

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102822\
 Data File : VU051593.D
 Acq On : 29 Oct 2022 02:19
 Operator : JC/MD
 Sample : N5276-13
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW4X3

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.1

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU051593.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.482	35	44	58	rBV	208987	513933	60.10%	7.003%
2	1.729	115	121	132	rVB	306880	384260	44.93%	5.236%
3	1.912	173	178	194	rVB	88262	117407	13.73%	1.600%
4	2.565	369	381	396	rVB	132962	214393	25.07%	2.922%
5	2.790	441	451	459	rBV	7676	15390	1.80%	0.210%
6	3.186	565	574	580	rBV5	4575	9176	1.07%	0.125%
7	3.594	686	701	704	rBV4	4292	9304	1.09%	0.127%
8	3.870	755	787	789	rBV	15872	52744	6.17%	0.719%
9	4.639	1004	1026	1066	rBV2	106625	373587	43.69%	5.091%
10	5.063	1141	1158	1184	rBV	153853	353467	41.33%	4.817%
11	5.722	1343	1363	1398	rBV4	277943	744389	87.05%	10.144%
12	6.247	1513	1526	1543	rBV	251953	487469	57.00%	6.643%
13	6.690	1650	1664	1683	rBV	187331	367259	42.95%	5.005%
14	7.166	1800	1812	1838	rBV2	44774	96883	11.33%	1.320%
15	7.565	1923	1936	1962	rBV	62007	109035	12.75%	1.486%
16	7.710	1969	1981	1995	rBV8	5240	10519	1.23%	0.143%
17	7.825	2000	2017	2027	rBV7	13261	32096	3.75%	0.437%
18	7.896	2027	2039	2055	rVV	275656	485135	56.73%	6.611%
19	7.970	2055	2062	2073	rVB	12144	21651	2.53%	0.295%
20	8.179	2114	2127	2142	rBV2	34986	61663	7.21%	0.840%
21	8.484	2210	2222	2234	rVV7	6959	16156	1.89%	0.220%
22	8.636	2253	2269	2305	rBV	422554	855150	100.00%	11.653%
23	8.783	2309	2315	2329	rVB	4999	10697	1.25%	0.146%
24	9.417	2499	2512	2535	rBV	386524	648144	75.79%	8.832%
25	9.690	2588	2597	2611	rBV4	5597	9890	1.16%	0.135%
26	10.754	2918	2928	2945	rVB	162528	261917	30.63%	3.569%
27	10.893	2956	2971	2980	rBV2	6735	11454	1.34%	0.156%
28	11.809	3244	3256	3280	rBV	317152	522535	61.10%	7.121%
29	12.060	3323	3334	3350	rBV3	16285	31534	3.69%	0.430%
30	12.192	3363	3375	3396	rVB	263888	432738	50.60%	5.897%
31	14.423	4057	4069	4087	rBV2	32376	58389	6.83%	0.796%
32	15.111	4271	4283	4291	rBV4	12213	19964	2.33%	0.272%

