion monitoring, SPE – solid-phase

Sklerov, J.H., Magluilo, J. Jr, Shannon, K.K., Smith, M.L. Liquid chromatography-electrospray ionization mass spectrometry for the detection of lysergide and a major metabolite, 2-oxo-3-hydroxy-LSD, in urine and blood. *J Anal Toxicol.* **2000,** 24(7) 543-9. doi: 10.1093/jat/24.7.543.

Canezin, J., Cailleux, A., Turcant, A., Le Bouil, A., Harry, P., Allain, P. Determination of LSD and its metabolites in human biological fluids by high-performance liquid chromatography with electrospray tandem mass spectrometry. *J Chromatogr B Biomed Sci Appl*. **2001** 765(1), 15-27. doi: 10.1016/s0378-4347(01)00386-3.

Hoja, H., Marquet, P., Verneuil, B., Lotfi, H., Dupuy, J.L., Lachâtre, G. Determination of LSD and N-demethyl-LSD in urine by liquid chromatography coupled to electrospray ionization mass spectrometry. *J Chromatogr B Biomed Sci Appl*. **1997,** 692(2), 329-35. doi: 10.1016/s0378-4347(97)00008-x.

Lesne, E., Muñoz-Bartual, M., Esteve-Turrillas, F.A. Determination of synthetic hallucinogens in oral fluids by microextraction by packed sorbent and liquid chromatography–tandem mass spectrometry. *Anal Bioanal Chem.* **2023**, 415, 3607–3617. https://doi.org/10.1007/s00216-023-04751-2.

Jang, M., Kim, J., Han, I., Yang, W. Simultaneous determination of LSD and 2-oxo-3-hydroxy LSD in hair and urine by LC-MS/MS and its application to forensic cases. *J Pharm Biomed Anal.* **2015**, 115, 138-43. doi: 10.1016/j.jpba.2015.07.001.

Johansen, S.S., Jensen, J.L. Liquid chromatography-tandem mass spectrometry determination of LSD, ISO-LSD, and the main metabolite 2-oxo-3-hydroxy-LSD in forensic samples and application in a forensic case. *J Chromatogr B Analyt Technol Biomed Life Sci.* **2005**, 825(1), 21-8. doi: 10.1016/j.jchromb.2004.12.040.

Chung, A., Hudson, J., McKay, G. Validated ultra-performance liquid chromatography-tandem mass spectrometry method for analyzing LSD, iso-LSD, nor-LSD, and O-H-LSD in blood and urine. *J Anal Toxicol*. **2009**, 33(5), 253-9. doi: 10.1093/jat/33.5.253.

Dimitrova, A., Di Milia, M.G., Rensi, R., Grassi, S., Gualco, B., Vaiano, F. Determination of Lysergic Acid Diethylamide and 2-Oxo-3-Hydroxy-LSD in Blood: Validation and Comparison of Two Liquid Chromatography–Tandem Mass Spectrometry Methods. *Separations* **2023**, 10, 502. https://doi.org/10.3390/separations10090502.

Martin, R., Schürenkamp, J., Gasse, A., Pfeiffer, H., Köhler, H. Determination of psilocin, bufotenine, LSD and its metabolites in serum, plasma and urine by SPE-LC-MS/MS. *Int J Legal Med*. **2013**, 127(3), 593-601. doi: 10.1007/s00414-012-0796-1.

L10	Urine Blood Vitreous humor (2 mL)	LSD Iso-LSD Nor-LSD 2-oxo-3-OH-LSD	LSD-d_3	LLE	HPLC-QTRAP-MS/MS	ESI	10	2007	Favretto et al.
L11	Plasma (100 µL)	LSD Iso-LSD Nor-LSD 2-oxo-3-OH-LSD	LSD-d_3	Precipitation with ACN	HPLC-MS/MS (SRM)	APCI	50	2017	Dolder et al.
L12	Serum (100 µL)	LSD 2-oxo-3-OH-LSD	LSD-d_3	Precipitation with ACN	HPLC-MS/MS (SRM)	APCI	100	2014	Dolder et al.
L13	Plasma (0.5 mL)	LSD Iso-LSD Nor-LSD 2-oxo-3-OH-LSD	LSD-d_3	SPE	HPLC-QTRAP-MS/MS (MRM)	ESI	10	2017	Steuer et al.
L14	Blood (0.5 mL)	LSD	LSD-d_3	LLE	UPLC-MS/MS (MRM)	ESI	94	2013	Berg et al.

Table S7.2. Summarization of modern gas chromatographic methods coupled with mass spectrometry for determination of LSD in biological samples

No	Biological sample	Determined substances [a]	Internal standard	Sample preparation	Method	Mode	LOQ [pg/mL] [b]	Year	Reference
G1	Serum (1 mL)	LSD	LSD-d_3	Derivatization with MSTFA	GC-MS (SIM)	EI	100	1997	Musshoff et al.
G2	Urine (4 mL)	LSD 2-oxo-3-OH-LSD	LAMPA OH-LAMPA	SPE and derivatization with BSTFA	GC-MS/MS (SRM)	CI	10	1999	Reuschel et al.
G3	Urine (4 mL) Blood Plasma (5 mL)	LSD Iso-LSD Nor-LSD	LAMPA	LLE and derivatization with BSTFA or TFAI	GC-MS/MS (MRM)	CI	10	1992	Nelson et al.
G4	Blood (2 mL)	LSD	LAMPA	SPE	GC-IT-MS	CI	20	2003	Libong et al.

[a] LSD analogs, [b] the lowest limit of quantification in the group of determined LSD analogs; LOQ – limit of quantification, GC – gas chromatography, MS/MS – tandem mass spectrometry, IT – ion trap, SIM – single ion monitoring, SRM – selected reaction monitoring, MRM – multiple reaction monitoring, SPE – solid-phase extraction, LLE – liquid liquid extraction, MSTFA – N-Methyl-N-(trimethylsilyl)-trifluoroacetamide, TFAI – trifluoroacetylimidazole; BSTFA – *N*,*O*-bis(trimethylsilyl)trifluoroacetamide

Favretto, D., Frison, G., Maietti, S., Ferrara, S.D. LC-ESI-MS/MS on an ion trap for the determination of LSD, iso-LSD, nor-LSD and 2-oxo-3-hydroxy-LSD in blood, urine and vitreous humor. *Int J Legal Med.* **2007**, 121(4):259-65. doi: 10.1007/s00414-006-0078-x.

Dolder, P.C., Liechti, M.E., Rentsch, K.M. Development and validation of an LC-MS/MS method to quantify lysergic acid diethylamide (LSD), iso-LSD, 2-oxo-3-hydroxy-LSD, and nor-LSD and identify novel metabolites in plasma samples in a controlled clinical trial. *J Clin Lab Anal.* **2018**, 32(2):e22265. doi: 10.1002/jcla.22265.

Dolder, P.C., Liechti, M.E., Rentsch, K.M. Development and validation of a rapid turboflow LC-MS/MS method for the quantification of LSD and 2-oxo-3-hydroxy LSD in serum and urine samples of emergency toxicological cases. *Anal Bioanal Chem.* **2015** 407(6), 1577-84. doi: 10.1007/s00216-014-8388-1.

Steuer, A.E., Poetzsch, M., Stock, L., Eisenbeiss, L., Schmid, Y., Liechti, M.E., Kraemer, T. Development and validation of an ultra-fast and sensitive microflow liquid chromatography-tandem mass spectrometry (MFLC-MS/MS) method for quantification of LSD and its metabolites in plasma and application to a controlled LSD administration study in humans. *Drug Test Anal*. **2017**, 9(5), 788-797. doi: 10.1002/dta.2042.

Berg, T., Jørgenrud, B., Strand, D.H. Determination of buprenorphine, fentanyl and LSD in whole blood by UPLC-MS-MS. *J Anal Toxicol.* **2013**, 37(3), 159-65. doi: 10.1093/jat/bkt005.

Musshoff, F., Daldrup, T. Gas chromatographic/mass spectrometric determination of lysergic acid diethylamide (LSD) in serum samples. *Forensic Sci Int.* **1997**, 88(2), 133-40. doi: 10.1016/s0379-0738(97)00063-7.

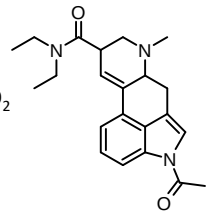
Reuschel, S.A., Percey, S.E., Liu, S., Eades, D.M., Foltz, R.L. Quantitative determination of LSD and a major metabolite, 2-oxo-3-hydroxy-LSD, in human urine by solid-phase extraction and gas chromatography-tandem mass spectrometry. *J Anal Toxicol.* **1999**, 23(5), 306-12. doi: 10.1093/jat/23.5.306.

Nelson, C.C., Foltz, R.L. Determination of lysergic acid diethylamide (LSD), iso-LSD, and N-demethyl-LSD in body fluids by gas chromatography/tandem mass spectrometry. *Anal Chem*. **1992**, 64(14), 1578-85. doi: 10.1021/ac00038a014.

Libong, D., Bouchonnet, S., Ricordel, I. A selective and sensitive method for quantitation of lysergic acid diethylamide (LSD) in whole blood by gas chromatography-ion trap tandem mass spectrometry. *J Anal Toxicol.* **2003**, 27(1), 24-9. doi: 10.1093/jat/27.1.24.

S8: Mass spectra of determined substances

ALD-52

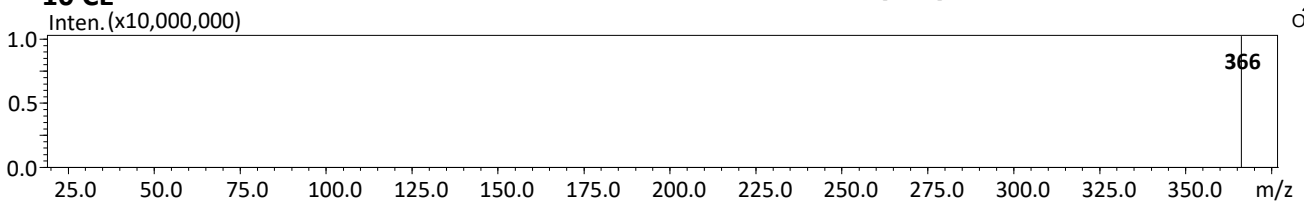


Molecular Formula: $C_{22}H_{27}N_3O_2$

Formula Weight: 365.5

[M+H]$^+$: 366.217604 Da

10 CE



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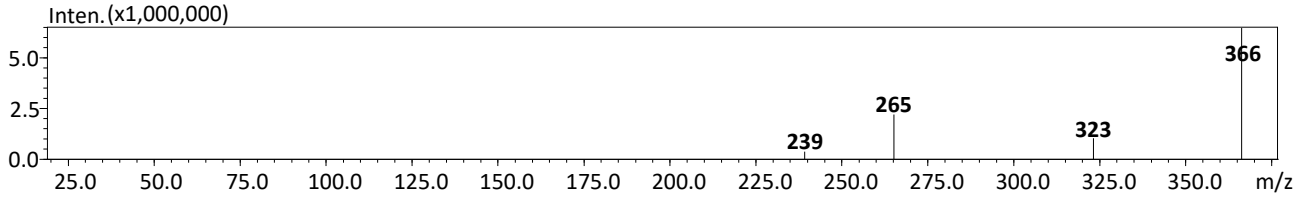

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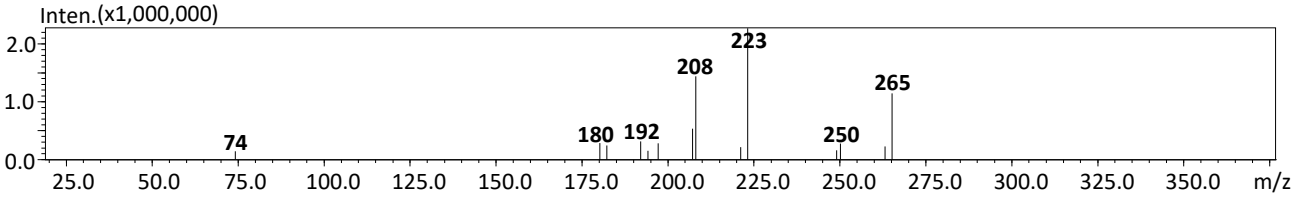

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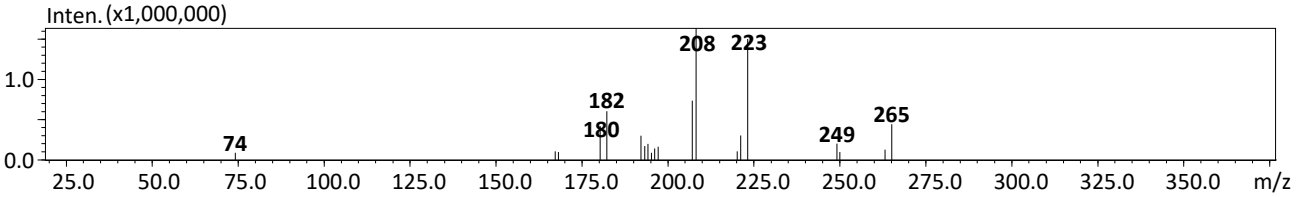

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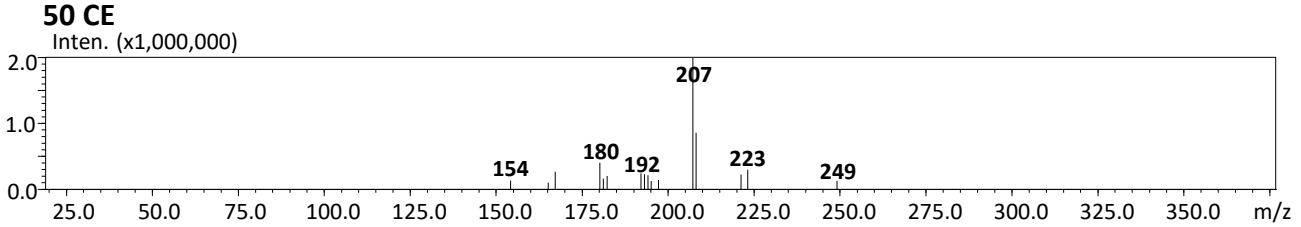
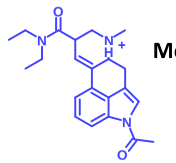


QqQ-MS/MS: Detection of the investigated compounds was achieved with the use of a triple quadrupole mass spectrometer (QqQ, Shimadzu 8060, Kyoto, Japan) in positive mode. The spectrometer was equipped with an electrospray ionization (ESI) sourceThe following MS parameters were fixed: nebulizing gas flow, 3 L/min; heating gas flow, 10 L/min; interface temperature, 250 °C; desolvation line temperature, 200 °C; heat block temperature, 350 °C; and drying gas flow, 10 L/min. Fragmentation MS/MS spectra were acquired by conducting a product ion scan experiment at five collision energies (CE: –10, –20, –35,–40 and –50 V).

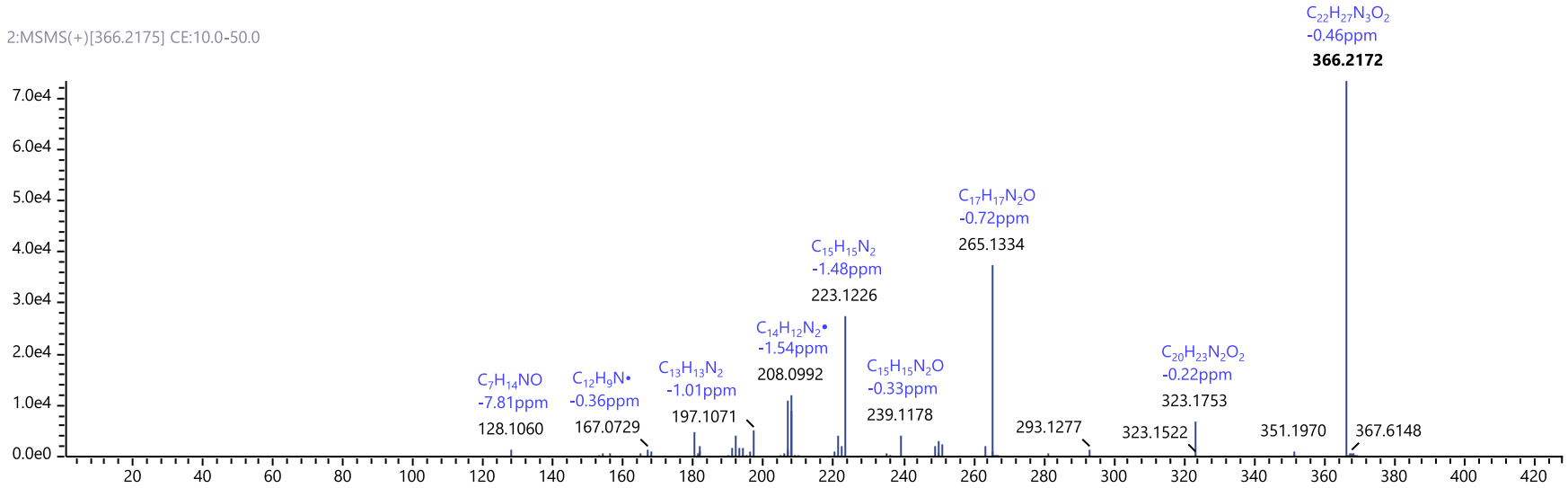
ALD-52



Molecular Formula: $C_{22}H_{27}N_3O_2$

Formula Weight: 365.5

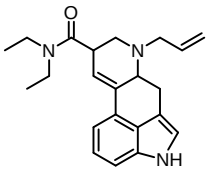
$[M+H]^+$: 366.217604 Da



Experimental m/z	Intensity	Molecular Formula	Charge	Predicted m/z	Δ ppm	Experimental m/z	Intensity	Molecular Formula	Charge	Predicted m/z	Δ ppm
366.2174	–	$C_{22}H_{27}N_3O_2$	$[M+H]^+$	366.2176	-0.46	**208.0992**	12074	$C_{14}H_{12}N_2^•$	$[+H]^+$	208.0995	-1.54
351.1970	1149	–	–	–	–	**208.0755**	8781	$C_{14}H_{10}NO$	+	208.0757	-1.11
323.1753	6990	$C_{20}H_{23}N_2O_2$	+	323.1754	-0.22	**207.0917**	10815	$C_{14}H_{11}N_2$	$[+H]^+$	207.0917	-0.05
293.1278	1299	$C_{18}H_{17}N_2O_2$	+	293.1285	-2.39	**197.1071**	5245	$C_{13}H_{13}N_2$	$[+H]^+$	197.1073	-1.02
281.1665	676	–	–	–	–	**194.0960**	1741	$C_{14}H_{12}N$	+	194.0964	-1.44
265.1334	37176	$C_{17}H_{17}N_2O$	$[+H]^+$	265.1335	-0.72	**192.0810**	4121	$C_{14}H_{10}N$	+	192.0808	1.35
251.1173	2252	$C_{16}H_{15}N_2O$	+	251.1179	-2.47	**182.0969**	1885	$C_{13}H_{12}N$	$[+H]^+$	182.0964	2.42
249.1006	2168	–	–	–	–	**180.0810**	4706	$C_{13}H_{10}N$	$[+H]^+$	180.0808	1.06
239.1178	4176	$C_{15}H_{15}N_2O$	$[+H]^+$	239.1179	-0.34	**167.0729**	1219	$C_{12}H_9N^•$	+	167.0730	-0.36
223.1226	27549	$C_{15}H_{15}N_2$	$[+H]^+$	223.1230	-1.48	**154.0648**	772	$C_{11}H_8N$	+	154.0651	-2.47
221.1071	4161	$C_{15}H_{13}N_2$	$[+H]^+$	221.1073	-1.09	**128.1060**	1385	$C_7H_{14}NO$	$[+H]^+$	128.1070	-7.81

QTOF-MS/MS: The QTOF Shimadzu 9050 (Kyoto, Japan) spectrometer was equipped with an electrospray ionization (ESI) source. The following QTOF parameters were fixed: nebulizing gas flow, 3 L/min; heating gas flow, 10 L/min; interface temperature, 250 ◦C; desolvation line temperature, 200 ◦C; interface voltage (+), 4.50 kV; heat block temperature, 350 ◦C; and drying gas flow, 10 L/min. MS/MS spectra for all substances were acquired by conducting datadependent acquisition (DDA) function. DDA data were acquired in the range 40–500 m/z and collision energies from − 10 V to − 50 V.

AL-LAD

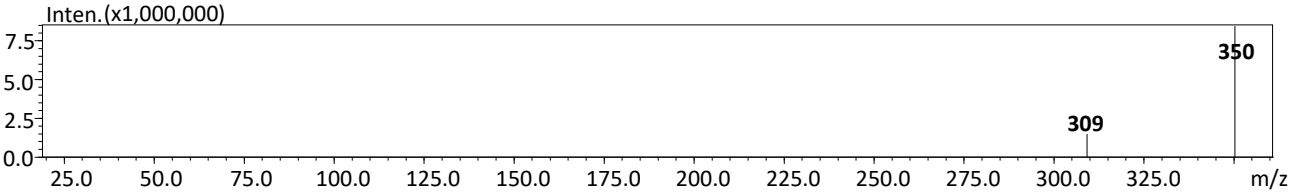


Molecular Formula: $C_{22}H_{27}N_3O$

Formula Weight: 349.5

$[M+H]^+$: 350.222689 Da

10 CE



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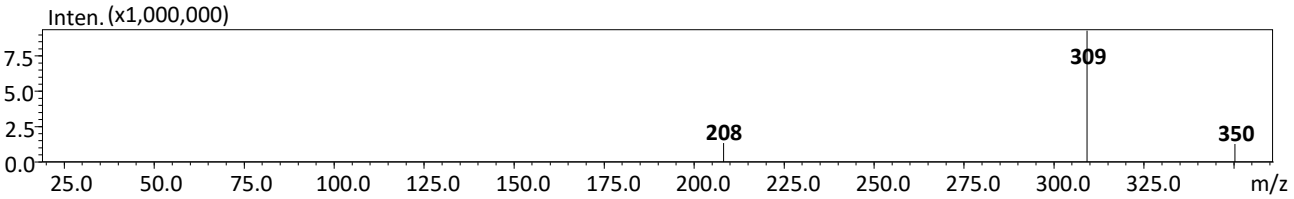

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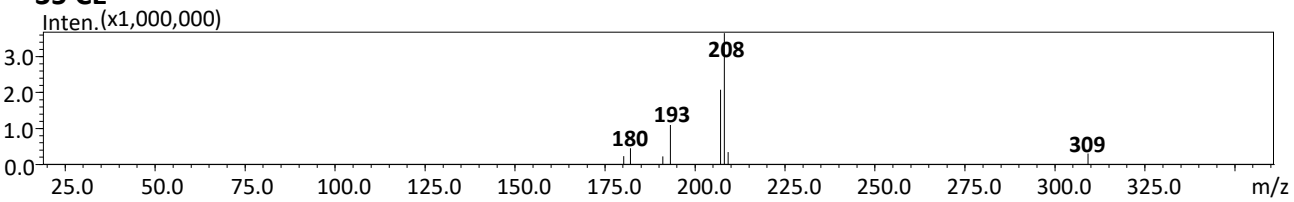

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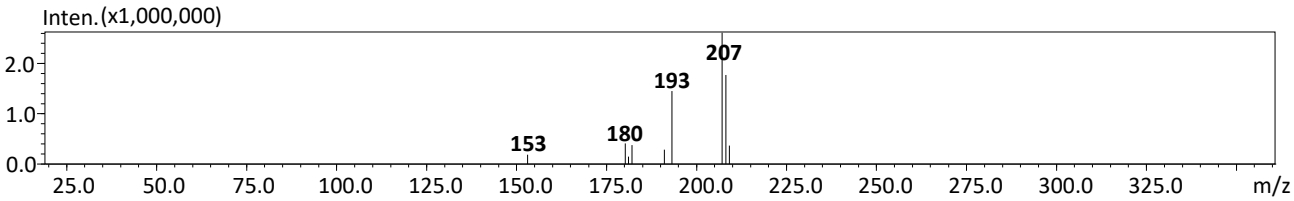

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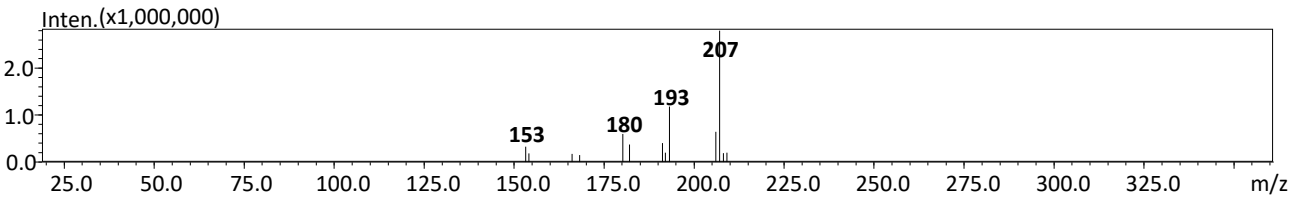

QqQ-MS/MS: Detection of the investigated compounds was achieved with the use of a triple quadrupole mass spectrometer (QqQ, Shimadzu 8060, Kyoto, Japan) in positive mode. The spectrometer was equipped with an electrospray ionization (ESI) sourceThe following MS parameters were fixed: nebulizing gas flow, 3 L/min; heating gas flow, 10 L/min; interface temperature, 250 °C; desolvation line temperature, 200 °C; heat block temperature, 350 °C; and drying gas flow, 10 L/min. Fragmentation MS/MS spectra were acquired by conducting a product ion scan experiment at five collision energies (CE: –10, –20, –35,–40 and –50 V).

AL-LAD

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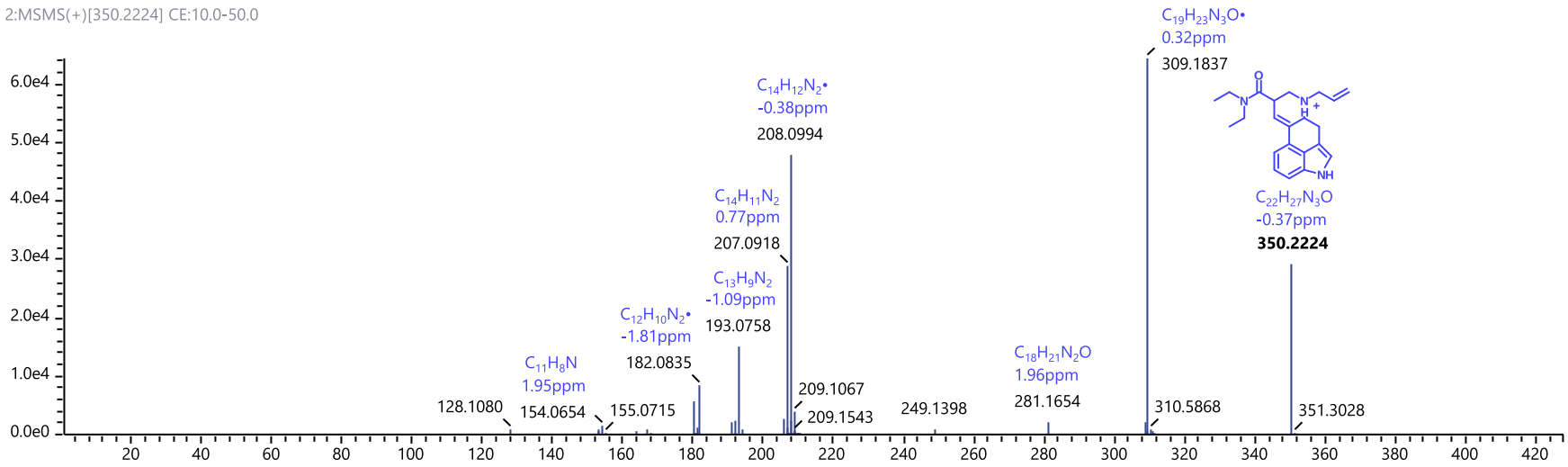
Formula Weight: 349.5

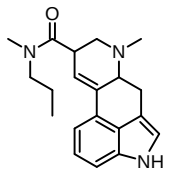
$[M+H]^+$: 350.222689 Da



Experimental m/z	Intensity	Molecular Formula	Charge	Predicted m/z	Δ ppm	Experimental m/z	Intensity	Molecular Formula	Charge	Predicted m/z	Δ ppm
350.2226	–	$C_{22}H_{27}N_3O$	$[M+H]^+$	349.2154	-0.37	**193.0758**	14964	$C_{13}H_9N_2$	$[+H]^+$	193.0760	-1.09
309.1837	64399	$C_{19}H_{23}N_3O^•$	$[+H]^+$	309.1836	0.32	**182.0835**	8278	$C_{12}H_{10}N_2^•$	$[+H]^+$	182.0839	-1.81
281.1654	2124	$C_{18}H_{21}N_2O$	+	281.1648	1.96	**180.0810**	5845	$C_{13}H_{10}N$	$[+H]^+$	180.0810	0.94
249.1398	766	–	–	–	–	**167.0727**	982	$C_{12}H_9N^•$	+	167.0730	-1.62
209.1067	3870	$C_{14}H_{13}N_2$	$[+H]^+$	209.1073	-2.77	**154.0654**	1515	$C_{11}H_8N$	+	154.0651	1.95
208.0994	47757	$C_{14}H_{12}N_2^•$	$[+H]^+$	208.0995	-0.38	**128.1080**	881	–	–	–	–
207.0918	29030	$C_{14}H_{11}N_2$	$[+H]^+$	207.0917	0.77						

QTOF-MS/MS: The QTOF Shimadzu 9050 (Kyoto, Japan) spectrometer was equipped with an electrospray ionization (ESI) source. The following QTOF parameters were fixed: nebulizing gas flow, 3 L/min; heating gas flow, 10 L/min; interface temperature, 250 ◦C; desolvation line temperature, 200 ◦C; interface voltage (+), 4.50 kV; heat block temperature, 350 ◦C; and drying gas flow, 10 L/min. MS/MS spectra for all substances were acquired by conducting datadependent acquisition (DDA) function. DDA data were acquired in the range 40–500 m/z and collision energies from − 10 V to − 50 V.

