

Acquisition Method Report

Acquisition Method Info

Method Name Pyrimidine_13CGLn_10-8-20.m

Method Path D:\MassHunter\methods\Thomas\Pyrimidine_13CGLn_10-8-20.m

Method Description Default Method

Device List

Sampler
Binary Pump
Column Oven
QQQ

MS QQQ Mass Spectrometer

Ion Source AJS ESI **Tune File** D:\MassHunter\Tune\QQQ\G6470A\atunes.TUNE.XML

Stop Mode By StopTime **Stop Time (min)** 40

Time Filter On **Time Filter Width (min)** 0.1

Time Segments

Index	Start Time (min)	Scan Type	Ion Mode	Div Valve	Delta EMV (+)	Delta EMV (-)	Store
1	0	MRM	ESI+Agilent Jet Stream	To MS	300	300	Yes

Time Segment 1

Scan Segments

Cpd Group	Cpd Name	ISTD?	Prec Ion	MS1 Res	Prod Ion	MS2 Res	Dwell	Frag (V)	CE (V)	Cell Acc (V)	Polarity
	GMP	No	364	Unit/Enh (6490)	152	Unit/Enh (6490)	10	40	18	5	Positive
	IMP	No	349	Unit/Enh (6490)	137	Unit/Enh (6490)	10	40	19	5	Positive
	AMP	No	348	Unit/Enh (6490)	136	Unit/Enh (6490)	10	40	21	5	Positive
	UMP M+3	No	328	Unit/Enh (6490)	97	Unit/Enh (6490)	10	30	14	5	Positive
	UMP	No	325	Unit/Enh (6490)	97	Unit/Enh (6490)	10	30	14	5	Positive
	Guanosine	No	284	Unit/Enh (6490)	152	Unit/Enh (6490)	10	30	20	5	Positive
	Inosine	No	269	Unit/Enh (6490)	137	Unit/Enh (6490)	10	35	20	5	Positive
	deoxyguanosine	No	268.1	Unit/Enh (6490)	152	Unit/Enh (6490)	10	30	14	5	Positive
	Adenosine	No	268	Unit/Enh (6490)	136	Unit/Enh (6490)	10	40	18	5	Positive
	deoxyadenosine	No	252	Unit/Enh (6490)	136	Unit/Enh (6490)	10	35	20	5	Positive
	Uridine M+3	No	248.2	Unit/Enh (6490)	115.96	Unit/Enh (6490)	10	30	14	5	Positive
	Cytidine M+3	No	247.22	Unit/Enh (6490)	111.92	Unit/Enh (6490)	10	28	10	5	Positive
	Uridine	No	245.2	Unit/Enh (6490)	112.96	Unit/Enh (6490)	10	30	14	5	Positive
	Cytidine	No	244.22	Unit/Enh (6490)	111.92	Unit/Enh (6490)	10	28	10	5	Positive
	deoxyuridine M+3	No	232.1	Unit/Enh (6490)	116	Unit/Enh (6490)	10	28	20	5	Positive
	deoxycytidine M+3	No	231.1	Unit/Enh (6490)	115	Unit/Enh (6490)	10	28	20	5	Positive
	deoxyuridine	No	229.1	Unit/Enh (6490)	113	Unit/Enh (6490)	10	28	20	5	Positive
	deoxycytidine	No	228.1	Unit/Enh (6490)	112	Unit/Enh (6490)	10	28	20	5	Positive

