

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012825\
 Data File : VU063070.D
 Acq On : 28 Jan 2025 16:28
 Operator : MD/SY
 Sample : Q1174-18
 Misc : 25mL/MSVOA_U/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 E2952

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\SFAMUTR012725WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VU063070.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.460	45	53	81	rBV	40326	84568	24.85%	2.482%
2	1.592	86	94	109	rVB	22941	33476	9.84%	0.982%
3	1.904	183	191	200	rBV	18588	24143	7.09%	0.709%
4	2.554	381	393	405	rBV	46425	75642	22.22%	2.220%
5	2.615	405	412	425	rVB	6004	10084	2.96%	0.296%
6	2.878	486	494	507	rBV3	3515	7153	2.10%	0.210%
7	4.608	1022	1032	1055	rBV	40974	102383	30.08%	3.005%
8	5.049	1154	1169	1189	rBV	67378	149926	44.05%	4.400%
9	5.711	1357	1375	1398	rBV3	108588	299372	87.96%	8.786%
10	6.235	1527	1538	1557	rBV	132860	252295	74.13%	7.405%
11	6.676	1663	1675	1697	rBV2	68785	137354	40.36%	4.031%
12	7.557	1939	1949	1966	rBV	43980	80358	23.61%	2.358%
13	7.888	2040	2052	2068	rBV	153453	270169	79.38%	7.929%
14	7.962	2069	2075	2086	rVB4	4512	7122	2.09%	0.209%
15	8.171	2129	2140	2159	rBV	25508	45614	13.40%	1.339%
16	8.621	2270	2280	2313	rBV	145904	291385	85.61%	8.552%
17	9.409	2513	2525	2543	rBV	198459	340364	100.00%	9.989%
18	9.495	2543	2552	2563	rVB4	15039	24488	7.19%	0.719%
19	9.688	2603	2612	2623	rBV5	2989	5741	1.69%	0.168%
20	10.746	2930	2941	2954	rBV2	72534	121011	35.55%	3.552%
21	11.804	3257	3270	3291	rBV	200721	339026	99.61%	9.950%
22	12.058	3339	3349	3368	rBV2	20193	51596	15.16%	1.514%
23	12.183	3376	3388	3410	rVB	182625	303975	89.31%	8.921%
24	12.884	3597	3606	3616	rBV4	6413	10000	2.94%	0.293%
25	14.023	3952	3960	3971	rVB5	3948	7125	2.09%	0.209%