LAMPA

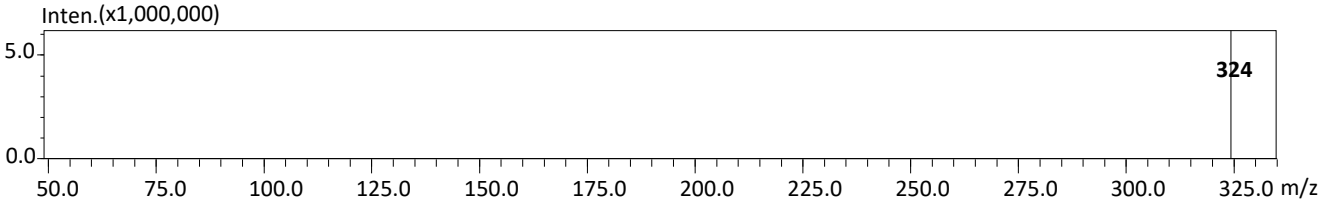


Molecular Formula: $C_{20}H_{25}N_3O$

Formula Weight: 323.4

[M+H]$^+$: 324.207039 Da

10 CE



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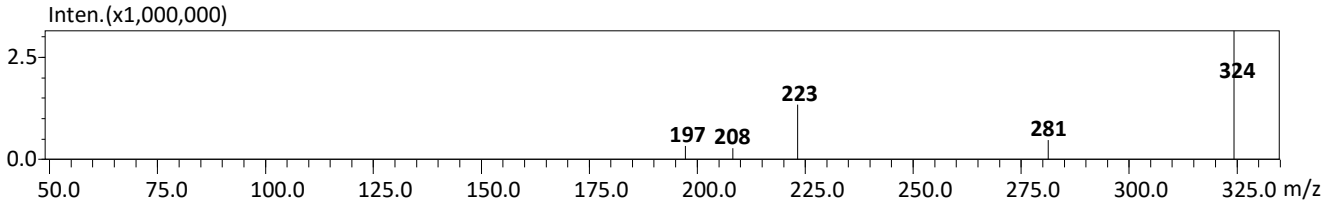

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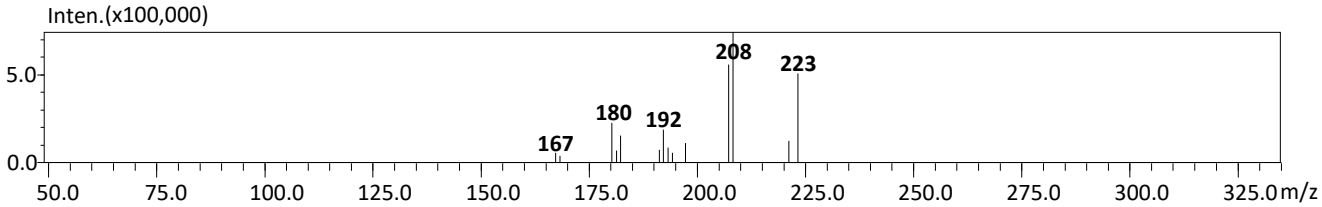

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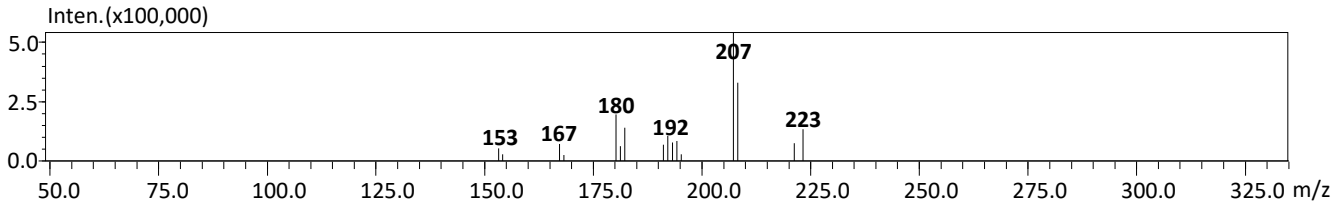

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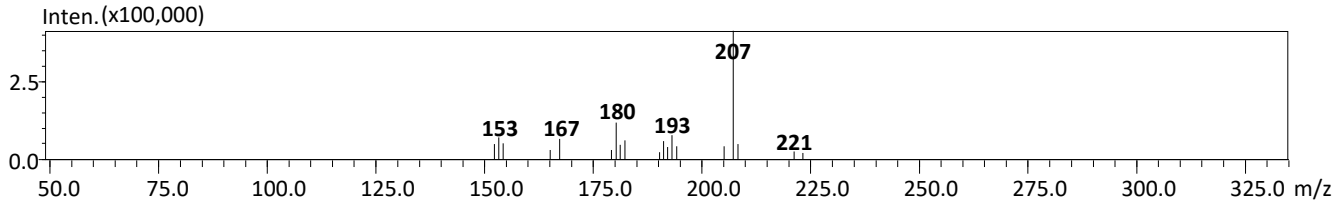

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LAMPA

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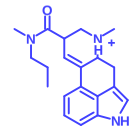
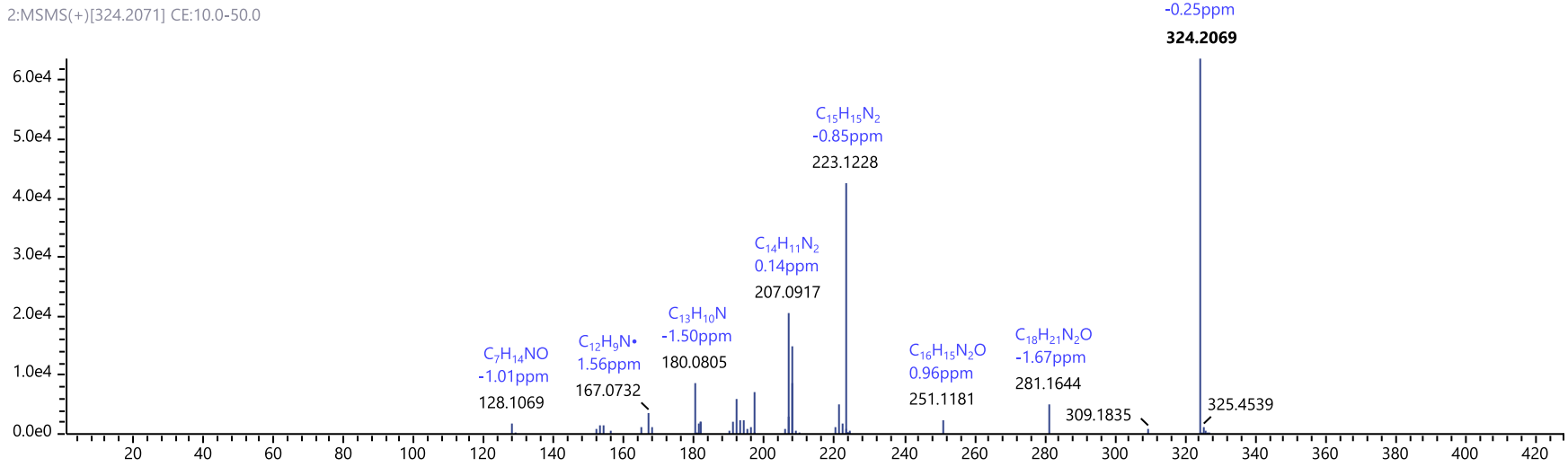
Formula Weight: 323.4

[M+H]⁺: 324.207039 Da

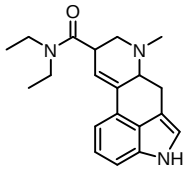




Experimental m/z	Intensity	Molecular Formula	Charge	Predicted m/z	Δ ppm	Experimental m/z	Intensity	Molecular Formula	Charge	Predicted m/z	Δ ppm
324.2070	–	$C_{20}H_{25}N_3O$	$[M+H]^+$	324.2070	-0.25	**197.1073**	7040	$C_{13}H_{13}N_2$	$[+H]^+$	197.1073	-0.05
309.1835	825	$C_{19}H_{23}N_3O^•$	$[+H]^+$	309.1836	-0.13	**194.0959**	2392	$C_{14}H_{12}N$	+	194.0964	-2.63
281.1644	5084	$C_{18}H_{21}N_2O$	+	281.1648	-1.67	**192.0810**	5844	$C_{14}H_{10}N$	+	192.0808	1.25
251.1181	2257	$C_{16}H_{15}N_2O$	+	251.1179	0.96	**182.0964**	2033	$C_{13}H_{12}N$	$[+H]^+$	182.0964	0.06
223.1228	42597	$C_{15}H_{15}N_2$	$[+H]^+$	223.1230	-0.85	**180.0805**	8748	$C_{13}H_{10}N$	$[+H]^+$	180.0808	-1.50
221.1077	4924	$C_{15}H_{13}N_2$	$[+H]^+$	221.1073	1.81	**167.0732**	3609	$C_{12}H_9N^•$	+	167.0730	1.56
208.0995	14968	$C_{14}H_{12}N_2^•$	$[+H]^+$	208.0995	-0.14	**154.0657**	1434	$C_{11}H_8N$	+	154.0651	3.57
208.0758	8647	$C_{14}H_{10}NO$	+	208.0757	0.34	**128.1069**	1731	$C_7H_{14}NO$	$[+H]^+$	128.1070	-1.02
207.0917	20585	$C_{14}H_{11}N_2$	$[+H]^+$	207.0917	0.15						

QTOF-MS/MS: The QTOF Shimadzu 9050 (Kyoto, Japan) spectrometer was equipped with an electrospray ionization (ESI) source. The following QTOF parameters were fixed: nebulizing gas flow, 3 L/min; heating gas flow, 10 L/min; interface temperature, 250 ◦C; desolvation line temperature, 200 ◦C; interface voltage (+), 4.50 kV; heat block temperature, 350 ◦C; and drying gas flow, 10 L/min. MS/MS spectra for all substances were acquired by conducting datadependent acquisition (DDA) function. DDA data were acquired in the range 40–500 m/z and collision energies from − 10 V to − 50 V.

LSD

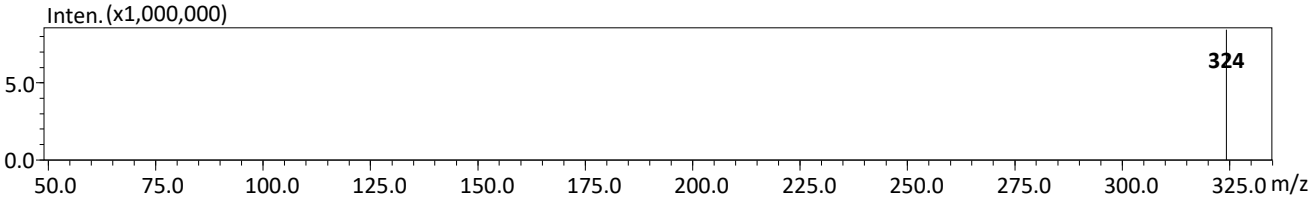


Molecular Formula: $C_{20}H_{25}N_3O$

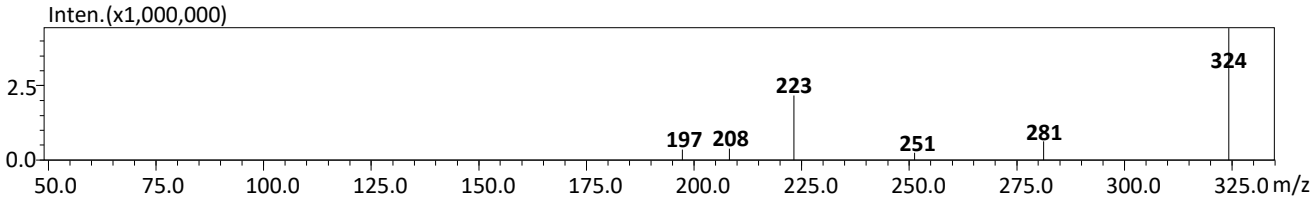
Formula Weight: 323.4

[M+H]$^+$: 324.207039 Da

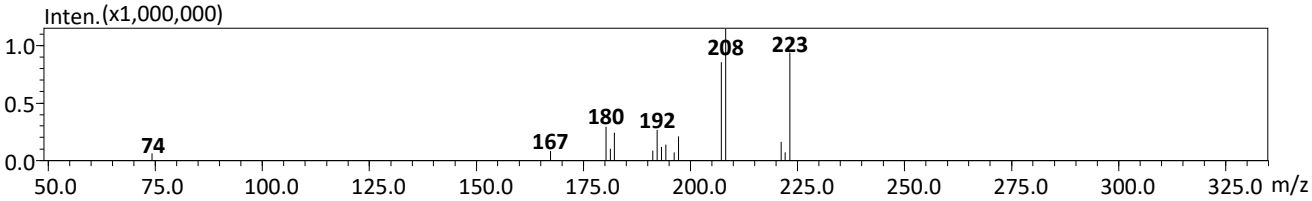
10 CE



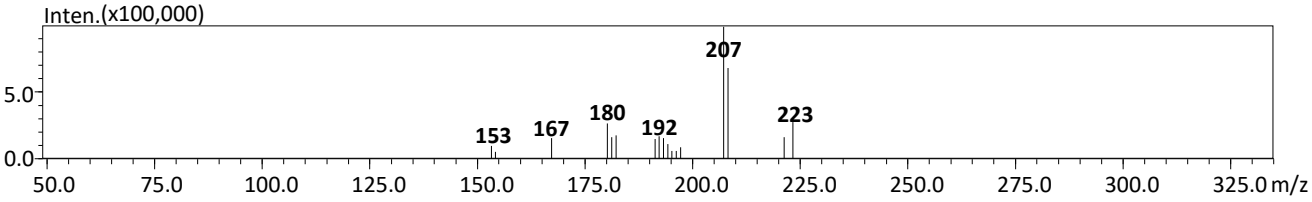
20 CE



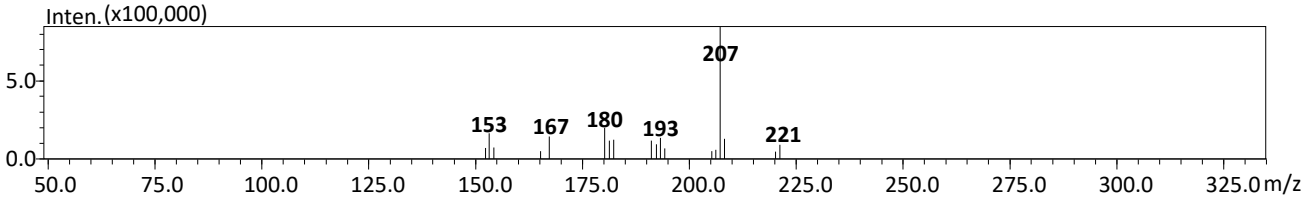
35 CE



40 CE



50 CE



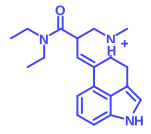
QqQ-MS/MS: Detection of the investigated compounds was achieved with the use of a triple quadrupole mass spectrometer (QqQ, Shimadzu 8060, Kyoto, Japan) in positive mode. The spectrometer was equipped with an electrospray ionization (ESI) sourceThe following MS parameters were fixed: nebulizing gas flow, 3 L/min; heating gas flow, 10 L/min; interface temperature, 250 °C; desolvation line temperature, 200 °C; heat block temperature, 350 °C; and drying gas flow, 10 L/min. Fragmentation MS/MS spectra were acquired by conducting a product ion scan experiment at five collision energies (CE: –10, –20, –35,–40 and –50 V).

LSD

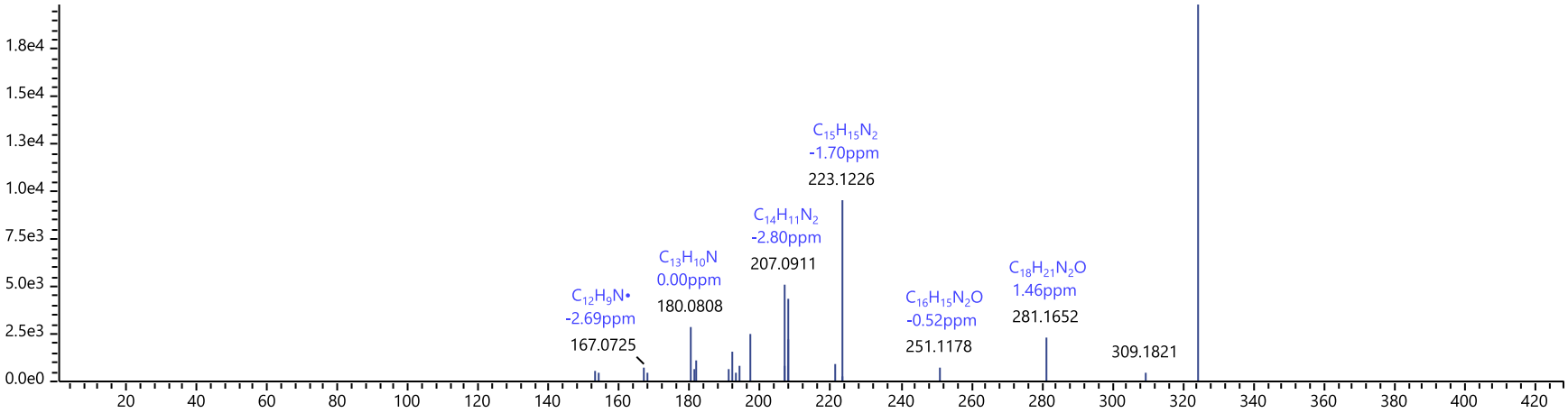
Molecular Formula: $C_{20}H_{25}N_3O$

Formula Weight: 323.4

$[M+H]^+$: 324.207039 Da



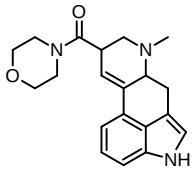
$C_{20}H_{25}N_3O$
-0.56ppm
324.2066



Experimental m/z	Intensity	Molecular Formula	Charge	Predicted m/z	Δ ppm	Experimental m/z	Intensity	Molecular Formula	Charge	Predicted m/z	Δ ppm
324.2069	–	$C_{20}H_{25}N_3O$	$[M+H]^+$	324.2070	-0.56	**207.0911**	5088	$C_{14}H_{11}N_2$	$[+H]^+$	207.0917	-2.80
309.1821	498	–	–	–	–	**197.1076**	2493	$C_{13}H_{13}N_2$	$[+H]^+$	197.1073	1.47
281.1653	2304	$C_{18}H_{21}N_2O$	+	281.1648	1.46	**194.0965**	825	$C_{14}H_{12}N$	+	194.0964	0.36
251.1178	741	$C_{16}H_{15}N_2O$	+	251.1179	-0.52	**192.0804**	1581	$C_{14}H_{10}N$	+	192.0808	-1.98
223.1226	9564	$C_{15}H_{15}N_2$	+	223.1230	-1.70	**182.0827**	1136	–	–	–	–
221.1074	912	$C_{15}H_{13}N_2$	$[+H]^+$	221.1073	0.36	**180.0808**	2884	$C_{13}H_{10}N$	$[+H]^+$	180.0808	0.0
208.0994	4316	$C_{14}H_{12}N_2•$	$[+H]^+$	208.0995	-0.38	**167.0725**	735	$C_{12}H_9N•$	+	167.0730	-2.69
208.0758	2246	$C_{14}H_{10}NO$	+	208.0757	0.48	**154.0638**	484	–	–	–	–

QTOF-MS/MS: The QTOF Shimadzu 9050 (Kyoto, Japan) spectrometer was equipped with an electrospray ionization (ESI) source. The following QTOF parameters were fixed: nebulizing gas flow, 3 L/min; heating gas flow, 10 L/min; interface temperature, 250 ◦C; desolvation line temperature, 200 ◦C; interface voltage (+), 4.50 kV; heat block temperature, 350 ◦C; and drying gas flow, 10 L/min. MS/MS spectra for all substances were acquired by conducting datadependent acquisition (DDA) function. DDA data were acquired in the range 40–500 m/z and collision energies from − 10 V to − 50 V.

LSM-775

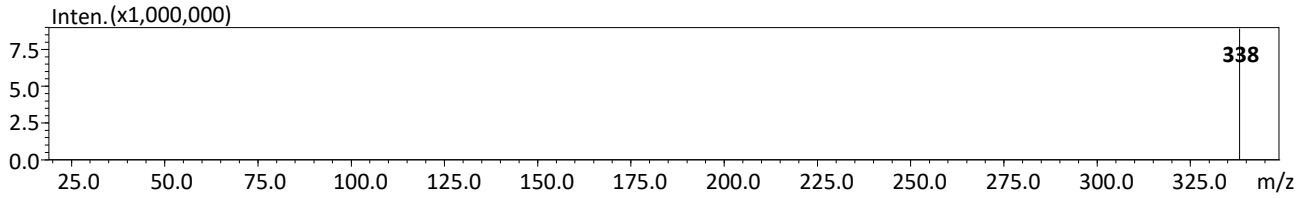


Molecular Formula: $C_{20}H_{23}N_3O_2$

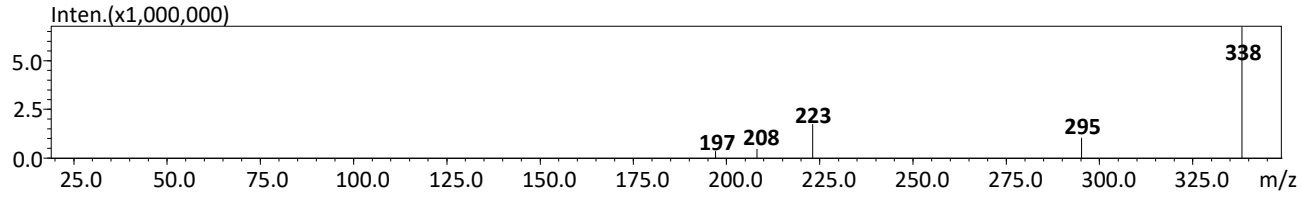
Formula Weight: 337.4

$[M+H]^+$: 338.186303 Da

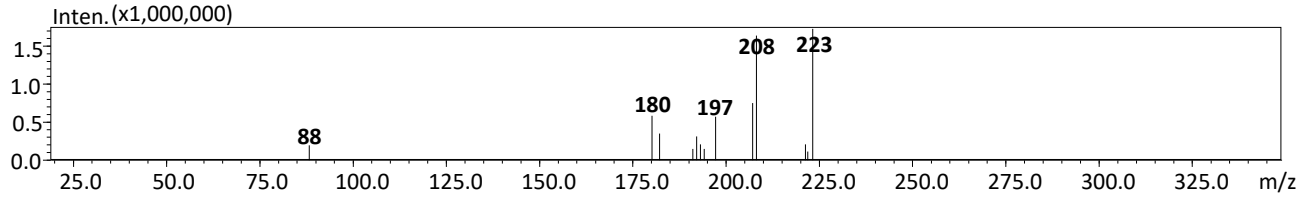
10 CE



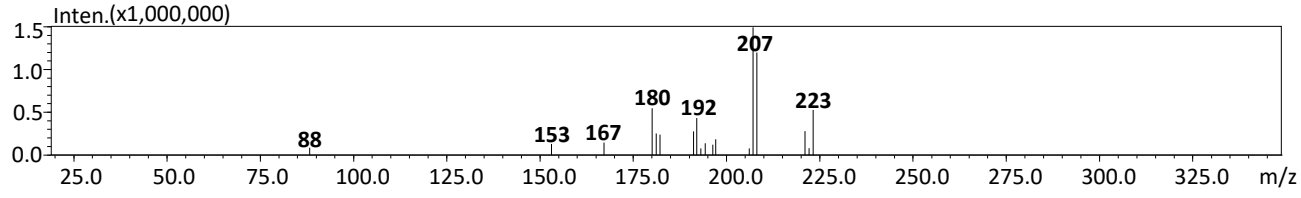
20 CE



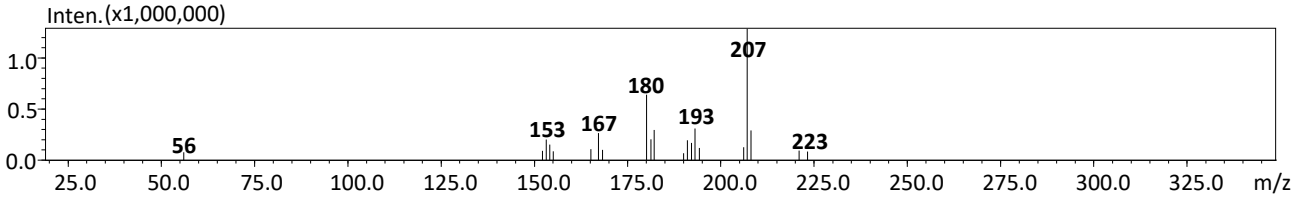
35 CE



40 CE



50 CE



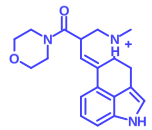
QqQ-MS/MS: Detection of the investigated compounds was achieved with the use of a triple quadrupole mass spectrometer (QqQ, Shimadzu 8060, Kyoto, Japan) in positive mode. The spectrometer was equipped with an electrospray ionization (ESI) sourceThe following MS parameters were fixed: nebulizing gas flow, 3 L/min; heating gas flow, 10 L/min; interface temperature, 250 °C; desolvation line temperature, 200 °C; heat block temperature, 350 °C; and drying gas flow, 10 L/min. Fragmentation MS/MS spectra were acquired by conducting a product ion scan experiment at five collision energies (CE: –10, –20, –35,–40 and –50 V).

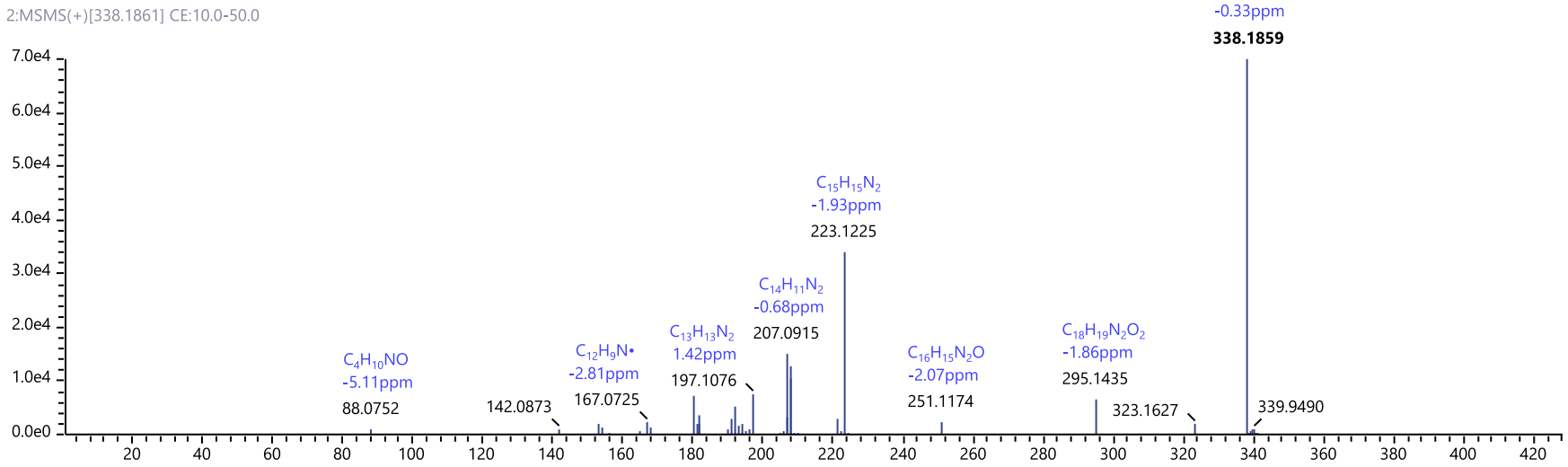
LSM-775

Molecular Formula: $C_{20}H_{23}N_3O_2$

Formula Weight: 337.4

$[M+H]^+$: 338.186303 Da

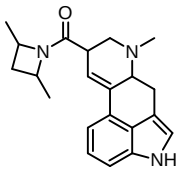




Experimental m/z	Intensity	Molecular Formula	Charge	Predicted m/z	Δ ppm	Experimental m/z	Intensity	Molecular Formula	Charge	Predicted m/z	Δ ppm
338.1862	–	$C_{20}H_{23}N_3O_2$	$[M+H]^+$	338.1863	-0.33	**194.0964**	1957	$C_{14}H_{12}N$	+	194.0964	0.0
323.1627	2011	$C_{19}H_{21}N_3O_2$•	$[+H]^+$	323.1628	-0.53	**192.0804**	5097	$C_{14}H_{10}N$	+	192.0808	-2.14
295.1436	6431	$C_{18}H_{19}N_2O_2$	+	295.1441	-1.86	**182.0962**	2034	$C_{13}H_{12}N$	$[+H]^+$	182.0964	-1.04
251.1174	2441	$C_{16}H_{15}N_2O$	+	251.1179	-2.07	**182.0833**	3442	$C_{12}H_{10}N_2$•	$[+H]^+$	182.0839	-3.13
223.1225	34108	$C_{15}H_{15}N_2$	$[+H]^+$	223.1230	-1.93	**180.0804**	7331	$C_{13}H_{10}N$	$[+H]^+$	180.0808	-2.39
221.1070	2893	$C_{15}H_{13}N_2$	$[+H]^+$	221.1073	-1.67	**167.0725**	2292	$C_{12}H_9N$•	+	167.0730	-2.81
208.0996	12610	$C_{14}H_{12}N_2$•	$[+H]^+$	208.0995	0.29	**154.0660**	1171	$C_{11}H_8N$	+	154.0651	5.52
208.0752	10511	$C_{14}H_{10}NO$	+	208.0757	-2.21	**142.0873**	904	–	–	–	–
207.0915	14996	$C_{14}H_{11}N_2$	$[+H]^+$	207.0917	-0.68	**88.0752**	832	$C_4H_{10}NO$	$[+H]^+$	88.0757	-5.11
197.1076	7508	$C_{13}H_{13}N_2$	$[+H]^+$	197.1073	1.42						

QTOF-MS/MS: The QTOF Shimadzu 9050 (Kyoto, Japan) spectrometer was equipped with an electrospray ionization (ESI) source. The following QTOF parameters were fixed: nebulizing gas flow, 3 L/min; heating gas flow, 10 L/min; interface temperature, 250 ◦C; desolvation line temperature, 200 ◦C; interface voltage (+), 4.50 kV; heat block temperature, 350 ◦C; and drying gas flow, 10 L/min. MS/MS spectra for all substances were acquired by conducting datadependent acquisition (DDA) function. DDA data were acquired in the range 40–500 m/z and collision energies from − 10 V to − 50 V.

