

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV020725\
 Data File : VV038654.D
 Acq On : 07 Feb 2025 18:39
 Operator : SY/MD
 Sample : Q1334-13
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 E29B4

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_V\Method\SFAMVTR020625WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VV038654.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.262	63	69	79	rBV2	455796	633526	3.66%	1.387%
2	1.326	80	89	101	rBV	301235	731399	4.22%	1.602%
3	2.050	306	314	335	rVB	267762	433147	2.50%	0.948%
4	3.104	627	642	657	rBV	124601	270179	1.56%	0.592%
5	3.828	850	867	923	rBV2	53096	307283	1.77%	0.673%
6	4.239	981	995	1028	rVB	152110	404701	2.34%	0.886%
7	4.947	1201	1215	1252	rBV2	375839	1030788	5.95%	2.257%
8	5.526	1385	1395	1420	rVV	272750	599083	3.46%	1.312%
9	5.641	1420	1431	1466	rVB2	166329	394471	2.28%	0.864%
10	5.982	1524	1537	1567	rBV	205477	470624	2.72%	1.031%
11	6.497	1682	1697	1731	rBV	468936	1061732	6.13%	2.325%
12	6.908	1816	1825	1847	rBV	95473	201887	1.16%	0.442%
13	7.156	1891	1902	1917	rBV2	142377	324620	1.87%	0.711%
14	7.236	1917	1927	1938	rVV	463101	849080	4.90%	1.859%
15	7.307	1938	1949	1973	rVB2	242955	600685	3.47%	1.315%
16	7.493	1997	2007	2018	rBV2	107656	201102	1.16%	0.440%
17	7.783	2084	2097	2112	rBV	183450	346911	2.00%	0.760%
18	7.860	2112	2121	2151	rVB	82187	199575	1.15%	0.437%
19	8.021	2160	2171	2191	rBV	428732	871888	5.03%	1.909%
20	8.776	2385	2406	2442	rBV	463607	927040	5.35%	2.030%
21	10.146	2822	2832	2847	rBV	173561	276674	1.60%	0.606%
22	11.094	3118	3127	3136	rBV	129931	199088	1.15%	0.436%
23	11.178	3144	3153	3163	rBV	466841	711038	4.10%	1.557%
24	11.464	3232	3242	3261	rBV	1766378	3155469	18.21%	6.910%
25	11.551	3262	3269	3292	rVB	495719	924017	5.33%	2.023%
26	13.429	3844	3853	3874	rVB	928307	1501318	8.66%	3.288%
27	13.528	3876	3884	3897	rBV2	228828	355580	2.05%	0.779%
28	13.618	3904	3912	3928	rVB	221944	382162	2.20%	0.837%
29	13.818	3963	3974	4004	rBV	2291730	3617338	20.87%	7.921%
30	14.223	4093	4100	4129	rVB4	83716	207483	1.20%	0.454%
31	14.496	4175	4185	4196	rBV	549586	863100	4.98%	1.890%
32	14.561	4197	4205	4215	rVB2	200746	329147	1.90%	0.721%
33	14.747	4254	4263	4273	rBV	111325	180477	1.04%	0.395%
34	14.866	4289	4300	4331	rBV	990412	1908540	11.01%	4.179%
35	15.091	4362	4370	4382	rVB	321730	485486	2.80%	1.063%
36	15.615	4520	4533	4566	rBV	10005492	17331682	100.00%	37.952%

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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_V\Method\SFAMVTR020625WMA.M
Title : TRACE VOA SFAM1.0

37	15.866	4603	4611	4637	rVB	1255815	2026731	11.69%	4.438%
38	16.226	4714	4723	4736	rVB5	168600	351970	2.03%	0.771%

