

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV062320\
 Data File : VV017032.D
 Acq On : 22 Jun 2020 21:21
 Operator : SY/MD
 Sample : L3067-13
 Misc : 25.0mL/MSVOA V/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BFXH0

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.1

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR061720WMA.M

Title : TRACE VOA SOM01.0

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.132	312	324	337	rBV4	361293	600681	3.25%	2.004%
2	3.209	643	659	681	rBV	1939073	4002829	21.69%	13.356%
3	3.933	869	884	919	rBV4	144836	465107	2.52%	1.552%
4	4.376	1006	1022	1042	rBV	108740	268805	1.46%	0.897%
5	4.637	1078	1103	1137	rBV	7368965	18456747	100.00%	61.584%
6	5.071	1219	1238	1252	rBV2	250296	618890	3.35%	2.065%
7	5.640	1397	1415	1438	rBV	222200	454497	2.46%	1.517%
8	6.096	1542	1557	1576	rBV	139391	286592	1.55%	0.956%
9	6.341	1619	1633	1649	rBV	101909	214979	1.16%	0.717%
10	7.338	1930	1943	1958	rBV	316029	540471	2.93%	1.803%
11	8.109	2173	2183	2211	rBV	295530	534229	2.89%	1.783%
12	8.874	2408	2421	2443	rBV	335129	609400	3.30%	2.033%
13	9.752	2682	2694	2706	rBV	193041	306578	1.66%	1.023%
14	10.501	2916	2927	2940	rVB	942155	1506518	8.16%	5.027%
15	11.270	3155	3166	3183	rBV	357910	559019	3.03%	1.865%
16	11.646	3272	3283	3304	rVV	326340	544741	2.95%	1.818%