LSZ

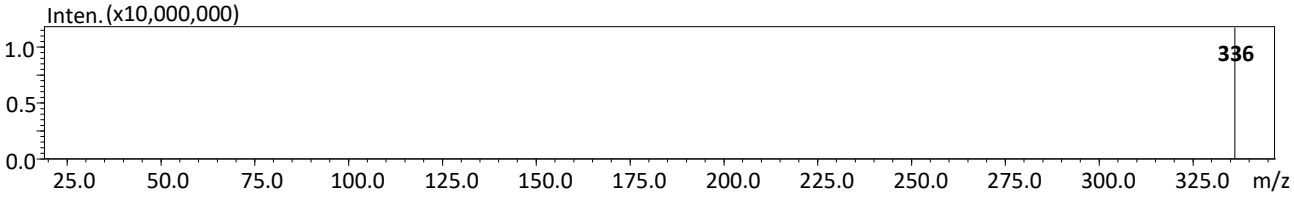


Molecular Formula: $C_{21}H_{25}N_3O$

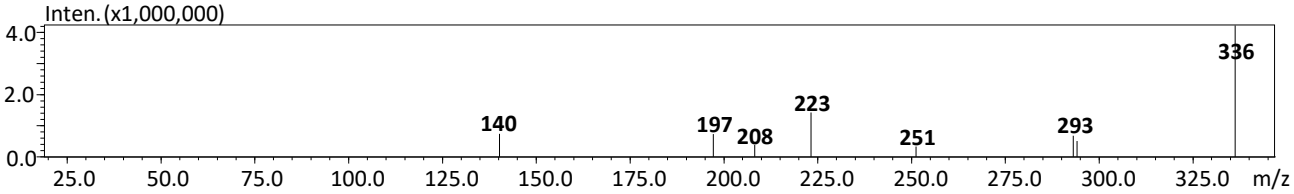
Formula Weight: 335.5

$[M+H]^+$: 336.207039 Da

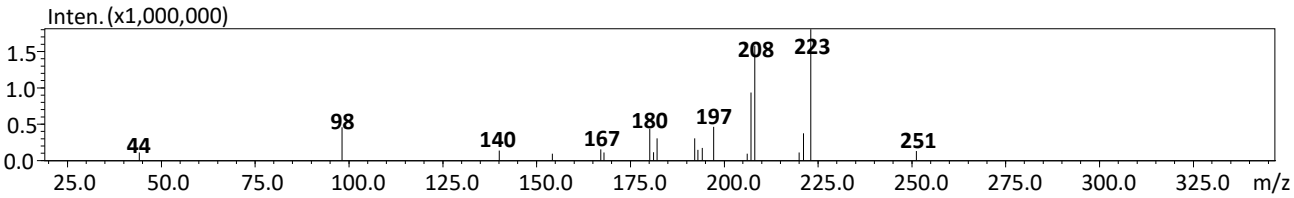
10 CE



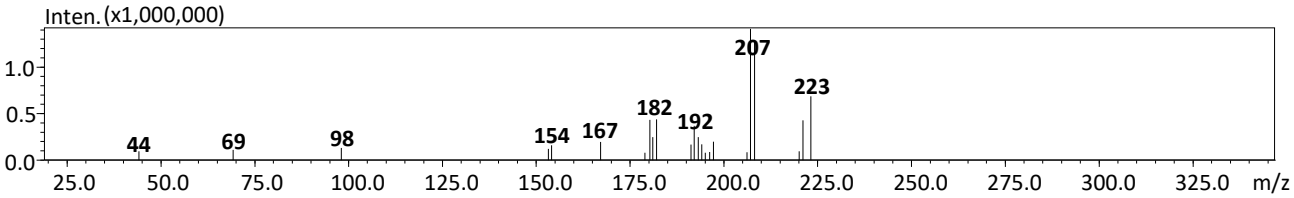
20 CE



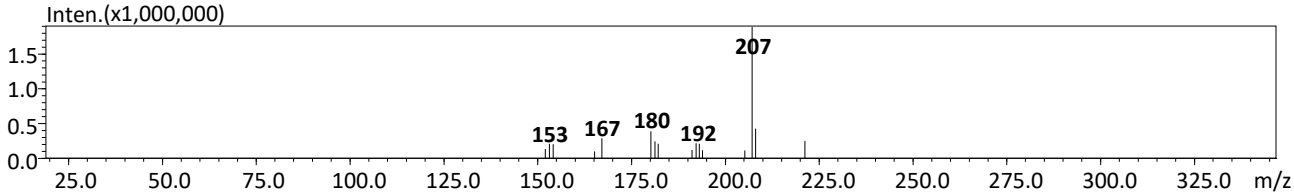
35 CE



40 CE



50 CE



QqQ-MS/MS: Detection of the investigated compounds was achieved with the use of a triple quadrupole mass spectrometer (QqQ, Shimadzu 8060, Kyoto, Japan) in positive mode. The spectrometer was equipped with an electrospray ionization (ESI) sourceThe following MS parameters were fixed: nebulizing gas flow, 3 L/min; heating gas flow, 10 L/min; interface temperature, 250 °C; desolvation line temperature, 200 °C; heat block temperature, 350 °C; and drying gas flow, 10 L/min. Fragmentation MS/MS spectra were acquired by conducting a product ion scan experiment at five collision energies (CE: –10, –20, –35,–40 and –50 V).

LSZ

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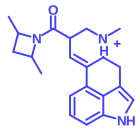

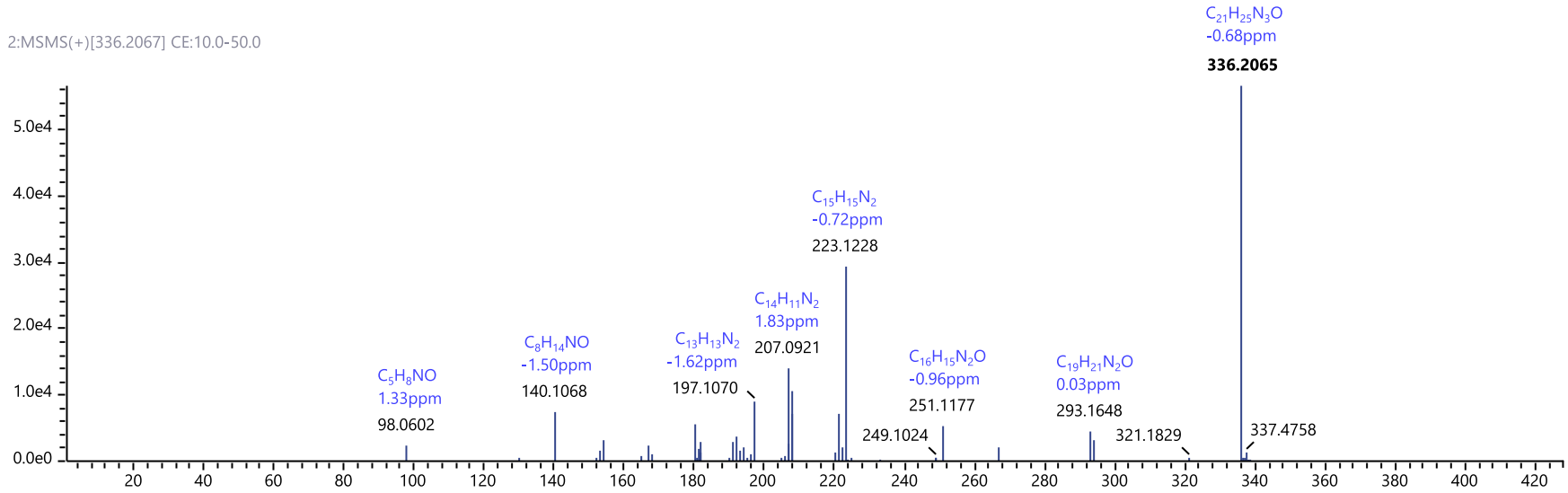

Experimental m/z	Intensity	Molecular Formula	Charge	Predicted m/z	Δ ppm	Experimental m/z	Intensity	Molecular Formula	Charge	Predicted m/z	Δ ppm
336.2068	–	$C_{21}H_{25}N_3O$	$[M+H]^+$	336.2070	-0.68	**197.1070**	9037	$C_{13}H_{13}N_2$	$[+H]^+$	197.1073	-1.62
321.1829	492	$C_{20}H_{23}N_3O^{\bullet}$	$[+H]^+$	321.1836	-1.93	**194.0962**	2091	$C_{14}H_{12}N$	+	194.0964	-0.98
293.1649	4579	$C_{19}H_{21}N_2O$	+	293.1648	0.03	**192.0809**	3611	$C_{14}H_{10}N$	+	192.0808	0.42
267.1370	2002	$C_{16}H_{17}N_3O^{\bullet}$	$[+H]^+$	267.1366	1.31	**182.0970**	1242	$C_{13}H_{12}N$	$[+H]^+$	182.0964	3.35
251.1177	5292	$C_{16}H_{15}N_2O$	+	251.1179	-0.96	**182.0840**	3034	$C_{12}H_{10}N_2^{\bullet}$	$[+H]^+$	182.0839	0.82
223.1228	29322	$C_{15}H_{15}N_2$	$[+H]^+$	223.1230	-0.72	**180.0806**	5516	$C_{13}H_{10}N$	$[+H]^+$	180.0808	-1.06
221.1072	7093	$C_{15}H_{13}N_2$	$[+H]^+$	221.1073	-0.77	**167.0727**	2450	$C_{12}H_9N^{\bullet}$	+	167.0730	-1.38
208.0995	10522	$C_{14}H_{12}N_2\bullet$	$[+H]^+$	208.0995	-0.10	**154.0652**	3163	$C_{11}H_8N$	+	154.0651	0.33
208.0753	7079	$C_{14}H_{10}NO$	+	208.0757	-1.78	**140.1068**	7287	$C_8H_{14}NO$	$[+H]^+$	140.1070	-1.50
207.0921	14125	$C_{14}H_{11}N_2$	$[+H]^+$	207.0917	1.84	**98.0602**	2273	C_5H_8NO	$[+H]^+$	98.0600	1.33

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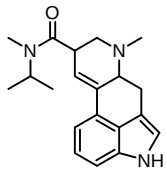
MiPLA

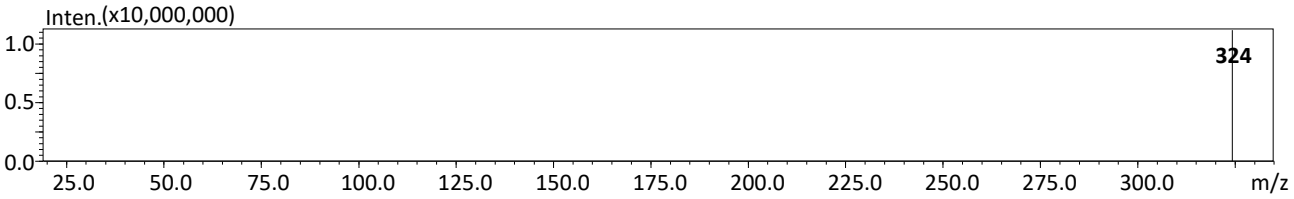


Molecular Formula: $C_{20}H_{25}N_3O$

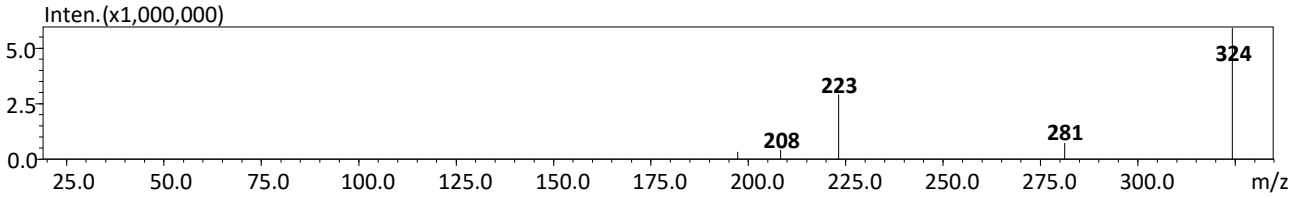
Formula Weight: 323.4

$[M+H]^+$: 324.207039 Da

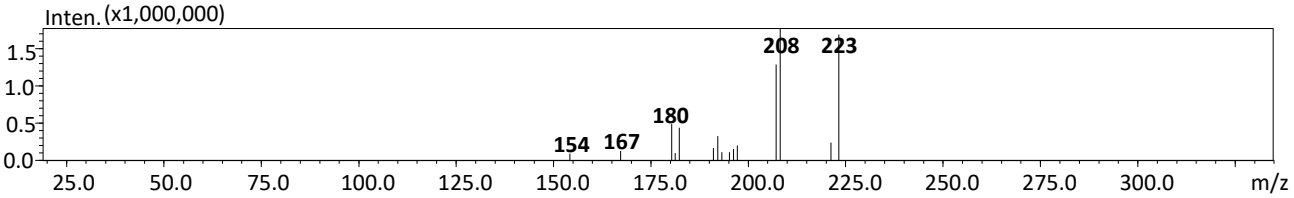
10 CE



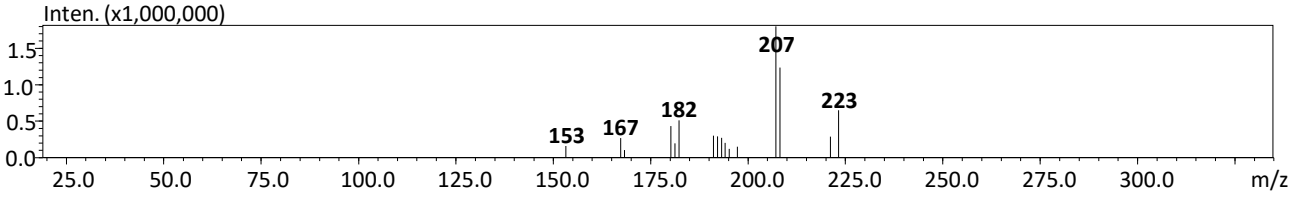
20 CE



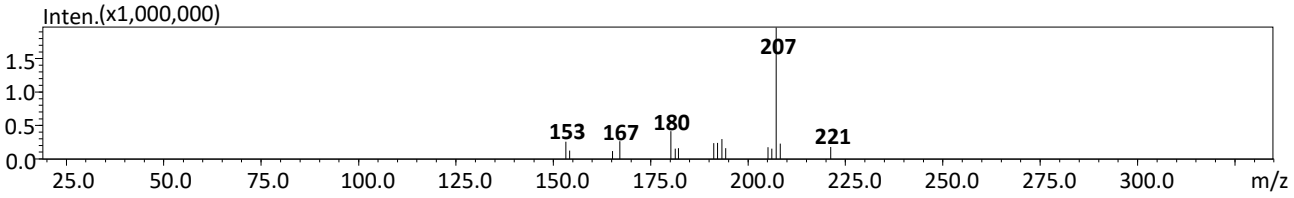
35 CE



40 CE



50 CE



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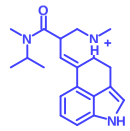
MiPLA

Molecular Formula: $C_{20}H_{25}N_3O$

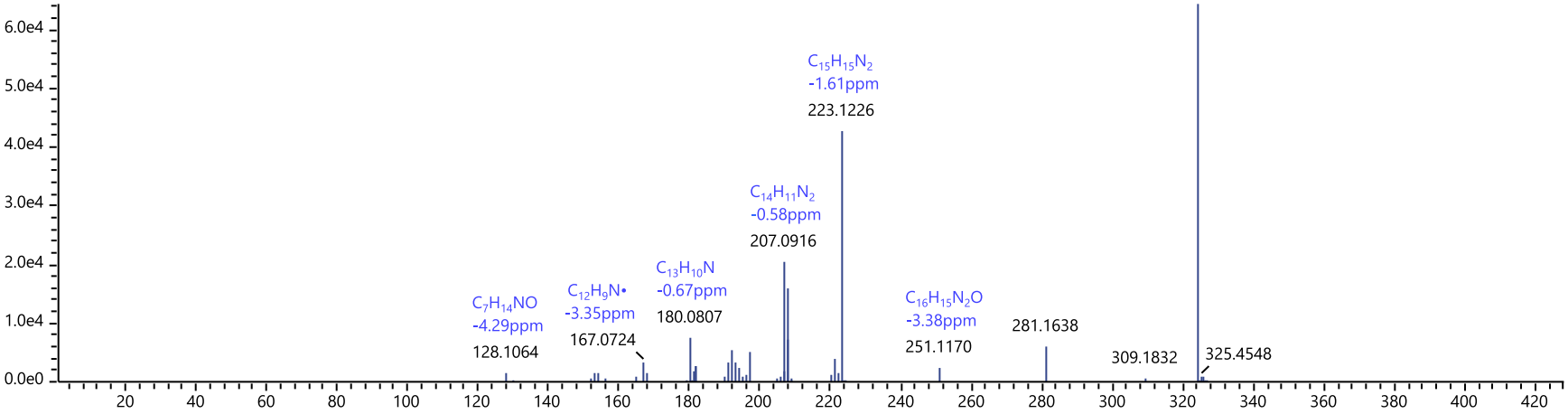
Formula Weight: 323.4

[M+H]⁺: 324.207039 Da



$C_{20}H_{25}N_3O$
-0.40ppm
324.2067

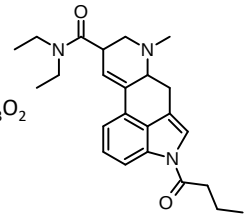
2:MSMS(+)[324.2069] CE:10.0-50.0



Experimental m/z	Intensity	Molecular Formula	Charge	Predicted m/z	Δ ppm	Experimental m/z	Intensity	Molecular Formula	Charge	Predicted m/z	Δ ppm
324.2069	–	$C_{20}H_{25}N_3O$	$[M+H]^+$	324.2070	-0.40	**197.1071**	5122	$C_{13}H_{13}N_2$	$[+H]^+$	197.1073	-1.22
309.1832	529	$C_{19}H_{23}N_3O^•$	$[+H]^+$	309.1836	-1.29	**194.0964**	2448	$C_{14}H_{12}N$	+	194.0964	0.0
281.1638	5953	–	–	–	–	**192.0811**	5399	$C_{14}H_{10}N$	+	192.0808	1.46
251.1170	2414	$C_{16}H_{15}N_2O$	+	251.1179	-3.39	**182.0962**	2565	$C_{13}H_{12}N$	$[+H]^+$	182.0964	-1.48
223.1226	42759	$C_{15}H_{15}N_2$	$[+H]^+$	223.1230	-1.61	**180.0807**	7459	$C_{13}H_{10}N$	$[+H]^+$	180.0808	-0.67
221.1072	3824	$C_{15}H_{13}N_2$	$[+H]^+$	221.1073	-0.50	**167.0724**	3397	$C_{12}H_9N^•$	+	167.0730	-3.35
208.0996	15828	$C_{14}H_{12}N_2^•$	$[+H]^+$	208.0995	0.24	**154.0650**	1464	$C_{11}H_8N$	+	154.0651	-0.65
208.0755	7244	$C_{14}H_{10}NO$	+	208.0757	-0.87	**128.1064**	1401	$C_7H_{14}NO$	$[+H]^+$	128.1070	-4.29
207.0916	20540	$C_{14}H_{11}N_2$	$[+H]^+$	207.0917	-0.58						

QTOF-MS/MS: The QTOF Shimadzu 9050 (Kyoto, Japan) spectrometer was equipped with an electrospray ionization (ESI) source. The following QTOF parameters were fixed: nebulizing gas flow, 3 L/min; heating gas flow, 10 L/min; interface temperature, 250 ◦C; desolvation line temperature, 200 ◦C; interface voltage (+), 4.50 kV; heat block temperature, 350 ◦C; and drying gas flow, 10 L/min. MS/MS spectra for all substances were acquired by conducting datadependent acquisition (DDA) function. DDA data were acquired in the range 40–500 m/z and collision energies from − 10 V to − 50 V.

1B-LSD

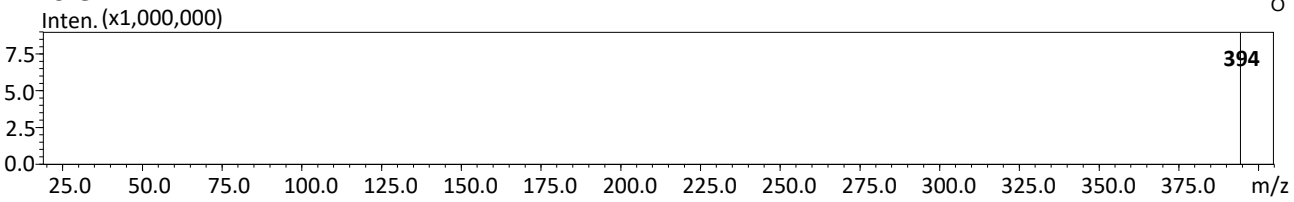


Molecular Formula: $C_{24}H_{31}N_3O_2$

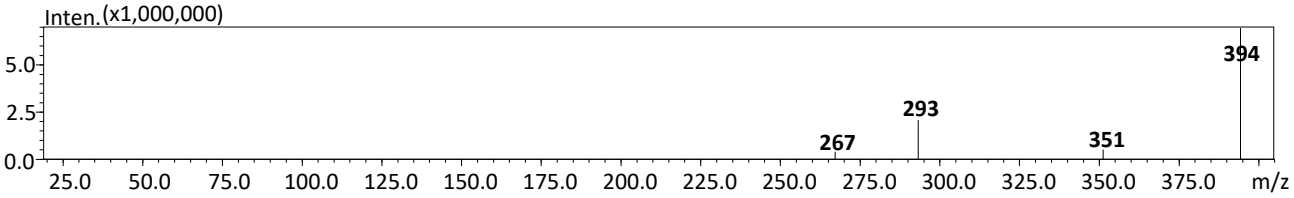
Formula Weight: 393.5

[M+H]$^+$: 394.248904 Da

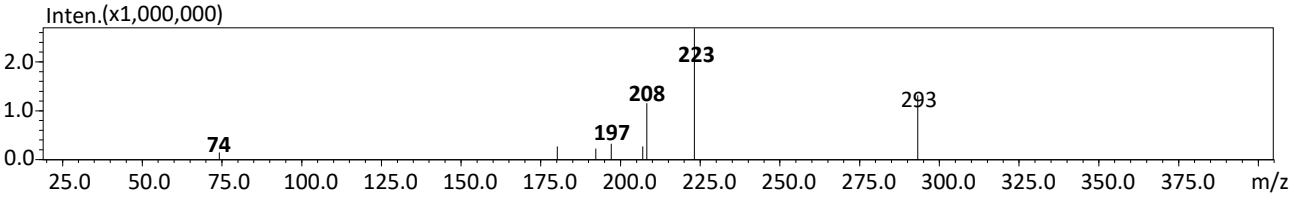
10 CE



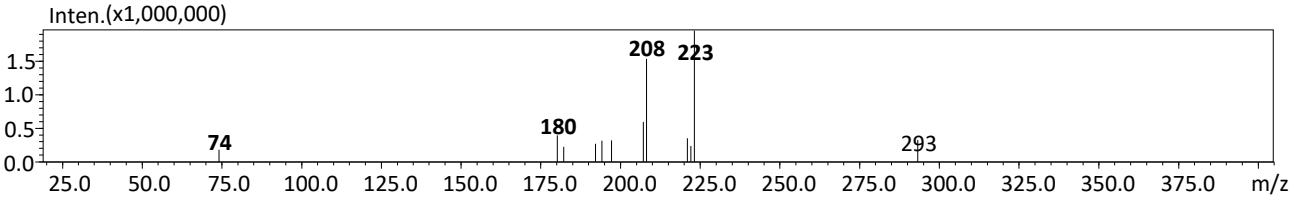
20 CE



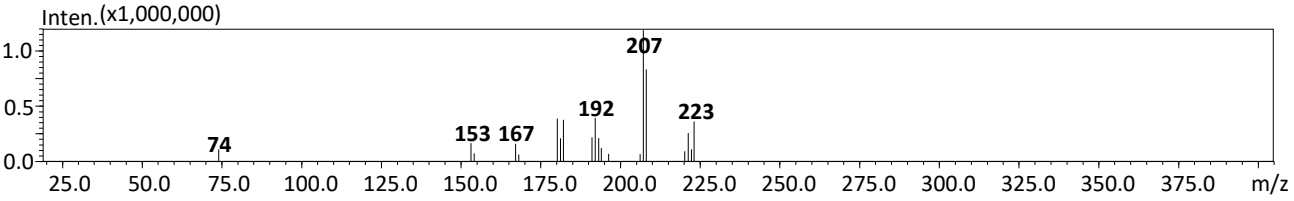
35 CE



40 CE

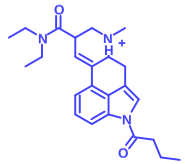


50 CE



QqQ-MS/MS: Detection of the investigated compounds was achieved with the use of a triple quadrupole mass spectrometer (QqQ, Shimadzu 8060, Kyoto, Japan) in positive mode. The spectrometer was equipped with an electrospray ionization (ESI) sourceThe following MS parameters were fixed: nebulizing gas flow, 3 L/min; heating gas flow, 10 L/min; interface temperature, 250 °C; desolvation line temperature, 200 °C; heat block temperature, 350 °C; and drying gas flow, 10 L/min. Fragmentation MS/MS spectra were acquired by conducting a product ion scan experiment at five collision energies (CE: –10, –20, –35,–40 and –50 V).

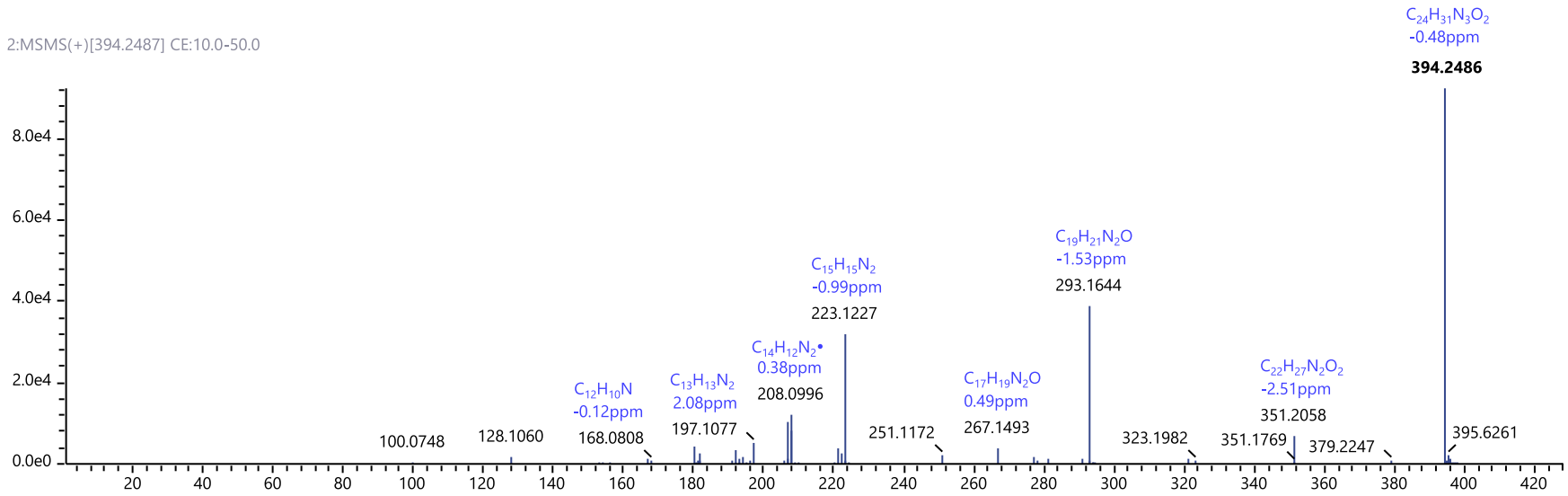
1B-LSD



Molecular Formula: $C_{24}H_{31}N_3O_2$

Formula Weight: 393.5

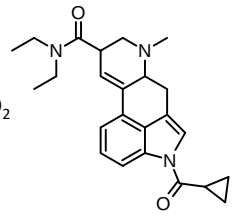
[M+H]⁺: 394.248904 Da



Experimental m/z	Intensity	Molecular Formula	Charge	Predicted m/z	Δ ppm	Experimental m/z	Intensity	Molecular Formula	Charge	Predicted m/z	Δ ppm
394.2487	–	$C_{24}H_{31}N_3O_2$	$[M+H]^+$	394.2489	-0.48	**208.0996**	11976	$C_{14}H_{12}N_2^•$	$[+H]^+$	208.0995	0.38
379.2247	969	$C_{23}H_{29}N_3O_2^•$	$[+H]^+$	379.2254	-1.93	**208.0755**	8371	$C_{14}H_{10}NO$	+	208.0757	-1.01
351.2058	6703	$C_{22}H_{27}N_2O_2$	+	351.2067	-2.51	**207.0914**	10153	$C_{14}H_{11}N_2$	$[+H]^+$	207.0917	-1.55
321.1585	1110	–	–	–	–	**197.1077**	5027	$C_{13}H_{13}N_2$	$[+H]^+$	197.1073	2.08
293.1644	38637	$C_{19}H_{21}N_2O$	$[+H]^+$	293.1648	-1.54	**194.0970**	1840	$C_{14}H_{12}N$	+	194.0964	2.99
281.1653	1251	$C_{18}H_{21}N_2O$	+	281.1648	1.74	**192.0802**	3614	$C_{14}H_{10}N$	+	192.0808	-3.23
277.1329	1537	$C_{18}H_{17}N_2O$	$[+H]^+$	277.1335	-2.42	**182.0967**	2489	$C_{13}H_{12}N$	$[+H]^+$	182.0964	1.32
267.1493	3759	$C_{17}H_{19}N_2O$	$[+H]^+$	267.1492	0.49	**180.0806**	4141	$C_{13}H_{10}N$	$[+H]^+$	180.0808	-0.89
251.1172	1966	$C_{16}H_{15}N_2O$	+	251.1179	-2.75	**167.0745**	1095	–	–	–	–
223.1228	31814	$C_{15}H_{15}N_2$	$[+H]^+$	223.1230	-0.99	**154.0635**	579	–	–	–	–
221.1071	3865	$C_{15}H_{13}N_2$	$[+H]^+$	221.1073	-1.0	**128.1060**	1835	–	–	–	–

QTOF-MS/MS: The QTOF Shimadzu 9050 (Kyoto, Japan) spectrometer was equipped with an electrospray ionization (ESI) source. The following QTOF parameters were fixed: nebulizing gas flow, 3 L/min; heating gas flow, 10 L/min; interface temperature, 250 ◦C; desolvation line temperature, 200 ◦C; interface voltage (+), 4.50 kV; heat block temperature, 350 ◦C; and drying gas flow, 10 L/min. MS/MS spectra for all substances were acquired by conducting datadependent acquisition (DDA) function. DDA data were acquired in the range 40–500 m/z and collision energies from – 10 V to – 50 V.

1cP-LSD

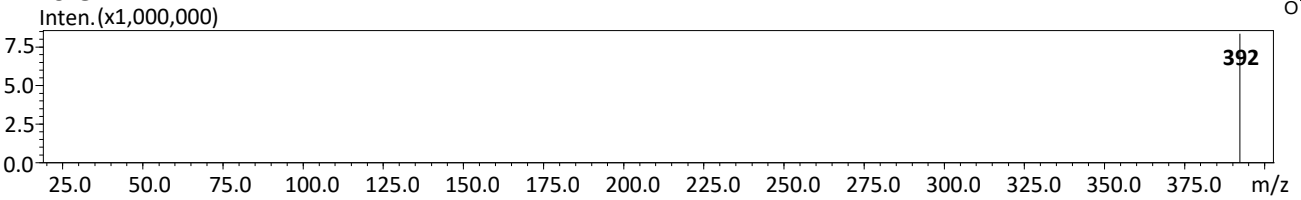


Molecular Formula: $C_{24}H_{29}N_3O_2$

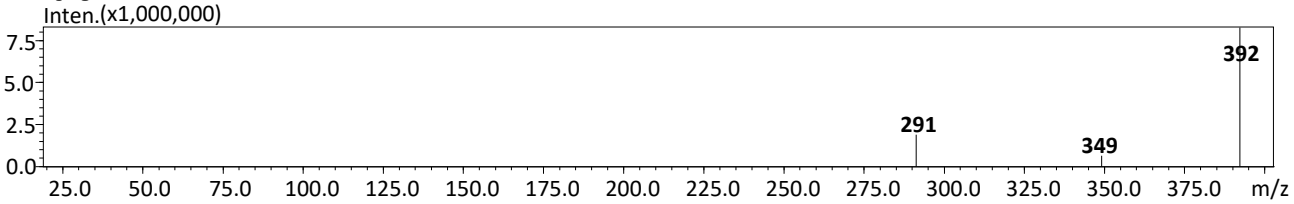
Formula Weight: 391.5

[M+H]$^+$: 392.233254 Da

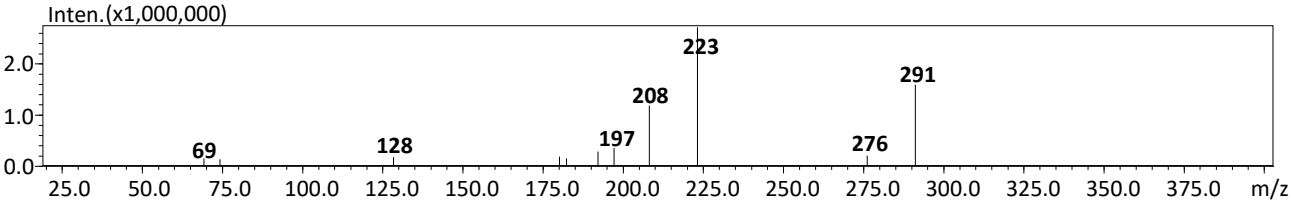
10 CE



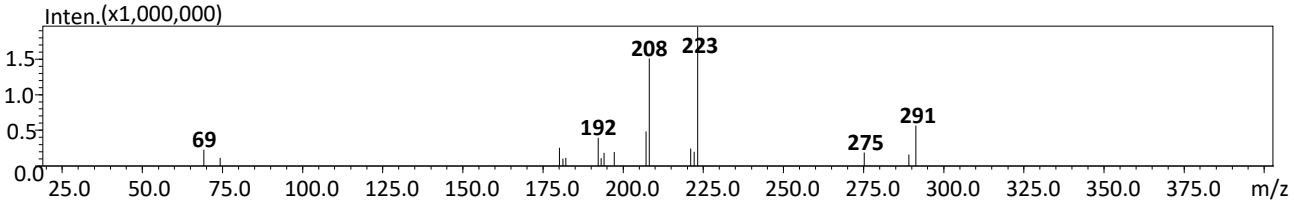
20 CE



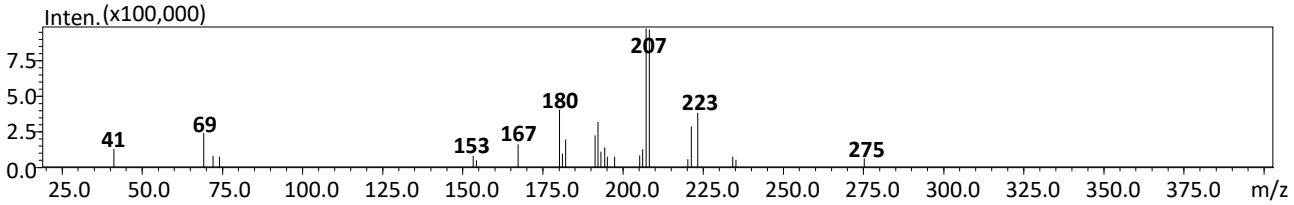
35 CE



40 CE



50 CE



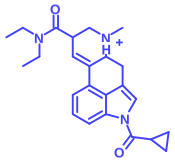
QqQ-MS/MS: Detection of the investigated compounds was achieved with the use of a triple quadrupole mass spectrometer (QqQ, Shimadzu 8060, Kyoto, Japan) in positive mode. The spectrometer was equipped with an electrospray ionization (ESI) sourceThe following MS parameters were fixed: nebulizing gas flow, 3 L/min; heating gas flow, 10 L/min; interface temperature, 250 °C; desolvation line temperature, 200 °C; heat block temperature, 350 °C; and drying gas flow, 10 L/min. Fragmentation MS/MS spectra were acquired by conducting a product ion scan experiment at five collision energies (CE: –10, –20, –35,–40 and –50 V).