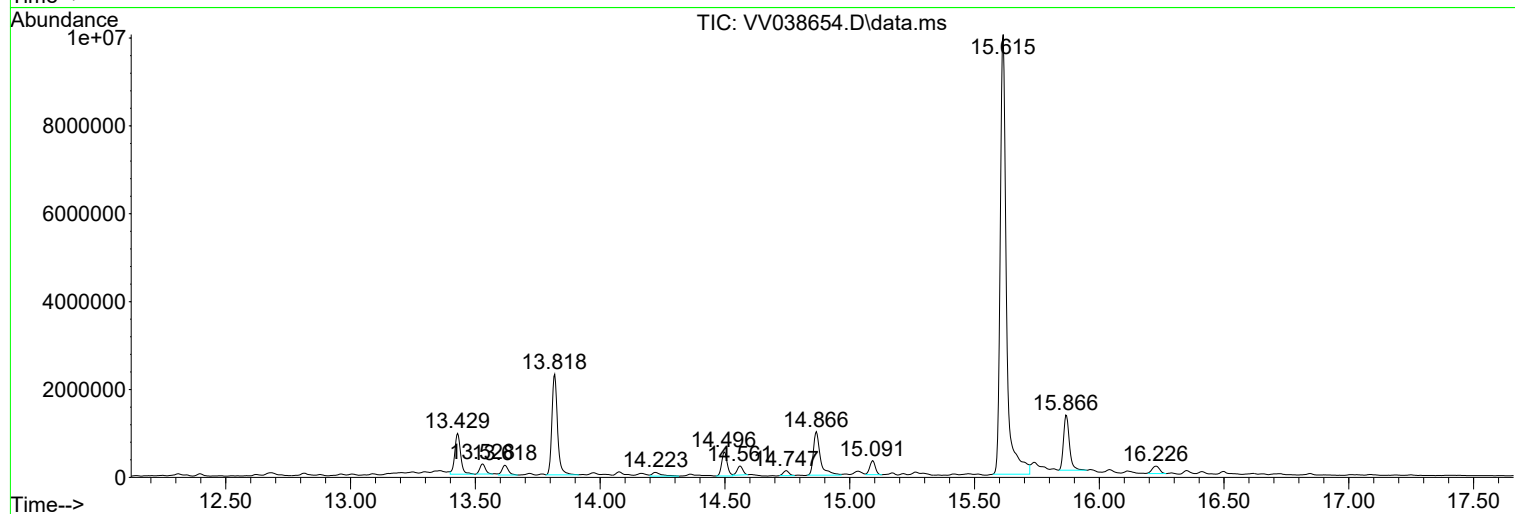
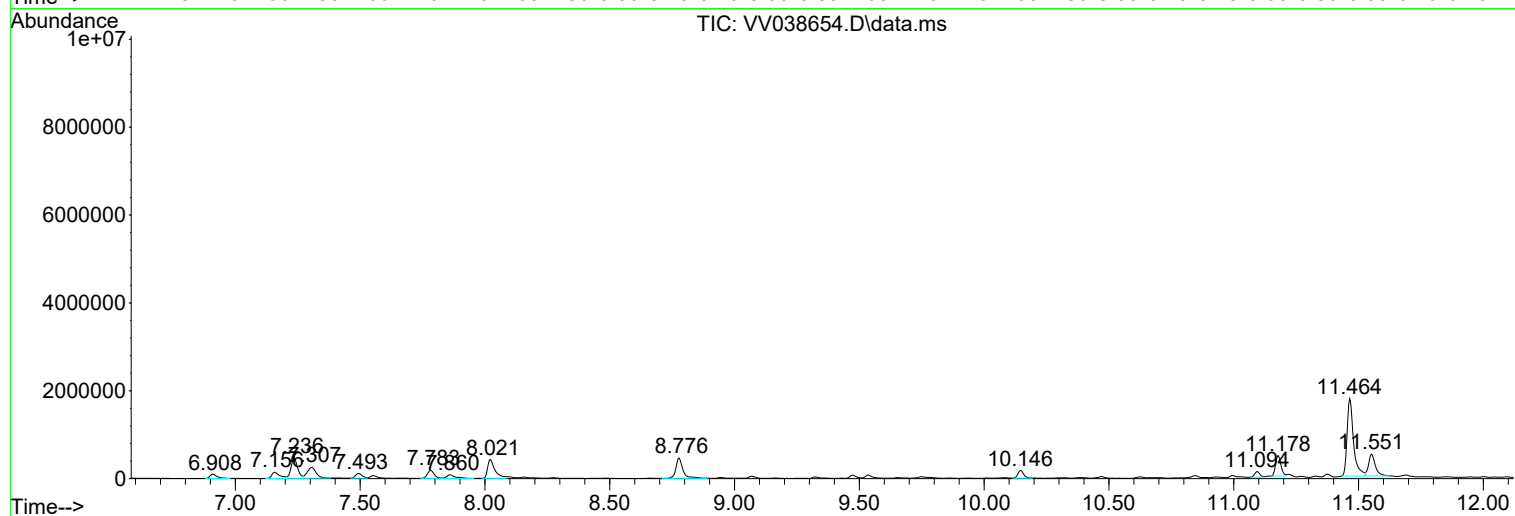
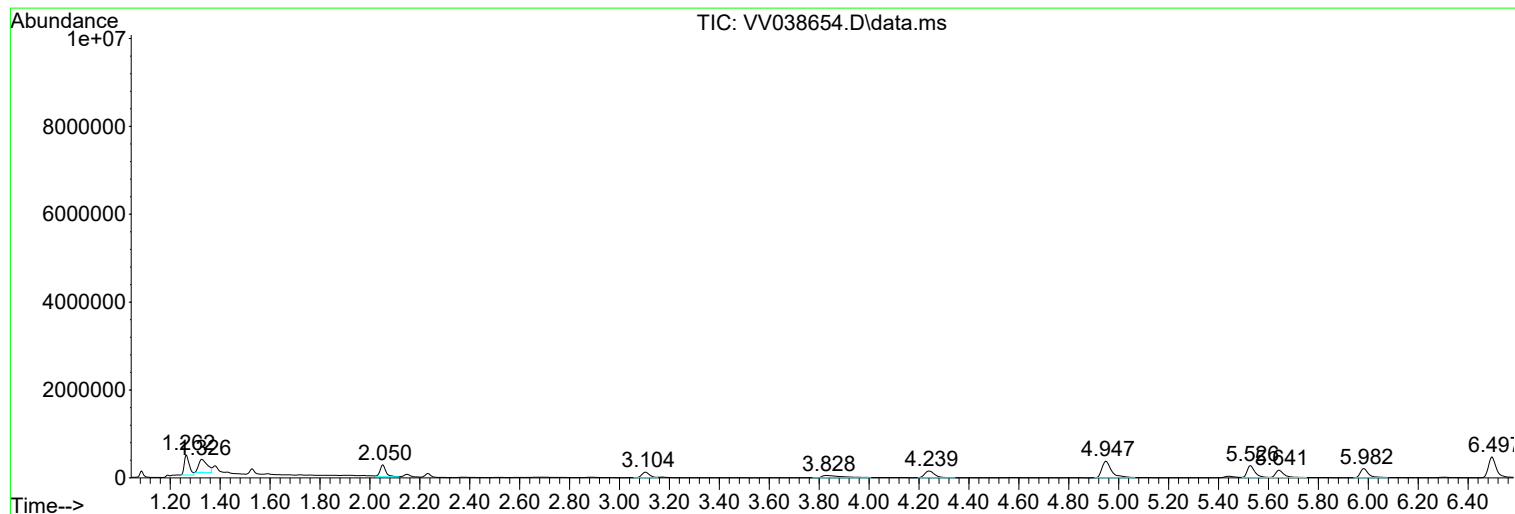
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR020625WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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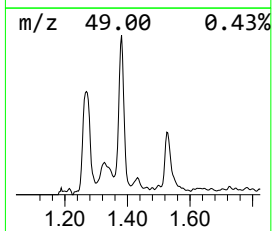
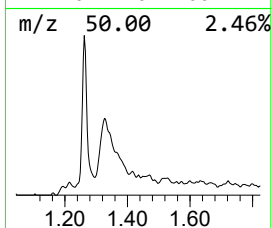
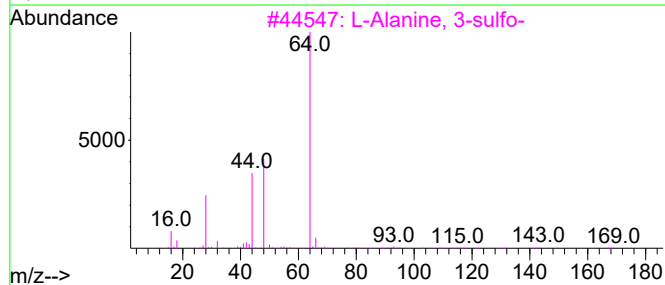
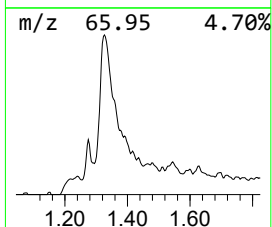
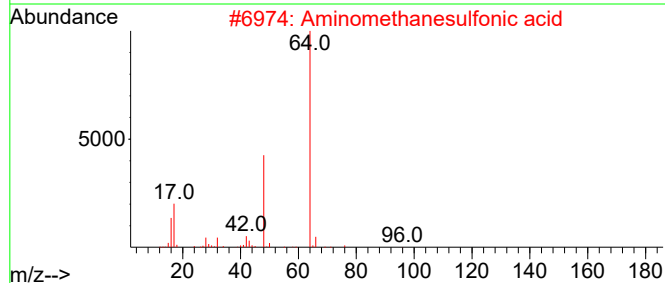
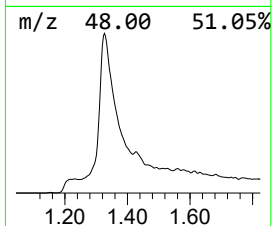
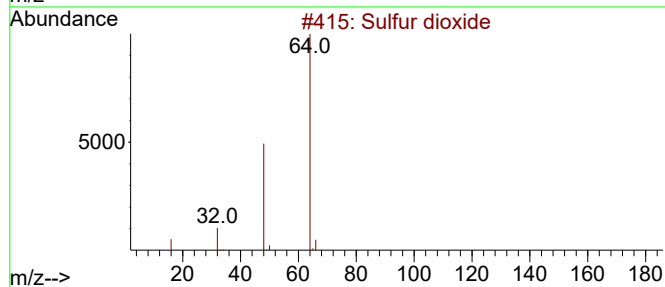
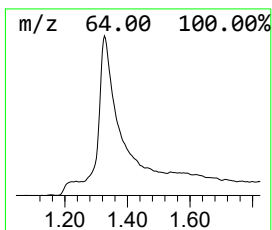
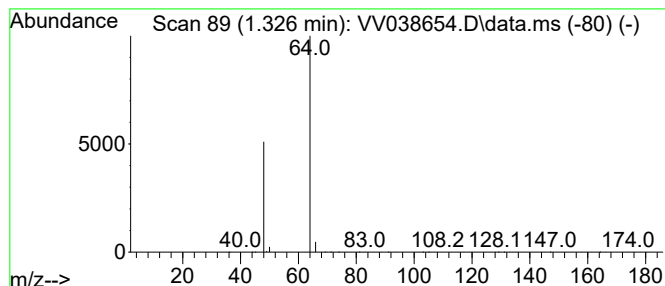
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Sulfur dioxide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.326	6.10 ug/L	731399	1,4-Difluorobenzene	5.529