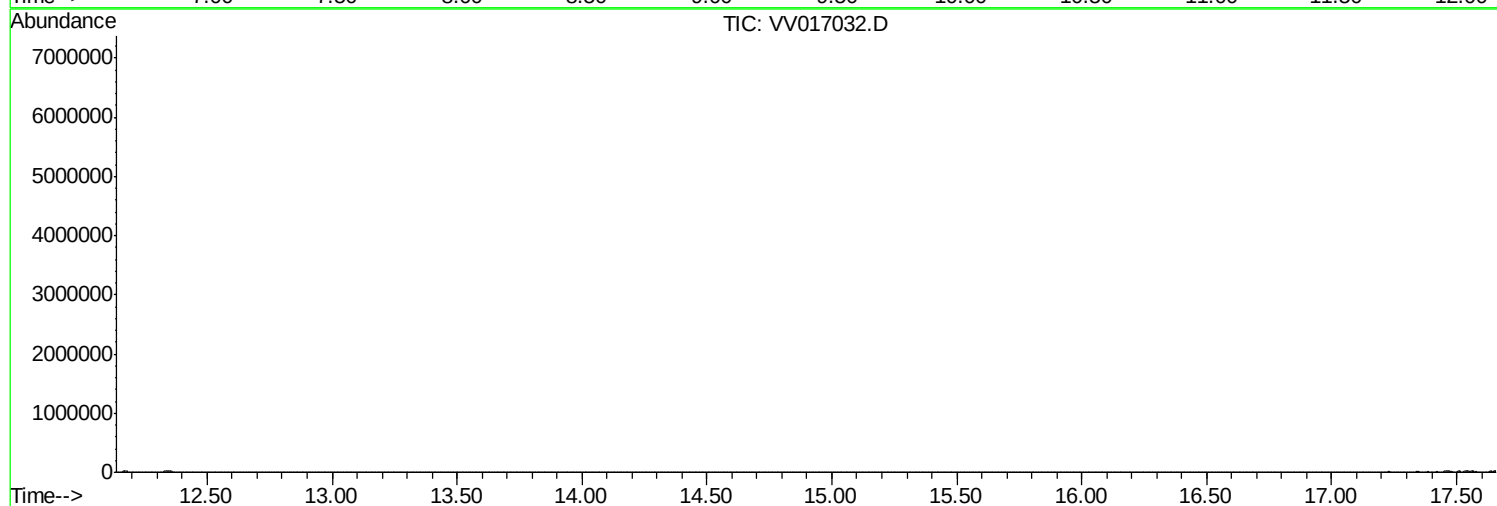
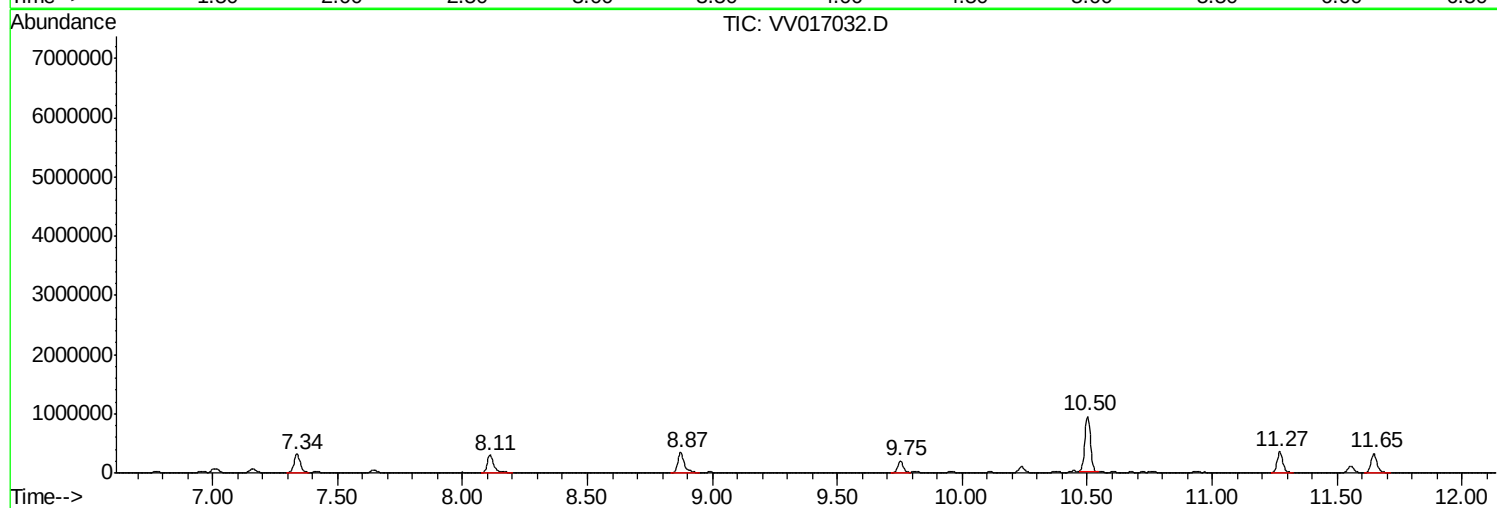
