

Acquisition Method Report

Acquisition Method Info

Method Name 56X13_dSRM_Final.m

Method Path D:\Chromosomes\X13_datapack\history_selection\peptides_56X13\56X13_dSRM_Final.m

Method Description Reserpine MS2scan (2000 Da/sec), 1 ul (50 pg/ul) on-column injection, LC-gradient, Zorbax SB-C18, 2.1 x 50 mm, 1.8 um, 80A (PN: 822700-902)

Device List

- HiP Sampler
- Binary Pump
- Column Comp.
- QQQ

MS QQQ Mass Spectrometer

Ion Source AJS ESI Tune File atunes.TUNE.XML

Stop Mode No Limit/As Pump Stop Time (min) 1

Time Filter On Time Filter Width (min) 0.07

LC->Waste Pre Row N/A LC->Waste Post Row N/A

Time Segments

Index	Start Time (min)	Scan Type	Ion Mode	Div Valve	Delta EMV	Store	Cycle Time (ms)	Triggered?	MRM Repeats
1	0	DynamicMRM	ESI+Agilent Jet Stream	To MS	300	Yes	250	No	3

Time Segment 1

Scan Segments

Cpd Name	ISTD?	Prec Ion	MS1 Res	Prod Ion	MS2 Res	Frag (V)	CE (V)	Cell Acc (V)	Ret Time (min)	Ret Window	Polarity
AIEYVHG YFSSEQV VDLLR.ligh	No	742.379	Unit/Enh (6490)	714.451	Unit/Enh (6490)	380	27.15	2.5	31.03	1	Positive
AIEYVHG YFSSEQV VDLLR.ligh	No	742.379	Unit/Enh (6490)	615.382	Unit/Enh (6490)	380	27.15	2	31.03	1	Positive
AIEYVHG YFSSEQV VDLLR.ligh	No	742.379	Unit/Enh (6490)	516.314	Unit/Enh (6490)	380	27.15	3.5	31.03	1	Positive
ALIFSTDD FFFR.ligh	No	739.869	Unit/Enh (6490)	1034.458	Unit/Enh (6490)	380	27.04	3.5	37.08	1	Positive
ALIFSTDD FFFR.ligh	No	739.869	Unit/Enh (6490)	947.426	Unit/Enh (6490)	380	27.04	3.5	37.08	1	Positive
ALIFSTDD FFFR.ligh	No	739.869	Unit/Enh (6490)	731.351	Unit/Enh (6490)	380	27.04	3.5	37.08	1	Positive
ALYNETE SLLVGR.li	No	732.888	Unit/Enh (6490)	773.452	Unit/Enh (6490)	380	26.74	3.5	21.7	1	Positive
ALYNETE SLLVGR.li	No	732.888	Unit/Enh (6490)	644.409	Unit/Enh (6490)	380	26.74	3.5	21.7	1	Positive
ALYNETE SLLVGR.li	No	732.888	Unit/Enh (6490)	557.377	Unit/Enh (6490)	380	26.74	3.5	21.7	1	Positive