26	14.415	4070	4082	4092	rBV2	6434	10642	3.13%	0.312%
27	15.103	4288	4296	4304	rVB9	2813	4345	1.28%	0.128%
28	15.476	4402	4412	4426	rBV2	13599	23652	6.95%	0.694%
29	15.714	4481	4486	4498	rVB6	4147	6093	1.79%	0.179%
30	16.225	4633	4645	4661	rBV	128081	228290	67.07%	6.700%
31	16.482	4716	4725	4741	rBV	35174	59908	17.60%	1.758%

Sum of corrected areas: 3407300

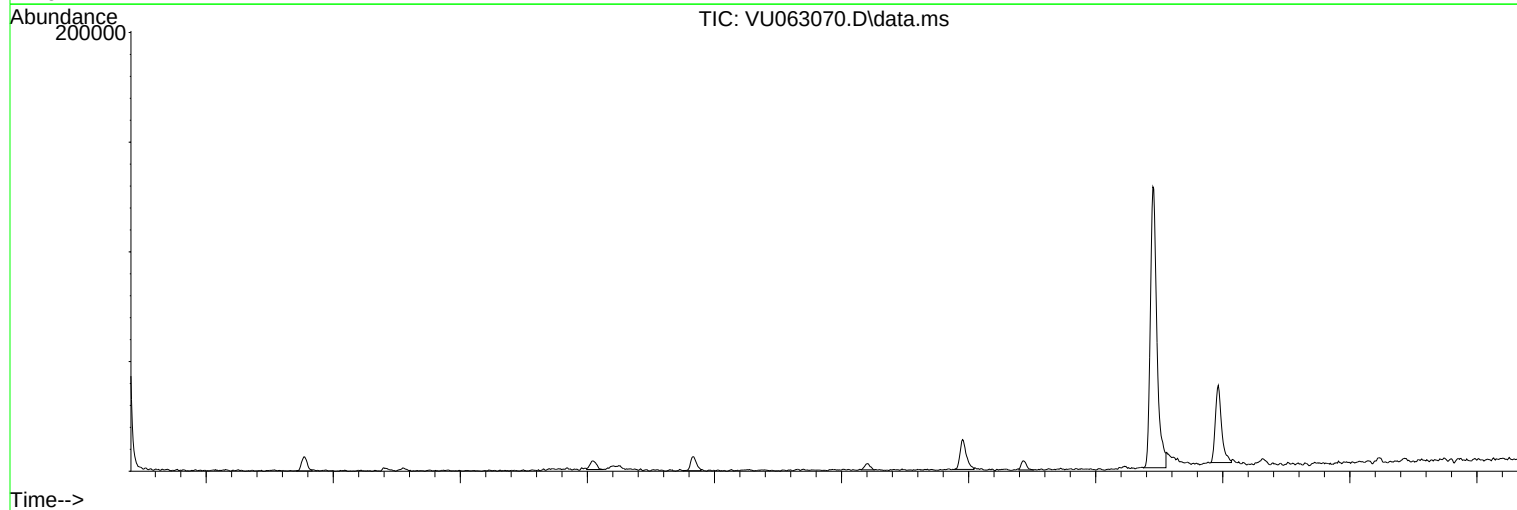
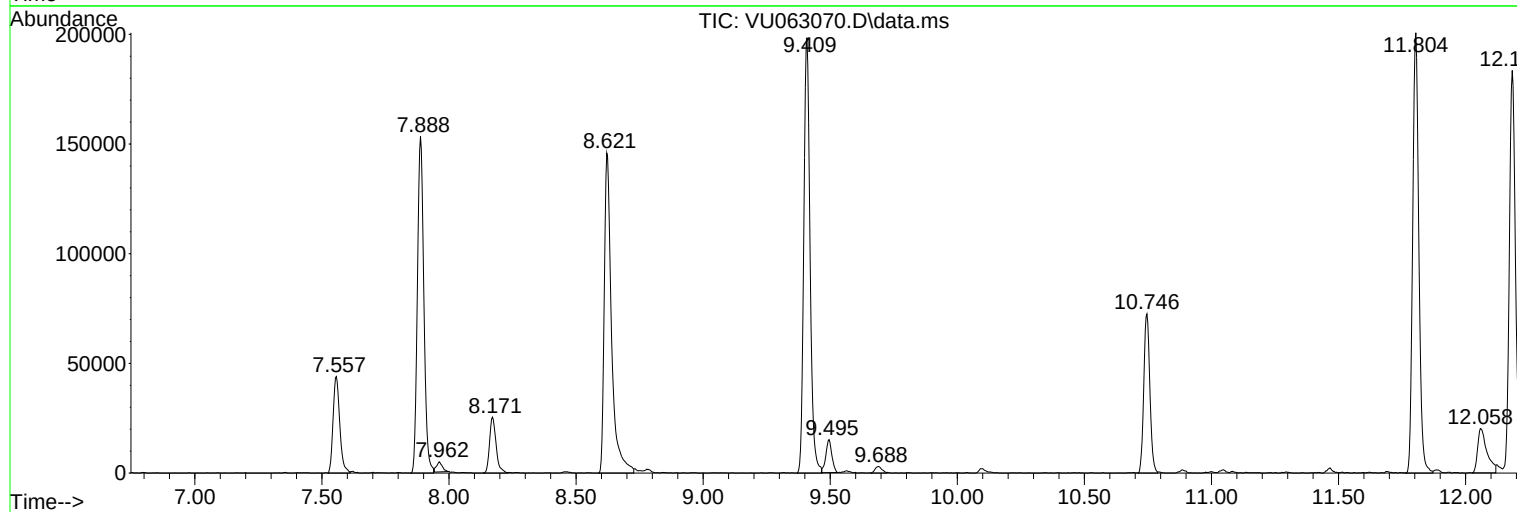
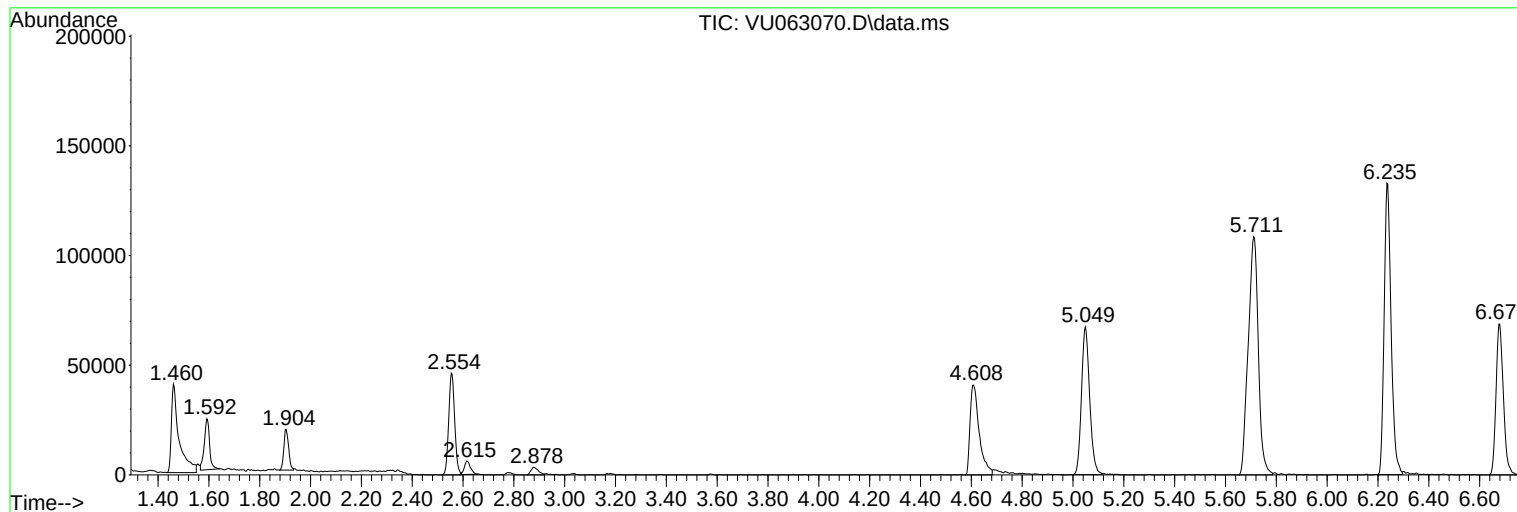
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012725WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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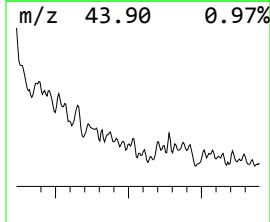
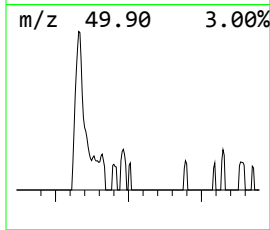
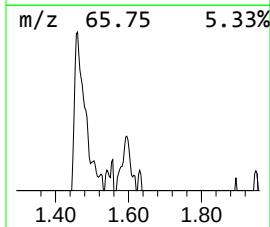
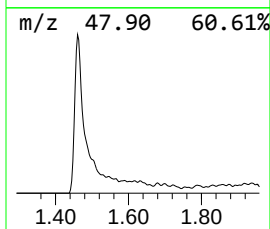
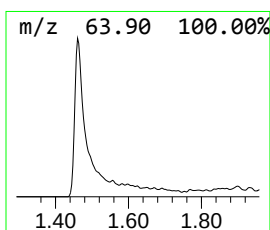
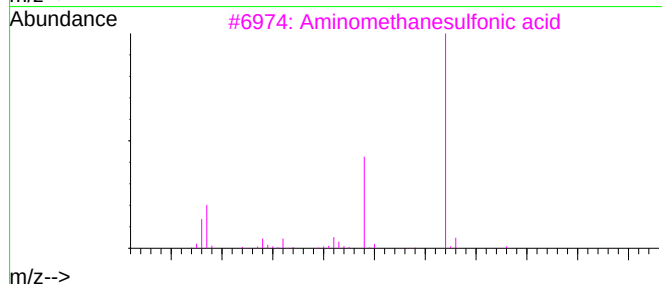