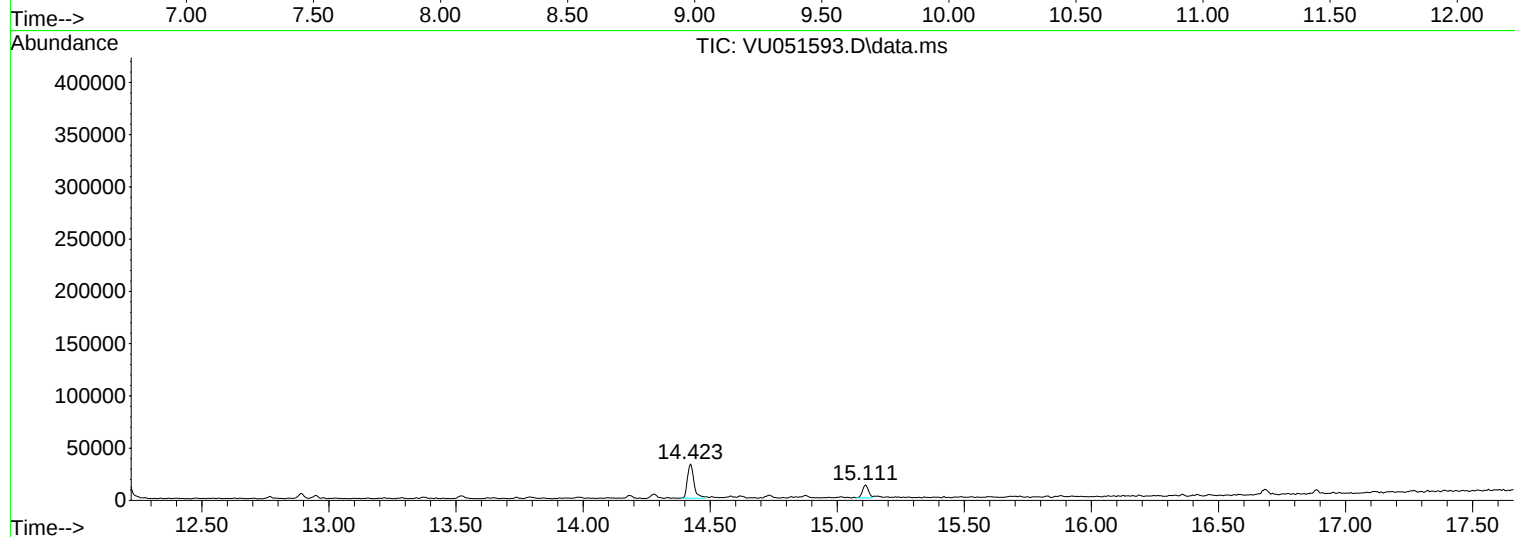
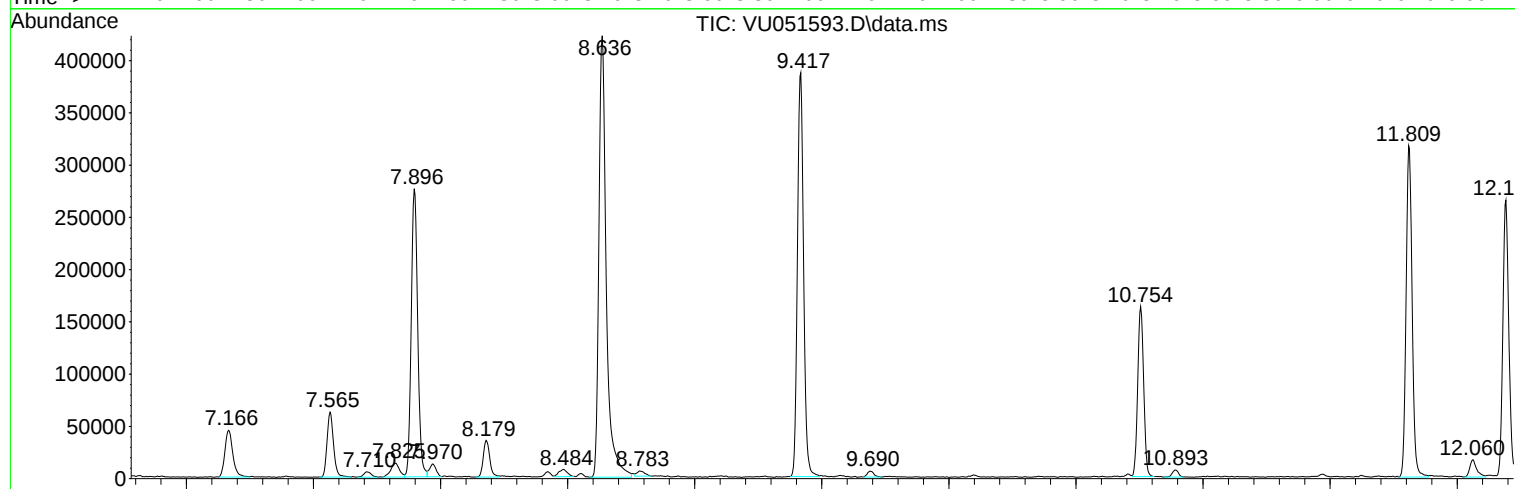
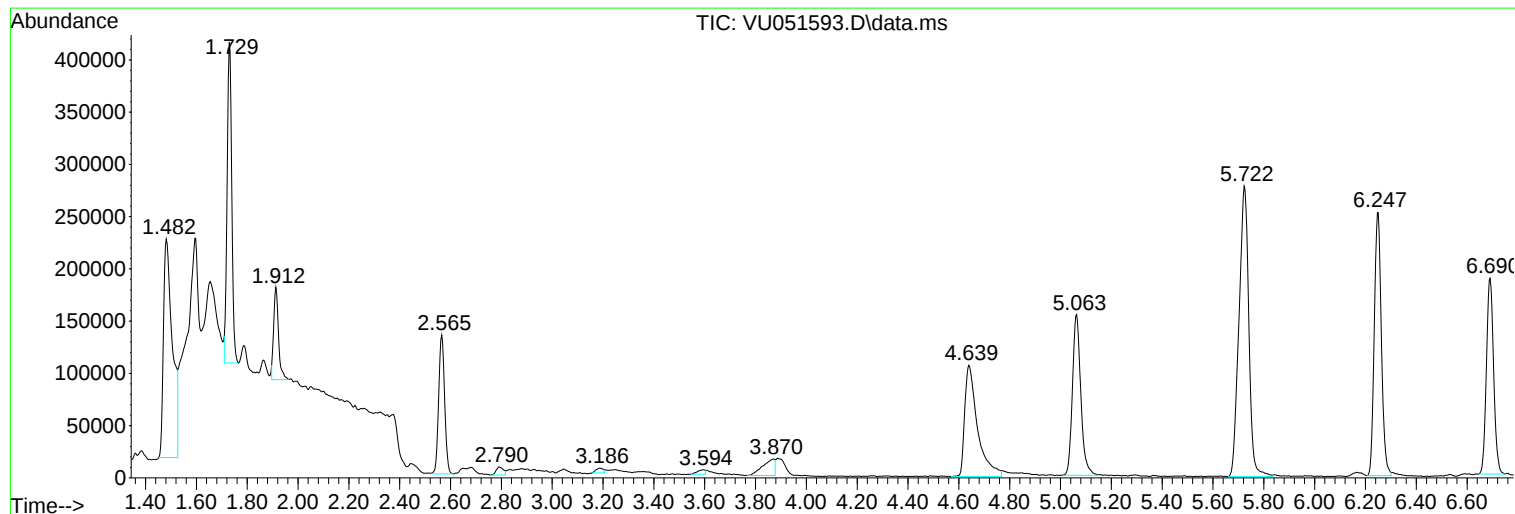
Sum of corrected areas: 7338328