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Cpd Name	ISTD?	Prec Ion	MS1 Res	Prod Ion	MS2 Res	Frag (V)	CE (V)	Cell Acc (V)	Ret Time (min)	Ret Window	Polarity
EFYLSNS EK.light	No	558.764	Unit/Enh (6490)	840.41	Unit/Enh (6490)	380	19.13	2	7.23	1	Positive
EFYLSNS EK.light	No	558.764	Unit/Enh (6490)	677.346	Unit/Enh (6490)	380	19.13	2	7.23	1	Positive
EFYLSNS EK.light	No	558.764	Unit/Enh (6490)	564.262	Unit/Enh (6490)	380	19.13	2	7.23	1	Positive
ELNESEN SVFQAVY GLQR.light	No	695.008	Unit/Enh (6490)	806.452	Unit/Enh (6490)	380	25.08	4.7	26.77	1	Positive
ELNESEN SVFQAVY GLQR.light	No	695.008	Unit/Enh (6490)	636.346	Unit/Enh (6490)	380	25.08	2	26.77	1	Positive
ELNESEN SVFQAVY GLQR.light	No	695.008	Unit/Enh (6490)	473.283	Unit/Enh (6490)	380	25.08	5	26.77	1	Positive
ENFWDGI TDESIDK.li ght	No	834.873	Unit/Enh (6490)	807.373	Unit/Enh (6490)	380	31.19	3.5	23.62	1	Positive
ENFWDGI TDESIDK.li ght	No	834.873	Unit/Enh (6490)	706.325	Unit/Enh (6490)	380	31.19	3.5	23.62	1	Positive
ENFWDGI TDESIDK.li ght	No	834.873	Unit/Enh (6490)	591.298	Unit/Enh (6490)	380	31.19	3.5	23.62	1	Positive
ENQEGAA NVNVR.lig ht	No	650.816	Unit/Enh (6490)	800.437	Unit/Enh (6490)	380	23.15	5	2.91	1	Positive
ENQEGAA NVNVR.lig ht	No	650.816	Unit/Enh (6490)	743.416	Unit/Enh (6490)	380	23.15	5	2.91	1	Positive
ENQEGAA NVNVR.lig ht	No	650.816	Unit/Enh (6490)	672.379	Unit/Enh (6490)	380	23.15	5	2.91	1	Positive
EPDSYDG ITTNQR.lig ht	No	748.337	Unit/Enh (6490)	904.448	Unit/Enh (6490)	380	27.41	4.8	4.78	1	Positive
EPDSYDG ITTNQR.lig ht	No	748.337	Unit/Enh (6490)	789.421	Unit/Enh (6490)	380	27.41	2.5	4.78	1	Positive
EPDSYDG ITTNQR.lig ht	No	748.337	Unit/Enh (6490)	619.316	Unit/Enh (6490)	380	27.41	2	4.78	1	Positive
FISPFQF NITR.light	No	735.891	Unit/Enh (6490)	1026.537	Unit/Enh (6490)	380	32.24	3.5	29.63	1	Positive
FISPFQF NITR.light	No	735.891	Unit/Enh (6490)	650.362	Unit/Enh (6490)	380	32.24	2	29.63	1	Positive
FISPFQF NITR.light	No	735.891	Unit/Enh (6490)	503.294	Unit/Enh (6490)	380	32.24	4.5	29.63	1	Positive
FSTDYEF LDK.light	No	632.79	Unit/Enh (6490)	1030.473	Unit/Enh (6490)	380	17.89	3.5	17.48	1	Positive
FSTDYEF LDK.light	No	632.79	Unit/Enh (6490)	929.425	Unit/Enh (6490)	380	17.89	3.5	17.48	1	Positive
FSTDYEF LDK.light	No	632.79	Unit/Enh (6490)	614.246	Unit/Enh (6490)	380	17.89	3.5	17.48	1	Positive
GEEAAPE SLDVYR. light	No	767.873	Unit/Enh (6490)	651.346	Unit/Enh (6490)	380	22.61	2	14.38	1	Positive
GEEAAPE SLDVYR. light	No	767.873	Unit/Enh (6490)	536.319	Unit/Enh (6490)	380	22.61	2	14.38	1	Positive