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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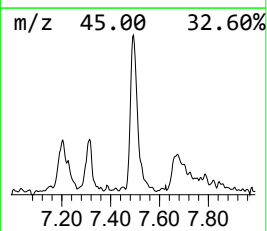
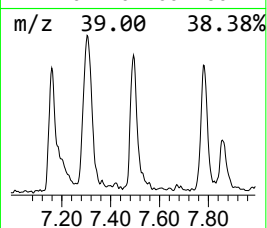
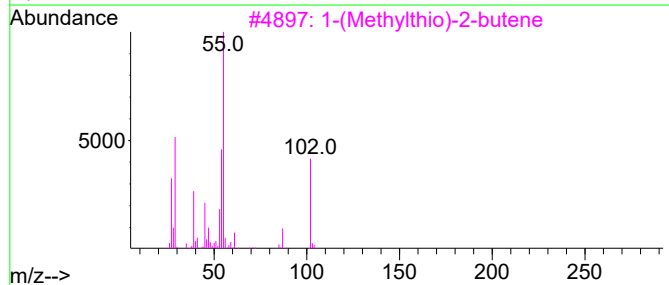
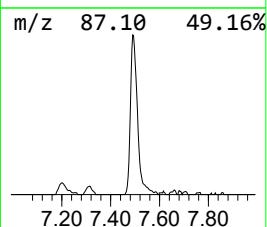
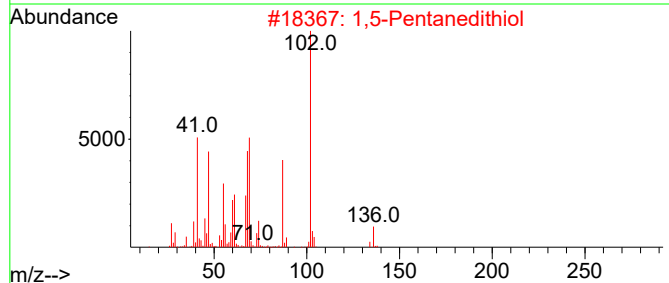
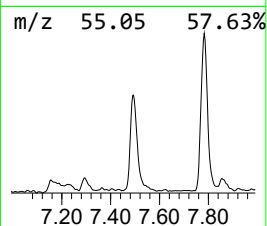
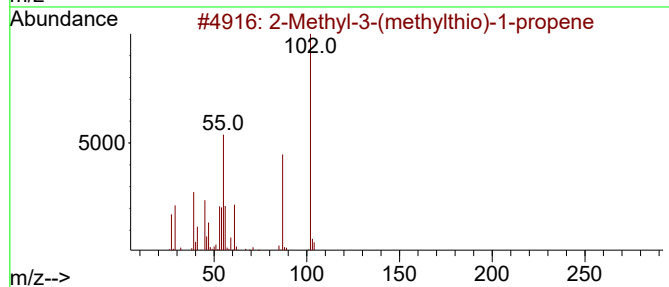
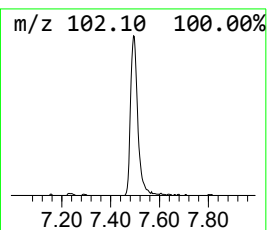
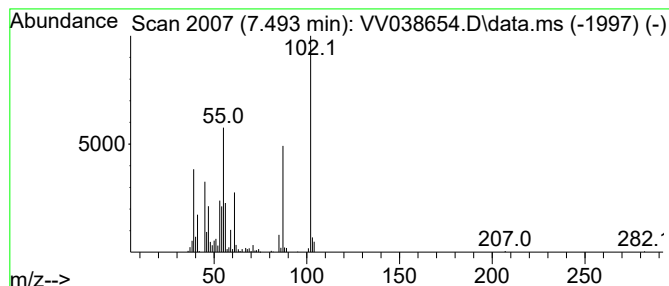
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR020625WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Methyl-3-(methylthio)-1-p... Concentration Rank 21

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.493	1.08 ug/L	201102	Chlorobenzene-d5	8.776