1cP-LSD

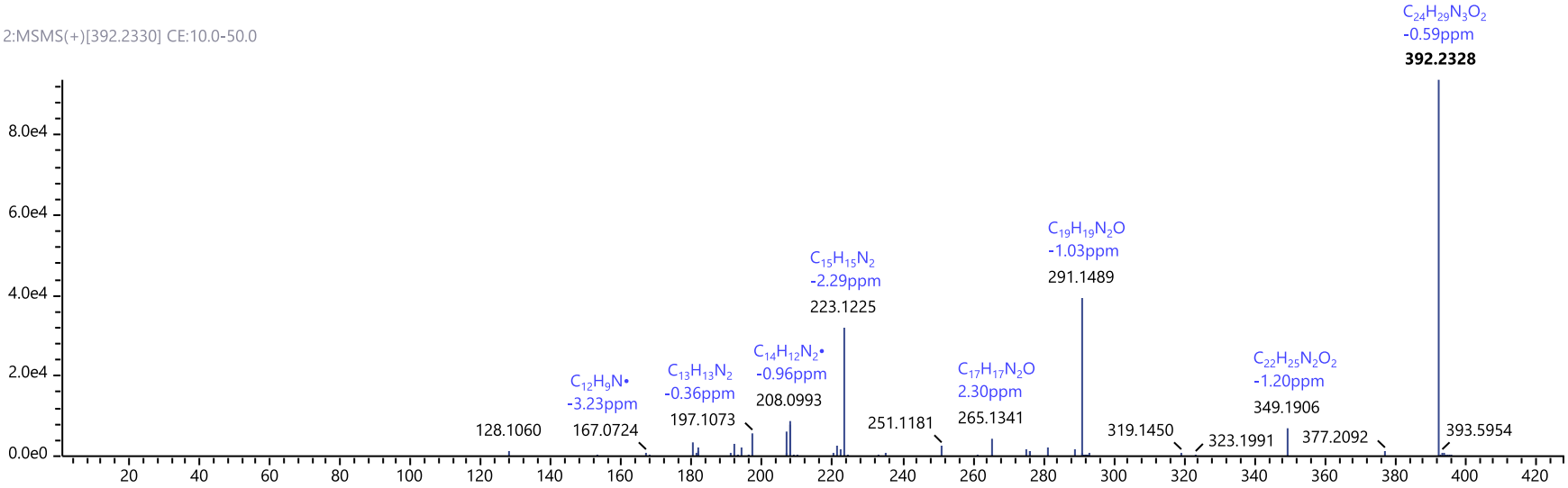
Molecular Formula: $C_{24}H_{29}N_3O_2$

Formula Weight: 391.5

$[M+H]^+$: 392.233254 Da



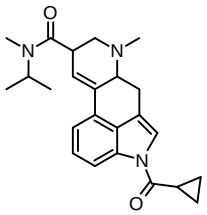
2:MSMS(+)[392.2330] CE:10.0-50.0



Experimental m/z	Intensity	Molecular Formula	Charge	Predicted m/z	Δ ppm	Experimental m/z	Intensity	Molecular Formula	Charge	Predicted m/z	Δ ppm
392.2330	–	$C_{24}H_{30}N_3O_2$	$[M+H]^+$	392.2333	-0.59	**208.0993**	8670	$C_{14}H_{12}N_2$•	$[+H]^+$	208.0995	-0.96
377.2092	1114	$C_{23}H_{27}N_3O_2$•	$[+H]^+$	377.2098	-1.56	**208.0756**	7731	$C_{14}H_{10}NO$	+	208.0757	-0.58
349.1906	7027	$C_{22}H_{25}N_2O_2$	+	349.1911	-1.20	**207.0915**	5990	$C_{14}H_{11}N_2$	$[+H]^+$	207.0917	-0.63
319.1426	1090	–	–	–	–	**197.1073**	5792	$C_{13}H_{13}N_2$	$[+H]^+$	197.1073	-0.36
291.1489	39237	$C_{19}H_{19}N_2O$	$[+H]^+$	291.1492	-1.03	**194.0963**	2235	$C_{14}H_{12}N$	+	194.0964	-0.82
281.1634	1990	–	–	–	–	**192.0802**	3089	$C_{14}H_{10}N$	+	192.0808	-2.81
275.1176	1759	$C_{18}H_{15}N_2O$	$[+H]^+$	275.1179	-1.05	**182.0966**	2023	$C_{13}H_{12}N$	$[+H]^+$	182.0964	1.15
265.1342	4587	$C_{17}H_{17}N_2O$	$[+H]^+$	265.1335	2.30	**180.0807**	3327	$C_{13}H_{10}N$	$[+H]^+$	180.0808	-0.22
251.1181	2774	$C_{16}H_{15}N_2O$	+	251.1179	0.72	**167.0724**	664	$C_{12}H_9N$•	+	167.0730	-3.23
223.1225	31801	$C_{15}H_{15}N_2$	$[+H]^+$	223.1230	-2.29	**128.1060**	1485	–	–	–	–
221.1074	2572	$C_{15}H_{13}N_2$	$[+H]^+$	221.1073	0.41						

QTOF-MS/MS: The QTOF Shimadzu 9050 (Kyoto, Japan) spectrometer was equipped with an electrospray ionization (ESI) source. The following QTOF parameters were fixed: nebulizing gas flow, 3 L/min; heating gas flow, 10 L/min; interface temperature, 250 ◦C; desolvation line temperature, 200 ◦C; interface voltage (+), 4.50 kV; heat block temperature, 350 ◦C; and drying gas flow, 10 L/min. MS/MS spectra for all substances were acquired by conducting datadependent acquisition (DDA) function. DDA data were acquired in the range 40–500 m/z and collision energies from − 10 V to − 50 V.

1cP-MiPLA

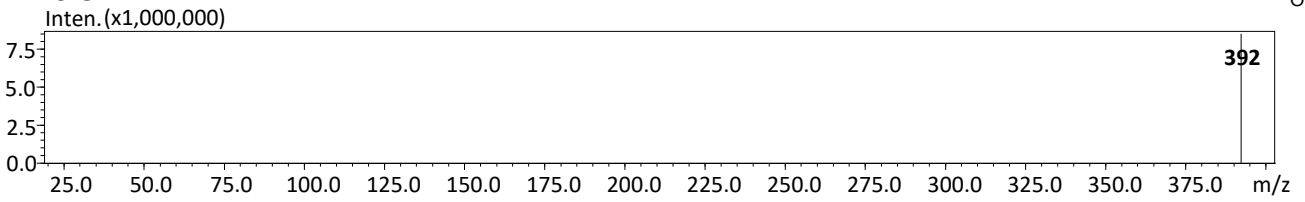


Molecular Formula: $C_{24}H_{29}N_3O_2$

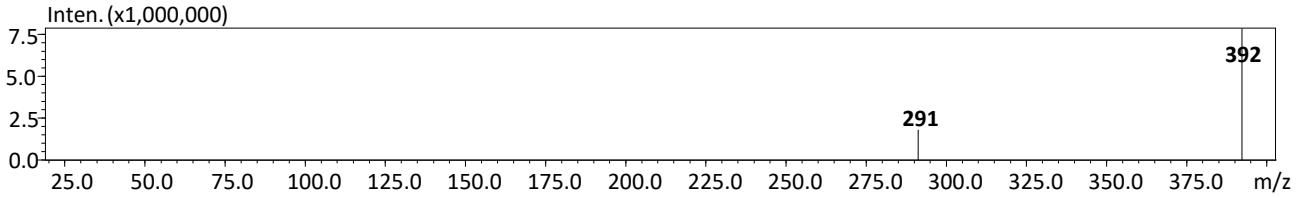
Formula Weight: 391.5

[M+H]$^+$: 392.233254 Da

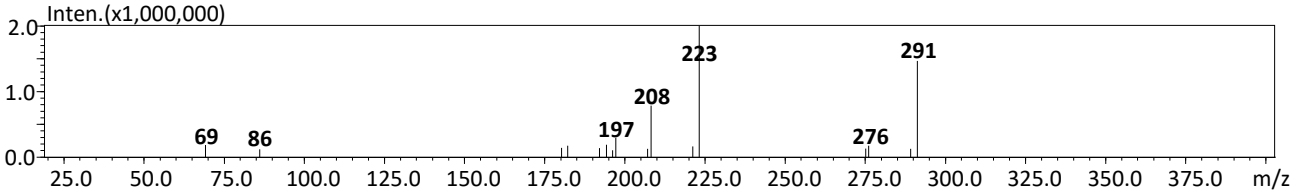
10 CE



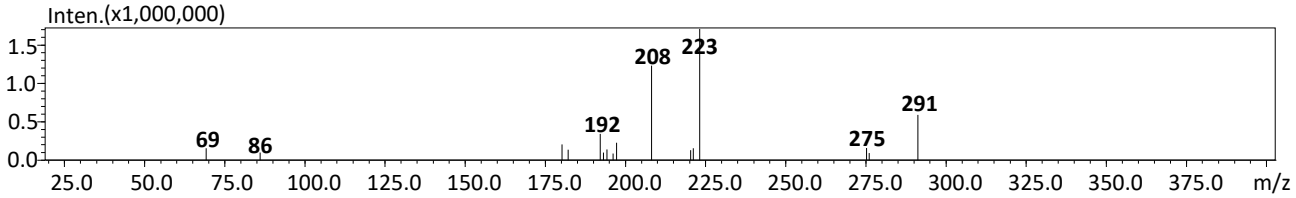
20 CE



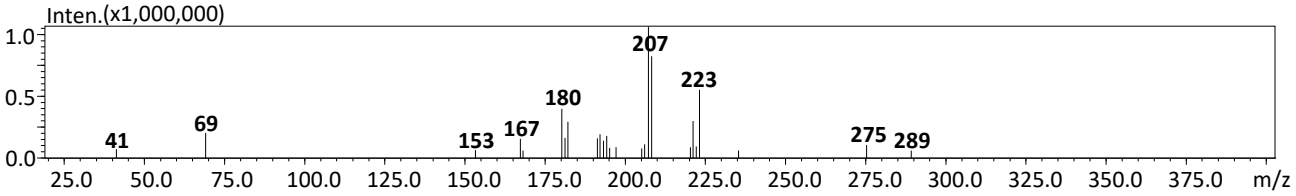
35 CE



40 CE



50 CE



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1cP-MiPLA

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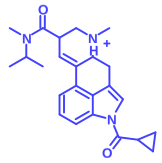
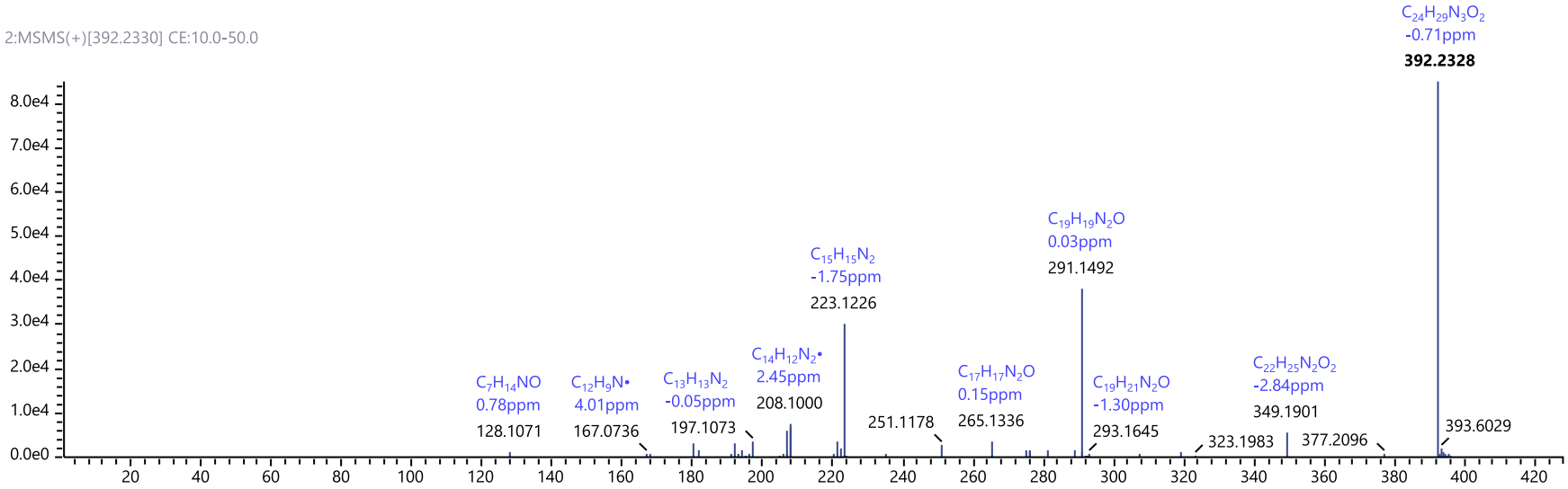
Formula Weight: 391.5

[M+H]$^+$: 392.233254 Da

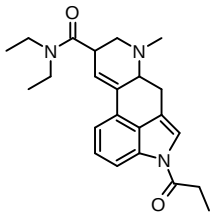




Experimental m/z	Intensity	Molecular Formula	Charge	Predicted m/z	Δ ppm	Experimental m/z	Intensity	Molecular Formula	Charge	Predicted m/z	Δ ppm
392.2330	–	$C_{24}H_{29}N_3O_2$	$[M+H]^+$	392.2333	-0.71	**208.1000**	7398	$C_{14}H_{12}N_2^•$	$[+H]^+$	208.0995	2.45
377.2097	658	$C_{23}H_{27}N_3O_2^•$	$[+H]^+$	377.2098	-0.35	**208.0755**	6770	$C_{14}H_{10}NO$	+	208.0757	-0.87
349.1901	5713	$C_{22}H_{25}N_2O_2$	+	349.1911	-2.84	**207.0911**	5825	$C_{14}H_{11}N_2$	$[+H]^+$	207.0917	-2.85
319.1450	1011	$C_{20}H_{19}N_2O_2$	+	319.1441	2.73	**197.1073**	3604	$C_{13}H_{13}N_2$	$[+H]^+$	197.1073	-0.05
291.1492	37975	$C_{19}H_{19}N_2O$	$[+H]^+$	291.1492	0.03	**194.0957**	1653	$C_{14}H_{12}N$	+	194.0964	-3.56
281.1657	1526	$C_{18}H_{21}N_2O$	+	281.1648	2.88	**192.0806**	3052	$C_{14}H_{10}N$	+	192.0808	-0.99
275.1177	1713	$C_{18}H_{15}N_2O$	$[+H]^+$	275.1179	-0.80	**182.0967**	1758	$C_{13}H_{12}N$	$[+H]^+$	182.0964	1.26
265.1336	3707	$C_{17}H_{17}N_2O$	$[+H]^+$	265.1335	0.15	**180.0810**	3031	$C_{13}H_{10}N$	$[+H]^+$	180.0808	1.22
251.1178	2768	$C_{16}H_{15}N_2O$	+	251.1179	-0.48	**167.0736**	696	$C_{12}H_9N^•$	+	167.0730	4.01
223.1226	30382	$C_{15}H_{15}N_2$	$[+H]^+$	223.1230	-1.75	**128.1071**	1062	$C_7H_{14}NO$	$[+H]^+$	128.1070	0.78
221.1077	3478	$C_{15}H_{13}N_2$	$[+H]^+$	221.1073	1.90						

QTOF-MS/MS: The QTOF Shimadzu 9050 (Kyoto, Japan) spectrometer was equipped with an electrospray ionization (ESI) source. The following QTOF parameters were fixed: nebulizing gas flow, 3 L/min; heating gas flow, 10 L/min; interface temperature, 250 ◦C; desolvation line temperature, 200 ◦C; interface voltage (+), 4.50 kV; heat block temperature, 350 ◦C; and drying gas flow, 10 L/min. MS/MS spectra for all substances were acquired by conducting datadependent acquisition (DDA) function. DDA data were acquired in the range 40–500 m/z and collision energies from – 10 V to – 50 V.

1P-LSD

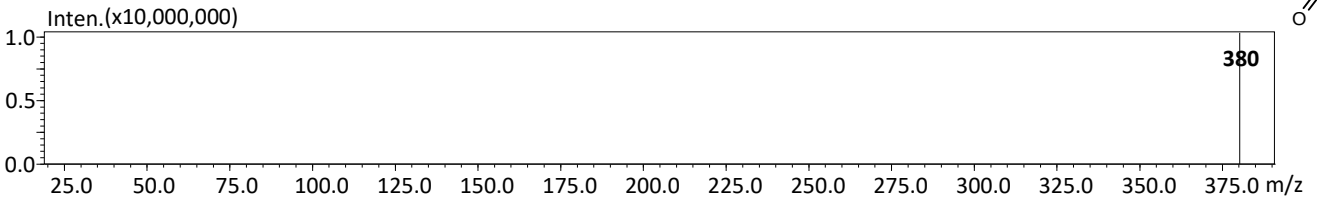


Molecular Formula: $C_{23}H_{29}N_3O_2$

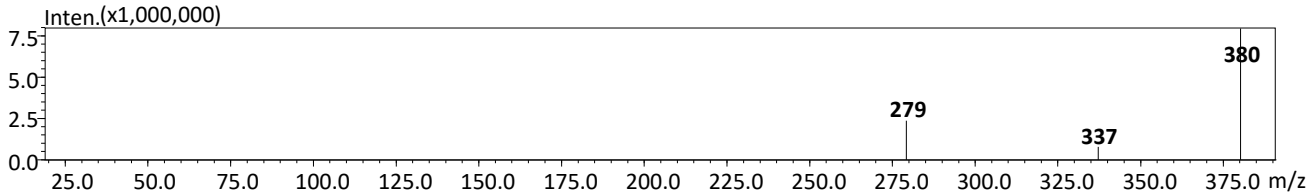
Formula Weight: 379.5

[M+H]$^+$: 380.233254 Da

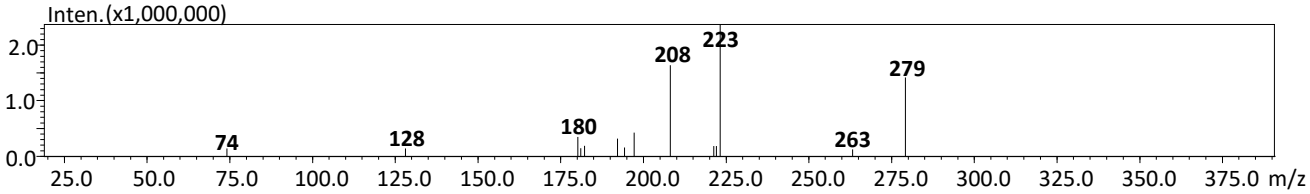
10 CE



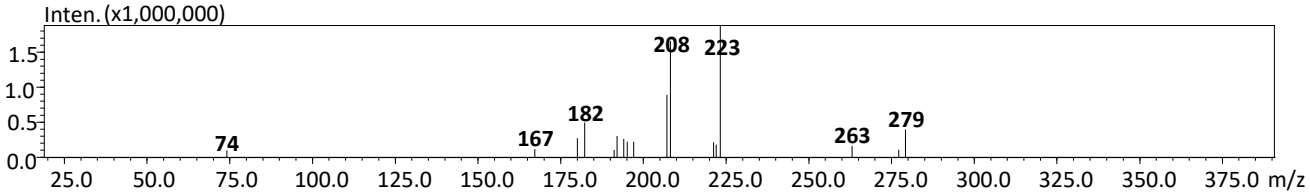
20 CE



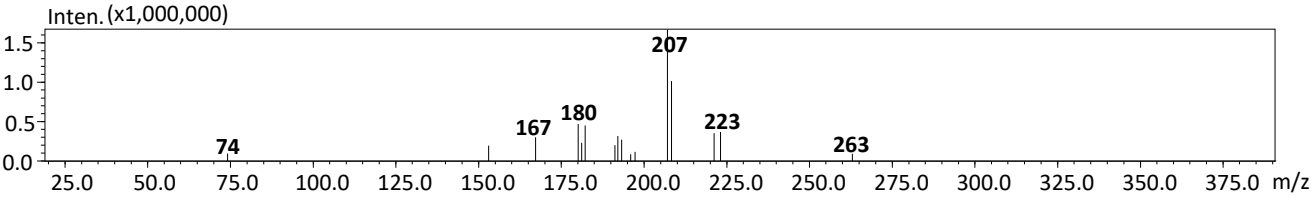
35 CE



40 CE



50 CE



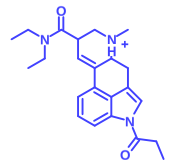
QqQ-MS/MS: Detection of the investigated compounds was achieved with the use of a triple quadrupole mass spectrometer (QqQ, Shimadzu 8060, Kyoto, Japan) in positive mode. The spectrometer was equipped with an electrospray ionization (ESI) sourceThe following MS parameters were fixed: nebulizing gas flow, 3 L/min; heating gas flow, 10 L/min; interface temperature, 250 °C; desolvation line temperature, 200 °C; heat block temperature, 350 °C; and drying gas flow, 10 L/min. Fragmentation MS/MS spectra were acquired by conducting a product ion scan experiment at five collision energies (CE: –10, –20, –35,–40 and –50 V).

1P-LSD

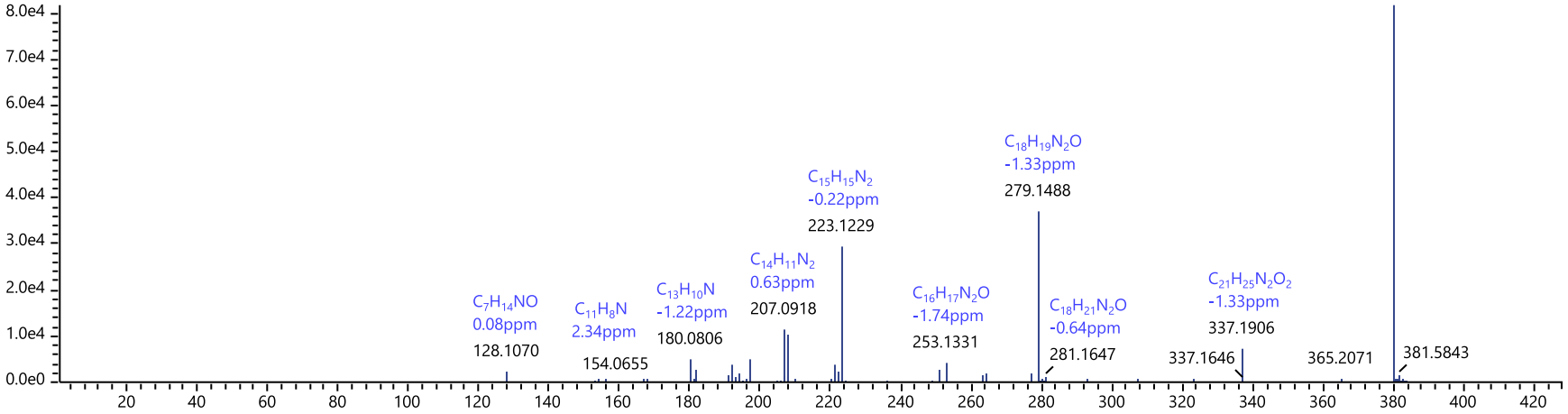
Molecular Formula: $C_{23}H_{29}N_3O_2$

Formula Weight: 379.5

[M+H]$^+$: 380.233254 Da



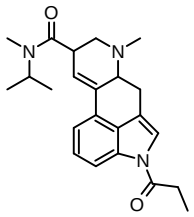
2:MSMS(+)[380.2331] CE:10.0-50.0



Experimental m/z	Intensity	Molecular Formula	Charge	Predicted m/z	Δ ppm	Experimental m/z	Intensity	Molecular Formula	Charge	Predicted m/z	Δ ppm
380.2330	–	$C_{23}H_{29}N_3O_2$	$[M+H]^+$	380.2333	-0.58	**208.0995**	10338	$C_{14}H_{12}N_2^{\bullet}$	$[+H]^+$	208.0995	-0.24
365.2071	729	–	–	–	–	**208.0754**	9731	$C_{14}H_{10}NO$	+	208.0757	-1.30
337.1906	7447	$C_{21}H_{25}N_2O_2$	+	337.1911	-1.34	**207.0918**	11433	$C_{14}H_{11}N_2$	$[+H]^+$	207.0917	0.63
307.1447	628	$C_{19}H_{19}N_2O_2$	+	307.1441	2.08	**197.1062**	4938	–	–	–	–
281.1647	1090	$C_{18}H_{21}N_2O$	+	281.1648	-0.64	**194.0966**	2044	$C_{14}H_{12}N$	+	194.0964	0.62
279.1488	37251	$C_{18}H_{19}N_2O$	$[+H]^+$	279.1492	-1.33	**192.0808**	3908	$C_{14}H_{10}N$	+	192.0808	0.05
263.1173	1573	$C_{17}H_{15}N_2O$	$[+H]^+$	263.1179	-2.32	**182.0958**	2497	$C_{13}H_{12}N$	$[+H]^+$	182.0958	-3.73
253.1331	4386	$C_{16}H_{17}N_2O$	$[+H]^+$	253.1335	-1.74	**180.0806**	5063	$C_{13}H_{10}N$	$[+H]^+$	180.0808	-1.22
251.1184	2641	$C_{16}H_{15}N_2O$	+	251.1179	1.91	**167.0709**	896	–	–	–	–
223.1229	29424	$C_{15}H_{15}N_2$	$[+H]^+$	223.1230	-0.22	**154.0655**	725	$C_{11}H_8N$	+	154.0651	2.34
221.1082	3999	$C_{15}H_{13}N_2$	$[+H]^+$	221.1073	3.89	**128.1070**	2156	$C_7H_{14}NO$	$[+H]^+$	128.1070	0.08

QTOF-MS/MS: The QTOF Shimadzu 9050 (Kyoto, Japan) spectrometer was equipped with an electrospray ionization (ESI) source. The following QTOF parameters were fixed: nebulizing gas flow, 3 L/min; heating gas flow, 10 L/min; interface temperature, 250 ◦C; desolvation line temperature, 200 ◦C; interface voltage (+), 4.50 kV; heat block temperature, 350 ◦C; and drying gas flow, 10 L/min. MS/MS spectra for all substances were acquired by conducting datadependent acquisition (DDA) function. DDA data were acquired in the range 40–500 m/z and collision energies from − 10 V to − 50 V.