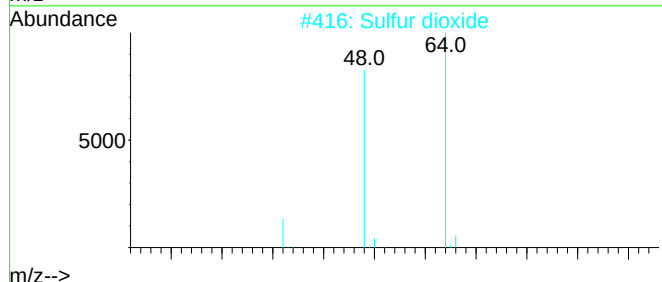
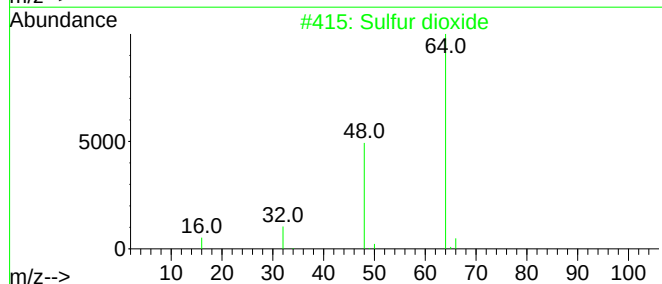
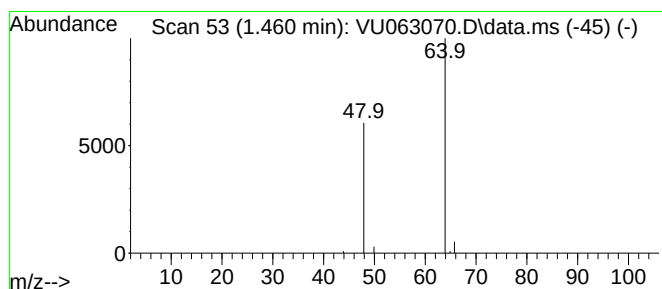
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.460	1.68 ug/L	84568	1,4-Difluorobenzene	6.238

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	90
2	Sulfur dioxide	64	O2S	007446-09-5	74
3	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
4	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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ClientSampleId :
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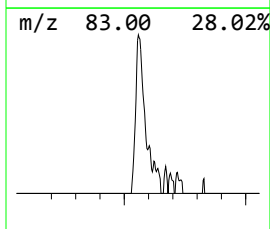
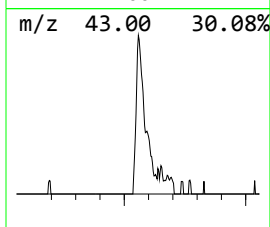
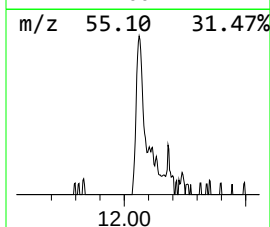
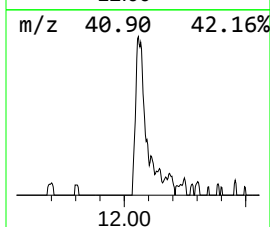
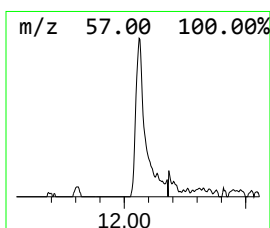
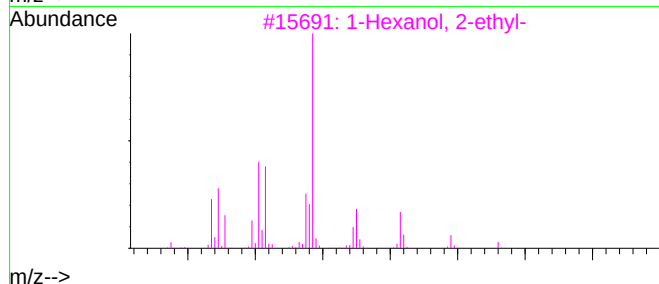
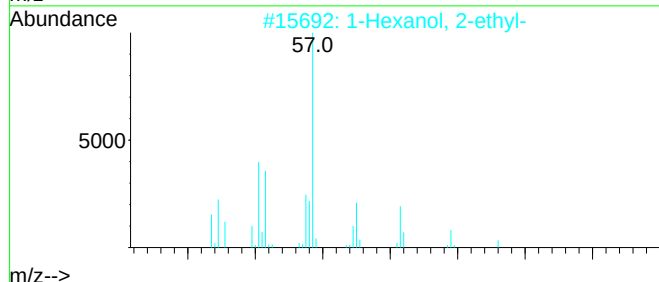
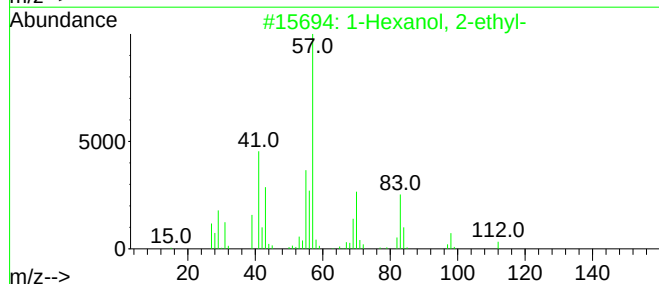