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methyl-3-(methylthio)-1-propene	102	C5H10S	052326-10-0	96
2			1,5-Pentanedithiol	136	C5H12S2	000928-98-3	38
3			1-(Methylthio)-2-butene	102	C5H10S	032931-14-9	38
4			Thiophene, tetrahydro-3-methyl-	102	C5H10S	004740-00-5	37
5			Methyl 2,2-dimethyl-3-hydroxypro...	132	C6H12O3	014002-80-3	32



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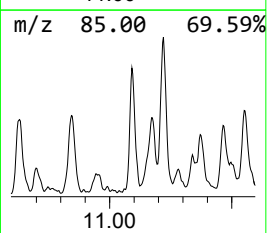
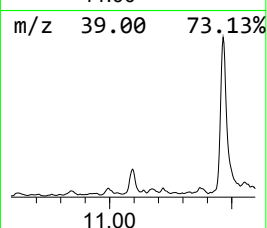
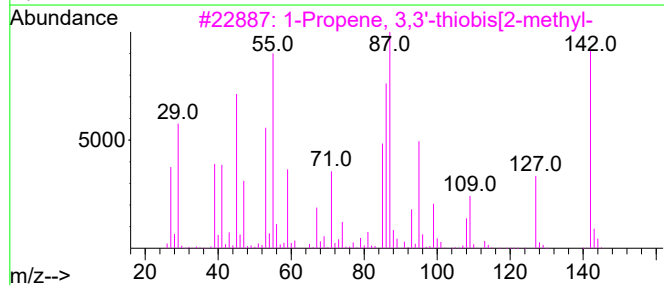
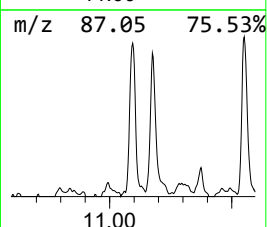
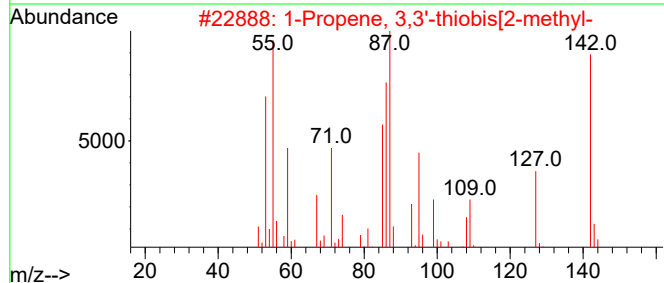
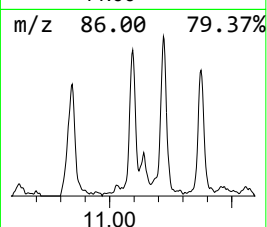
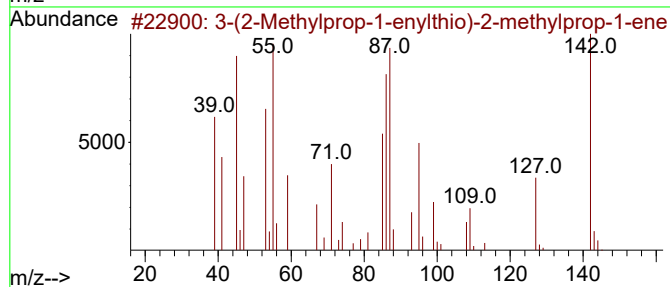
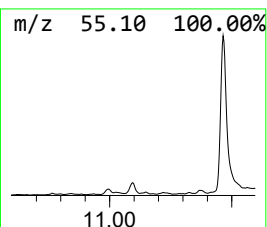
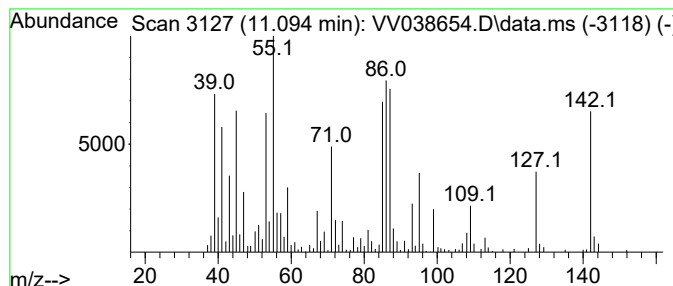
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR020625WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 3-(2-Methylprop-1-enylthio)... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.095	1.40 ug/L	199088	1,4-Dichlorobenzene-d4	11.178

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-(2-Methylprop-1-enylthio)-2-me...	142	C8H14S	1000122-39-8	95
2			1-Propene, 3,3'-thiobis[2-methyl-	142	C8H14S	023973-54-8	87
3			1-Propene, 3,3'-thiobis[2-methyl-	142	C8H14S	023973-54-8	78
4			1-Propene, 3,3'-thiobis[2-methyl-	142	C8H14S	023973-54-8	50
5			Tetrazole-5-thiole, 1-allyl-	142	C4H6N4S	007624-33-1	35