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102822\
Data File : VU051593.D
Acq On : 29 Oct 2022 02:19
Operator : JC/MD
Sample : N5276-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4X3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102822\
Data File : VU051593.D
Acq On : 29 Oct 2022 02:19
Operator : JC/MD
Sample : N5276-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4X3

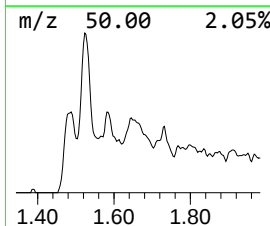
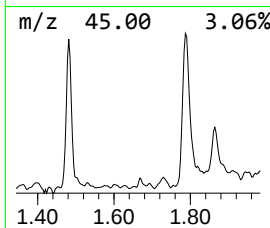
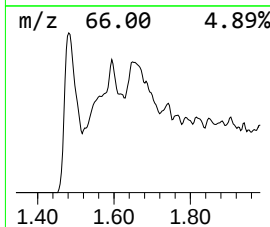
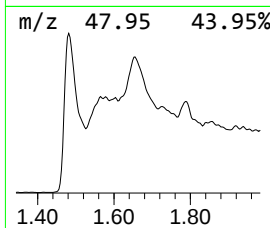
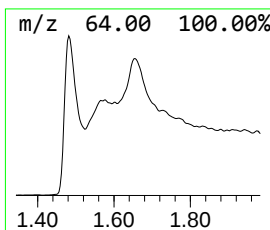
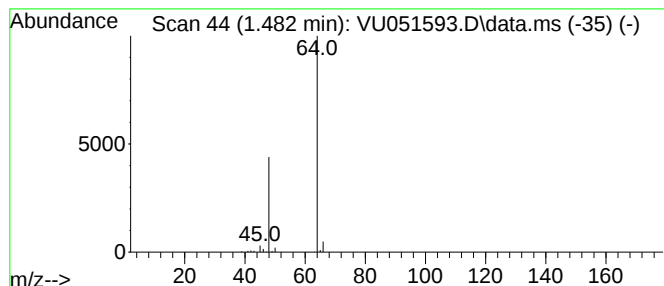
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.482	5.27 ug/L	513933	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	7
5			Sulfur dioxide	64	O2S	007446-09-5	5



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102822\
Data File : VU051593.D
Acq On : 29 Oct 2022 02:19
Operator : JC/MD
Sample : N5276-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4X3