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Cpd Name	ISTD?	Prec Ion	MS1 Res	Prod Ion	MS2 Res	Frag (V)	CE (V)	Cell Acc (V)	Ret Time (min)	Ret Window	Polarity
GEEAAPE SLDVVYR. light	No	767.873	Unit/Enh (6490)	458.188	Unit/Enh (6490)	380	22.61	2	14.38	1	Positive
GPLSPQE VEYWILIG ESSR.light	No	720.704	Unit/Enh (6490)	761.415	Unit/Enh (6490)	380	26.2	3.5	34.58	1	Positive
GPLSPQE VEYWILIG ESSR.light	No	720.704	Unit/Enh (6490)	648.331	Unit/Enh (6490)	380	26.2	3.5	34.58	1	Positive
GPLSPQE VEYWILIG ESSR.light	No	720.704	Unit/Enh (6490)	535.247	Unit/Enh (6490)	380	26.2	3.5	34.58	1	Positive
GPVNYNV TTEFEK.li ght	No	749.365	Unit/Enh (6490)	967.473	Unit/Enh (6490)	380	27.46	3.5	14.92	1	Positive
GPVNYNV TTEFEK.li ght	No	749.365	Unit/Enh (6490)	853.43	Unit/Enh (6490)	380	27.46	3.5	14.92	1	Positive
GPVNYNV TTEFEK.li ght	No	749.365	Unit/Enh (6490)	531.256	Unit/Enh (6490)	380	27.46	3.5	14.92	1	Positive
HVDALNA WR.light	No	541.281	Unit/Enh (6490)	944.495	Unit/Enh (6490)	380	22.04	3.7	9.35	1	Positive
HVDALNA WR.light	No	541.281	Unit/Enh (6490)	845.426	Unit/Enh (6490)	380	22.04	3.7	9.35	1	Positive
HVDALNA WR.light	No	541.281	Unit/Enh (6490)	730.399	Unit/Enh (6490)	380	22.04	3.7	9.35	1	Positive
ILYDLHSE VQTLK.lig ht	No	779.927	Unit/Enh (6490)	941.505	Unit/Enh (6490)	380	33.82	3.5	17.29	1	Positive
ILYDLHSE VQTLK.lig ht	No	779.927	Unit/Enh (6490)	804.446	Unit/Enh (6490)	380	33.82	3.5	17.29	1	Positive
ILYDLHSE VQTLK.lig ht	No	779.927	Unit/Enh (6490)	588.372	Unit/Enh (6490)	380	33.82	3.5	17.29	1	Positive
IQSSLSSA SPSK.light	No	596.314	Unit/Enh (6490)	776.415	Unit/Enh (6490)	380	24.92	3.5	3.19	1	Positive
IQSSLSSA SPSK.light	No	596.314	Unit/Enh (6490)	663.331	Unit/Enh (6490)	380	24.92	2	3.19	1	Positive
IQSSLSSA SPSK.light	No	596.314	Unit/Enh (6490)	576.299	Unit/Enh (6490)	380	24.92	3.5	3.19	1	Positive
LQVSEPQI R.light	No	968.002	Unit/Enh (6490)	956.516	Unit/Enh (6490)	380	37.01	3.5	22.91	1	Positive
LQVSEPQI R.light	No	968.002	Unit/Enh (6490)	828.457	Unit/Enh (6490)	380	37.01	3.5	22.91	1	Positive
LQVSEPQI R.light	No	968.002	Unit/Enh (6490)	513.314	Unit/Enh (6490)	380	37.01	4.8	22.91	1	Positive
LNDTTLQ VLNTWYT K.light	No	905.473	Unit/Enh (6490)	925.478	Unit/Enh (6490)	380	34.28	5	27.99	1	Positive
LNDTTLQ VLNTWYT K.light	No	905.473	Unit/Enh (6490)	597.303	Unit/Enh (6490)	380	34.28	2	27.99	1	Positive
LNDTTLQ VLNTWYT K.light	No	905.473	Unit/Enh (6490)	545.257	Unit/Enh (6490)	380	34.28	3.5	27.99	1	Positive
LPLTLVPG ER.light	No	547.832	Unit/Enh (6490)	557.304	Unit/Enh (6490)	380	18.65	3.5	18.74	1	Positive