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Cpd Group	Cpd Name	ISTD?	Prec Ion	MS1 Res	Prod Ion	MS2 Res	Dwell	Frag (V)	CE (V)	Cell Acc (V)	Polarity
	Citrulline	No	176.1	Unit/Enh (6490)	70	Unit/Enh (6490)	10	35	13	5	Positive
	Arginine	No	175.2	Unit/Enh (6490)	60	Unit/Enh (6490)	10	40	14	5	Positive
	Xanthene	No	153	Unit/Enh (6490)	110	Unit/Enh (6490)	10	30	20	5	Positive
	Aspartate M +4	No	138	Unit/Enh (6490)	76	Unit/Enh (6490)	10	40	15	5	Positive
	Hypoxanthine	No	137.1	Unit/Enh (6490)	109.9	Unit/Enh (6490)	10	44	20	5	Positive
	Aspartate	No	134	Unit/Enh (6490)	74	Unit/Enh (6490)	10	40	15	5	Positive
	Ornithine	No	133	Unit/Enh (6490)	70	Unit/Enh (6490)	10	35	12	5	Positive
	d2_ND	No	127	Unit/Enh (6490)	84	Unit/Enh (6490)	10	100	20	5	Positive
	Proline M+5	No	121	Unit/Enh (6490)	74.1	Unit/Enh (6490)	10	80	20	5	Positive
	Proline	No	116	Unit/Enh (6490)	70	Unit/Enh (6490)	10	80	20	5	Positive
	Serine Standard	No	109	Unit/Enh (6490)	63	Unit/Enh (6490)	10	40	13	5	Positive
	Serine	No	106	Unit/Enh (6490)	60	Unit/Enh (6490)	10	40	13	5	Positive
	Beta- Aminolsobuty rate M+3	No	105	Unit/Enh (6490)	39	Unit/Enh (6490)	10	40	30	5	Positive
	Beta- Aminolsobuty rate	No	104	Unit/Enh (6490)	39	Unit/Enh (6490)	10	40	30	5	Positive
	Alanine M+2	No	92	Unit/Enh (6490)	45	Unit/Enh (6490)	10	40	17	5	Positive
	Alanine	No	90	Unit/Enh (6490)	44	Unit/Enh (6490)	10	40	17	5	Positive
	Glycine	No	76	Unit/Enh (6490)	30	Unit/Enh (6490)	10	40	20	5	Positive
	ATP Standard	No	542.9	Unit/Enh (6490)	158.9	Unit/Enh (6490)	10	80	50	5	Negative
	GTP	No	522.2	Unit/Enh (6490)	159	Unit/Enh (6490)	10	30	32	5	Negative
	dGTP	No	506	Unit/Enh (6490)	159	Unit/Enh (6490)	10	30	32	5	Negative
	ATP	No	506	Unit/Enh (6490)	159	Unit/Enh (6490)	10	35	40	5	Negative
	dATP	No	490.1	Unit/Enh (6490)	159	Unit/Enh (6490)	10	35	32	5	Negative
	UTP M+3	No	486	Unit/Enh (6490)	159	Unit/Enh (6490)	10	30	26	5	Negative
	CTP M+3	No	485.16	Unit/Enh (6490)	159	Unit/Enh (6490)	10	34	26	5	Negative
	dTTP M+3	No	484	Unit/Enh (6490)	159	Unit/Enh (6490)	10	30	36	5	Negative
	UTP	No	483	Unit/Enh (6490)	159	Unit/Enh (6490)	10	30	26	5	Negative
	CTP	No	482.16	Unit/Enh (6490)	159	Unit/Enh (6490)	10	34	26	5	Negative
	dTTP	No	481	Unit/Enh (6490)	159	Unit/Enh (6490)	10	30	36	5	Negative
	dUTP M+3	No	470	Unit/Enh (6490)	159	Unit/Enh (6490)	10	30	36	5	Negative
	dCTP M+3	No	469	Unit/Enh (6490)	159	Unit/Enh (6490)	10	34	35	5	Negative
	dUTP	No	467	Unit/Enh (6490)	159	Unit/Enh (6490)	10	30	36	5	Negative
	dCTP	No	466	Unit/Enh (6490)	159	Unit/Enh (6490)	10	34	35	5	Negative
	GDP	No	442	Unit/Enh (6490)	150	Unit/Enh (6490)	10	35	24	5	Negative

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Trusted Answers

Cpd Group	Cpd Name	ISTD?	Prec Ion	MS1 Res	Prod Ion	MS2 Res	Dwell	Frag (V)	CE (V)	Cell Acc (V)	Polarity
	ADP	No	426	Unit/Enh (6490)	134	Unit/Enh (6490)	10	135	20	5	Negative
	UDP M+3	No	406.16	Unit/Enh (6490)	159	Unit/Enh (6490)	10	30	26	5	Negative
	CDP M+3	No	405.18	Unit/Enh (6490)	159	Unit/Enh (6490)	10	30	26	5	Negative
	dTDP M+3	No	404	Unit/Enh (6490)	79	Unit/Enh (6490)	10	36	44	5	Negative
	UDP	No	403.16	Unit/Enh (6490)	159	Unit/Enh (6490)	10	30	26	5	Negative
	CDP	No	402.18	Unit/Enh (6490)	159	Unit/Enh (6490)	10	30	26	5	Negative
	dTDP	No	401	Unit/Enh (6490)	79	Unit/Enh (6490)	10	36	44	5	Negative
	OMP M+3	No	370	Unit/Enh (6490)	79	Unit/Enh (6490)	10	35	36	5	Negative
	OMP	No	367	Unit/Enh (6490)	79	Unit/Enh (6490)	10	35	36	5	Negative
	AMP Neg	No	346	Unit/Enh (6490)	79	Unit/Enh (6490)	10	40	21	5	Negative
	UMP Neg M +3	No	326	Unit/Enh (6490)	79	Unit/Enh (6490)	10	40	30	5	Negative
	CMP M+3	No	325	Unit/Enh (6490)	79	Unit/Enh (6490)	10	35	30	5	Negative
	dTMP M+3	No	324.2	Unit/Enh (6490)	79	Unit/Enh (6490)	10	30	30	5	Negative
	UMP Neg	No	323	Unit/Enh (6490)	79	Unit/Enh (6490)	10	40	30	5	Negative
	CMP	No	322	Unit/Enh (6490)	79	Unit/Enh (6490)	10	35	30	5	Negative
	dTMP	No	321	Unit/Enh (6490)	79	Unit/Enh (6490)	10	30	30	5	Negative
	dUMP M+3	No	307	Unit/Enh (6490)	79	Unit/Enh (6490)	10	40	30	5	Negative
	dUMP	No	307	Unit/Enh (6490)	79	Unit/Enh (6490)	10	40	30	5	Negative
	Thymidine M +3	No	244	Unit/Enh (6490)	44	Unit/Enh (6490)	10	35	10	5	Negative
	Thymidine	No	241	Unit/Enh (6490)	42	Unit/Enh (6490)	10	35	10	5	Negative
	Carbomoyl Aspartate	No	175	Unit/Enh (6490)	79	Unit/Enh (6490)	10	40	20	5	Negative
	Dihydroorotate M+3	No	160	Unit/Enh (6490)	116	Unit/Enh (6490)	10	35	12	5	Negative
	Orotate M+3	No	158	Unit/Enh (6490)	114	Unit/Enh (6490)	10	35	12	5	Negative
	Dihydroorotate	No	157	Unit/Enh (6490)	113	Unit/Enh (6490)	10	35	12	5	Negative
	Orotate	No	155	Unit/Enh (6490)	111	Unit/Enh (6490)	10	35	12	5	Negative
	Carbamoyl-phosphate	No	140	Unit/Enh (6490)	79	Unit/Enh (6490)	10	70	20	5	Negative
	Fumaric acid d2 Std	No	117	Unit/Enh (6490)	72.8	Unit/Enh (6490)	10	50	20	5	Negative
	Uracil M+3	No	114	Unit/Enh (6490)	44	Unit/Enh (6490)	10	30	20	5	Negative
	Uracil	No	111	Unit/Enh (6490)	42	Unit/Enh (6490)	10	30	20	5	Negative
	Lactate	No	89	Unit/Enh (6490)	43	Unit/Enh (6490)	10	40	16	5	Negative