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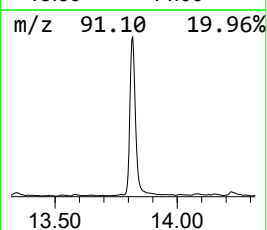
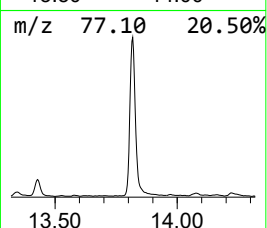
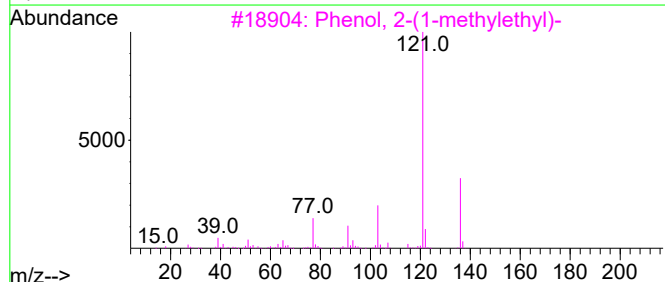
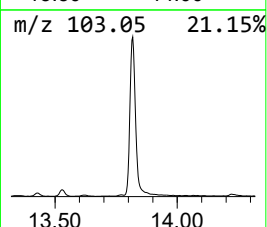
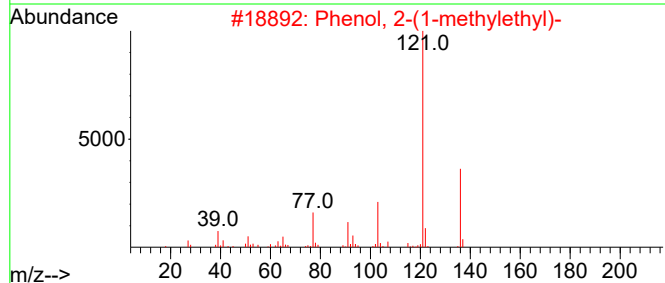
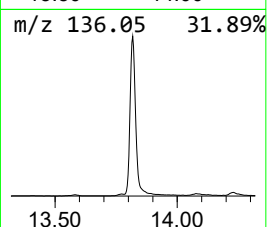
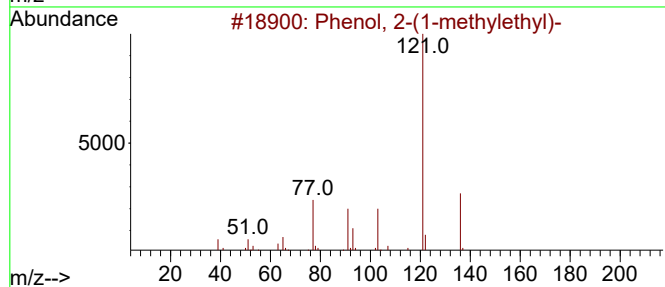
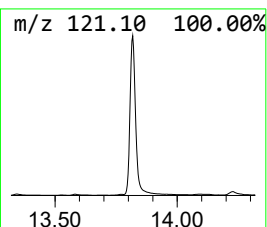
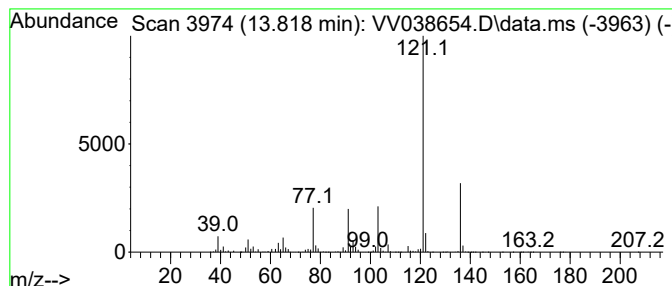
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 12 Phenol, 2-(1-methylethyl)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.818	25.44 ug/L	3617340	1,4-Dichlorobenzene-d4	11.178

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2-(1-methylethyl)-	136	C9H12O	000088-69-7	94
2			Phenol, 2-(1-methylethyl)-	136	C9H12O	000088-69-7	93
3			Phenol, 2-(1-methylethyl)-	136	C9H12O	000088-69-7	91
4			Phenol, 3-(1-methylethyl)-	136	C9H12O	000618-45-1	90
5			Phenol, 3-(1-methylethyl)-	136	C9H12O	000618-45-1	90



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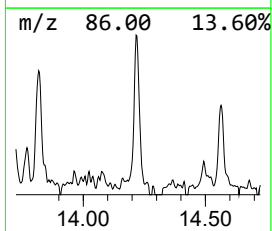
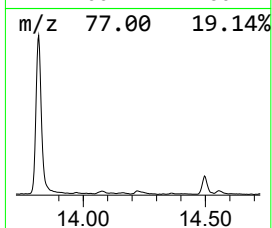
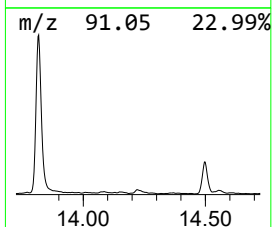
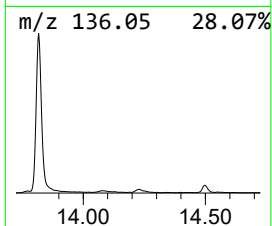
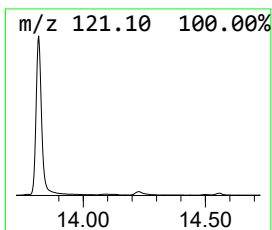
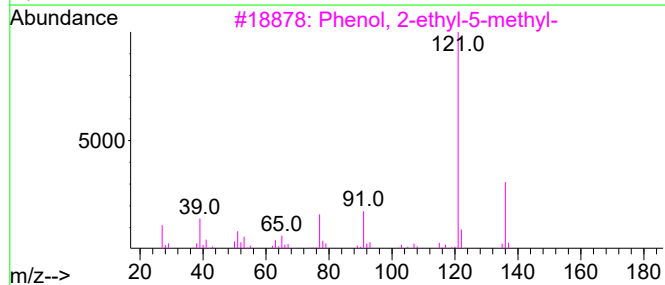
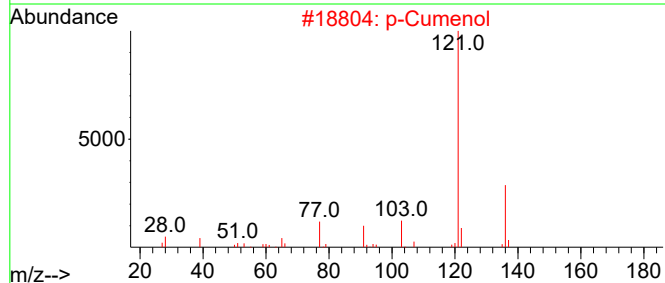
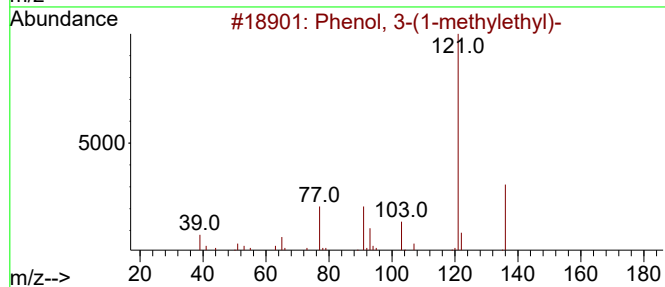
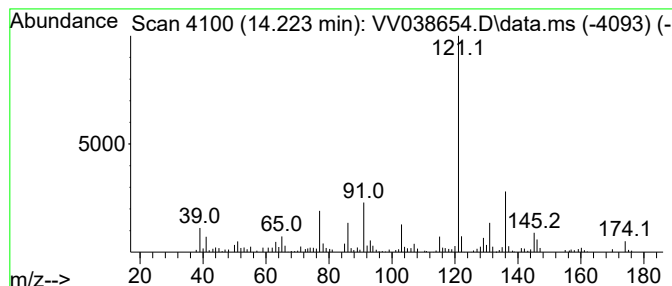
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 13 Phenol, 3-(1-methylethyl)- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.223	1.46 ug/L	207483	1,4-Dichlorobenzene-d4	11.178