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Cpd Name	ISTD?	Prec Ion	MS1 Res	Prod Ion	MS2 Res	Frag (V)	CE (V)	Cell Acc (V)	Ret Time (min)	Ret Window	Polarity
LPLTLVPG ER.light	No	547.832	Unit/Enh (6490)	538.36	Unit/Enh (6490)	380	18.65	4.7	18.74	1	Positive
LPLTLVPG ER.light	No	547.832	Unit/Enh (6490)	458.236	Unit/Enh (6490)	380	18.65	5	18.74	1	Positive
LQEQNELI ITQR.light	No	742.907	Unit/Enh (6490)	986.563	Unit/Enh (6490)	380	27.18	3.5	12	1	Positive
LQEQNELI ITQR.light	No	742.907	Unit/Enh (6490)	630.393	Unit/Enh (6490)	380	27.18	2	12	1	Positive
LQEQNELI ITQR.light	No	742.907	Unit/Enh (6490)	517.309	Unit/Enh (6490)	380	27.18	5	12	1	Positive
LYLFQAQ EWLK.light	No	719.89	Unit/Enh (6490)	1049.541	Unit/Enh (6490)	380	26.17	2.2	32.82	1	Positive
LYLFQAQ EWLK.light	No	719.89	Unit/Enh (6490)	902.473	Unit/Enh (6490)	380	26.17	5	32.82	1	Positive
LYLFQAQ EWLK.light	No	719.89	Unit/Enh (6490)	774.414	Unit/Enh (6490)	380	26.17	2.5	32.82	1	Positive
NTITDLQP SVK.light	No	608.333	Unit/Enh (6490)	887.483	Unit/Enh (6490)	380	18.52	5	10.01	1	Positive
NTITDLQP SVK.light	No	608.333	Unit/Enh (6490)	671.409	Unit/Enh (6490)	380	18.52	3.5	10.01	1	Positive
NTITDLQP SVK.light	No	608.333	Unit/Enh (6490)	558.325	Unit/Enh (6490)	380	18.52	3.5	10.01	1	Positive
NVFIIVIE TFAEIR.lig ht	No	867.993	Unit/Enh (6490)	865.441	Unit/Enh (6490)	380	26.11	4.5	51.86	1	Positive
NVFIIVIE TFAEIR.lig ht	No	867.993	Unit/Enh (6490)	644.377	Unit/Enh (6490)	380	26.11	2	51.86	1	Positive
NVFIIVIE TFAEIR.lig ht	No	867.993	Unit/Enh (6490)	545.308	Unit/Enh (6490)	380	26.11	5	51.86	1	Positive
SWLTATS ASQDIEK.I ght	No	768.881	Unit/Enh (6490)	790.394	Unit/Enh (6490)	380	22.65	2.5	15.79	1	Positive
SWLTATS ASQDIEK.I ght	No	768.881	Unit/Enh (6490)	719.357	Unit/Enh (6490)	380	22.65	2.5	15.79	1	Positive
SWLTATS ASQDIEK.I ght	No	768.881	Unit/Enh (6490)	632.325	Unit/Enh (6490)	380	22.65	2.5	15.79	1	Positive
TGAVYVA EIGAK.ligh t	No	589.824	Unit/Enh (6490)	850.467	Unit/Enh (6490)	380	20.49	3.5	10.69	1	Positive
TGAVYVA EIGAK.ligh t	No	589.824	Unit/Enh (6490)	687.404	Unit/Enh (6490)	380	20.49	3.5	10.69	1	Positive
TGAVYVA EIGAK.ligh t	No	589.824	Unit/Enh (6490)	517.298	Unit/Enh (6490)	380	20.49	3.5	10.69	1	Positive
THQLSLD AFLVALK.I ght	No	778.446	Unit/Enh (6490)	761.492	Unit/Enh (6490)	380	28.73	3.5	34.32	1	Positive
THQLSLD AFLVALK.I ght	No	778.446	Unit/Enh (6490)	567.289	Unit/Enh (6490)	380	28.73	3.5	34.32	1	Positive
THQLSLD AFLVALK.I ght	No	778.446	Unit/Enh (6490)	480.257	Unit/Enh (6490)	380	28.73	3.5	34.32	1	Positive
TSLWEEE NALWEEE R.light	No	960.934	Unit/Enh (6490)	1046.49	Unit/Enh (6490)	380	36.7	2.7	26.74	1	Positive