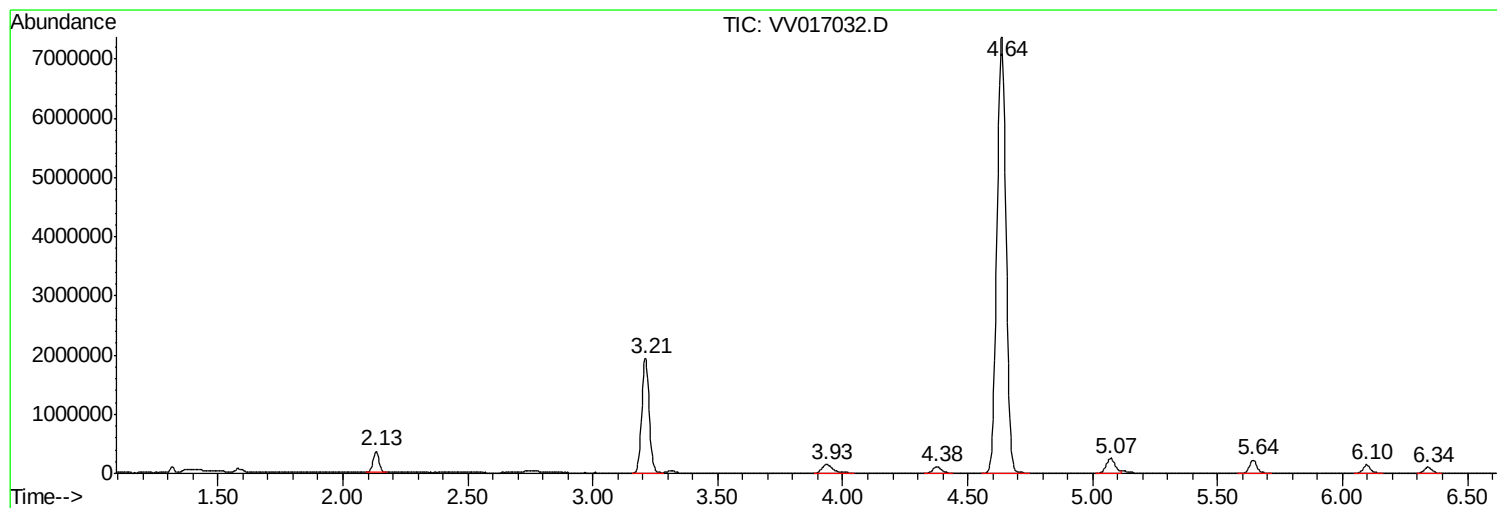
Sum of corrected areas: 29970083