1P-MiPLA

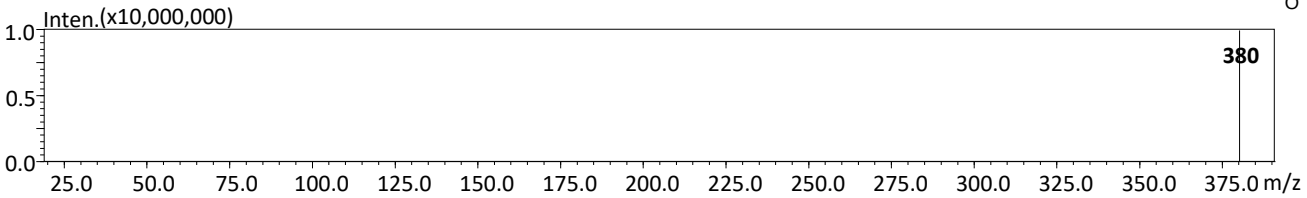


Molecular Formula: $C_{23}H_{29}N_3O_2$

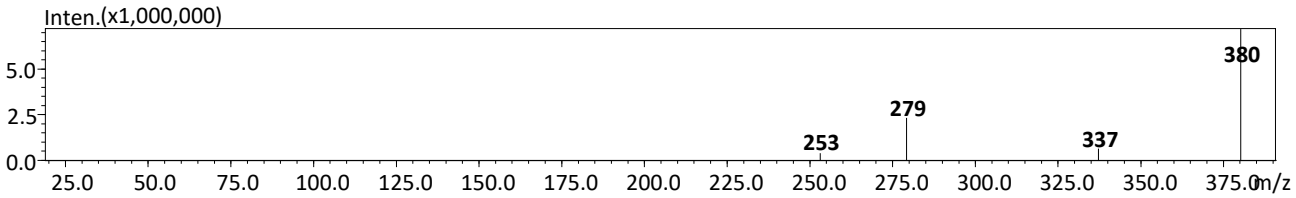
Formula Weight: 379.5

$[M+H]^+$: 380.233254 Da

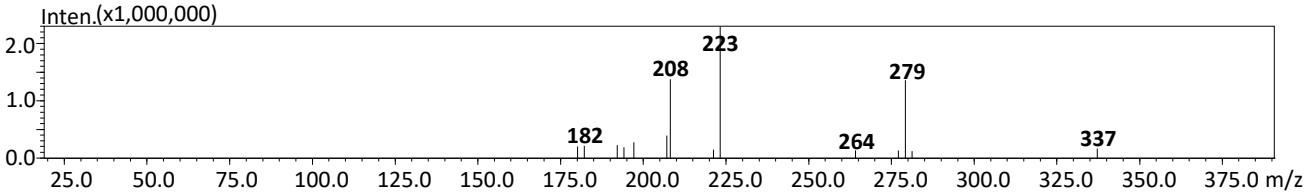
10 CE



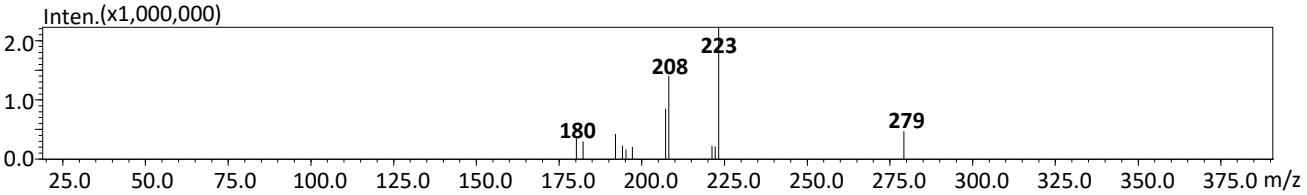
20 CE



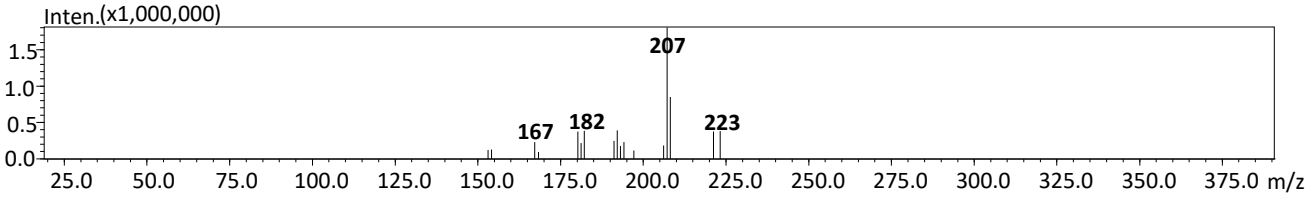
35 CE



40 CE



50 CE



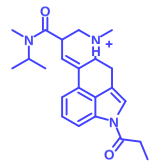
QqQ-MS/MS: Detection of the investigated compounds was achieved with the use of a triple quadrupole mass spectrometer (QqQ, Shimadzu 8060, Kyoto, Japan) in positive mode. The spectrometer was equipped with an electrospray ionization (ESI) sourceThe following MS parameters were fixed: nebulizing gas flow, 3 L/min; heating gas flow, 10 L/min; interface temperature, 250 °C; desolvation line temperature, 200 °C; heat block temperature, 350 °C; and drying gas flow, 10 L/min. Fragmentation MS/MS spectra were acquired by conducting a product ion scan experiment at five collision energies (CE: –10, –20, –35,–40 and –50 V).

1P-MiPLA

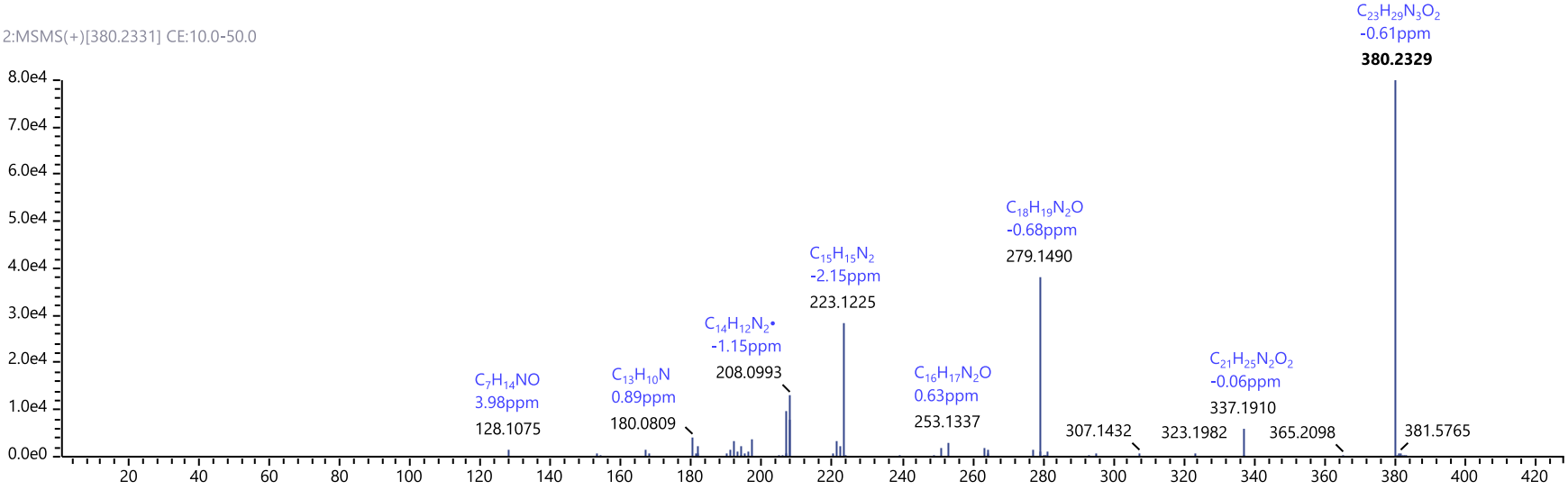
Molecular Formula: $C_{23}H_{29}N_3O_2$

Formula Weight: 379.5

[M+H]$^+$: 380.233254 Da



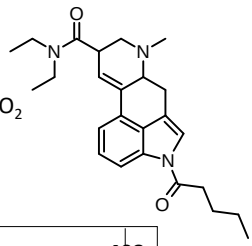
2:MSMS(+)[380.2331] CE:10.0-50.0



Experimental m/z	Intensity	Molecular Formula	Charge	Predicted m/z	Δ ppm	Experimental m/z	Intensity	Molecular Formula	Charge	Predicted m/z	Δ ppm
380.2330	–	$C_{23}H_{29}N_3O_2$	$[M+H]^+$	380.2333	-0.61	**208.0993**	13144	$C_{14}H_{12}N_2$•	$[+H]^+$	208.0995	-1.15
365.2098	373	$C_{22}H_{27}N_3O_2$•	$[+H]^+$	365.2098	-0.03	**208.0754**	7865	$C_{14}H_{10}NO$	+	208.0757	-1.54
337.1910	5841	$C_{21}H_{25}N_2O_2$	+	337.1911	-0.06	**207.0916**	9854	$C_{14}H_{11}N_2$	$[+H]^+$	207.0917	-0.48
307.1432	875	$C_{19}H_{19}N_2O_2$	+	307.1441	-2.90	**197.1066**	3657	$C_{13}H_{13}N_2$	$[+H]^+$	197.1073	-3.65
281.1628	1045	–	–	–	–	**194.0967**	2152	$C_{14}H_{12}N$	+	194.0964	1.24
279.1490	38013	$C_{18}H_{19}N_2O$	$[+H]^+$	279.1492	-0.68	**192.0810**	3268	$C_{14}H_{10}N$	+	192.0808	1.09
263.1185	1709	$C_{17}H_{15}N_2O$	$[+H]^+$	263.1179	2.24	**182.0967**	2273	$C_{13}H_{12}N$	$[+H]^+$	182.0964	1.48
253.1337	3095	$C_{16}H_{17}N_2O$	$[+H]^+$	253.1335	0.63	**180.0809**	4118	$C_{13}H_{10}N$	$[+H]^+$	180.0808	0.89
251.1181	1969	$C_{16}H_{15}N_2O$	+	251.1179	0.84	**167.0726**	1543	$C_{12}H_9N$•	+	167.0730	-1.98
223.1225	28469	$C_{15}H_{15}N_2$	$[+H]^+$	223.1230	-2.15	**154.0659**	487	$C_{11}H_8N$	+	154.0651	4.93
221.1075	3415	$C_{15}H_{13}N_2$	$[+H]^+$	221.1073	0.86	**128.1075**	1590	$C_7H_{14}NO$	$[+H]^+$	128.1070	3.98

QTOF-MS/MS: The QTOF Shimadzu 9050 (Kyoto, Japan) spectrometer was equipped with an electrospray ionization (ESI) source. The following QTOF parameters were fixed: nebulizing gas flow, 3 L/min; heating gas flow, 10 L/min; interface temperature, 250 ◦C; desolvation line temperature, 200 ◦C; interface voltage (+), 4.50 kV; heat block temperature, 350 ◦C; and drying gas flow, 10 L/min. MS/MS spectra for all substances were acquired by conducting datadependent acquisition (DDA) function. DDA data were acquired in the range 40–500 m/z and collision energies from – 10 V to – 50 V.

1V-LSD

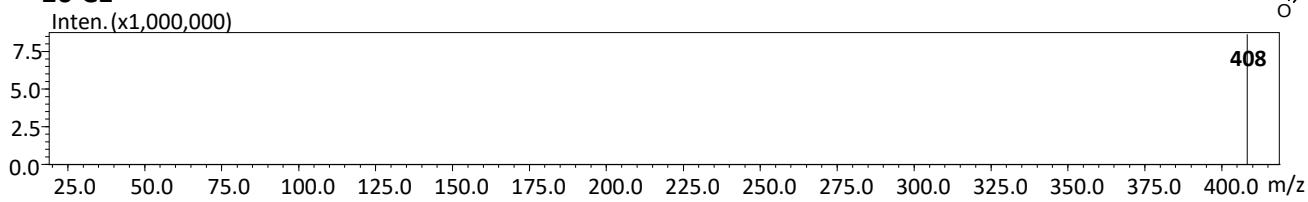


Molecular Formula: $C_{25}H_{33}N_3O_2$

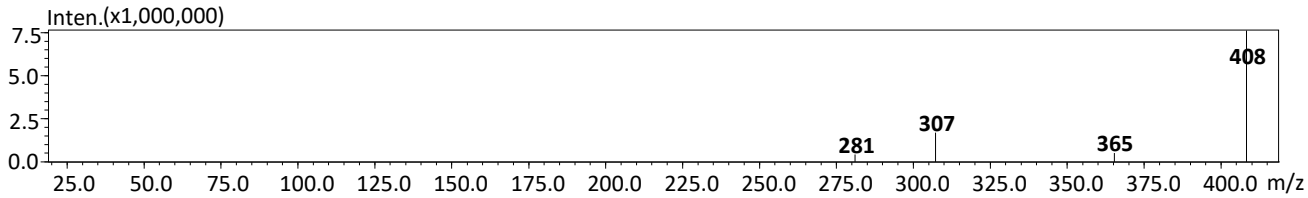
Formula Weight: 407.6

[M+H]$^+$: 408.264554 Da

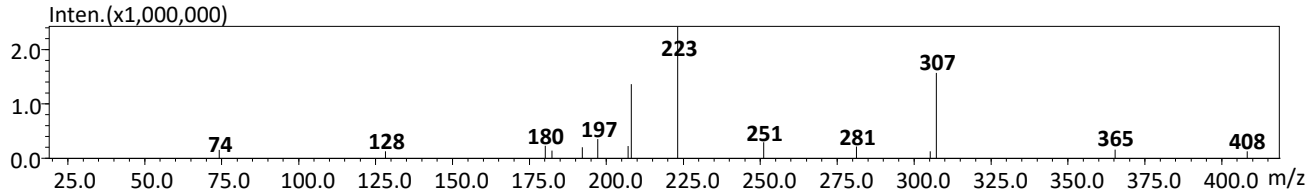
10 CE



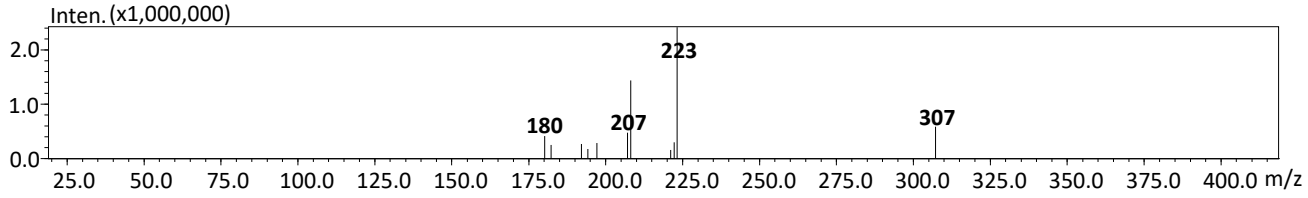
20 CE



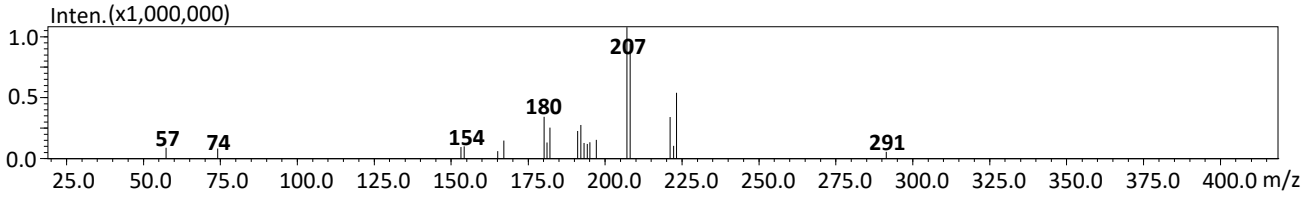
35 CE



40 CE



50 CE



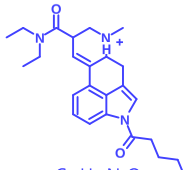
QqQ-MS/MS: Detection of the investigated compounds was achieved with the use of a triple quadrupole mass spectrometer (QqQ, Shimadzu 8060, Kyoto, Japan) in positive mode. The spectrometer was equipped with an electrospray ionization (ESI) sourceThe following MS parameters were fixed: nebulizing gas flow, 3 L/min; heating gas flow, 10 L/min; interface temperature, 250 °C; desolvation line temperature, 200 °C; heat block temperature, 350 °C; and drying gas flow, 10 L/min. Fragmentation MS/MS spectra were acquired by conducting a product ion scan experiment at five collision energies (CE: –10, –20, –35,–40 and –50 V).

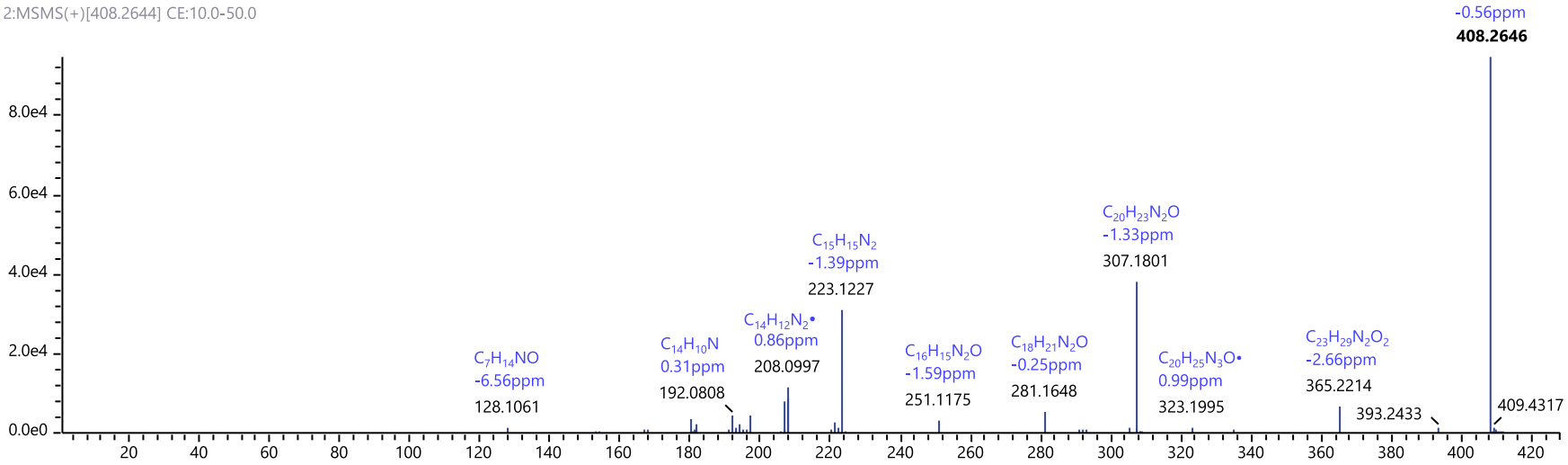
1V-LSD

Molecular Formula: $C_{25}H_{33}N_3O_2$

Formula Weight: 407.6

[M+H]⁺: 408.264554 Da

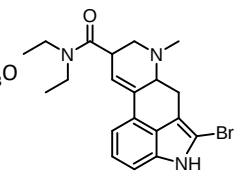




Experimental m/z	Intensity	Molecular Formula	Charge	Predicted m/z	Δ ppm	Experimental m/z	Intensity	Molecular Formula	Charge	Predicted m/z	Δ ppm
408.2643	–	$C_{25}H_{33}N_3O_2$	$[M+H]^+$	408.2646	-0.56	**208.0758**	8679	$C_{14}H_{10}NO$	+	208.0757	0.63
393.2433	1126	–	–	–	–	**207.0911**	8107	$C_{14}H_{11}N_2$	$[+H]^+$	207.0917	-2.80
365.2214	6585	$C_{23}H_{29}N_2O_2$	+	365.2224	-2.66	**197.1075**	4416	$C_{13}H_{13}N_2$	$[+H]^+$	197.1073	0.71
335.1758	753	$C_{21}H_{23}N_2O_2$	+	335.1754	1.07	**194.0969**	2032	$C_{14}H_{12}N$	+	194.0964	2.37
307.1801	38068	$C_{20}H_{23}N_2O$	$[+H]^+$	307.1805	-1.34	**192.0808**	4387	$C_{14}H_{10}N$	+	192.0808	0.31
291.1493	799	$C_{19}H_{19}N_2O$	$[+H]^+$	291.1492	0.24	**182.0970**	2321	$C_{13}H_{12}N$	$[+H]^+$	182.0964	3.24
281.1648	5399	$C_{18}H_{21}N_2O$	+ / [+H]+	281.1648	-0.25	**180.0803**	3538	$C_{13}H_{10}N$	$[+H]^+$	180.0808	-2.55
251.1175	2976	$C_{16}H_{15}N_2O$	+	251.1179	-1.59	**167.0732**	939	$C_{12}H_9N^•$	+	167.0730	1.56
223.1227	30788	$C_{15}H_{15}N_2$	$[+H]^+$	223.1230	-1.39	**154.0656**	421	$C_{11}H_8N$	+	154.0651	2.73
221.1075	2858	$C_{15}H_{13}N_2$	$[+H]^+$	221.1073	0.91	**128.1062**	1459	$C_7H_{14}NO$	$[+H]^+$	128.1070	-6.56
208.0997	11598	$C_{14}H_{12}N_2^•$	$[+H]^+$	208.0995	0.87						

QTOF-MS/MS: The QTOF Shimadzu 9050 (Kyoto, Japan) spectrometer was equipped with an electrospray ionization (ESI) source. The following QTOF parameters were fixed: nebulizing gas flow, 3 L/min; heating gas flow, 10 L/min; interface temperature, 250 ◦C; desolvation line temperature, 200 ◦C; interface voltage (+), 4.50 kV; heat block temperature, 350 ◦C; and drying gas flow, 10 L/min. MS/MS spectra for all substances were acquired by conducting datadependent acquisition (DDA) function. DDA data were acquired in the range 40–500 m/z and collision energies from − 10 V to − 50 V.

2-Bromo-LSD

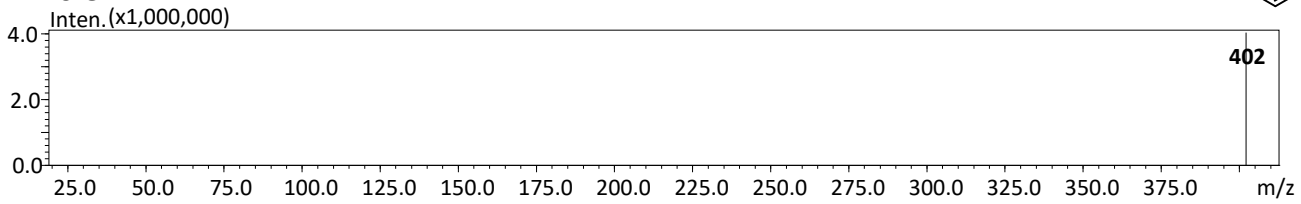


Molecular Formula: $C_{20}H_{24}BrN_3O$

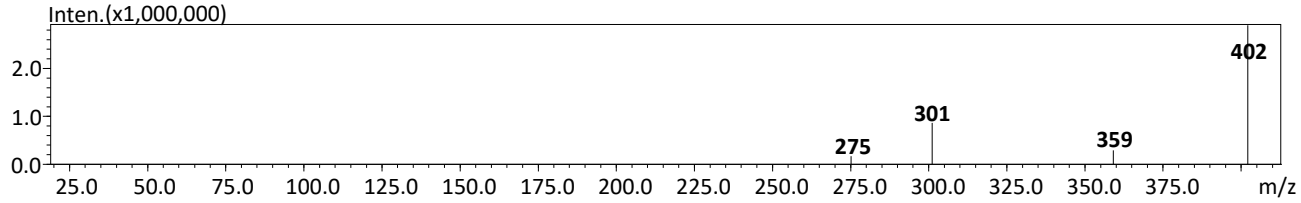
Formula Weight: 402.3

[M+H]$^+$: 402.117544 Da

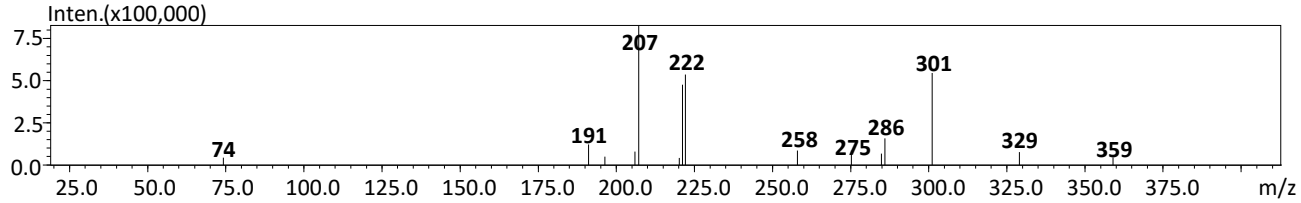
10 CE



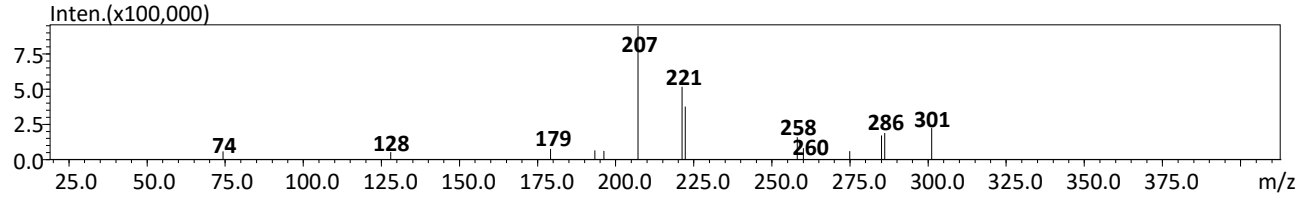
20 CE



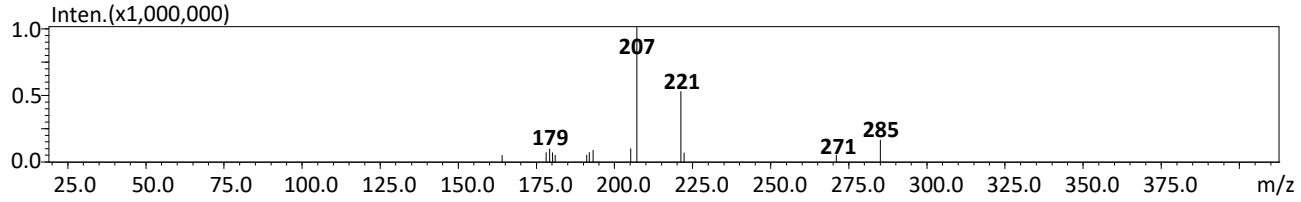
35 CE



40 CE



50 CE



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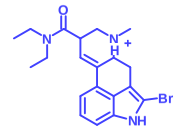
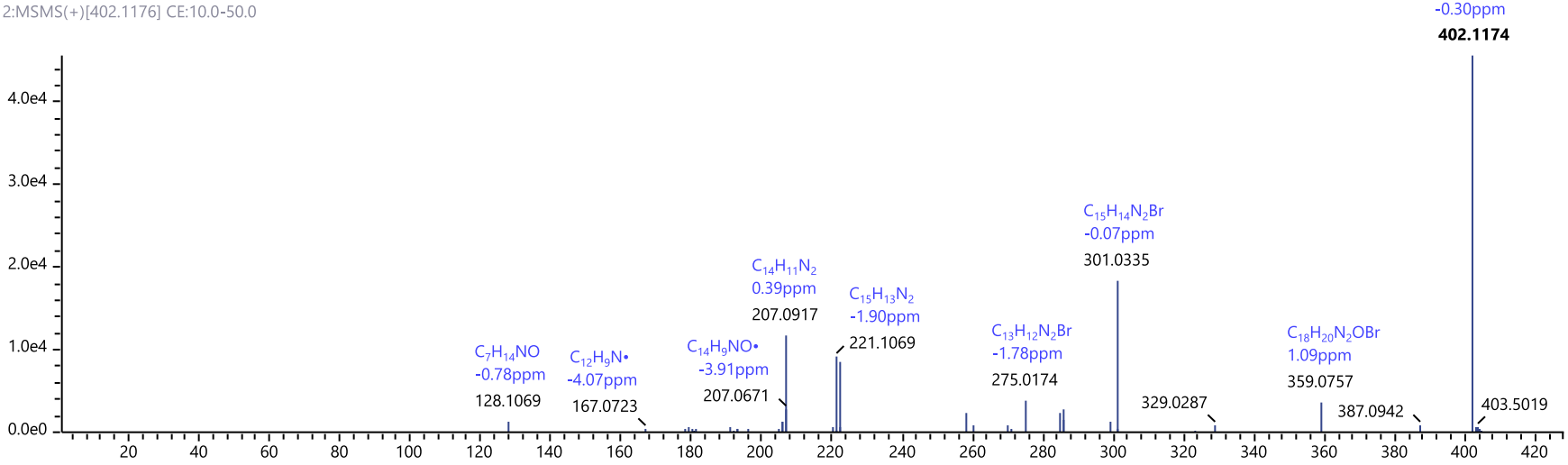
Formula Weight: 402.3

[M+H]$^+$: 402.117544 Da

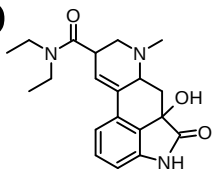




Experimental m/z	Intensity	Molecular Formula	Charge	Predicted m/z	Δ ppm	Experimental m/z	Intensity	Molecular Formula	Charge	Predicted m/z	Δ ppm
402.1174	–	$C_{20}H_{24}N_3OBr$	$[M+H]^+$	402.1176	-0.30	**275.0174**	3777	$C_{13}H_{12}N_2Br$	$[+H]^+$	275.0178	-1.78
387.0942	789	$C_{19}H_{22}N_3OBr^•$	$[+H]^+$	387.0941	0.21	**257.9912**	2328	$C_{13}H_9NBr$	+	257.9913	-0.43
359.0757	3722	$C_{18}H_{20}N_2OBr$	+	359.0754	1.09	**222.1147**	8471	$C_{15}H_{14}N_2^•$	$[+H]^+$	222.1152	-1.85
329.0287	872	$C_{16}H_{14}N_2OBr$	+	329.0284	1.03	**221.1069**	9237	$C_{15}H_{13}N_2$	$[+H]^+$	221.1073	-1.90
301.0335	18343	$C_{15}H_{14}N_2Br$	$[+H]^+$	301.0335	-0.07	**207.0918**	11651	$C_{14}H_{11}N_2$	$[+H]^+$	207.0917	0.39
286.0103	2837	$C_{14}H_{11}N_2Br^•$	$[+H]^+$	286.0100	1.15	**167.0723**	517	$C_{12}H_9N^•$	+	167.0730	-4.07
285.0013	2258	$C_{14}H_{10}N_2Br$	$[+H]^+$	285.0022	-3.23	**128.1069**	1310	$C_7H_{14}NO$	$[+H]^+$	128.1070	-0.78

QTOF-MS/MS: The QTOF Shimadzu 9050 (Kyoto, Japan) spectrometer was equipped with an electrospray ionization (ESI) source. The following QTOF parameters were fixed: nebulizing gas flow, 3 L/min; heating gas flow, 10 L/min; interface temperature, 250 ◦C; desolvation line temperature, 200 ◦C; interface voltage (+), 4.50 kV; heat block temperature, 350 ◦C; and drying gas flow, 10 L/min. MS/MS spectra for all substances were acquired by conducting datadependent acquisition (DDA) function. DDA data were acquired in the range 40–500 m/z and collision energies from − 10 V to − 50 V.