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Cpd Name	ISTD?	Prec Ion	MS1 Res	Prod Ion	MS2 Res	Frag (V)	CE (V)	Cell Acc (V)	Ret Time (min)	Ret Window	Polarity
TSLWEEE NALWEEE R.light	No	960.934	Unit/Enh (6490)	748.326	Unit/Enh (6490)	380	36.7	2.7	26.74	1	Positive
TSLWEEE NALWEEE R.light	No	960.934	Unit/Enh (6490)	562.247	Unit/Enh (6490)	380	36.7	2.7	26.74	1	Positive
VATGQEL SNNILDTV FK.light	No	924.989	Unit/Enh (6490)	949.535	Unit/Enh (6490)	380	35.13	2	25.93	1	Positive
VATGQEL SNNILDTV FK.light	No	924.989	Unit/Enh (6490)	722.408	Unit/Enh (6490)	380	35.13	2	25.93	1	Positive
VATGQEL SNNILDTV FK.light	No	924.989	Unit/Enh (6490)	609.324	Unit/Enh (6490)	380	35.13	2	25.93	1	Positive
VESPEEQ WFADK.lig ht	No	789.378	Unit/Enh (6490)	1036.51	Unit/Enh (6490)	380	33.17	3.5	21.57	1	Positive
VESPEEQ WFADK.lig ht	No	789.378	Unit/Enh (6490)	907.467	Unit/Enh (6490)	380	33.17	5	21.57	1	Positive
VESPEEQ WFADK.lig ht	No	789.378	Unit/Enh (6490)	666.325	Unit/Enh (6490)	380	33.17	2	21.57	1	Positive
VLNLSST SPEK.light	No	587.819	Unit/Enh (6490)	848.436	Unit/Enh (6490)	380	20.4	4.5	6.94	1	Positive
VLNLSST SPEK.light	No	587.819	Unit/Enh (6490)	735.352	Unit/Enh (6490)	380	20.4	3.5	6.94	1	Positive
VLNLSST SPEK.light	No	587.819	Unit/Enh (6490)	460.24	Unit/Enh (6490)	380	20.4	3.5	6.94	1	Positive
YAHGLISD YIPK.light	No	688.864	Unit/Enh (6490)	835.456	Unit/Enh (6490)	380	24.81	5	17.47	1	Positive
YAHGLISD YIPK.light	No	688.864	Unit/Enh (6490)	542.272	Unit/Enh (6490)	380	24.81	5	17.47	1	Positive
YAHGLISD YIPK.light	No	688.864	Unit/Enh (6490)	520.313	Unit/Enh (6490)	380	24.81	5	17.47	1	Positive
YDNYADS LR.light	No	558.751	Unit/Enh (6490)	838.405	Unit/Enh (6490)	380	19.13	4.3	6.14	1	Positive
YDNYADS LR.light	No	558.751	Unit/Enh (6490)	724.362	Unit/Enh (6490)	380	19.13	4.3	6.14	1	Positive
YDNYADS LR.light	No	558.751	Unit/Enh (6490)	561.299	Unit/Enh (6490)	380	19.13	4.3	6.14	1	Positive
YHAISAD GER.light	No	559.765	Unit/Enh (6490)	818.4	Unit/Enh (6490)	380	23.01	3.5	2.68	1	Positive
YHAISAD GER.light	No	559.765	Unit/Enh (6490)	747.363	Unit/Enh (6490)	380	23.01	3.5	2.68	1	Positive
YHAISAD GER.light	No	559.765	Unit/Enh (6490)	634.279	Unit/Enh (6490)	380	23.01	3.5	2.68	1	Positive