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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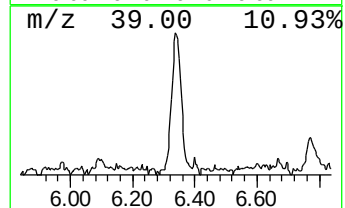
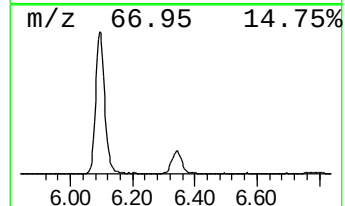
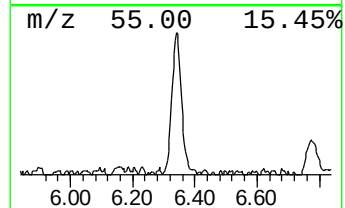
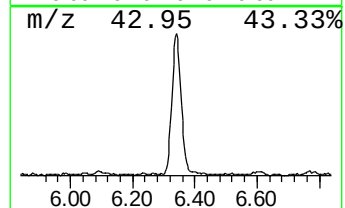
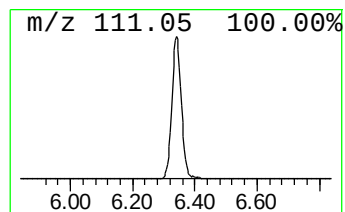
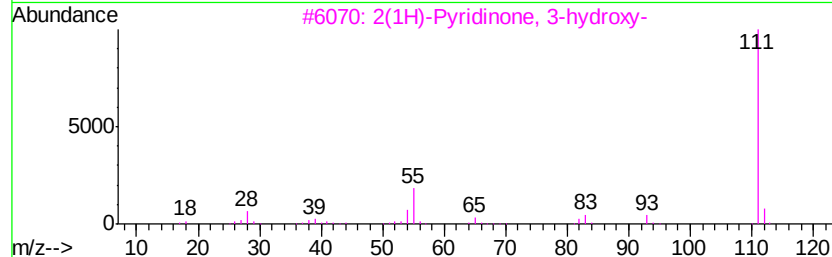
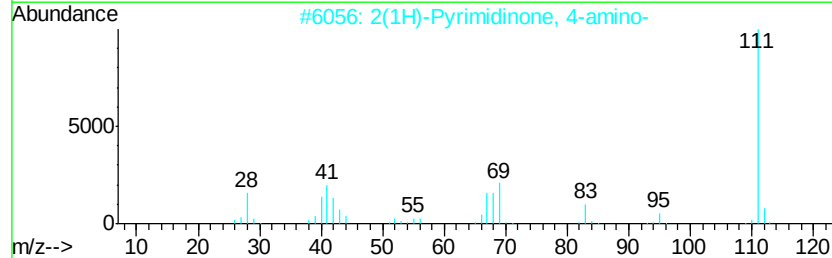
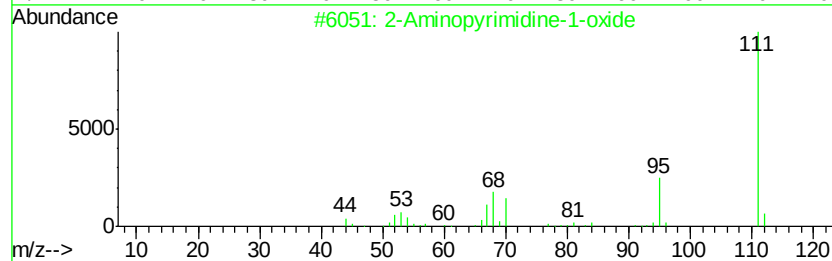
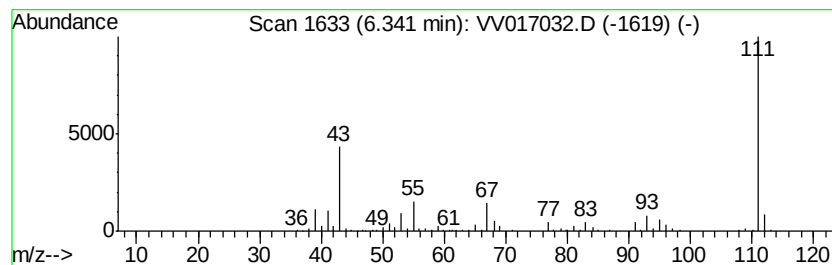
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Aminopyrimidine-1-oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	2.37 ug/L	214979	1,4-Difluorobenzene	5.64