2-oxo-3-OH-LSD

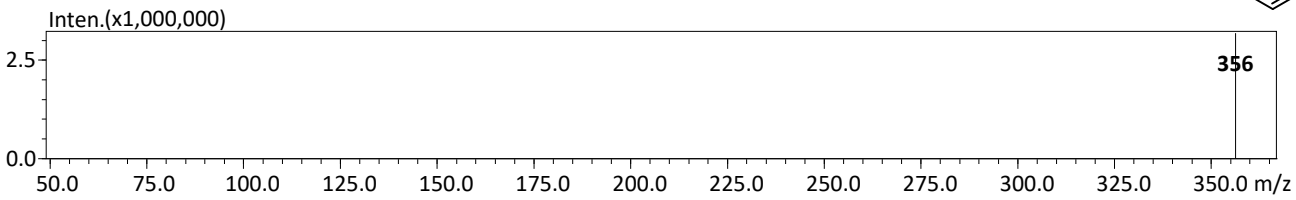


Molecular Formula: $C_{20}H_{25}N_3O_3$

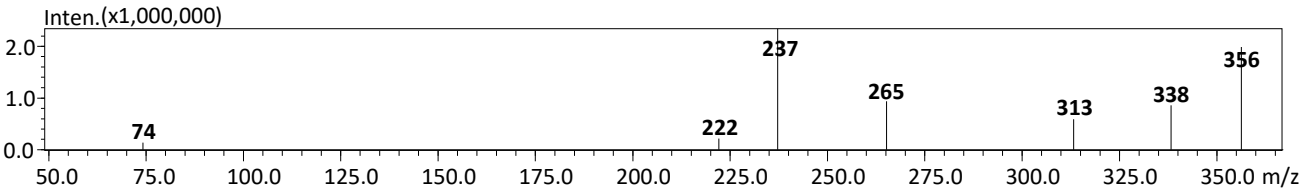
Formula Weight: 355.4

$[M+H]^+$: 356.196868 Da

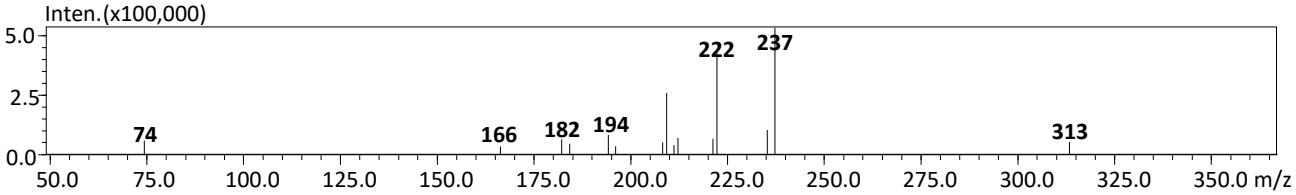
10 CE



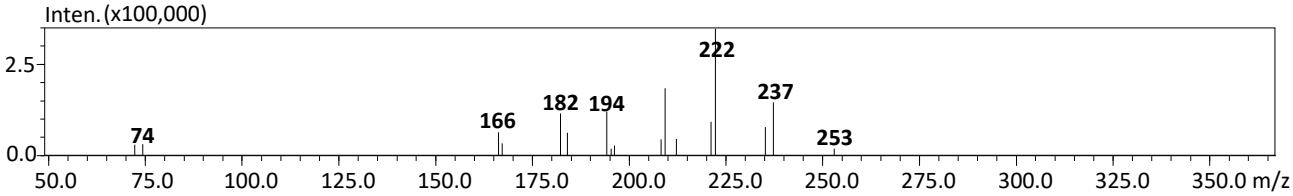
20 CE



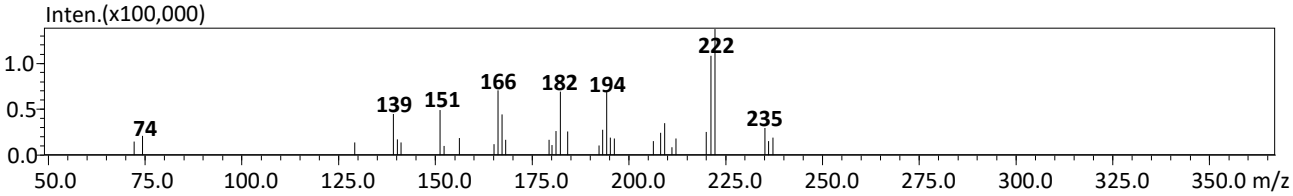
35 CE



40 CE



50 CE



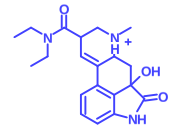
QqQ-MS/MS: Detection of the investigated compounds was achieved with the use of a triple quadrupole mass spectrometer (QqQ, Shimadzu 8060, Kyoto, Japan) in positive mode. The spectrometer was equipped with an electrospray ionization (ESI) sourceThe following MS parameters were fixed: nebulizing gas flow, 3 L/min; heating gas flow, 10 L/min; interface temperature, 250 °C; desolvation line temperature, 200 °C; heat block temperature, 350 °C; and drying gas flow, 10 L/min. Fragmentation MS/MS spectra were acquired by conducting a product ion scan experiment at five collision energies (CE: –10, –20, –35,–40 and –50 V).

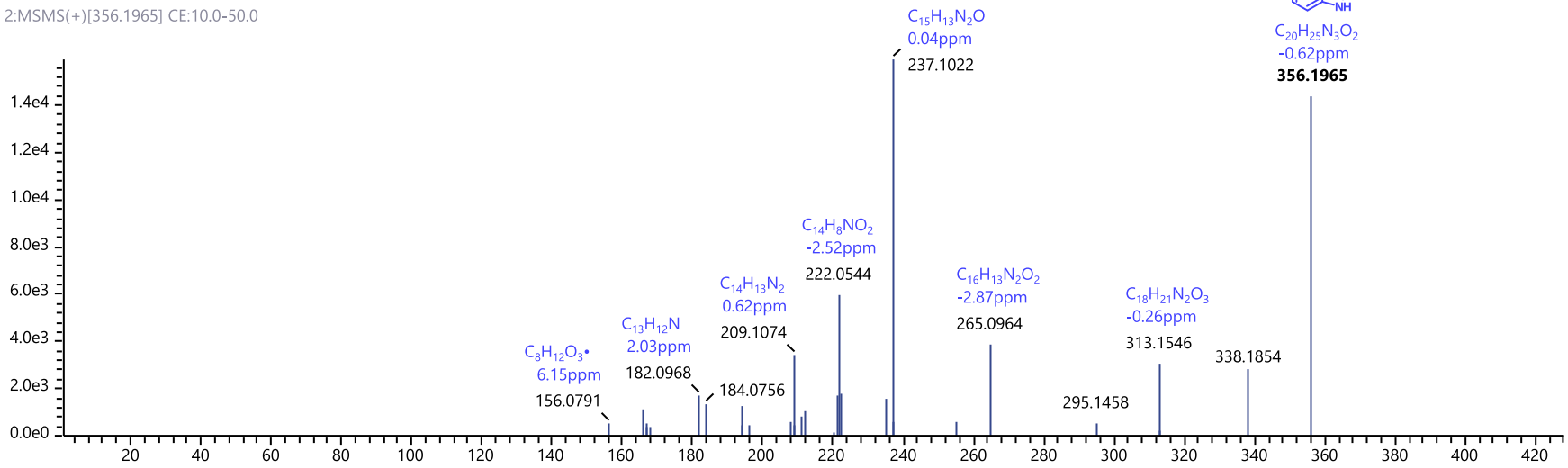
2-oxo-3-OH-LSD

Molecular Formula: $C_{20}H_{25}N_3O_3$

Formula Weight: 355.4

[M+H]$^+$: 356.196868 Da



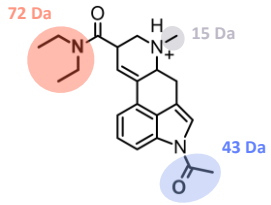
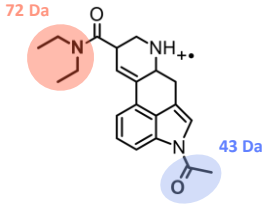
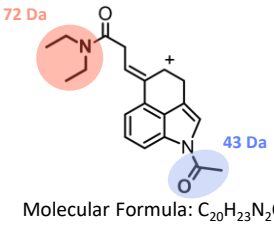
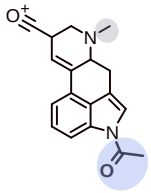
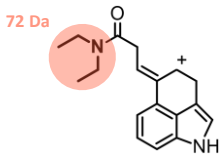
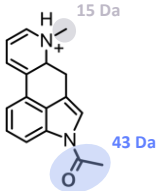
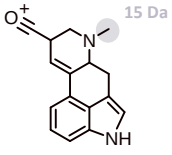


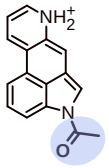
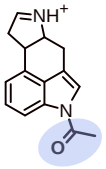
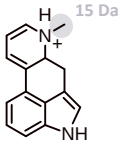
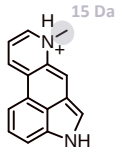
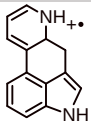
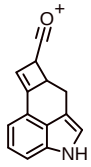
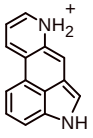
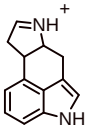
Experimental m/z	Intensity	Molecular Formula	Charge	Predicted m/z	Δ ppm	Experimental m/z	Intensity	Molecular Formula	Charge	Predicted m/z	Δ ppm
356.1965	–	$C_{20}H_{25}N_3O_3$	$[M+H]^+$	356.19665	-0.62	**237.1023**	15947	$C_{15}H_{13}N_2O$	$[+H]^+$	237.1022	0.04
338.1854	2865	$C_{20}H_{24}N_3O_2$	$[+H]^+$	338.1863	-2.54	**222.0544**	5993	$C_{14}H_8NO_2$	+	222.0550	-2.52
313.1546	3062	$C_{18}H_{21}N_2O_3$	+	313.1547	-0.26	**209.1075**	3455	$C_{14}H_{13}N_2$	$[+H]^+$	209.1073	0.62
295.1458	555	–	–	–	–	**184.0756**	1336	$C_{12}H_{10}NO$	$[+H]^+$	184.0757	-0.33
265.0964	3912	$C_{16}H_{13}N_2O_2$	+	265.0972	-2.87	**182.0968**	1688	$C_{13}H_{12}N$	$[+H]^+$	182.0964	2.03
255.1125	600	$C_{15}H_{15}N_2O_2$	$[+H]^+$	255.1128	-1.37	**166.0649**	1122	$C_{12}H_8N$	+	166.0651	-1.45

QTOF-MS/MS: The QTOF Shimadzu 9050 (Kyoto, Japan) spectrometer was equipped with an electrospray ionization (ESI) source. The following QTOF parameters were fixed: nebulizing gas flow, 3 L/min; heating gas flow, 10 L/min; interface temperature, 250 ◦C; desolvation line temperature, 200 ◦C; interface voltage (+), 4.50 kV; heat block temperature, 350 ◦C; and drying gas flow, 10 L/min. MS/MS spectra for all substances were acquired by conducting datadependent acquisition (DDA) function. DDA data were acquired in the range 40–500 m/z and collision energies from – 10 V to – 50 V.

S9. Fragmentation of LSD analogs with the use of QTOF-MS/MS.

Table S9.1. Fragment ions of ALD-52 (1A-LSD)

No	Experimental m/z	Intensity	Structure of ion	Molecular Formula	Charge	Predicted m/z	Δ ppm
Precursor Ion	366.2174	–	 Molecular Formula: $C_{22}H_{28}N_3O_2^+$ Monoisotopic Mass: **366.217604 Da**	$C_{22}H_{27}N_3O_2$	$[M+H]^+$	366.2176	-0.46
1.	351.1970	1149	 Molecular Formula: $C_{21}H_{25}N_3O_2^+$ Monoisotopic Mass: **351.194128 Da**	–	–	–	–
2.	323.1753	6990	 Molecular Formula: $C_{20}H_{23}N_2O_2^+$ Monoisotopic Mass: **323.175404 Da**	$C_{20}H_{23}N_2O_2$	+	323.1754	-0.22
3.	293.1278	1299	 Molecular Formula: $C_{18}H_{17}N_2O_2^+$ Monoisotopic Mass: **293.128454 Da**	$C_{18}H_{17}N_2O_2$	+	293.1285	-2.39
4.	281.1665	676	 Molecular Formula: $C_{18}H_{21}N_2O^+$ Monoisotopic Mass: **281.16484 Da**	–	–	–	–
5.	265.1334	37176	 Molecular Formula: $C_{17}H_{17}N_2O^+$ Monoisotopic Mass: **265.13354 Da**	$C_{17}H_{17}N_2O$	$[+H]^+$	265.1335	-0.72
6.	251.1173	2252	 Molecular Formula: $C_{16}H_{15}N_2O^+$ Monoisotopic Mass: **251.11789 Da**	$C_{16}H_{15}N_2O$	+	251.1179	-2.47

7.	249.1006	2168	 Molecular Formula: $C_{16}H_{13}N_2O^+$ Monoisotopic Mass: **249.102239 Da**	–	–	–	–
8.	239.1178	4176	 Molecular Formula: $C_{15}H_{15}N_2O^+$ Monoisotopic Mass: **239.11789 Da**	$C_{15}H_{15}N_2O$	$[+H]^+$	239.1179	-0.34
9.	223.1226	27549	 Molecular Formula: $C_{15}H_{15}N_2^+$ Monoisotopic Mass: **223.122975 Da**	$C_{15}H_{15}N_2$	$[+H]^+$	223.1230	-1.48
10.	221.1071	4161	 Molecular Formula: $C_{15}H_{13}N_2^+$ Monoisotopic Mass: **221.107325 Da**	$C_{15}H_{13}N_2$	$[+H]^+$	221.1073	-1.09
11.	208.0992	12074	 Molecular Formula: $C_{14}H_{12}N_2^+$ Monoisotopic Mass: **208.0995 Da**	$C_{14}H_{12}N_2^{\bullet}$	$[+H]^+$	208.0995	-1.54
12.	208.0755	8781	 Molecular Formula: $C_{14}H_{10}NO^+$ Monoisotopic Mass: **208.07569 Da**	$C_{14}H_{10}NO$	+	208.0757	-1.11
13.	207.0917	10815	 Molecular Formula: $C_{14}H_{11}N_2^+$ Monoisotopic Mass: **207.091675 Da**	$C_{14}H_{11}N_2$	$[+H]^+$	207.0917	-0.05
14.	197.1071	5245	 Molecular Formula: $C_{13}H_{13}N_2^+$ Monoisotopic Mass: **197.107325 Da**	$C_{13}H_{13}N_2$	$[+H]^+$	197.1073	-1.02

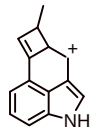
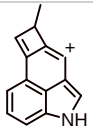
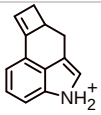
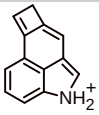
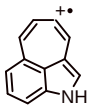
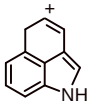
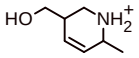
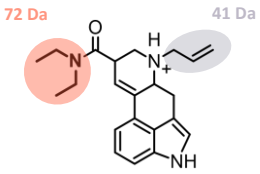
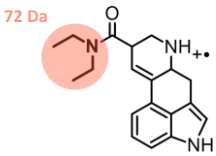
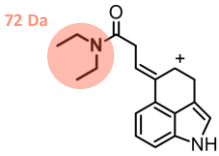
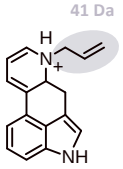
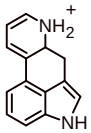
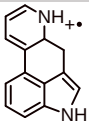
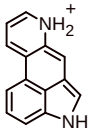
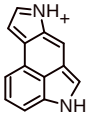
15.	194.0960	1741	 Molecular Formula: $C_{14}H_{12}N^+$ Monoisotopic Mass: **194.096426 Da**	$C_{14}H_{12}N$	+	194.0964	-1.44
16.	192.0810	4121	 Molecular Formula: $C_{14}H_{10}N^+$ Monoisotopic Mass: **192.080776 Da**	$C_{14}H_{10}N$	+	192.0808	1.35
17.	182.0969	1885	 Molecular Formula: $C_{13}H_{12}N^+$ Monoisotopic Mass: **182.096426 Da**	$C_{13}H_{12}N$	$[+H]^+$	182.0964	2.42
18.	180.0810	4706	 Molecular Formula: $C_{13}H_{10}N^+$ Monoisotopic Mass: **180.080776 Da**	$C_{13}H_{10}N$	$[+H]^+$	180.0808	1.06
19.	167.0729	1219	 Molecular Formula: $C_{12}H_9N^+$ Monoisotopic Mass: **167.072951 Da**	$C_{12}H_9N^{\bullet}$	+	167.0730	-0.36
20.	154.0648	772	 Molecular Formula: $C_{11}H_8N^+$ Monoisotopic Mass: **154.065126 Da**	$C_{11}H_8N$	+	154.0651	-2.47
21.	128.1060	1385	 Molecular Formula: $C_7H_{14}NO^+$ Monoisotopic Mass: **128.10699 Da**	$C_7H_{14}NO$	$[+H]^+$	128.1070	-7.81

Table S9.2. Fragment ions of AL-LAD

No	Experimental m/z	Intensity	Structure of ion	Molecular Formula	Charge	Predicted m/z	Δ ppm
Precursor Ion	350.2226	–	 Molecular Formula: $C_{22}H_{28}N_3O^+$ Monoisotopic Mass: **350.222689 Da**	$C_{22}H_{27}N_3O$	$[M+H]^+$	349.2154	-0.37
1.	309.1837	64399	 Molecular Formula: $C_{19}H_{23}N_3O^+$ Monoisotopic Mass: **309.183564 Da**	$C_{19}H_{23}N_3O^{\bullet}$	$[+H]^+$	309.1836	0.32
2.	281.1654	2124	 Molecular Formula: $C_{18}H_{21}N_2O^+$ Monoisotopic Mass: **281.16484 Da**	$C_{18}H_{21}N_2O$	+	281.1648	1.96
3.	249.1398	766	 Molecular Formula: $C_{17}H_{17}N_2^+$ Monoisotopic Mass: **249.138625 Da**	–	–	–	–
4.	209.1067	3870	 Molecular Formula: $C_{14}H_{13}N_2^+$ Monoisotopic Mass: **209.107325 Da**	$C_{14}H_{13}N_2$	$[+H]^+$	209.1073	-2.77
5.	208.0994	47757	 Molecular Formula: $C_{14}H_{12}N_2^+$ Monoisotopic Mass: **208.0995 Da**	$C_{14}H_{12}N_2^{\bullet}$	$[+H]^+$	208.0995	-0.38
6.	207.0918	29030	 Molecular Formula: $C_{14}H_{11}N_2^+$ Monoisotopic Mass: **207.091675 Da**	$C_{14}H_{11}N_2$	$[+H]^+$	207.0917	0.77
7.	193.0758	14964	 Molecular Formula: $C_{13}H_9N_2^+$ Monoisotopic Mass: **193.076025 Da**	$C_{13}H_9N_2$	$[+H]^+$	193.0760	-1.09

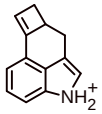
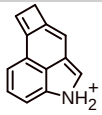
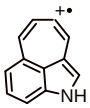
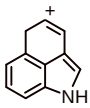
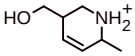
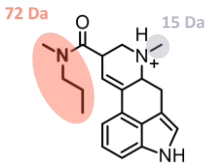
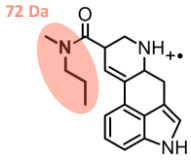
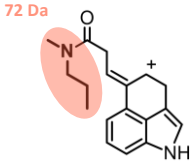
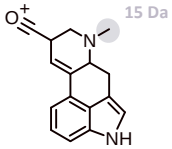
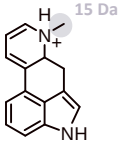
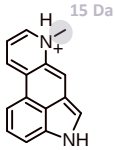
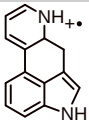
8.	182.0835	8278	 Molecular Formula: $C_{13}H_{12}N^+$ Monoisotopic Mass: **182.096426 Da**	$C_{12}H_{10}N_2^{\bullet}$	$[+H]^+$	182.0839	-1.81
9.	180.0810	5845	 Molecular Formula: $C_{13}H_{10}N^+$ Monoisotopic Mass: **180.080776 Da**	$C_{13}H_{10}N$	$[+H]^+$	180.0810	0.94
10.	167.0727	982	 Molecular Formula: $C_{12}H_9N^+$ Monoisotopic Mass: **167.072951 Da**	$C_{12}H_9N^{\bullet}$	+	167.0730	-1.62
11.	154.0654	1515	 Molecular Formula: $C_{11}H_8N^+$ Monoisotopic Mass: **154.065126 Da**	$C_{11}H_8N$	+	154.0651	1.95
12.	128.1080	881	 Molecular Formula: $C_7H_{14}NO^+$ Monoisotopic Mass: **128.10699 Da**	–	–	–	–

Table S9.3. Fragment ions of LAMPA

No	Experimental m/z	Intensity	Structure of ion	Molecular Formula	Charge	Predicted m/z	Δ ppm
Precursor Ion	324.2070	–	 Molecular Formula: $C_{20}H_{26}N_3O^+$ Monoisotopic Mass: **324.207039 Da**	$C_{20}H_{25}N_3O$	$[M+H]^+$	324.2070	-0.25
1.	309.1835	825	 Molecular Formula: $C_{19}H_{23}N_3O^+$ Monoisotopic Mass: **309.183564 Da**	$C_{19}H_{23}N_3O^{\bullet}$	$[+H]^+$	309.1836	-0.13
2.	281.1644	5084	 Molecular Formula: $C_{18}H_{21}N_2O^+$ Monoisotopic Mass: **281.16484 Da**	$C_{18}H_{21}N_2O$	+	281.1648	-1.67
3.	251.1181	2257	 Molecular Formula: $C_{16}H_{15}N_2O^+$ Monoisotopic Mass: **251.11789 Da**	$C_{16}H_{15}N_2O$	+	251.1179	0.96
4.	223.1228	42597	 Molecular Formula: $C_{15}H_{15}N_2^+$ Monoisotopic Mass: **223.122975 Da**	$C_{15}H_{15}N_2$	$[+H]^+$	223.1230	-0.85
5.	221.1077	4924	 Molecular Formula: $C_{15}H_{13}N_2^+$ Monoisotopic Mass: **221.107325 Da**	$C_{15}H_{13}N_2$	$[+H]^+$	221.1073	1.81
6.	208.0995	14968	 Molecular Formula: $C_{14}H_{12}N_2^+$ Monoisotopic Mass: **208.0995 Da**	$C_{14}H_{12}N_2^{\bullet}$	$[+H]^+$	208.0995	-0.14

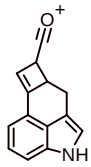
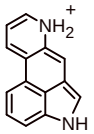
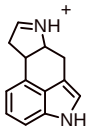
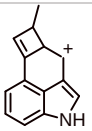
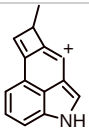
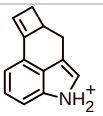
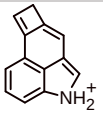
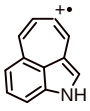
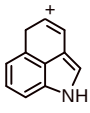
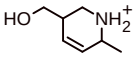
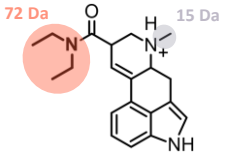
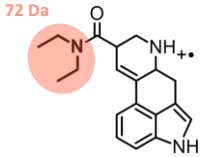
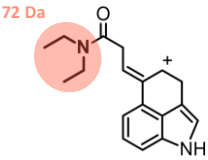
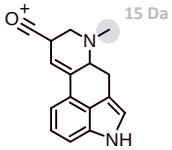
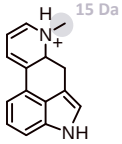
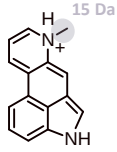
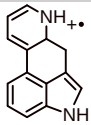
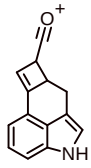
7.	208.0758	8647	 Molecular Formula: $C_{14}H_{10}NO^+$ Monoisotopic Mass: **208.07569 Da**	$C_{14}H_{10}NO$	+	208.0757	0.34
8.	207.0917	20585	 Molecular Formula: $C_{14}H_{11}N_2^+$ Monoisotopic Mass: **207.091675 Da**	$C_{14}H_{11}N_2$	$[+H]^+$	207.0917	0.15
9.	197.1073	7040	 Molecular Formula: $C_{13}H_{13}N_2^+$ Monoisotopic Mass: **197.107325 Da**	$C_{13}H_{13}N_2$	$[+H]^+$	197.1073	-0.05
10.	194.0959	2392	 Molecular Formula: $C_{14}H_{12}N^+$ Monoisotopic Mass: **194.096426 Da**	$C_{14}H_{12}N$	+	194.0964	-2.63
11.	192.0810	5844	 Molecular Formula: $C_{14}H_{10}N^+$ Monoisotopic Mass: **192.080776 Da**	$C_{14}H_{10}N$	+	192.0808	1.25
12.	182.0964	2033	 Molecular Formula: $C_{13}H_{12}N^+$ Monoisotopic Mass: **182.096426 Da**	$C_{13}H_{12}N$	$[+H]^+$	182.0964	0.06
13.	180.0805	8748	 Molecular Formula: $C_{13}H_{10}N^+$ Monoisotopic Mass: **180.080776 Da**	$C_{13}H_{10}N$	$[+H]^+$	180.0808	-1.50
14.	167.0732	3609	 Molecular Formula: $C_{12}H_9N^+$ Monoisotopic Mass: **167.072951 Da**	$C_{12}H_9N^{\bullet}$	+	167.0730	1.56
15.	154.0657	1434	 Molecular Formula: $C_{11}H_8N^+$ Monoisotopic Mass: **154.065126 Da**	$C_{11}H_8N$	+	154.0651	3.57
16.	128.1069	1731	 Molecular Formula: $C_7H_{14}NO^+$ Monoisotopic Mass: **128.10699 Da**	$C_7H_{14}NO$	$[+H]^+$	128.1070	-1.02

Table S9.4. Fragment ions of LSD

No	Experimental m/z	Intensity	Structure of ion	Molecular Formula	Charge	Predicted m/z	Δ ppm
Precursor Ion	324.2069	–	 Molecular Formula: $C_{20}H_{26}N_3O^+$ Monoisotopic Mass: **324.207039 Da**	$C_{20}H_{25}N_3O$	$[M+H]^+$	324.2070	-0.56
1.	309.1821	498	 Molecular Formula: $C_{19}H_{23}N_3O^+$ Monoisotopic Mass: **309.183564 Da**	–	–	–	–
2.	281.1653	2304	 Molecular Formula: $C_{18}H_{21}N_2O^+$ Monoisotopic Mass: **281.16484 Da**	$C_{18}H_{21}N_2O$	+	281.1648	1.46
3.	251.1178	741	 Molecular Formula: $C_{16}H_{15}N_2O^+$ Monoisotopic Mass: **251.11789 Da**	$C_{16}H_{15}N_2O$	+	251.1179	-0.52
4.	223.1226	9564	 Molecular Formula: $C_{15}H_{15}N_2^+$ Monoisotopic Mass: **223.122975 Da**	$C_{15}H_{15}N_2$	+	223.1230	-1.70
5.	221.1074	912	 Molecular Formula: $C_{15}H_{13}N_2^+$ Monoisotopic Mass: **221.107325 Da**	$C_{15}H_{13}N_2$	$[+H]^+$	221.1073	0.36
6.	208.0994	4316	 Molecular Formula: $C_{14}H_{12}N_2^+$ Monoisotopic Mass: **208.0995 Da**	$C_{14}H_{12}N_2^{\bullet}$	$[+H]^+$	208.0995	-0.38
7.	208.0758	2246	 Molecular Formula: $C_{14}H_{10}NO^+$ Monoisotopic Mass: **208.07569 Da**	$C_{14}H_{10}NO$	+	208.0757	0.48

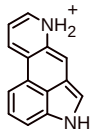
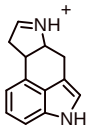
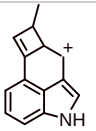
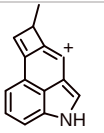
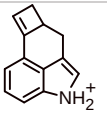
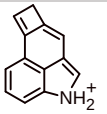
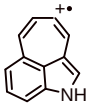
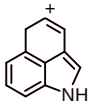
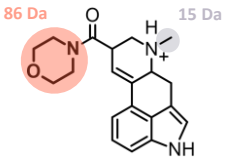
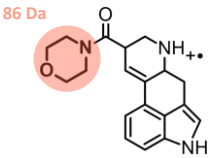
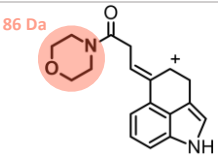
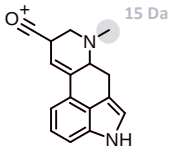
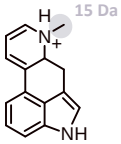
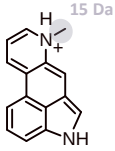
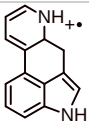
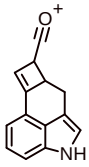
8.	207.0911	5088	 Molecular Formula: $C_{14}H_{11}N_2^+$ Monoisotopic Mass: **207.091675 Da**	$C_{14}H_{11}N_2$	$[+H]^+$	207.0917	-2.80
9.	197.1076	2493	 Molecular Formula: $C_{13}H_{13}N_2^+$ Monoisotopic Mass: **197.107325 Da**	$C_{13}H_{13}N_2$	$[+H]^+$	197.1073	1.47
10.	194.0965	825	 Molecular Formula: $C_{14}H_{12}N^+$ Monoisotopic Mass: **194.096426 Da**	$C_{14}H_{12}N$	+	194.0964	0.36
11.	192.0804	1581	 Molecular Formula: $C_{14}H_{10}N^+$ Monoisotopic Mass: **192.080776 Da**	$C_{14}H_{10}N$	+	192.0808	-1.98
12.	182.0827	1136	 Molecular Formula: $C_{13}H_{12}N^+$ Monoisotopic Mass: **182.096426 Da**	–	–	–	–
13.	180.0808	2884	 Molecular Formula: $C_{13}H_{10}N^+$ Monoisotopic Mass: **180.080776 Da**	$C_{13}H_{10}N$	$[+H]^+$	180.0808	0.0
14.	167.0725	735	 Molecular Formula: $C_{12}H_9N^+$ Monoisotopic Mass: **167.072951 Da**	$C_{12}H_9N^{\bullet}$	+	167.0730	-2.69
15.	154.0638	484	 Molecular Formula: $C_{11}H_8N^+$ Monoisotopic Mass: **154.065126 Da**	–	–	–	–

Table S9.5. Fragment ions of LSM-775

No	Experimental m/z	Intensity	Structure of ion	Molecular Formula	Charge	Predicted m/z	Δ ppm
Precursor Ion	338.1862	–	 Molecular Formula: $C_{24}H_{30}N_3O_2^+$ Monoisotopic Mass: **392.233254 Da**	$C_{20}H_{23}N_3O_2$	$[M+H]^+$	338.1863	-0.33
1.	323.1627	2011	 Molecular Formula: $C_{19}H_{21}N_3O_2^+$ Monoisotopic Mass: **323.162828 Da**	$C_{19}H_{21}N_3O_2•$	$[+H]^+$	323.1628	-0.53
2.	295.1436	6431	 Molecular Formula: $C_{18}H_{19}N_2O_2^+$ Monoisotopic Mass: **295.144104 Da**	$C_{18}H_{19}N_2O_2$	+	295.1441	-1.86
3.	251.1174	2441	 Molecular Formula: $C_{16}H_{15}N_2O^+$ Monoisotopic Mass: **251.11789 Da**	$C_{16}H_{15}N_2O$	+	251.1179	-2.07
4.	223.1225	34108	 Molecular Formula: $C_{15}H_{15}N_2^+$ Monoisotopic Mass: **223.122975 Da**	$C_{15}H_{15}N_2$	$[+H]^+$	223.1230	-1.93
5.	221.1070	2893	 Molecular Formula: $C_{15}H_{13}N_2^+$ Monoisotopic Mass: **221.107325 Da**	$C_{15}H_{13}N_2$	$[+H]^+$	221.1073	-1.67
6.	208.0996	12610	 Molecular Formula: $C_{14}H_{12}N_2^+$ Monoisotopic Mass: **208.0995 Da**	$C_{14}H_{12}N_2•$	$[+H]^+$	208.0995	0.29
7.	208.0752	10511	 Molecular Formula: $C_{14}H_{10}NO^+$ Monoisotopic Mass: **208.07569 Da**	$C_{14}H_{10}NO$	+	208.0757	-2.21