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 3-(1-methylethyl)-	136	C9H12O	000618-45-1	89
2			p-Cumenol	136	C9H12O	000099-89-8	76
3			Phenol, 2-ethyl-5-methyl-	136	C9H12O	001687-61-2	76
4			Phenol, 3-(1-methylethyl)-	136	C9H12O	000618-45-1	76
5			p-Cumenol	136	C9H12O	000099-89-8	76



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV020725\
Data File : VV038654.D
Acq On : 07 Feb 2025 18:39
Operator : SY/MD
Sample : Q1334-13
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
E29B4

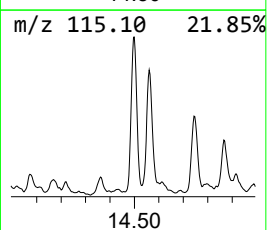
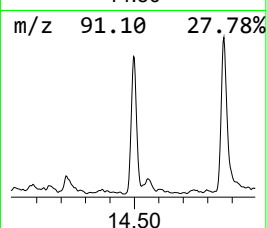
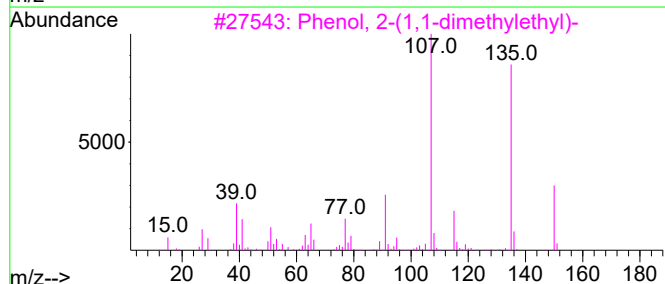
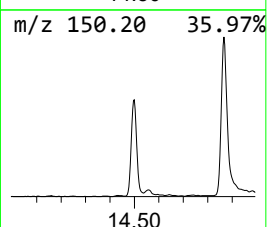
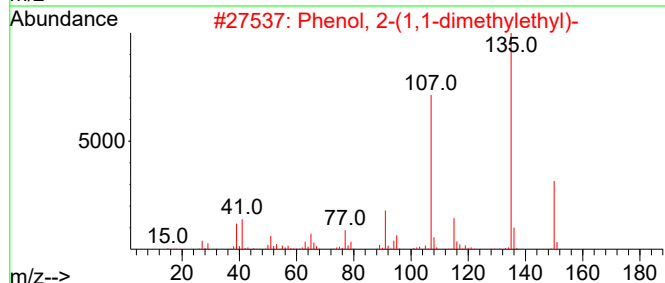
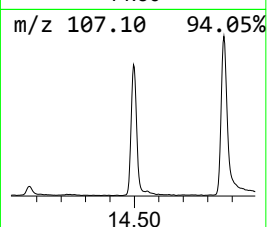
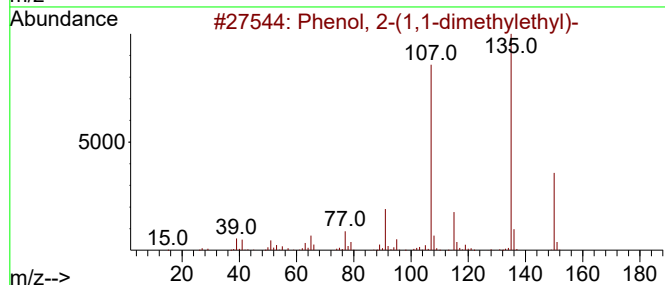
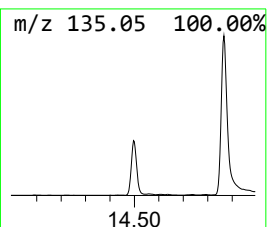
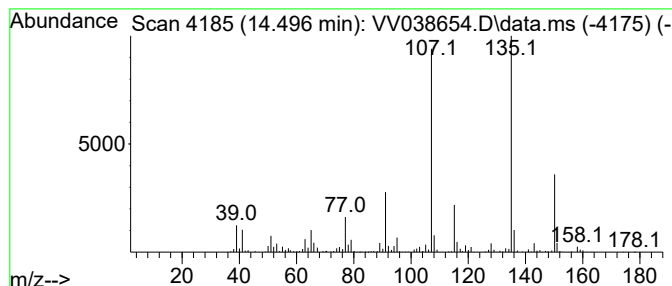
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 14 Phenol, 2-(1,1-dimethylethyl)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.496	6.07 ug/L	863100	1,4-Dichlorobenzene-d4	11.178

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	96
2			Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	91
3			Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	87
4			Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	64
5			Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV020725\
Data File : VV038654.D
Acq On : 07 Feb 2025 18:39
Operator : SY/MD
Sample : Q1334-13
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
E29B4