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Aminopyrimidine-1-oxide	111	C4H5N3O	035034-15-2	72
2			2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	59
3			2(1H)-Pyridinone, 3-hydroxy-	111	C5H5N2O	016867-04-2	53
4			Bruceantin	548	C28H36O11	041451-75-6	45
5			2(1H)-Pyridinone, 3-hydroxy-	111	C5H5N2O	016867-04-2	45



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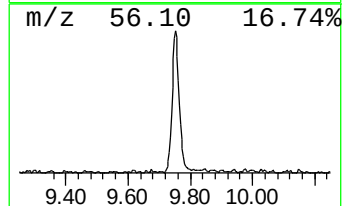
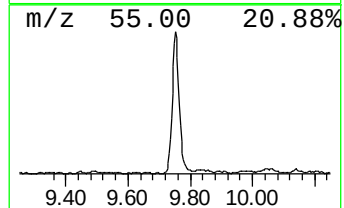
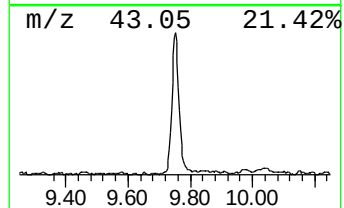
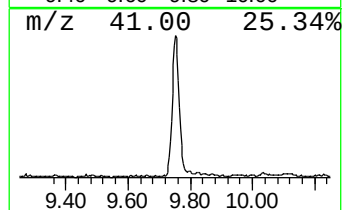
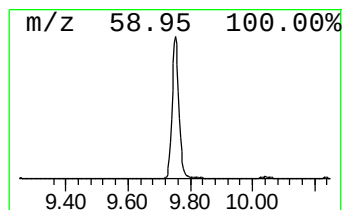
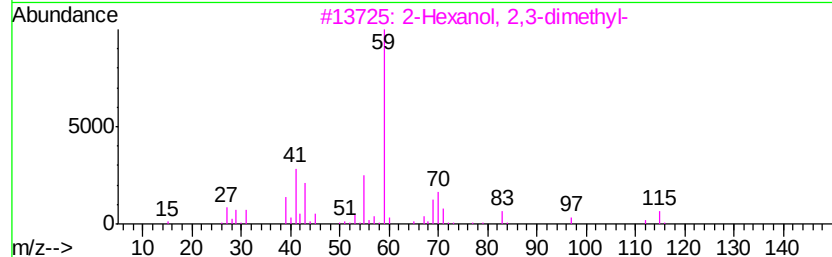
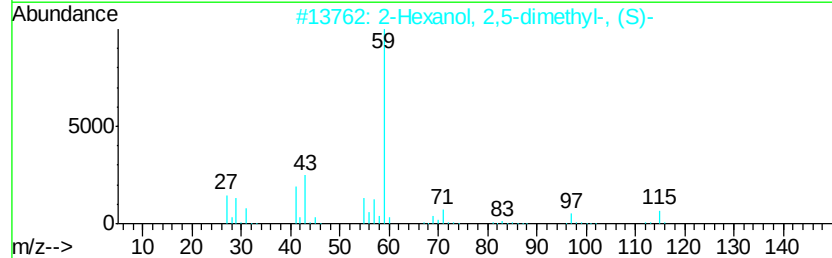
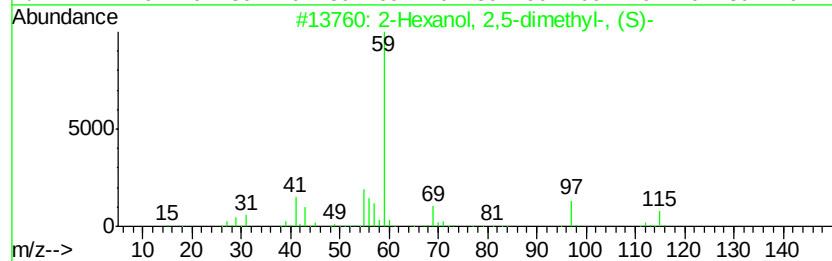
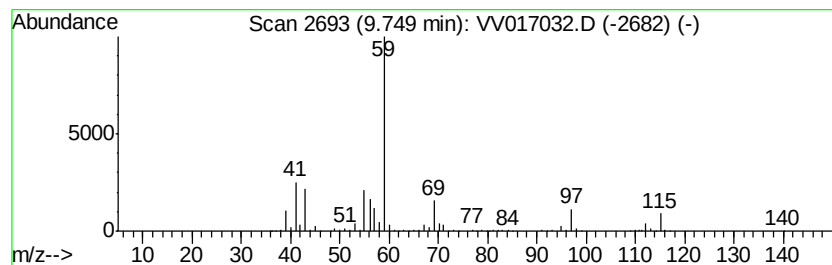
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Hexanol, 2,5-dimethyl-, (S)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.75	2.52 ug/L	306578	Chlorobenzene-d5	8.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	90
2		2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	72
3		2-Hexanol, 2,3-dimethyl-	130	C8H18O	019550-03-9	50
4		2-Octanol, 2,6-dimethyl-	158	C10H22O	018479-57-7	45
5		Hexanamide, 4-ethyl-5,5-dimethyl-	171	C10H21NO	054789-39-8	40