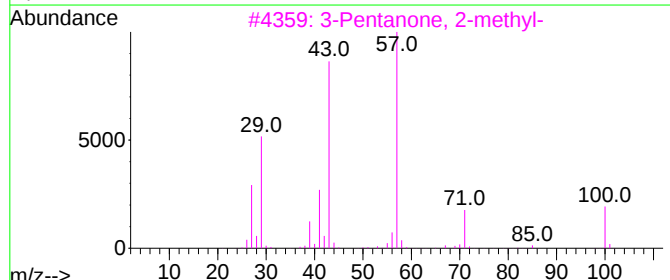
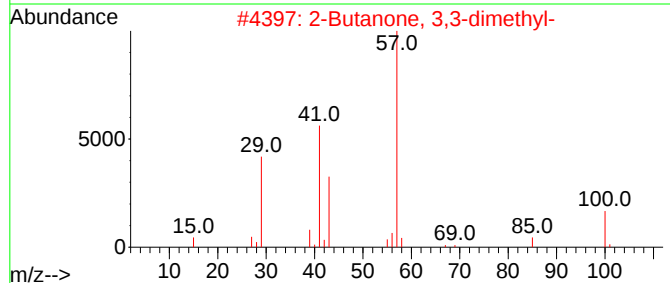
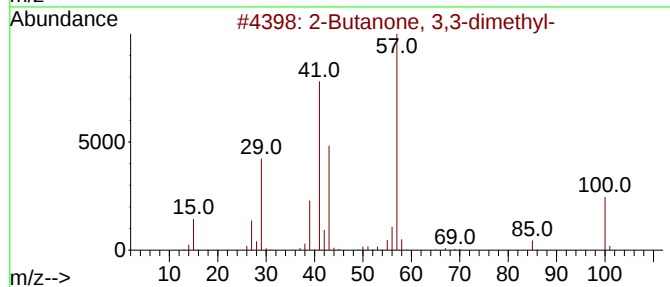
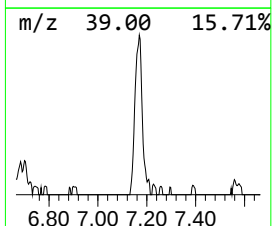
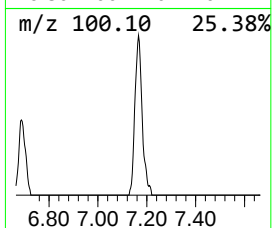
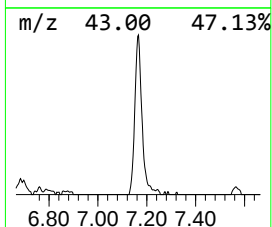
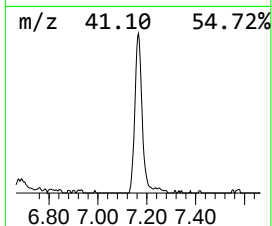
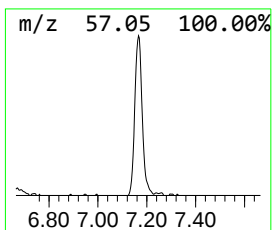
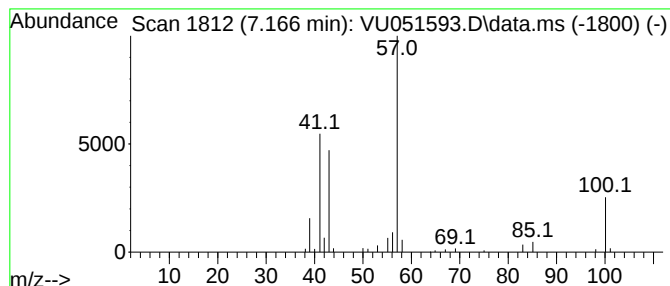
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Butanone, 3,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.166	0.99 ug/L	96883	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3,3-dimethyl-		100	C6H12O	000075-97-8	90	
2	2-Butanone, 3,3-dimethyl-		100	C6H12O	000075-97-8	64	
3	3-Pentanone, 2-methyl-		100	C6H12O	000565-69-5	64	
4	2-Butanone, 3,3-dimethyl-		100	C6H12O	000075-97-8	59	
5	3-Pentanone, 2-methyl-		100	C6H12O	000565-69-5	53	



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102822\
Data File : VU051593.D
Acq On : 29 Oct 2022 02:19
Operator : JC/MD
Sample : N5276-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4X3