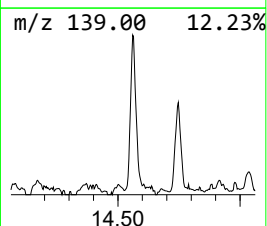
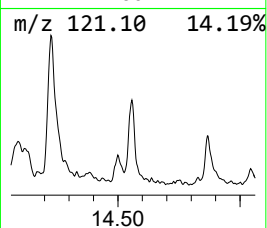
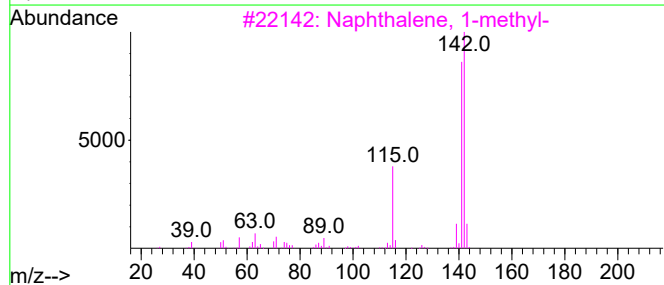
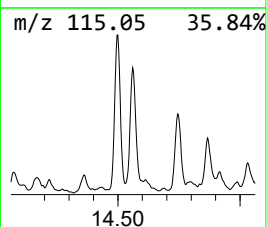
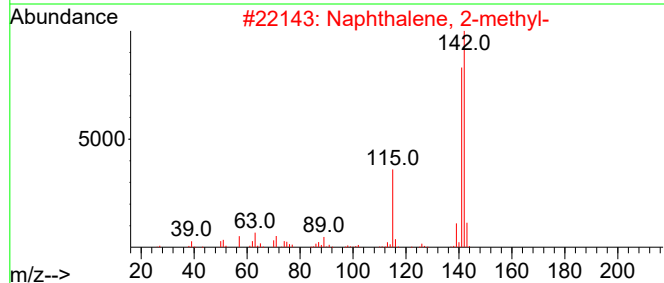
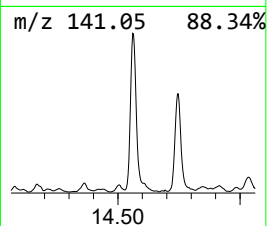
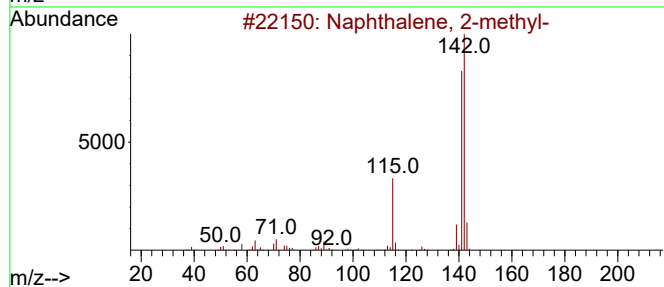
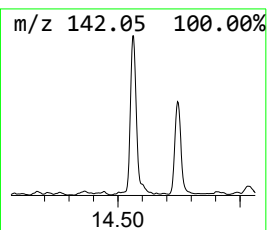
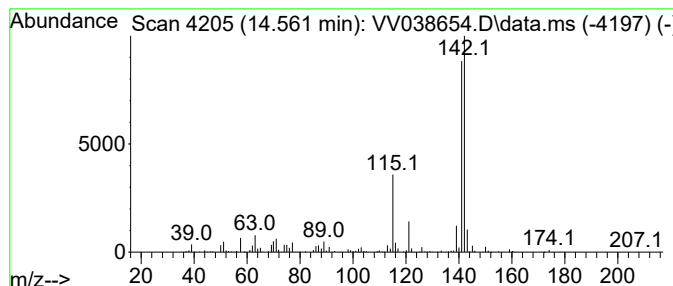
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 15 Naphthalene, 2-methyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.561	2.31 ug/L	329147	1,4-Dichlorobenzene-d4	11.178

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	97
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	93
5			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV020725\
Data File : VV038654.D
Acq On : 07 Feb 2025 18:39
Operator : SY/MD
Sample : Q1334-13
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
E29B4

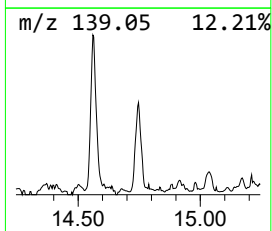
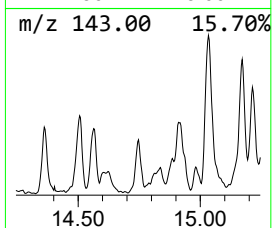
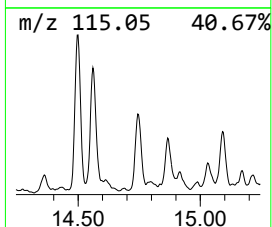
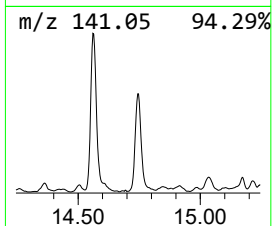
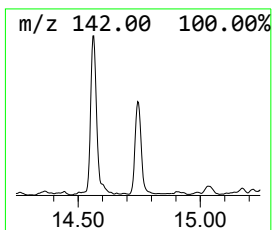
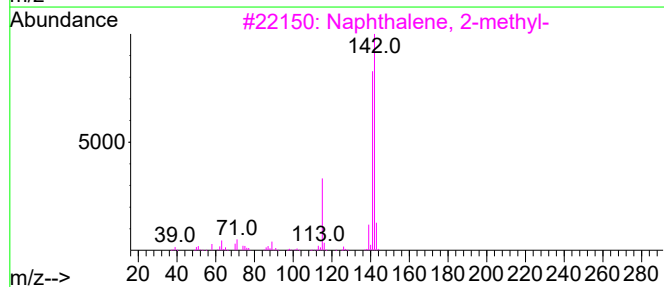
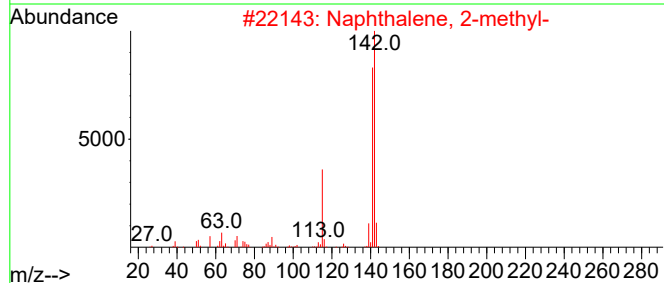
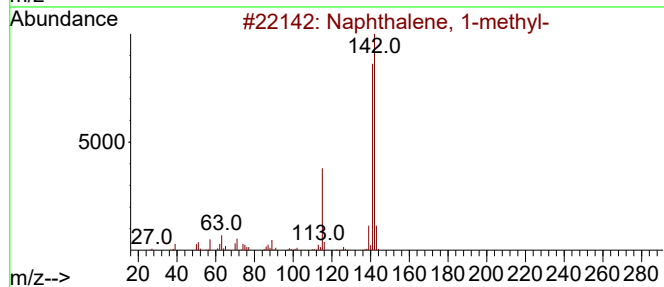
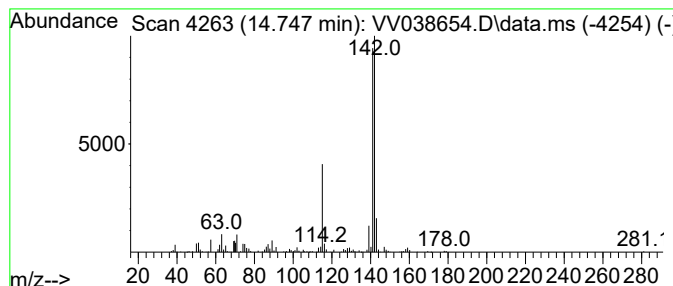
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 16 Naphthalene, 1-methyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.747	1.27 ug/L	180477	1,4-Dichlorobenzene-d4	11.178