Source Parameters

Parameter	Value (+)	Value (-)
Gas Temp (°C)	350	350
Gas Flow (l/min)	9	9
Nebulizer (psi)	50	50
SheathGasHeater	375	375

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SheathGasFlow	12	12
Capillary (V)	3500	3500
VCharging	1000	1000

Scan Parameters

Data Stg	Threshold
Centroid	0

Chromatograms

Chrom Type	Label	Offset	Y-Range
TIC	TIC	0	10000000

Instrument Curves

Actual

Name: Sampler

Module: G7129B

Auxiliary

Draw Speed	100 µL/min
Eject Speed	400 µL/min
Wait Time After Draw	1.2 s
Needle Height Offset	0.0 mm

Injection

Injection Mode	Standard injection
Injection Volume	10.00 µL

High throughput

Sample Flush-Out Factor	5.0
Injection Valve to Bypass for Delay Volume Reduction	No

Overlapped Injection

Overlapped Injection Mode	Off
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Stop Time

Stoptime Mode	As pump/No limit
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Post Time

Posttime Mode	Off
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Name: Binary Pump

Module: G7120A

Flow	0.350 mL/min
Use Solvent Types	Yes
Stroke Mode	Synchronized
Low Pressure Limit	0.00 bar
High Pressure Limit	700.00 bar
Max. Flow Ramp Up	100.000 mL/min ²
Max. Flow Ramp Down	100.000 mL/min ²
Expected Mixer	No check

Stroke A

Automatic Stroke Calculation A	Yes
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Stop Time

Stoptime Mode	Time set
Stoptime	40.00 min

Post Time

Posttime Mode	Off
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Solvent Composition

	Channel	Ch. 1 Solv.	Name 1	Ch2 Solv.	Name 2	Selected	Used	Percent (%)
1	A	100.0 % Water V.02		100.0 % Water V.02		Ch. 1	Yes	15.00 %
2	B	100.0 % Acetonitrile V.02		100.0 % Acetonitrile V.02		Ch. 1	Yes	85.00 %



Timetable

	Time (min)	A (%)	B (%)	Flow (mL/min)
1	5.00 min	70.00 %	30.00 %	0.350 mL/min
2	30.00 min	98.00 %	2.00 %	0.350 mL/min
3	35.00 min	98.00 %	2.00 %	0.350 mL/min
4	40.00 min	15.00 %	85.00 %	0.350 mL/min
5	45.00 min	15.00 %	85.00 %	0.350 mL/min

Name: Column Oven

Module: G7130A

Temperature Control

Temperature Control Mode

Not Controlled

Temperature Not Ready Limit

Temperature Not Ready Limit On

Yes

Temperature Not Ready Limit Value

0.8 °C

Temperature Equilibration Time

0.0 min

Enforce column for run

Enforce column for run enabled

No

Stop Time

Stoptime Mode

As pump/injector

Post Time

Posttime Mode

Off

Timetable



	Pressure (bar)
1	700.00 bar
2	700.00 bar
3	700.00 bar
4	700.00 bar
5	700.00 bar