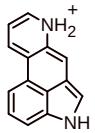
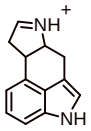
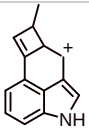
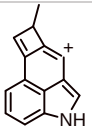
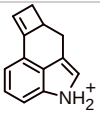
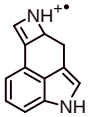
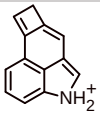
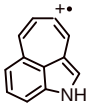
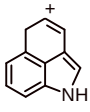
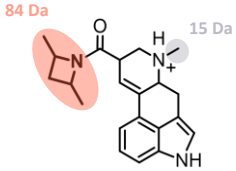
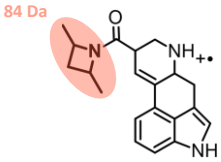
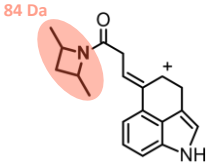
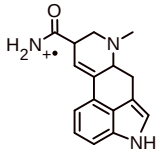
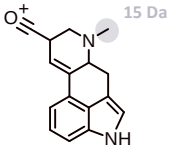
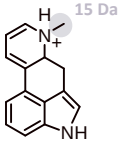
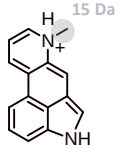
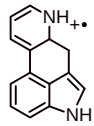
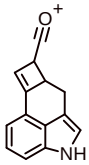
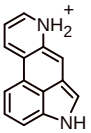
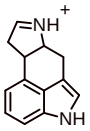
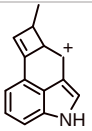
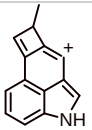
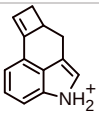
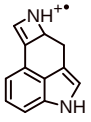
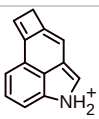
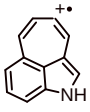
8.	207.0915	14996	 Molecular Formula: $C_{14}H_{11}N_2^+$ Monoisotopic Mass: **207.091675 Da**	$C_{14}H_{11}N_2$	$[+H]^+$	207.0917	-0.68
9.	197.1076	7508	 Molecular Formula: $C_{13}H_{13}N_2^+$ Monoisotopic Mass: **197.107325 Da**	$C_{13}H_{13}N_2$	$[+H]^+$	197.1073	1.42
10.	194.0964	1957	 Molecular Formula: $C_{14}H_{12}N^+$ Monoisotopic Mass: **194.096426 Da**	$C_{14}H_{12}N$	+	194.0964	0.0
11.	192.0804	5097	 Molecular Formula: $C_{14}H_{10}N^+$ Monoisotopic Mass: **192.080776 Da**	$C_{14}H_{10}N$	+	192.0808	-2.14
12.	182.0962	2034	 Molecular Formula: $C_{13}H_{12}N^+$ Monoisotopic Mass: **182.096426 Da**	$C_{13}H_{12}N$	$[+H]^+$	182.0964	-1.04
13.	182.0833	3442	 Molecular Formula: $C_{12}H_{10}N_2^+$ Monoisotopic Mass: **182.08385 Da**	$C_{12}H_{10}N_2^{\bullet}$	$[+H]^+$	182.0839	-3.13
14.	180.0804	7331	 Molecular Formula: $C_{13}H_{10}N^+$ Monoisotopic Mass: **180.080776 Da**	$C_{13}H_{10}N$	$[+H]^+$	180.0808	-2.39
15.	167.0725	2292	 Molecular Formula: $C_{12}H_9N^+$ Monoisotopic Mass: **167.072951 Da**	$C_{12}H_9N^{\bullet}$	+	167.0730	-2.81
16.	154.0660	1171	 Molecular Formula: $C_{11}H_8N^+$ Monoisotopic Mass: **154.065126 Da**	$C_{11}H_8N$	+	154.0651	5.52
17.	142.0873	904	 Molecular Formula: $C_7H_{12}NO_2^+$ Monoisotopic Mass: **142.086255 Da**	–	–	–	–
18.	88.0752	832	 Molecular Formula: $C_4H_{10}NO^+$ Monoisotopic Mass: **88.07569 Da**	$C_4H_{10}NO$	$[+H]^+$	88.0757	-5.11

Table S9.6. Fragment ions of LSZ

No	Experimental m/z	Intensity	Structure of ion	Molecular Formula	Charge	Predicted m/z	Δ ppm
Precursor Ion	336.2068	–	 Molecular Formula: $C_{21}H_{26}N_3O^+$ Monoisotopic Mass: **336.207039 Da**	$C_{21}H_{25}N_3O$	$[M+H]^+$	336.2070	-0.68
1.	321.1829	492	 Molecular Formula: $C_{20}H_{23}N_3O^+$ Monoisotopic Mass: **321.183564 Da**	$C_{20}H_{23}N_3O^{\bullet}$	$[+H]^+$	321.1836	-1.93
2.	293.1649	4579	 Molecular Formula: $C_{19}H_{21}N_2O^+$ Monoisotopic Mass: **293.16484 Da**	$C_{19}H_{21}N_2O$	+	293.1648	0.03
3.	267.1370	2002	 Molecular Formula: $C_{16}H_{17}N_3O^+$ Monoisotopic Mass: **267.136614 Da**	$C_{16}H_{17}N_3O^{\bullet}$	$[+H]^+$	267.1366	1.31
4.	251.1177	5292	 Molecular Formula: $C_{16}H_{15}N_2O^+$ Monoisotopic Mass: **251.11789 Da**	$C_{16}H_{15}N_2O$	+	251.1179	-0.96
5.	223.1228	29322	 Molecular Formula: $C_{15}H_{15}N_2^+$ Monoisotopic Mass: **223.122975 Da**	$C_{15}H_{15}N_2$	$[+H]^+$	223.1230	-0.72
6.	221.1072	7093	 Molecular Formula: $C_{15}H_{13}N_2^+$ Monoisotopic Mass: **221.107325 Da**	$C_{15}H_{13}N_2$	$[+H]^+$	221.1073	-0.77

7.	208.0995	10522	 Molecular Formula: $C_{14}H_{12}N_2^+$ Monoisotopic Mass: **208.0995 Da**	$C_{14}H_{12}N_2\bullet$	$[+H]^+$	208.0995	-0.10
8.	208.0753	7079	 Molecular Formula: $C_{14}H_{10}NO^+$ Monoisotopic Mass: **208.07569 Da**	$C_{14}H_{10}NO$	+	208.0757	-1.78
9.	207.0921	14125	 Molecular Formula: $C_{14}H_{11}N_2^+$ Monoisotopic Mass: **207.091675 Da**	$C_{14}H_{11}N_2$	$[+H]^+$	207.0917	1.84
10.	197.1070	9037	 Molecular Formula: $C_{13}H_{13}N_2^+$ Monoisotopic Mass: **197.107325 Da**	$C_{13}H_{13}N_2$	$[+H]^+$	197.1073	-1.62
11.	194.0962	2091	 Molecular Formula: $C_{14}H_{12}N^+$ Monoisotopic Mass: **194.096426 Da**	$C_{14}H_{12}N$	+	194.0964	-0.98
12.	192.0809	3611	 Molecular Formula: $C_{14}H_{10}N^+$ Monoisotopic Mass: **192.080776 Da**	$C_{14}H_{10}N$	+	192.0808	0.42
13.	182.0970	1242	 Molecular Formula: $C_{13}H_{12}N^+$ Monoisotopic Mass: **182.096426 Da**	$C_{13}H_{12}N$	$[+H]^+$	182.0964	3.35
14.	182.0840	3034	 Molecular Formula: $C_{12}H_{10}N_2^+$ Monoisotopic Mass: **182.08385 Da**	$C_{12}H_{10}N_2\bullet$	$[+H]^+$	182.0839	0.82
15.	180.0806	5516	 Molecular Formula: $C_{13}H_{10}N^+$ Monoisotopic Mass: **180.080776 Da**	$C_{13}H_{10}N$	$[+H]^+$	180.0808	-1.06
16.	167.0727	2450	 Molecular Formula: $C_{12}H_9N^+$ Monoisotopic Mass: **167.072951 Da**	$C_{12}H_9N\bullet$	+	167.0730	-1.38

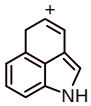
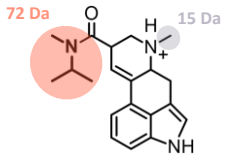
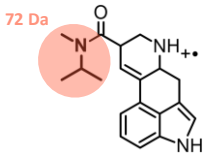
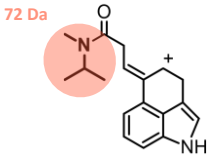
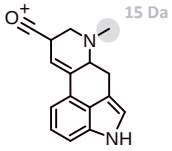
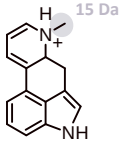
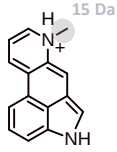
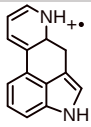
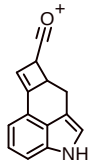
17.	154.0652	3163	 Molecular Formula: $C_{11}H_8N^+$ Monoisotopic Mass: **154.065126 Da**	$C_{11}H_8N$	+	154.0651	0.33
18.	140.1068	7287	 Molecular Formula: $C_8H_{14}NO^+$ Monoisotopic Mass: **140.10699 Da**	$C_8H_{14}NO$	$[+H]^+$	140.1070	-1.50
19.	98.0602	2273	 Molecular Formula: $C_5H_8NO^+$ Monoisotopic Mass: **98.06004 Da**	C_5H_8NO	$[+H]^+$	98.0600	1.33

Table S9.7. Fragment ions of MiPLA

No	Experimental m/z	Intensity	Structure of ion	Molecular Formula	Charge	Predicted m/z	Δ ppm
Precursor Ion	324.2069	–	 Molecular Formula: $C_{20}H_{26}N_3O^+$ Monoisotopic Mass: **324.207039 Da**	$C_{20}H_{25}N_3O$	$[M+H]^+$	324.2070	-0.40
1.	309.1832	529	 Molecular Formula: $C_{19}H_{23}N_3O^+$ Monoisotopic Mass: **309.183564 Da**	$C_{19}H_{23}N_3O^{\bullet}$	$[+H]^+$	309.1836	-1.29
2.	281.1638	5953	 Molecular Formula: $C_{18}H_{21}N_2O^+$ Monoisotopic Mass: **281.16484 Da**	–	–	–	–
3.	251.1170	2414	 Molecular Formula: $C_{16}H_{15}N_2O^+$ Monoisotopic Mass: **251.11789 Da**	$C_{16}H_{15}N_2O$	+	251.1179	-3.39
4.	223.1226	42759	 Molecular Formula: $C_{15}H_{15}N_2^+$ Monoisotopic Mass: **223.122975 Da**	$C_{15}H_{15}N_2$	$[+H]^+$	223.1230	-1.61
5.	221.1072	3824	 Molecular Formula: $C_{15}H_{13}N_2^+$ Monoisotopic Mass: **221.107325 Da**	$C_{15}H_{13}N_2$	$[+H]^+$	221.1073	-0.50
6.	208.0996	15828	 Molecular Formula: $C_{14}H_{12}N_2^+$ Monoisotopic Mass: **208.0995 Da**	$C_{14}H_{12}N_2^{\bullet}$	$[+H]^+$	208.0995	0.24
7.	208.0755	7244	 Molecular Formula: $C_{14}H_{10}NO^+$ Monoisotopic Mass: **208.07569 Da**	$C_{14}H_{10}NO$	+	208.0757	-0.87

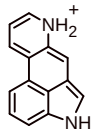
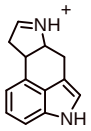
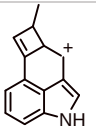
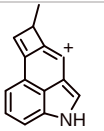
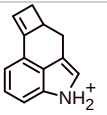
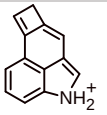
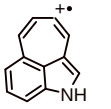
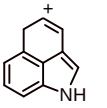
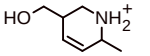
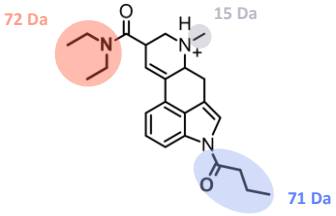
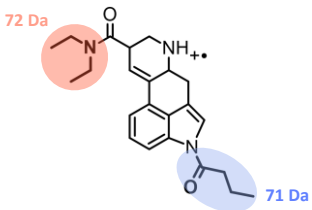
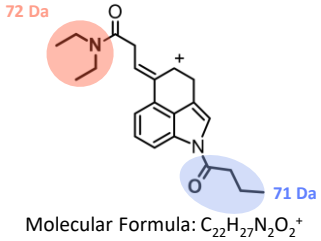
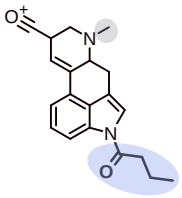
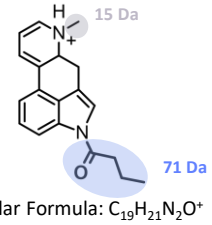
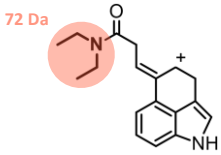
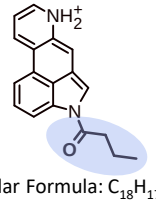
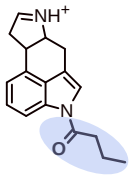
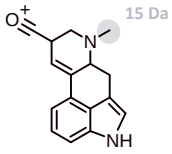
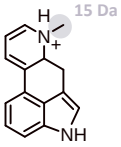
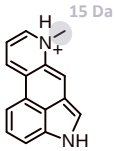
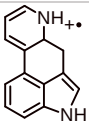
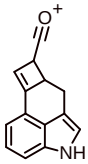
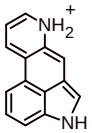
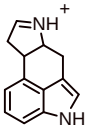
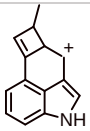
8.	207.0916	20540	 Molecular Formula: $C_{14}H_{11}N_2^+$ Monoisotopic Mass: **207.091675 Da**	$C_{14}H_{11}N_2$	$[+H]^+$	207.0917	-0.58
9.	197.1071	5122	 Molecular Formula: $C_{13}H_{13}N_2^+$ Monoisotopic Mass: **197.107325 Da**	$C_{13}H_{13}N_2$	$[+H]^+$	197.1073	-1.22
10.	194.0964	2448	 Molecular Formula: $C_{14}H_{12}N^+$ Monoisotopic Mass: **194.096426 Da**	$C_{14}H_{12}N$	+	194.0964	0.0
11.	192.0811	5399	 Molecular Formula: $C_{14}H_{10}N^+$ Monoisotopic Mass: **192.080776 Da**	$C_{14}H_{10}N$	+	192.0808	1.46
12.	182.0962	2565	 Molecular Formula: $C_{13}H_{12}N^+$ Monoisotopic Mass: **182.096426 Da**	$C_{13}H_{12}N$	$[+H]^+$	182.0964	-1.48
13.	180.0807	7459	 Molecular Formula: $C_{13}H_{10}N^+$ Monoisotopic Mass: **180.080776 Da**	$C_{13}H_{10}N$	$[+H]^+$	180.0808	-0.67
14.	167.0724	3397	 Molecular Formula: $C_{12}H_9N^+$ Monoisotopic Mass: **167.072951 Da**	$C_{12}H_9N^{\bullet}$	+	167.0730	-3.35
15.	154.0650	1464	 Molecular Formula: $C_{11}H_8N^+$ Monoisotopic Mass: **154.065126 Da**	$C_{11}H_8N$	+	154.0651	-0.65
16.	128.1064	1401	 Molecular Formula: $C_7H_{14}NO^+$ Monoisotopic Mass: **128.10699 Da**	$C_7H_{14}NO$	$[+H]^+$	128.1070	-4.29

Table S9.8. Fragment ions of 1B-LSD

No	Experimental m/z	Intensity	Structure of ion	Molecular Formula	Charge	Predicted m/z	Δ ppm
Precursor Ion	394.2487	–	 Molecular Formula: $C_{24}H_{32}N_3O_2^+$ Monoisotopic Mass: **394.248904 Da**	$C_{24}H_{31}N_3O_2$	$[M+H]^+$	394.2489	-0.48
1.	379.2247	969	 Molecular Formula: $C_{23}H_{29}N_3O_2^+$ Monoisotopic Mass: **379.225429 Da**	$C_{23}H_{29}N_3O_2^{\bullet}$	$[+H]^+$	379.2254	-1.93
2.	351.2058	6703	 Molecular Formula: $C_{22}H_{27}N_2O_2^+$ Monoisotopic Mass: **351.206705 Da**	$C_{22}H_{27}N_2O_2$	+	351.2067	-2.51
3.	321.1585	1110	 Molecular Formula: $C_{20}H_{21}N_2O_2^+$ Monoisotopic Mass: **321.159754 Da**	–	–	–	–
4.	293.1644	38637	 Molecular Formula: $C_{19}H_{21}N_2O^+$ Monoisotopic Mass: **293.16484 Da**	$C_{19}H_{21}N_2O$	$[+H]^+$	293.1648	-1.54
5.	281.1653	1251	 Molecular Formula: $C_{18}H_{21}N_2O^+$ Monoisotopic Mass: **281.16484 Da**	$C_{18}H_{21}N_2O$	+	281.1648	1.74
6.	277.1329	1537	 Molecular Formula: $C_{18}H_{17}N_2O^+$ Monoisotopic Mass: **277.13354 Da**	$C_{18}H_{17}N_2O$	$[+H]^+$	277.1335	-2.42

7.	267.1493	3759	 Molecular Formula: $C_{17}H_{19}N_2O^+$ Monoisotopic Mass: **267.14919 Da**	$C_{17}H_{19}N_2O$	$[+H]^+$	267.1492	0.49
8.	251.1172	1966	 Molecular Formula: $C_{16}H_{15}N_2O^+$ Monoisotopic Mass: **251.11789 Da**	$C_{16}H_{15}N_2O$	+	251.1179	-2.75
9.	223.1228	31814	 Molecular Formula: $C_{15}H_{15}N_2^+$ Monoisotopic Mass: **223.122975 Da**	$C_{15}H_{15}N_2$	$[+H]^+$	223.1230	-0.99
10.	221.1071	3865	 Molecular Formula: $C_{15}H_{13}N_2^+$ Monoisotopic Mass: **221.107325 Da**	$C_{15}H_{13}N_2$	$[+H]^+$	221.1073	-1.0
11.	208.0996	11976	 Molecular Formula: $C_{14}H_{12}N_2^+$ Monoisotopic Mass: **208.0995 Da**	$C_{14}H_{12}N_2^{\bullet}$	$[+H]^+$	208.0995	0.38
12.	208.0755	8371	 Molecular Formula: $C_{14}H_{10}NO^+$ Monoisotopic Mass: **208.07569 Da**	$C_{14}H_{10}NO$	+	208.0757	-1.01
13.	207.0914	10153	 Molecular Formula: $C_{14}H_{11}N_2^+$ Monoisotopic Mass: **207.091675 Da**	$C_{14}H_{11}N_2$	$[+H]^+$	207.0917	-1.55
14.	197.1077	5027	 Molecular Formula: $C_{13}H_{13}N_2^+$ Monoisotopic Mass: **197.107325 Da**	$C_{13}H_{13}N_2$	$[+H]^+$	197.1073	2.08
15.	194.0970	1840	 Molecular Formula: $C_{14}H_{12}N^+$ Monoisotopic Mass: **194.096426 Da**	$C_{14}H_{12}N$	+	194.0964	2.99

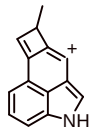
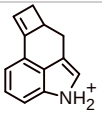
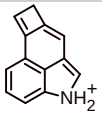
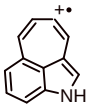
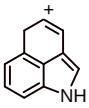
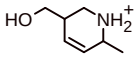
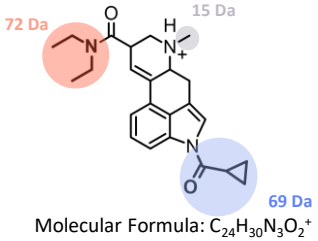
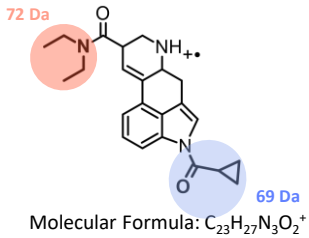
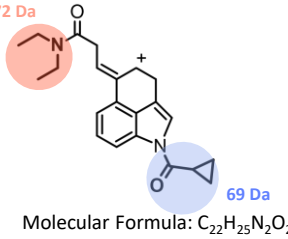
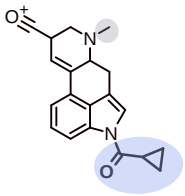
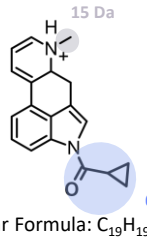
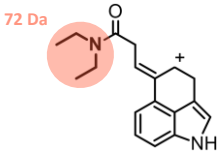
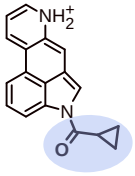
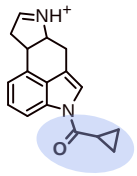
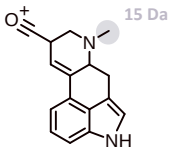
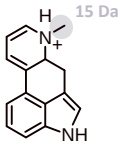
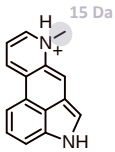
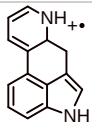
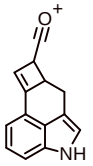
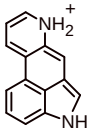
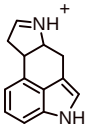
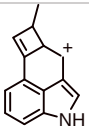
16.	192.0802	3614	 Molecular Formula: $C_{14}H_{10}N^+$ Monoisotopic Mass: **192.080776 Da**	$C_{14}H_{10}N$	+	192.0808	-3.23
17.	182.0967	2489	 Molecular Formula: $C_{13}H_{12}N^+$ Monoisotopic Mass: **182.096426 Da**	$C_{13}H_{12}N$	$[+H]^+$	182.0964	1.32
18.	180.0806	4141	 Molecular Formula: $C_{13}H_{10}N^+$ Monoisotopic Mass: **180.080776 Da**	$C_{13}H_{10}N$	$[+H]^+$	180.0808	-0.89
19.	167.0745	1095	 Molecular Formula: $C_{12}H_9N^+$ Monoisotopic Mass: **167.072951 Da**	–	–	–	–
20.	154.0635	579	 Molecular Formula: $C_{11}H_8N^+$ Monoisotopic Mass: **154.065126 Da**	–	–	–	–
21.	128.1060	1835	 Molecular Formula: $C_7H_{14}NO^+$ Monoisotopic Mass: **128.10699 Da**	–	–	–	–

Table S9.9. Fragment ions of 1cP-LSD

No	Experimental m/z	Intensity	Structure of ion	Molecular Formula	Charge	Predicted m/z	Δ ppm
Precursor Ion	392.2330	–	 Molecular Formula: $C_{24}H_{30}N_3O_2^+$ Monoisotopic Mass: **392.233254 Da**	$C_{24}H_{30}N_3O_2$	$[M+H]^+$	392.2333	-0.59
1.	377.2092	1114	 Molecular Formula: $C_{23}H_{27}N_3O_2^+$ Monoisotopic Mass: **377.209779 Da**	$C_{23}H_{27}N_3O_2^{\bullet}$	$[+H]^+$	377.2098	-1.56
2.	349.1906	7027	 Molecular Formula: $C_{22}H_{25}N_2O_2^+$ Monoisotopic Mass: **349.191054 Da**	$C_{22}H_{25}N_2O_2$	+	349.1911	-1.20
3.	319.1426	1090	 Molecular Formula: $C_{20}H_{19}N_2O_2^+$ Monoisotopic Mass: **319.144104 Da**	–	–	–	–
4.	291.1489	39237	 Molecular Formula: $C_{19}H_{19}N_2O^+$ Monoisotopic Mass: **291.14919 Da**	$C_{19}H_{19}N_2O$	$[+H]^+$	291.1492	-1.03
5.	281.1634	1990	 Molecular Formula: $C_{18}H_{21}N_2O^+$ Monoisotopic Mass: **281.16484 Da**	–	–	–	–
6.	275.1176	1759	 Molecular Formula: $C_{18}H_{15}N_2O^+$ Monoisotopic Mass: **275.11789 Da**	$C_{18}H_{15}N_2O$	$[+H]^+$	275.1179	-1.05

7.	265.1342	4587	 Molecular Formula: $C_{17}H_{17}N_2O^+$ Monoisotopic Mass: **265.13354 Da**	$C_{17}H_{17}N_2O$	$[+H]^+$	265.1335	2.30
8.	251.1181	2774	 Molecular Formula: $C_{16}H_{15}N_2O^+$ Monoisotopic Mass: **251.11789 Da**	$C_{16}H_{15}N_2O$	+	251.1179	0.72
9.	223.1225	31801	 Molecular Formula: $C_{15}H_{15}N_2^+$ Monoisotopic Mass: **223.122975 Da**	$C_{15}H_{15}N_2$	$[+H]^+$	223.1230	-2.29
10.	221.1074	2572	 Molecular Formula: $C_{15}H_{13}N_2^+$ Monoisotopic Mass: **221.107325 Da**	$C_{15}H_{13}N_2$	$[+H]^+$	221.1073	0.41
11.	208.0993	8670	 Molecular Formula: $C_{14}H_{12}N_2^+$ Monoisotopic Mass: **208.0995 Da**	$C_{14}H_{12}N_2^\bullet$	$[+H]^+$	208.0995	-0.96
12.	208.0756	7731	 Molecular Formula: $C_{14}H_{10}NO^+$ Monoisotopic Mass: **208.07569 Da**	$C_{14}H_{10}NO$	+	208.0757	-0.58
13.	207.0915	5990	 Molecular Formula: $C_{14}H_{11}N_2^+$ Monoisotopic Mass: **207.091675 Da**	$C_{14}H_{11}N_2$	$[+H]^+$	207.0917	-0.63
14.	197.1073	5792	 Molecular Formula: $C_{13}H_{13}N_2^+$ Monoisotopic Mass: **197.107325 Da**	$C_{13}H_{13}N_2$	$[+H]^+$	197.1073	-0.36
15.	194.0963	2235	 Molecular Formula: $C_{14}H_{12}N^+$ Monoisotopic Mass: **194.096426 Da**	$C_{14}H_{12}N$	+	194.0964	-0.82

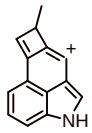
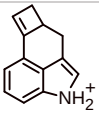
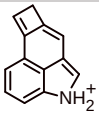
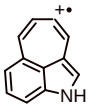
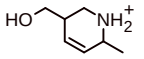
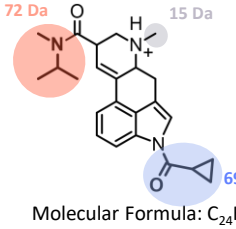
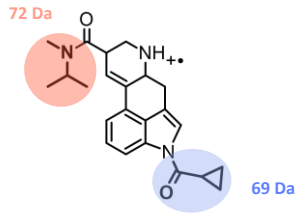
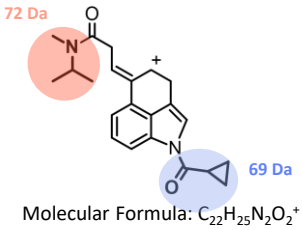
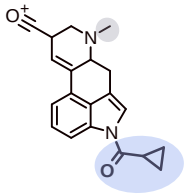
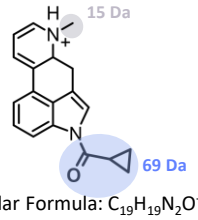
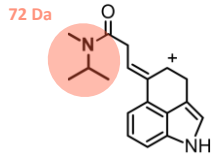
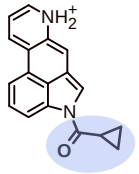
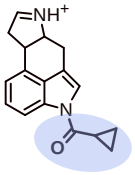
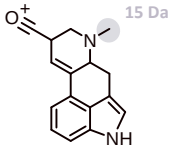
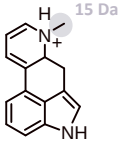
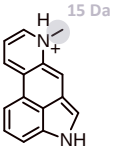
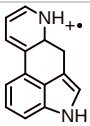
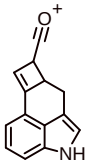
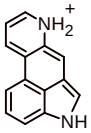
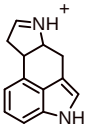
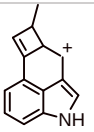
16.	192.0802	3089	 Molecular Formula: $C_{14}H_{10}N^+$ Monoisotopic Mass: **192.080776 Da**	$C_{14}H_{10}N$	+	192.0808	-2.81
17.	182.0966	2023	 Molecular Formula: $C_{13}H_{12}N^+$ Monoisotopic Mass: **182.096426 Da**	$C_{13}H_{12}N$	$[+H]^+$	182.0964	1.15
18.	180.0807	3327	 Molecular Formula: $C_{13}H_{10}N^+$ Monoisotopic Mass: **180.080776 Da**	$C_{13}H_{10}N$	$[+H]^+$	180.0808	-0.22
19.	167.0724	664	 Molecular Formula: $C_{12}H_9N^+$ Monoisotopic Mass: **167.072951 Da**	$C_{12}H_9N^{\bullet}$	+	167.0730	-3.23
20.	128.1060	1485	 Molecular Formula: $C_7H_{14}NO^+$ Monoisotopic Mass: **128.10699 Da**	–	–	–	–

Table S9.10. Fragment ions of 1cP-MiPLA

No	Experimental m/z	Intensity	Structure of ion	Molecular Formula	Charge	Predicted m/z	Δ ppm
Precursor Ion	392.2330	–	 Molecular Formula: $C_{24}H_{30}N_3O_2^+$ Monoisotopic Mass: **392.233254 Da**	$C_{24}H_{29}N_3O_2$	$[M+H]^+$	392.2333	-0.71
1.	377.2097	658	 Molecular Formula: $C_{23}H_{27}N_3O_2^+$ Monoisotopic Mass: **377.209779 Da**	$C_{23}H_{27}N_3O_2^{\bullet}$	$[+H]^+$	377.2098	-0.35
2.	349.1901	5713	 Molecular Formula: $C_{22}H_{25}N_2O_2^+$ Monoisotopic Mass: **349.191054 Da**	$C_{22}H_{25}N_2O_2$	+	349.1911	-2.84
3.	319.1450	1011	 Molecular Formula: $C_{20}H_{19}N_2O_2^+$ Monoisotopic Mass: **319.144104 Da**	$C_{20}H_{19}N_2O_2$	+	319.1441	2.73
4.	291.1492	37975	 Molecular Formula: $C_{19}H_{19}N_2O^+$ Monoisotopic Mass: **291.14919 Da**	$C_{19}H_{19}N_2O$	$[+H]^+$	291.1492	0.03
5.	281.1657	1526	 Molecular Formula: $C_{18}H_{21}N_2O^+$ Monoisotopic Mass: **281.16484 Da**	$C_{18}H_{21}N_2O$	+	281.1648	2.88
6.	275.1177	1713	 Molecular Formula: $C_{18}H_{15}N_2O^+$ Monoisotopic Mass: **275.11789 Da**	$C_{18}H_{15}N_2O$	$[+H]^+$	275.1179	-0.80

7.	265.1336	3707	 Molecular Formula: $C_{17}H_{17}N_2O^+$ Monoisotopic Mass: **265.13354 Da**	$C_{17}H_{17}N_2O$	$[+H]^+$	265.1335	0.15
8.	251.1178	2768	 Molecular Formula: $C_{16}H_{15}N_2O^+$ Monoisotopic Mass: **251.11789 Da**	$C_{16}H_{15}N_2O$	+	251.1179	-0.48
9.	223.1226	30382	 Molecular Formula: $C_{15}H_{15}N_2^+$ Monoisotopic Mass: **223.122975 Da**	$C_{15}H_{15}N_2$	$[+H]^+$	223.1230	-1.75
10.	221.1077	3478	 Molecular Formula: $C_{15}H_{13}N_2^+$ Monoisotopic Mass: **221.107325 Da**	$C_{15}H_{13}N_2$	$[+H]^+$	221.1073	1.90
11.	208.1000	7398	 Molecular Formula: $C_{14}H_{12}N_2^+$ Monoisotopic Mass: **208.0995 Da**	$C_{14}H_{12}N_2^\bullet$	$[+H]^+$	208.0995	2.45
12.	208.0755	6770	 Molecular Formula: $C_{14}H_{10}NO^+$ Monoisotopic Mass: **208.07569 Da**	$C_{14}H_{10}NO$	+	208.0757	-0.87
13.	207.0911	5825	 Molecular Formula: $C_{14}H_{11}N_2^+$ Monoisotopic Mass: **207.091675 Da**	$C_{14}H_{11}N_2$	$[+H]^+$	207.0917	-2.85
14.	197.1073	3604	 Molecular Formula: $C_{13}H_{13}N_2^+$ Monoisotopic Mass: **197.107325 Da**	$C_{13}H_{13}N_2$	$[+H]^+$	197.1073	-0.05
15.	194.0957	1653	 Molecular Formula: $C_{14}H_{12}N^+$ Monoisotopic Mass: **194.096426 Da**	$C_{14}H_{12}N$	+	194.0964	-3.56