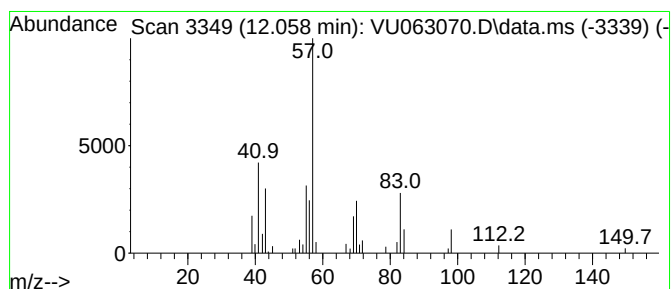
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012725WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.058	0.76 ug/L	51596	1,4-Dichlorobenzene-d4		11.804	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-		130	C8H18O	000104-76-7	90
2	1-Hexanol, 2-ethyl-		130	C8H18O	000104-76-7	78
3	1-Hexanol, 2-ethyl-		130	C8H18O	000104-76-7	72
4	2-Propyl-1-pentanol		130	C8H18O	058175-57-8	59
5	2-Propyl-1-pentanol		130	C8H18O	058175-57-8	59



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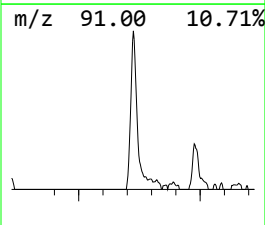
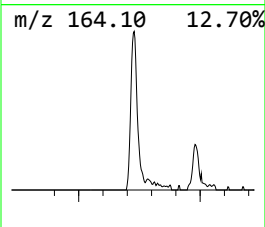
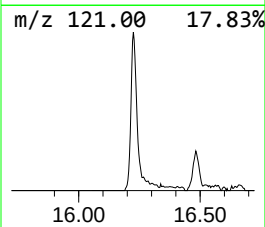
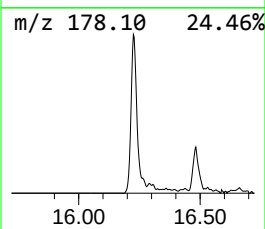
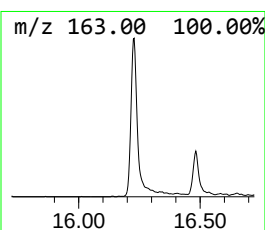
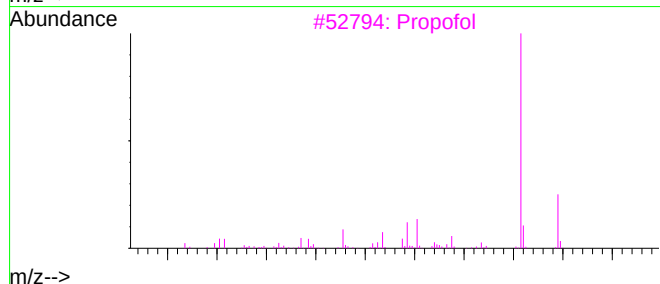
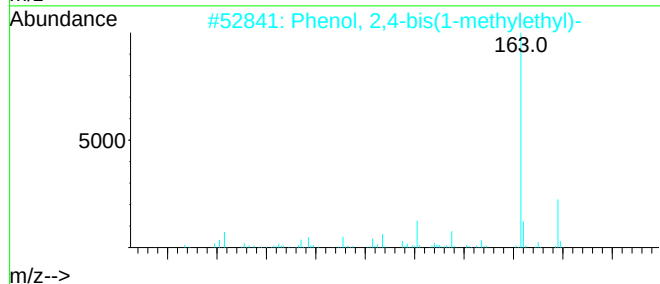
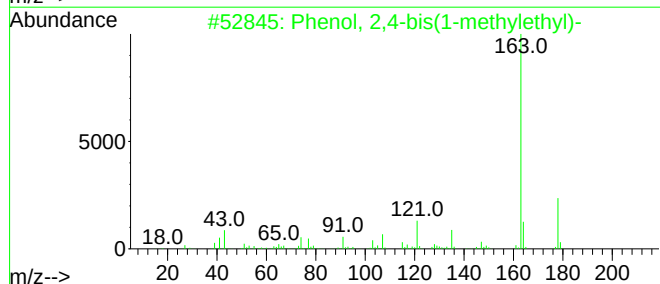