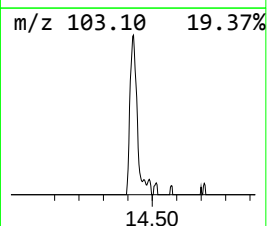
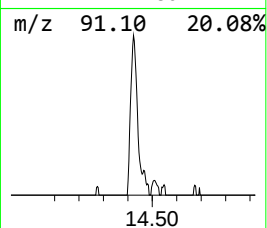
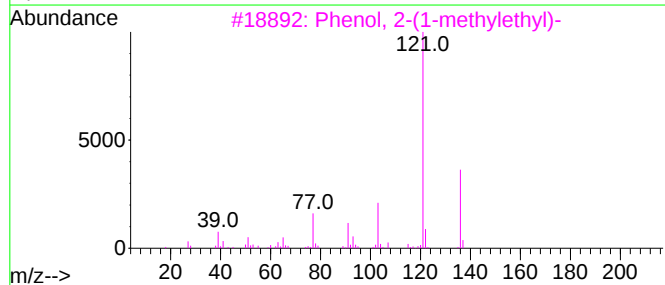
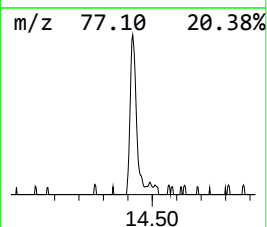
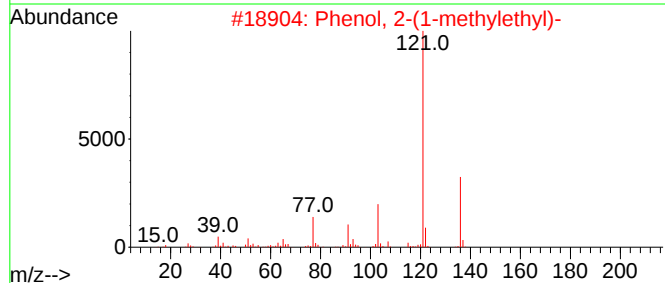
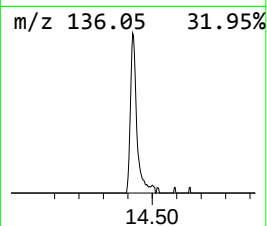
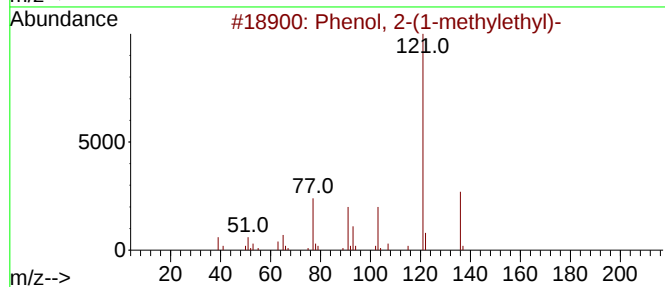
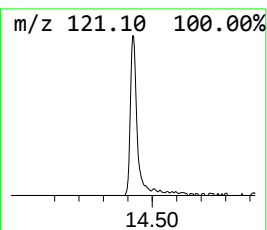
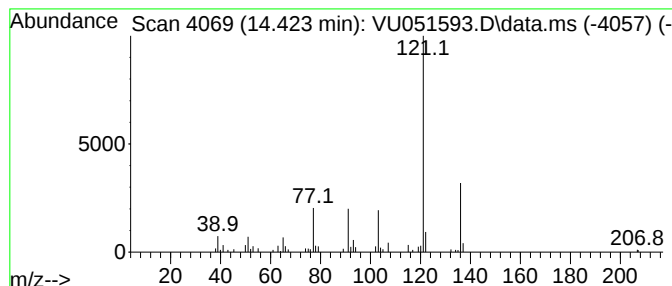
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Phenol, 2-(1-methylethyl)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.423	0.56 ug/L	58389	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2-(1-methylethyl)-	136	C9H12O	000088-69-7	91
2			Phenol, 2-(1-methylethyl)-	136	C9H12O	000088-69-7	91
3			Phenol, 2-(1-methylethyl)-	136	C9H12O	000088-69-7	91
4			p-Cumenol	136	C9H12O	000099-89-8	90
5			Phenol, 3-(1-methylethyl)-	136	C9H12O	000618-45-1	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102822\
Data File : VU051593.D
Acq On : 29 Oct 2022 02:19
Operator : JC/MD
Sample : N5276-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4X3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.482	5.3	ug/L	513933	1	6.250	487469	5.0
2-Butanone, 3,3...	7.166	1.0	ug/L	96883	1	6.250	487469	5.0
Phenol, 2-(1-me...	14.423	0.6	ug/L	58389	3	11.809	522535	5.0