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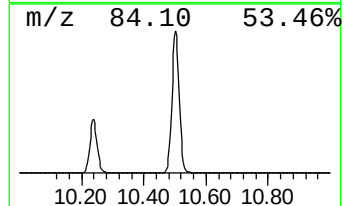
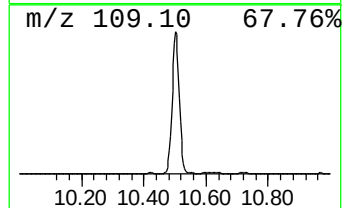
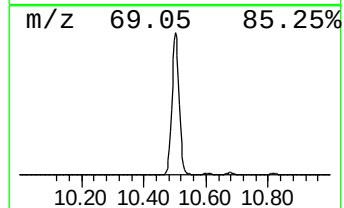
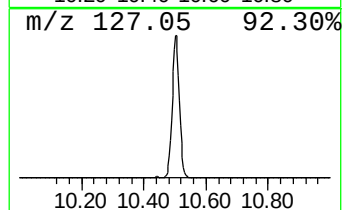
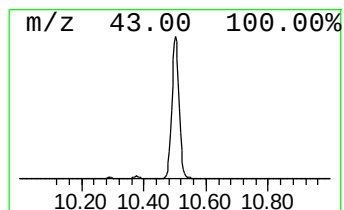
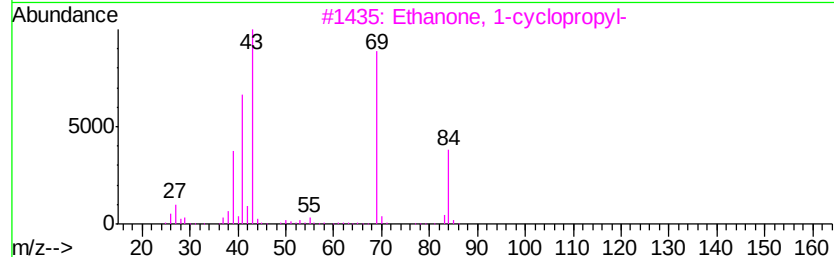
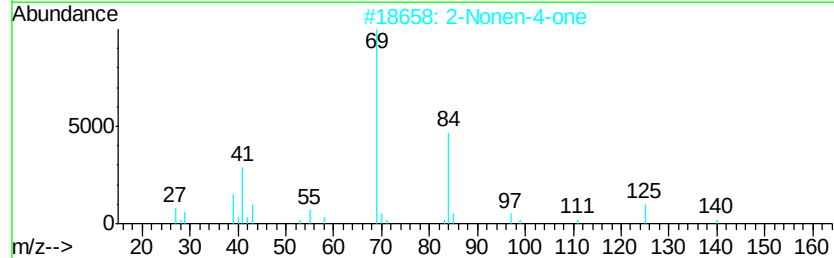
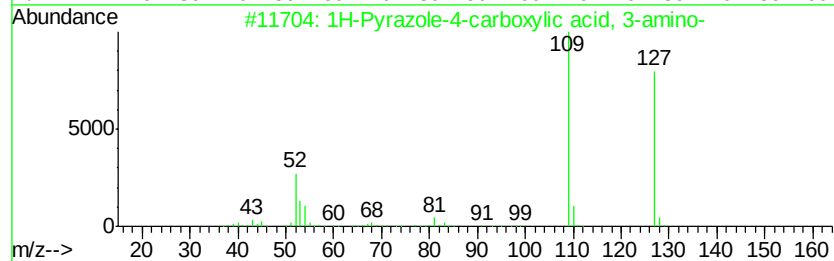
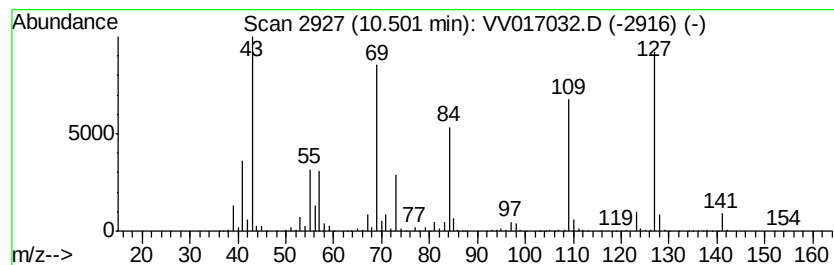
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Peak Number 3 1H-Pyrazole-4-carboxylic ac... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.50	13.47 ug/L	1506520	1,4-Dichlorobenzene-d4	11.27
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1H-Pyrazole-4-carboxylic acid, 3-amino-	127 C4H5N3O2	041680-34-6 35
2		2-Nonen-4-one	140 C9H16O	032064-72-5 27
3		Ethanone, 1-cyclopropyl-	84 C5H8O	000765-43-5 27
4		Pentane, 2-chloro-4-methyl-	120 C6H13Cl	025346-32-1 27
5		Furan, 2,3-dihydro-3-methyl-	84 C5H8O	001708-27-6 27



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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Aminopyrimidine...	6.34	2.4	ug/L	214979	1	5.64	454497	5.0
2-Hexanol, 2,5-di...	9.75	2.5	ug/L	306578	2	8.87	609400	5.0
1H-Pyrazole-4-car...	10.50	13.5	ug/L	1506520	3	11.27	559019	5.0