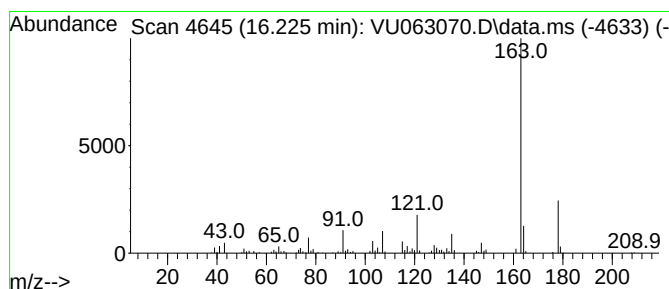
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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 Phenol, 2,4-bis(1-methylethyl) Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.225	3.37 ug/L	228290	1,4-Dichlorobenzene-d4	11.804	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,4-bis(1-methylethyl)-	178	C12H18O	002934-05-6	96
2	Phenol, 2,4-bis(1-methylethyl)-	178	C12H18O	002934-05-6	95
3	Propofol	178	C12H18O	002078-54-8	93
4	Propofol	178	C12H18O	002078-54-8	91
5	Propofol	178	C12H18O	002078-54-8	91



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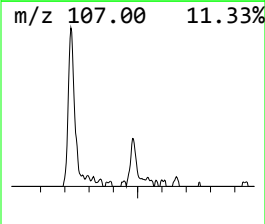
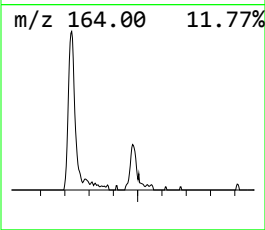
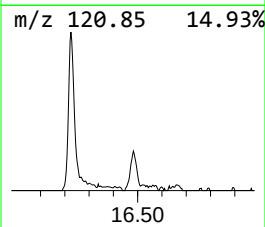
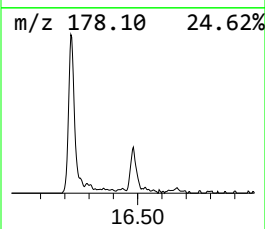
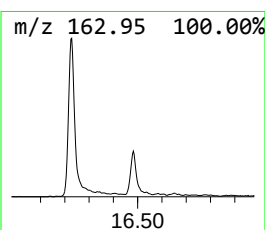
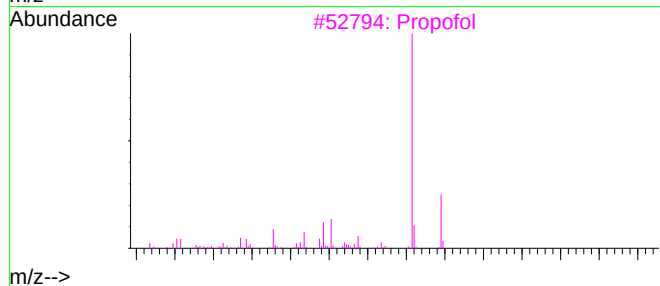
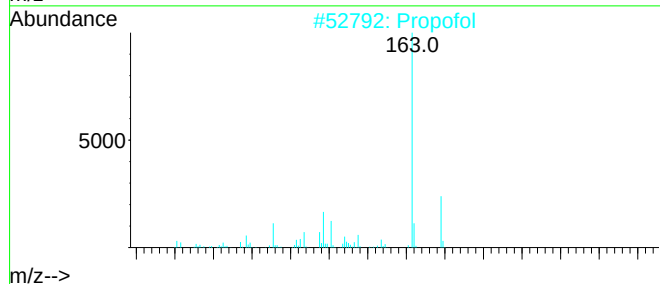
