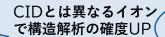
高分解能質量分析計を用いた 新モダリティ医薬品の構造解析

新モダリティに対応すべく、新たに高分解能質量分析装置を導入しました。新たな開裂法である電子励起解離(EAD, Electron Activated Dissociation)により、これまで困難であった環状ペプチド、LNP及びmRNAのCQAs等の詳細な構造解析が可能となりました。



<ZenoTOF7600の利点>

- · 新規解列方式 EAD (電子励起解離) を搭載
- · Zeno Trap pulsing でさらに高感度に
- · 広いマスレンジ:40~40KDa
- ・分解能:48,691 (FWHM, at m/z 1007.4[M+2H]²⁺)
- ・革新的なソフトウエアで迅速にご報告

従来機比較500倍以上 濃縮・分取せずに微量 成分の構造解析が可能

従来機比較3.4倍



代謝物の網羅的検索

	Report	Peak ID	Name	Formula	Assigned	Neutral Mass Averag	je Mass	m/z	Charge	ppm	R.T. (min)	Peak Area	% Area 5	Score	MS/MS Spect	
1	V	M69	Hydrogenation [M+H]+	C20H25CIN2O5	V	408.15	391.66	409,1526	1	0.3	19.22	4.56E+06	1/18	75.7	- 1	AB SCIEX社
2	~	M58	Loss of C2H4 and C2H5N [M+H]+	C16H14CINO5	V	335.06	335.58	336.0635	1	0.4	17.89	2.47E+06	0.64	85.7	- 1	
3	V		Parent (M+2H)2+	C20H23CIN2O5	V.	406.13	406.66	204.0724	2	1.5	17.05	6.23E+05	0.16	62.0	1	± ± 0.71 = 10.24145
4		M90	Amine to Carbonylic Acid [M+H]+	C21H22CIN07	4	435.11	435.69	436.1158	1	0.1		3.51E+06	0.91	86.2	1	未変化体の代謝物
5			Parent [M+H]+	C20H23CIN2O5	1	406.13	406.71	407.1374	1	1.5		dpine 5000 re	AME			^{∞∞ •} *∞ [∞] • [™] ™™ の構造式を推定
6		M78	Loss of C2H5N+Glucuronidation [M+H]+	4	Н	72.22	539.75	540.1268	1	0.2	The second second	Metabolites: 7	B of 97 Pea		Formula	Anapoel Books Mans Annap Mans on: Overproper S.L.(col) Facilities School
7		M6S	Loss of CI->H and C2H5N+Glucose Conjugation	H ₃ C	N_	O NH ₂	491.40	492.1865	1	0.1	0.4	MSS Line of CON			CORPOSOROOS CHIRITAGROS	/ 4815 3916 48152 1 55 1922 4595-96 138 757 1
8		M57	Demethylation to Carboxylic Acid [M+H]+	H ₃ C ⁻ O	人	O CH ₃	436.70	437.1112	1	0.5	3 4	Favor (61-21)	24		CONCOCNOS	7 205.04 205.08 206.00 1 64 17.08 2705-06 644 86.7 1 7 46.03 86.64 204.024 2 15 17.05 6.200-06 616 62.0 1
9	~	M66	Loss of CH2 and NH+Di-Oxidation and Ketone F	H ₃ C H	Ţ		423.61	424.0795	1	0.4		MSO Arms to Carb Farent (M-11)-			CZ9HZDONOF CZ9HZDONOOS	/ GS.11 GS.60 GS.708 1 S1 2301 3310-04 S01 862 1 / GS.13 40671 487/32N 1 15 1762 1310-07 332 965 1
10		M49	Ethyl to Carboxylic Acid (M+H)+	U	1 6	,	422.65	423.0958	1	1.1	Toronto Control	NAME OF THE OWNER OWNER OF THE OWNER OWNE			-	
11		M09	Loss of NH+Demethylation to Carboxylic Acid [M				421.68	422.1002	1	0.2	Interpretat	et of etc. t	Property	Options.	areas Apply	Removal Manu Selected neutral formula: C19H1BCINO7
12		M59	Loss of CI->H and C2H5N+Phosphorylation [M+H]				409.25	410.1004	1	1.2	g reference parer	ENSAS				201 CORE - 401 EDRO - Companion CHRISCHOT Man 407 6727, Swinsing C15113CROS, Man 302 6431
13	V	M75	Loss of CH2 and NH+Oxidation and Ketone For	アム	□÷)	ピン	407.61	408.0848	1	0.8	9 2000 9 2000 9 1000				268 0018 %	V 200.0007
14		M67	Loss of CH2+Oxidative Dearmination to Alcohol [393.70	394.1060	1	2.1	, , ,	80 100 120	140 190	190 200	230 240 260 mit. Da	280 300 320 340 3MR 380 480 5 F
15		M39	Loss of CH2 [M+H]+	(分子	量Z	108)	392.68	393.1220	1	2.0) peaks, score for 25 p		ortic 529.0	.0000	1 10
16	~	M38	Loss of CH2 [M+H]+	,,,,		•	392 65	393.1224	1	3.0	Fragments: 2	5 of 44 Proposed		ry son P	reposed Score	* Shustier Dirella for CTITAZON.
17		M68	Loss of NH [M+H]+	同定代謝物	迷け	10化合物	חל	392.1259	1	0.0	The state of the s	CHAS CERTIFICS	12	817 85	8 58	X X X
18		M06	Loss of C2H5NO+Demethylation to Carboxyl	וייאנים ו	JAYIO	попода	n	378.0739	1	0.0	1000	2.0342 C14H10NO2 2.0364 C14H9ONO	-02	262 118	2 315	OF Y 3 04
19		MS7	Loss of C2H5N (M+H)+	C18H18CINO5	1	363.09	363.62	1945	1	0.3	Park House	SENS CHARGNOS	82	HSE1 11.0 HSTR 12.0	8 350 10 418	
20		M24	Loss of 194.0139 [M+H]+	C10H16N2O3		212.12	212.32	213.122	1	-2.0	\$1000 FE.3	LESTS CHRHICEGO	88 3	162 128	0 415	Contained linuxial Losses
											n 🗸 11	TORRE CTTHTSCHOOL	81	3965 11.0	6 650	s stractures Feet
											35	LINE CHRYSCHOL	-41	86.1 H.E.	1 311	

測定から解析・報告まで のスループットが向上

EADによる環状ペプチドの帰属

微量代謝物を迅速に検索が可能