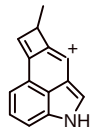
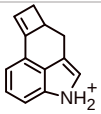
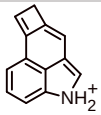
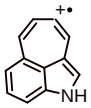
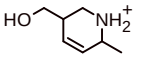
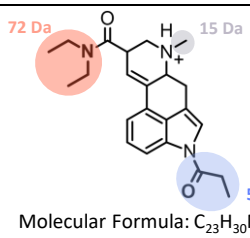
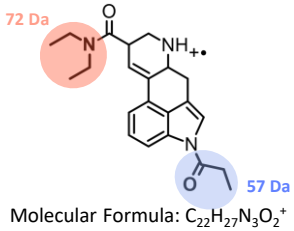
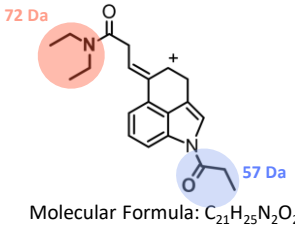
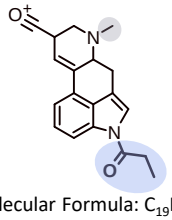
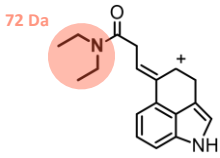
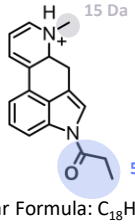
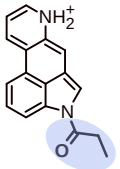
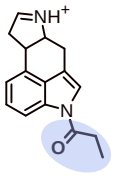
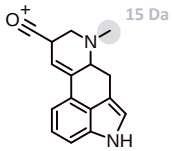
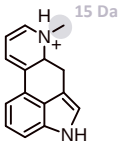
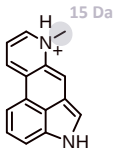
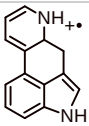
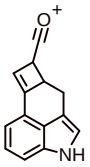
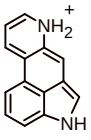
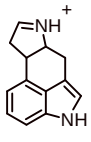
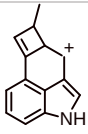
16.	192.0806	3052	 Molecular Formula: $C_{14}H_{10}N^+$ Monoisotopic Mass: **192.080776 Da**	$C_{14}H_{10}N$	+	192.0808	-0.99
17.	182.0967	1758	 Molecular Formula: $C_{13}H_{12}N^+$ Monoisotopic Mass: **182.096426 Da**	$C_{13}H_{12}N$	$[+H]^+$	182.0964	1.26
18.	180.0810	3031	 Molecular Formula: $C_{13}H_{10}N^+$ Monoisotopic Mass: **180.080776 Da**	$C_{13}H_{10}N$	$[+H]^+$	180.0808	1.22
19.	167.0736	696	 Molecular Formula: $C_{12}H_9N^+$ Monoisotopic Mass: **167.072951 Da**	$C_{12}H_9N^{\bullet}$	+	167.0730	4.01
20.	128.1071	1062	 Molecular Formula: $C_7H_{14}NO^+$ Monoisotopic Mass: **128.10699 Da**	$C_7H_{14}NO$	$[+H]^+$	128.1070	0.78

Table S9.11. Fragment ions of 1P-LSD

No	Experimental m/z	Intensity	Structure of ion	Molecular Formula	Charge	Predicted m/z	Δ ppm
Precursor Ion	380.2330	–	 Molecular Formula: $C_{23}H_{30}N_3O_2^+$ Monoisotopic Mass: **380.233254 Da**	$C_{23}H_{29}N_3O_2$	$[M+H]^+$	380.2333	-0.58
1.	365.2071	729	 Molecular Formula: $C_{22}H_{27}N_3O_2^+$ Monoisotopic Mass: **365.209779 Da**	–	–	–	–
2.	337.1906	7447	 Molecular Formula: $C_{21}H_{25}N_2O_2^+$ Monoisotopic Mass: **337.191054 Da**	$C_{21}H_{25}N_2O_2$	+	337.1911	-1.34
3.	307.1447	628	 Molecular Formula: $C_{19}H_{19}N_2O_2^+$ Monoisotopic Mass: **307.144104 Da**	$C_{19}H_{19}N_2O_2$	+	307.1441	2.08
4.	281.1647	1090	 Molecular Formula: $C_{18}H_{21}N_2O^+$ Monoisotopic Mass: **281.16484 Da**	$C_{18}H_{21}N_2O$	+	281.1648	-0.64
5.	279.1488	37251	 Molecular Formula: $C_{18}H_{19}N_2O^+$ Monoisotopic Mass: **279.14919 Da**	$C_{18}H_{19}N_2O$	$[+H]^+$	279.1492	-1.33
6.	263.1173	1573	 Molecular Formula: $C_{17}H_{15}N_2O^+$ Monoisotopic Mass: **263.11789 Da**	$C_{17}H_{15}N_2O$	$[+H]^+$	263.1179	-2.32

7.	253.1331	4386	 Molecular Formula: $C_{16}H_{17}N_2O^+$ Monoisotopic Mass: **253.13354 Da**	$C_{16}H_{17}N_2O$	$[+H]^+$	253.1335	-1.74
8.	251.1184	2641	 Molecular Formula: $C_{16}H_{15}N_2O^+$ Monoisotopic Mass: **251.11789 Da**	$C_{16}H_{15}N_2O$	+	251.1179	1.91
9.	223.1229	29424	 Molecular Formula: $C_{15}H_{15}N_2^+$ Monoisotopic Mass: **223.122975 Da**	$C_{15}H_{15}N_2$	$[+H]^+$	223.1230	-0.22
10.	221.1082	3999	 Molecular Formula: $C_{15}H_{13}N_2^+$ Monoisotopic Mass: **221.107325 Da**	$C_{15}H_{13}N_2$	$[+H]^+$	221.1073	3.89
11.	208.0995	10338	 Molecular Formula: $C_{14}H_{12}N_2^+$ Monoisotopic Mass: **208.0995 Da**	$C_{14}H_{12}N_2^{\bullet}$	$[+H]^+$	208.0995	-0.24
12.	208.0754	9731	 Molecular Formula: $C_{14}H_{10}NO^+$ Monoisotopic Mass: **208.07569 Da**	$C_{14}H_{10}NO$	+	208.0757	-1.30
13.	207.0918	11433	 Molecular Formula: $C_{14}H_{11}N_2^+$ Monoisotopic Mass: **207.091675 Da**	$C_{14}H_{11}N_2$	$[+H]^+$	207.0917	0.63
14.	197.1062	4938	 Molecular Formula: $C_{13}H_{13}N_2^+$ Monoisotopic Mass: **197.107325 Da**	–	–	–	–
15.	194.0966	2044	 Molecular Formula: $C_{14}H_{12}N^+$ Monoisotopic Mass: **194.096426 Da**	$C_{14}H_{12}N$	+	194.0964	0.62

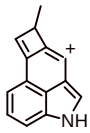
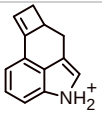
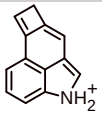
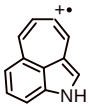
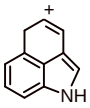
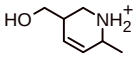
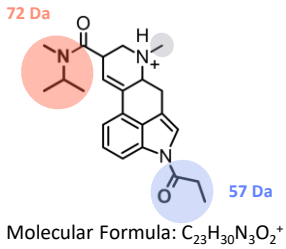
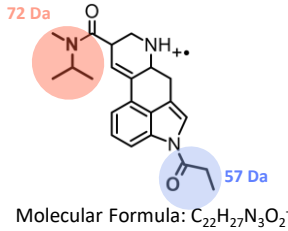
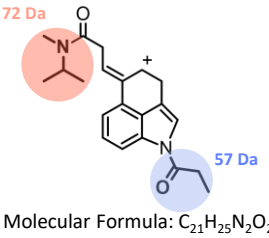
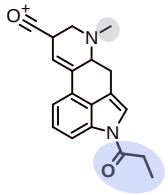
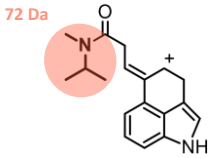
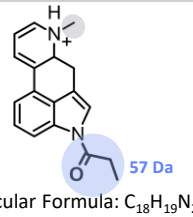
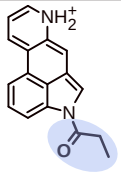
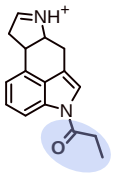
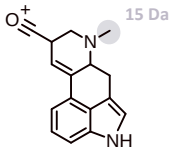
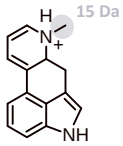
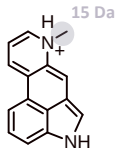
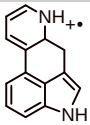
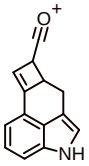
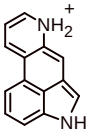
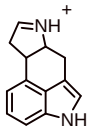
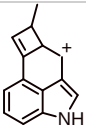
16.	192.0808	3908	 Molecular Formula: $C_{14}H_{10}N^+$ Monoisotopic Mass: **192.080776 Da**	$C_{14}H_{10}N$	+	192.0808	0.05
17.	182.0958	2497	 Molecular Formula: $C_{13}H_{12}N^+$ Monoisotopic Mass: **182.096426 Da**	$C_{13}H_{12}N$	$[+H]^+$	182.0958	-3.73
18.	180.0806	5063	 Molecular Formula: $C_{13}H_{10}N^+$ Monoisotopic Mass: **180.080776 Da**	$C_{13}H_{10}N$	$[+H]^+$	180.0808	-1.22
19.	167.0709	896	 Molecular Formula: $C_{12}H_9N^+$ Monoisotopic Mass: **167.072951 Da**	–	–	–	–
20.	154.0655	725	 Molecular Formula: $C_{11}H_8N^+$ Monoisotopic Mass: **154.065126 Da**	$C_{11}H_8N$	+	154.0651	2.34
21.	128.1070	2156	 Molecular Formula: $C_7H_{14}NO^+$ Monoisotopic Mass: **128.10699 Da**	$C_7H_{14}NO$	$[+H]^+$	128.1070	0.08

Table S9.12. Fragment ions of 1P-MiPLA

No	Experimental m/z	Intensity	Structure of ion	Molecular Formula	Charge	Predicted m/z	Δ ppm
Precursor Ion	380.2330	–	 Molecular Formula: $C_{23}H_{30}N_3O_2^+$ Monoisotopic Mass: **380.233254 Da**	$C_{23}H_{29}N_3O_2$	$[M+H]^+$	380.2333	-0.61
1.	365.2098	373	 Molecular Formula: $C_{22}H_{27}N_3O_2^+$ Monoisotopic Mass: **365.209779 Da**	$C_{22}H_{27}N_3O_2^{\bullet}$	$[+H]^+$	365.2098	-0.03
2.	337.1910	5841	 Molecular Formula: $C_{21}H_{25}N_2O_2^+$ Monoisotopic Mass: **337.191054 Da**	$C_{21}H_{25}N_2O_2$	+	337.1911	-0.06
3.	307.1432	875	 Molecular Formula: $C_{19}H_{19}N_2O_2^+$ Monoisotopic Mass: **307.144104 Da**	$C_{19}H_{19}N_2O_2$	+	307.1441	-2.90
4.	281.1628	1045	 Molecular Formula: $C_{18}H_{21}N_2O^+$ Monoisotopic Mass: **281.16484 Da**	–	–	–	–
5.	279.1490	38013	 Molecular Formula: $C_{18}H_{19}N_2O^+$ Monoisotopic Mass: **279.14919 Da**	$C_{18}H_{19}N_2O$	$[+H]^+$	279.1492	-0.68
6.	263.1185	1709	 Molecular Formula: $C_{17}H_{15}N_2O^+$ Monoisotopic Mass: **263.11789 Da**	$C_{17}H_{15}N_2O$	$[+H]^+$	263.1179	2.24

7.	253.1337	3095	 Molecular Formula: $C_{16}H_{17}N_2O^+$ Monoisotopic Mass: **253.13354 Da**	$C_{16}H_{17}N_2O$	$[+H]^+$	253.1335	0.63
8.	251.1181	1969	 Molecular Formula: $C_{16}H_{15}N_2O^+$ Monoisotopic Mass: **251.11789 Da**	$C_{16}H_{15}N_2O$	+	251.1179	0.84
9.	223.1225	28469	 Molecular Formula: $C_{15}H_{15}N_2^+$ Monoisotopic Mass: **223.122975 Da**	$C_{15}H_{15}N_2$	$[+H]^+$	223.1230	-2.15
10.	221.1075	3415	 Molecular Formula: $C_{15}H_{13}N_2^+$ Monoisotopic Mass: **221.107325 Da**	$C_{15}H_{13}N_2$	$[+H]^+$	221.1073	0.86
11.	208.0993	13144	 Molecular Formula: $C_{14}H_{12}N_2^+$ Monoisotopic Mass: **208.0995 Da**	$C_{14}H_{12}N_2^{\bullet}$	$[+H]^+$	208.0995	-1.15
12.	208.0754	7865	 Molecular Formula: $C_{14}H_{10}NO^+$ Monoisotopic Mass: **208.07569 Da**	$C_{14}H_{10}NO$	+	208.0757	-1.54
13.	207.0916	9854	 Molecular Formula: $C_{14}H_{11}N_2^+$ Monoisotopic Mass: **207.091675 Da**	$C_{14}H_{11}N_2$	$[+H]^+$	207.0917	-0.48
14.	197.1066	3657	 Molecular Formula: $C_{13}H_{13}N_2^+$ Monoisotopic Mass: **197.107325 Da**	$C_{13}H_{13}N_2$	$[+H]^+$	197.1073	-3.65
15.	194.0967	2152	 Molecular Formula: $C_{14}H_{12}N^+$ Monoisotopic Mass: **194.096426 Da**	$C_{14}H_{12}N$	+	194.0964	1.24

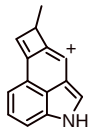
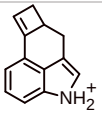
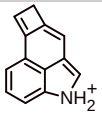
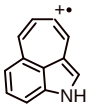
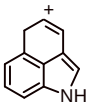
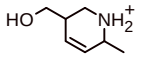
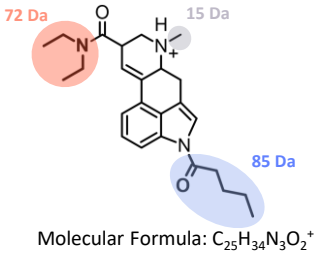
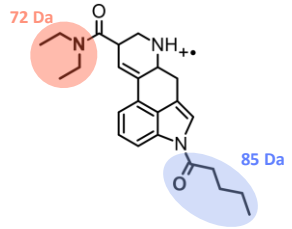
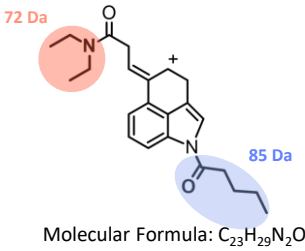
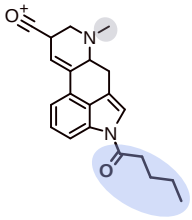
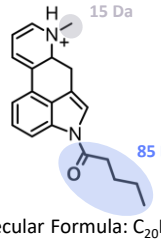
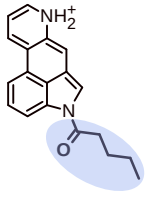
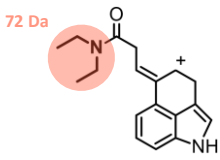
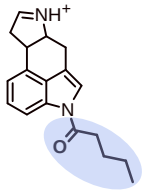
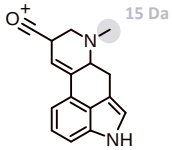
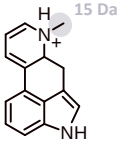
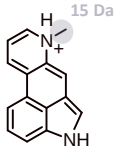
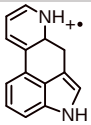
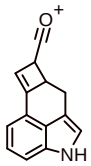
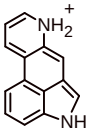
16.	192.0810	3268	 Molecular Formula: $C_{14}H_{10}N^+$ Monoisotopic Mass: **192.080776 Da**	$C_{14}H_{10}N$	+	192.0808	1.09
17.	182.0967	2273	 Molecular Formula: $C_{13}H_{12}N^+$ Monoisotopic Mass: **182.096426 Da**	$C_{13}H_{12}N$	$[+H]^+$	182.0964	1.48
18.	180.0809	4118	 Molecular Formula: $C_{13}H_{10}N^+$ Monoisotopic Mass: **180.080776 Da**	$C_{13}H_{10}N$	$[+H]^+$	180.0808	0.89
19.	167.0726	1543	 Molecular Formula: $C_{12}H_9N^+$ Monoisotopic Mass: **167.072951 Da**	$C_{12}H_9N^{\bullet}$	+	167.0730	-1.98
20.	154.0659	487	 Molecular Formula: $C_{11}H_8N^+$ Monoisotopic Mass: **154.065126 Da**	$C_{11}H_8N$	+	154.0651	4.93
21.	128.1075	1590	 Molecular Formula: $C_7H_{14}NO^+$ Monoisotopic Mass: **128.10699 Da**	$C_7H_{14}NO$	$[+H]^+$	128.1070	3.98

Table S9.13. Fragment ions of 1V-LSD

No	Experimental m/z	Intensity	Structure of ion	Molecular Formula	Charge	Predicted m/z	Δ ppm
Precursor Ion	408.2643	–	 Molecular Formula: $C_{25}H_{34}N_3O_2^+$ Monoisotopic Mass: **408.264554 Da**	$C_{25}H_{33}N_3O_2$	$[M+H]^+$	408.2646	-0.56
1.	393.2433	1126	 Molecular Formula: $C_{24}H_{31}N_3O_2^+$ Monoisotopic Mass: **393.241079 Da**	–	–	–	–
2.	365.2214	6585	 Molecular Formula: $C_{23}H_{29}N_2O_2^+$ Monoisotopic Mass: **365.222355 Da**	$C_{23}H_{29}N_2O_2$	+	365.2224	-2.66
3.	335.1758	753	 Molecular Formula: $C_{21}H_{23}N_2O_2^+$ Monoisotopic Mass: **335.175404 Da**	$C_{21}H_{23}N_2O_2$	+	335.1754	1.07
4.	307.1801	38068	 Molecular Formula: $C_{20}H_{23}N_2O^+$ Monoisotopic Mass: **307.18049 Da**	$C_{20}H_{23}N_2O$	$[+H]^+$	307.1805	-1.34
5.	291.1493	799	 Molecular Formula: $C_{19}H_{19}N_2O^+$ Monoisotopic Mass: **291.14919 Da**	$C_{19}H_{19}N_2O$	$[+H]^+$	291.1492	0.24

6.	281.1648	5399	 Molecular Formula: $C_{18}H_{21}N_2O^+$ Monoisotopic Mass: **281.16484 Da** and  Molecular Formula: $C_{18}H_{21}N_2O^+$ Monoisotopic Mass: **281.16484 Da**	$C_{18}H_{21}N_2O$	+ / [+H]+	281.1648	-0.25
7.	251.1175	2976	 Molecular Formula: $C_{16}H_{15}N_2O^+$ Monoisotopic Mass: **251.11789 Da**	$C_{16}H_{15}N_2O$	+	251.1179	-1.59
8.	223.1227	30788	 Molecular Formula: $C_{15}H_{15}N_2^+$ Monoisotopic Mass: **223.122975 Da**	$C_{15}H_{15}N_2$	$[+H]^+$	223.1230	-1.39
9.	221.1075	2858	 Molecular Formula: $C_{15}H_{13}N_2^+$ Monoisotopic Mass: **221.107325 Da**	$C_{15}H_{13}N_2$	$[+H]^+$	221.1073	0.91
10.	208.0997	11598	 Molecular Formula: $C_{14}H_{12}N_2^+$ Monoisotopic Mass: **208.0995 Da**	$C_{14}H_{12}N_2^{\bullet}$	$[+H]^+$	208.0995	0.87
11.	208.0758	8679	 Molecular Formula: $C_{14}H_{10}NO^+$ Monoisotopic Mass: **208.07569 Da**	$C_{14}H_{10}NO$	+	208.0757	0.63
12.	207.0911	8107	 Molecular Formula: $C_{14}H_{11}N_2^+$ Monoisotopic Mass: **207.091675 Da**	$C_{14}H_{11}N_2$	$[+H]^+$	207.0917	-2.80

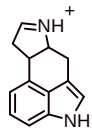
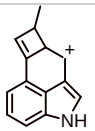
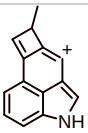
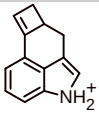
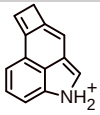
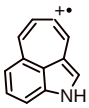
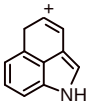
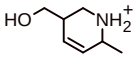
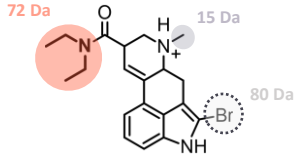
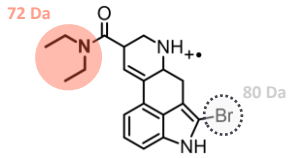
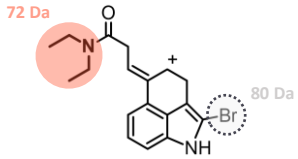
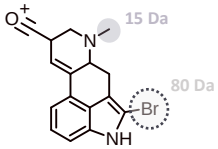
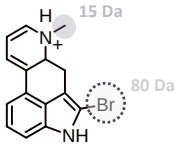
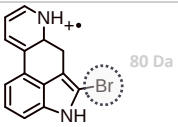
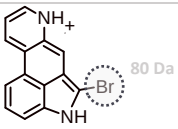
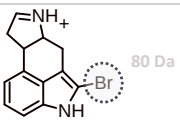
13.	197.1075	4416	 Molecular Formula: $C_{13}H_{13}N_2^+$ Monoisotopic Mass: **197.107325 Da**	$C_{13}H_{13}N_2$	$[+H]^+$	197.1073	0.71
14.	194.0969	2032	 Molecular Formula: $C_{14}H_{12}N^+$ Monoisotopic Mass: **194.096426 Da**	$C_{14}H_{12}N$	+	194.0964	2.37
15.	192.0808	4387	 Molecular Formula: $C_{14}H_{10}N^+$ Monoisotopic Mass: **192.080776 Da**	$C_{14}H_{10}N$	+	192.0808	0.31
16.	182.0970	2321	 Molecular Formula: $C_{13}H_{12}N^+$ Monoisotopic Mass: **182.096426 Da**	$C_{13}H_{12}N$	$[+H]^+$	182.0964	3.24
17.	180.0803	3538	 Molecular Formula: $C_{13}H_{10}N^+$ Monoisotopic Mass: **180.080776 Da**	$C_{13}H_{10}N$	$[+H]^+$	180.0808	-2.55
18.	167.0732	939	 Molecular Formula: $C_{12}H_9N^+$ Monoisotopic Mass: **167.072951 Da**	$C_{12}H_9N^{\bullet}$	+	167.0730	1.56
19.	154.0656	421	 Molecular Formula: $C_{11}H_8N^+$ Monoisotopic Mass: **154.065126 Da**	$C_{11}H_8N$	+	154.0651	2.73
20.	128.1062	1459	 Molecular Formula: $C_7H_{14}NO^+$ Monoisotopic Mass: **128.10699 Da**	$C_7H_{14}NO$	$[+H]^+$	128.1070	-6.56

Table S9.14. Fragment ions of 2-Bromo-LSD

No	Experimental m/z	Intensity	Structure of ion	Molecular Formula	Charge	Predicted m/z	Δ ppm
Precursor Ion	402.1174	–	 Molecular Formula: $C_{20}H_{25}BrN_3O^+$ Monoisotopic Mass: **402.117544 Da**	$C_{20}H_{24}N_3OBr$	$[M+H]^+$	402.1176	-0.30
1.	387.0942	789	 Molecular Formula: $C_{19}H_{22}BrN_3O^+$ Monoisotopic Mass: **387.094069 Da**	$C_{19}H_{22}N_3OBr^•$	$[+H]^+$	387.0941	0.21
2.	359.0757	3722	 Molecular Formula: $C_{18}H_{20}BrN_2O^+$ Monoisotopic Mass: **359.075345 Da**	$C_{18}H_{20}N_2OBr$	+	359.0754	1.09
3.	329.0287	872	 Molecular Formula: $C_{16}H_{14}BrN_2O^+$ Monoisotopic Mass: **329.028394 Da**	$C_{16}H_{14}N_2OBr$	+	329.0284	1.03
4.	301.0335	18343	 Molecular Formula: $C_{15}H_{14}BrN_2^+$ Monoisotopic Mass: **301.03348 Da**	$C_{15}H_{14}N_2Br$	$[+H]^+$	301.0335	-0.07
5.	286.0103	2837	 Molecular Formula: $C_{14}H_{11}BrN_2^+$ Monoisotopic Mass: **286.010005 Da**	$C_{14}H_{11}N_2Br^•$	$[+H]^+$	286.0100	1.15
6.	285.0013	2258	 Molecular Formula: $C_{14}H_{10}BrN_2^+$ Monoisotopic Mass: **285.00218 Da**	$C_{14}H_{10}N_2Br$	$[+H]^+$	285.0022	-3.23
7.	275.0174	3777	 Molecular Formula: $C_{13}H_{12}BrN_2^+$ Monoisotopic Mass: **275.01783 Da**	$C_{13}H_{12}N_2Br$	$[+H]^+$	275.0178	-1.78

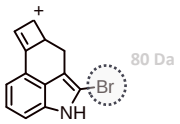
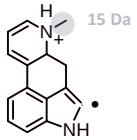
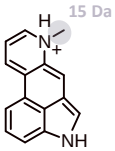
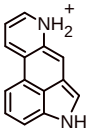
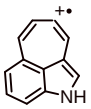
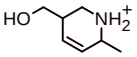
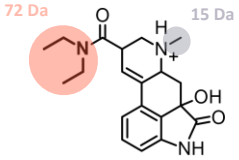
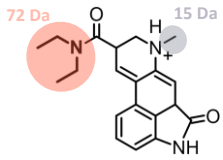
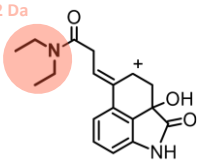
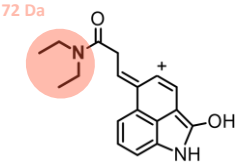
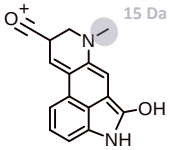
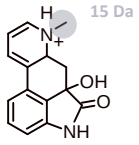
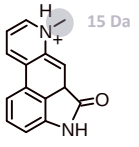
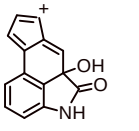
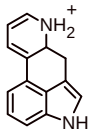
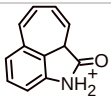
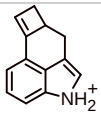
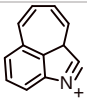
8.	257.9912	2328	 Molecular Formula: $C_{13}H_9BrN^+$ Monoisotopic Mass: **257.991281 Da**	$C_{13}H_9NBr$	+	257.9913	-0.43
9.	222.1147	8471	 Molecular Formula: $C_{15}H_{14}N_2^+$ Monoisotopic Mass: **222.11515 Da**	$C_{15}H_{14}N_2^{\bullet}$	$[+H]^+$	222.1152	-1.85
10.	221.1069	9237	 Molecular Formula: $C_{15}H_{13}N_2^+$ Monoisotopic Mass: **221.107325 Da**	$C_{15}H_{13}N_2$	$[+H]^+$	221.1073	-1.90
11.	207.0918	11651	 Molecular Formula: $C_{14}H_{11}N_2^+$ Monoisotopic Mass: **207.091675 Da**	$C_{14}H_{11}N_2$	$[+H]^+$	207.0917	0.39
12.	167.0723	517	 Molecular Formula: $C_{12}H_9N^+$ Monoisotopic Mass: **167.072951 Da**	$C_{12}H_9N^{\bullet}$	+	167.0730	-4.07
13.	128.1069	1310	 Molecular Formula: $C_7H_{14}NO^+$ Monoisotopic Mass: **128.10699 Da**	$C_7H_{14}NO$	$[+H]^+$	128.1070	-0.78

Table S9.15. Fragment ions of 2-oxo-3-OH-LSD

No	Experimental m/z	Intensity	Structure of ion	Molecular Formula	Charge	Predicted m/z	Δ ppm
Precursor Ion	356.1965	–	 Molecular Formula: $C_{20}H_{26}N_3O_3^+$ Monoisotopic Mass: **356.196868 Da**	$C_{20}H_{25}N_3O_3$	$[M+H]^+$	356.19665	-0.62
1.	338.1854	2865	 Molecular Formula: $C_{20}H_{24}N_3O_2^+$ Monoisotopic Mass: **338.186303 Da**	$C_{20}H_{24}N_3O_2$	$[+H]^+$	338.1863	-2.54
2.	313.1546	3062	 Molecular Formula: $C_{18}H_{21}N_2O_3^+$ Monoisotopic Mass: **313.154669 Da**	$C_{18}H_{21}N_2O_3$	+	313.1547	-0.26
3.	295.1458	555	 Molecular Formula: $C_{18}H_{19}N_2O_2^+$ Monoisotopic Mass: **295.144104 Da**	–	–	–	–
4.	265.0964	3912	 Molecular Formula: $C_{16}H_{13}N_2O_2^+$ Monoisotopic Mass: **265.097154 Da**	$C_{16}H_{13}N_2O_2$	+	265.0972	-2.87
5.	255.1125	600	 Molecular Formula: $C_{15}H_{15}N_2O_2^+$ Monoisotopic Mass: **255.112804 Da**	$C_{15}H_{15}N_2O_2$	$[+H]^+$	255.1128	-1.37
6.	237.1023	15947	 Molecular Formula: $C_{15}H_{13}N_2O^+$ Monoisotopic Mass: **237.102239 Da**	$C_{15}H_{13}N_2O$	$[+H]^+$	237.1022	0.04
7.	222.0544	5993	 Molecular Formula: $C_{14}H_8NO_2^+$ Monoisotopic Mass: **222.054955 Da**	$C_{14}H_8NO_2$	+	222.0550	-2.52

8.	209.1075	3455	 Molecular Formula: $C_{14}H_{13}N_2^+$ Monoisotopic Mass: **209.107325 Da**	$C_{14}H_{13}N_2$	$[+H]^+$	209.1073	0.62
9.	184.0756	1336	 Molecular Formula: $C_{12}H_{10}NO^+$ Monoisotopic Mass: **184.07569 Da**	$C_{12}H_{10}NO$	$[+H]^+$	184.0757	-0.33
10.	182.0968	1688	 Molecular Formula: $C_{13}H_{12}N^+$ Monoisotopic Mass: **182.096426 Da**	$C_{13}H_{12}N$	$[+H]^+$	182.0964	2.03
11.	166.0649	1122	 Molecular Formula: $C_{12}H_8N^+$ Monoisotopic Mass: **166.065126 Da**	$C_{12}H_8N$	+	166.0651	-1.45

S10: Analysis of mass spectra and fragmentation pattern