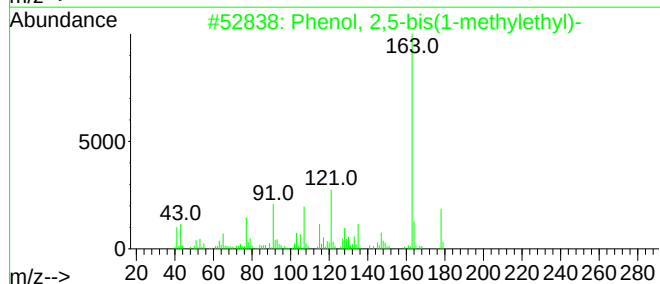
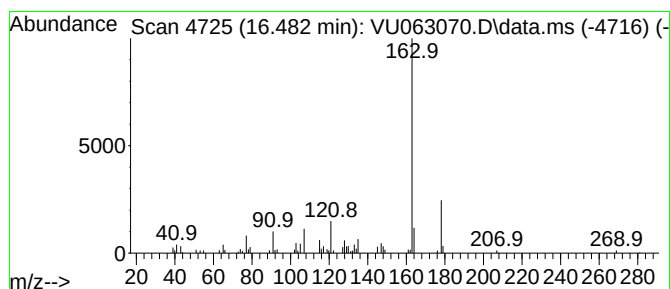
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TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 5 Phenol, 2,5-bis(1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.482	0.88 ug/L	59908	1,4-Dichlorobenzene-d4	11.804	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,5-bis(1-methylethyl)-	178	C12H18O	035946-91-9	95
2	Propofol	178	C12H18O	002078-54-8	94
3	Propofol	178	C12H18O	002078-54-8	94
4	Propofol	178	C12H18O	002078-54-8	91
5	Phenol, 2,4-bis(1-methylethyl)-	178	C12H18O	002934-05-6	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.460	1.7	ug/L	84568	1	6.238	252295	5.0
1-Hexanol, 2-et...	12.058	0.8	ug/L	51596	3	11.804	339026	5.0
Phenol, 2,4-bis...	16.225	3.4	ug/L	228290	3	11.804	339026	5.0
Phenol, 2,5-bis...	16.482	0.9	ug/L	59908	3	11.804	339026	5.0