Scan Parameters

Data Stg Threshold
Centroid 0

Acquisition Method Report

Source Parameters

Parameter	Value (+)	Value (-)
Gas Temp (°C)	250	250
Gas Flow (l/min)	14	14
Nebulizer (psi)	17	17
SheathGasHeater	280	280
SheathGasFlow	11	11
Capillary (V)	3500	3000
VCharging	450	1500

Ion Funnel Parameters

Pos High Pressure RF	150	Neg High Pressure RF	150
Pos Low Pressure RF	60	Neg Low Pressure RF	60

Chromatograms

Chrom Type	Label	Offset	Y-Range
TIC	Total Ion Chromatogram	10	100000

Instrument Curves

Actual

Name: HiP Sampler

Model: G4226A

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Auxiliary

Draw Speed	120.0 µL/min
Eject Speed	180.0 µL/min
Draw Position Offset	2.0 mm
Wait Time After Drawing	3.0 s
Sample Flush Out Factor	5.0
Vial/Well bottom sensing	Yes

Injection

Injection Mode	Injection with needle wash
Injection Volume	7.00 µL
Needle Wash	
Needle Wash Location	Flush Port
Wash Time	7.0 s

High throughput

Automatic Delay Volume Reduction	No
Overlapped Injection	
Enable Overlapped Injection	No

Valve Switching

Valve Movements	0
Valve Switch Time 1	
Switch Time 1 Enabled	No
Valve Switch Time 2	
Switch Time 2 Enabled	No
Valve Switch Time 3	
Switch Time 3 Enabled	No
Valve Switch Time 4	
Switch Time 4 Enabled	No

Stop Time

Stoptime Mode	As pump/No limit
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Post Time

Posttime Mode	Off
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Acquisition Method Report

Name: Binary Pump Model: G4220A

Flow 0.300 mL/min
 Use Solvent Types Yes
 Stroke Mode Synchronized
 Low Pressure Limit 0.00 bar
 High Pressure Limit 1000.00 bar
 Max. Flow Ramp Up 100.000 mL/min²
 Max. Flow Ramp Down 100.000 mL/min²
 Expected Mixer No check

Stroke A

Automatic Stroke Calculation A Yes

Stop Time

Stoptime Mode Time set
 Stoptime 60.00 min

Post Time

Posttime Mode Time set
 Posttime 5.00 min

Solvent Composition

	Channel	Ch. 1 Solv.	Name 1	Ch2 Solv.	Name 2	Selected	Used	Percent
1	A	100.0 % Water V.02	H2O w/ 0.1% formic acid	100.0 % Water V.02		Ch. 1	Yes	97.00 %
2	B	100.0 % Acetonitrile V.02	Acetonitrile w/ 0.1% formic	100.0 % Acetonitrile V.02		Ch. 1	Yes	3.00 %

Timetable

	Time	A	B	Flow	Pressure
1	2.00 min	91.50 %	8.50 %	--- mL/min	--- bar
2	50.00 min	68.00 %	32.00 %	--- mL/min	--- bar
3	52.00 min	46.40 %	53.60 %	--- mL/min	--- bar
4	53.00 min	20.00 %	80.00 %	--- mL/min	--- bar
5	58.00 min	20.00 %	80.00 %	--- mL/min	--- bar
6	60.00 min	97.00 %	3.00 %	--- mL/min	--- bar

Acquisition Method Report

Name: Column Comp. Model: G1316C

Valve Position Port 1 -> 2
Ready when front door open Yes

Left Temperature Control

Temperature Control Mode Not Controlled
Enable Analysis Left Temperature Yes
Enable Analysis Left Temperature Value 0.80 °C

Right Temperature Control

Right temperature Control Mode Temperature Set
Right temperature 42.00 °C
Enable Analysis Right Temperature Yes
Enable Analysis Right Temperature Value 0.80 °C

Stop Time

Stoptime Mode As pump/injector

Post Time

Posttime Mode Off