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	95
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	95
3			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	94
4			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	94
5			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV020725\
Data File : VV038654.D
Acq On : 07 Feb 2025 18:39
Operator : SY/MD
Sample : Q1334-13
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
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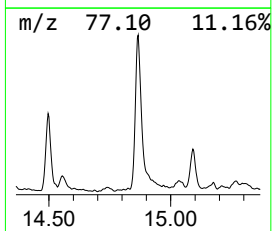
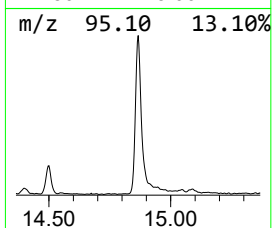
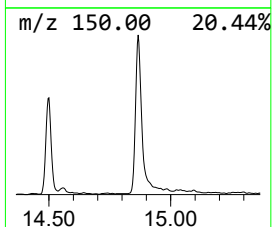
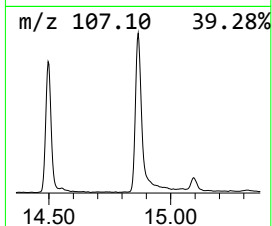
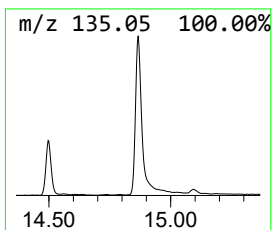
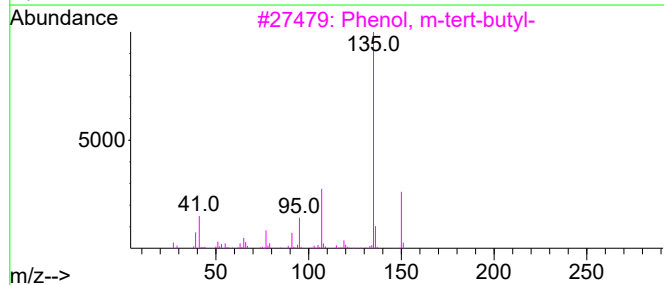
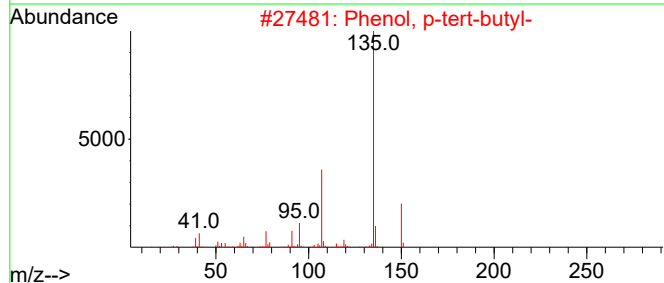
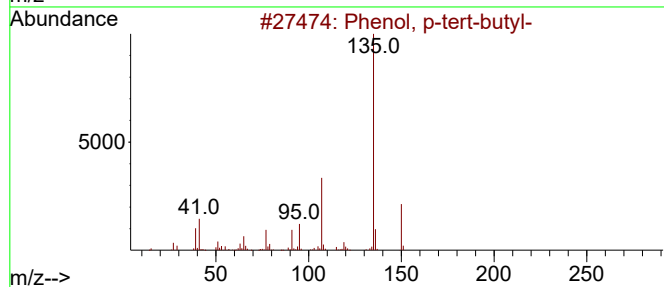
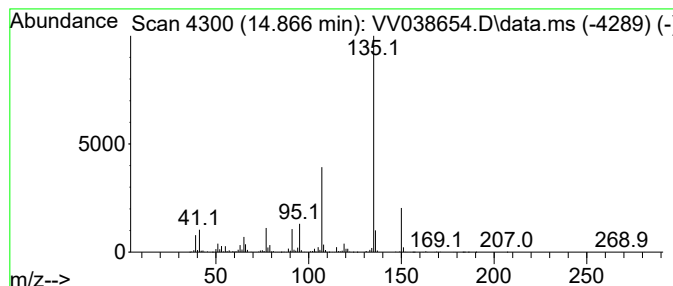
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 17 Phenol, p-tert-butyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.866	13.42 ug/L	1908540	1,4-Dichlorobenzene-d4	11.178

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	96
2			Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	96
3			Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	94
4			Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	94
5			Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV020725\
Data File : VV038654.D
Acq On : 07 Feb 2025 18:39
Operator : SY/MD
Sample : Q1334-13
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
E29B4

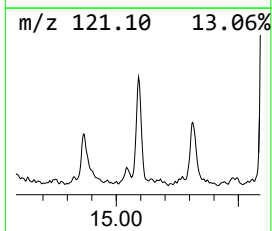
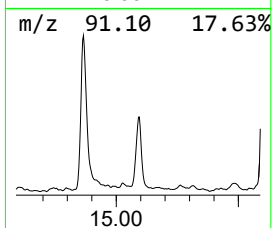
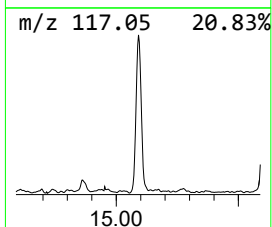
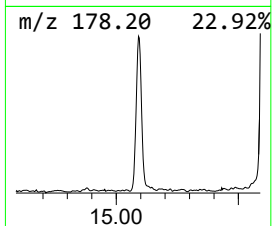
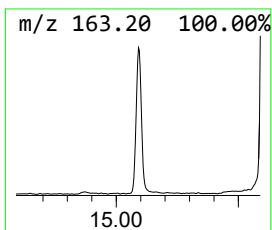
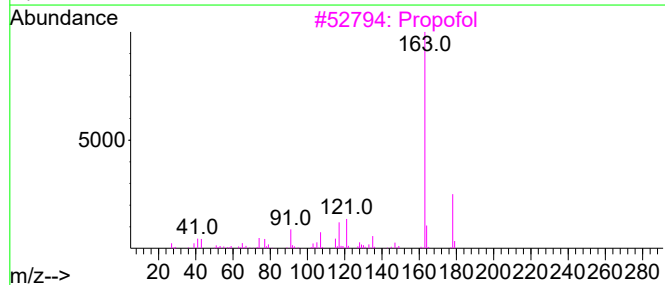
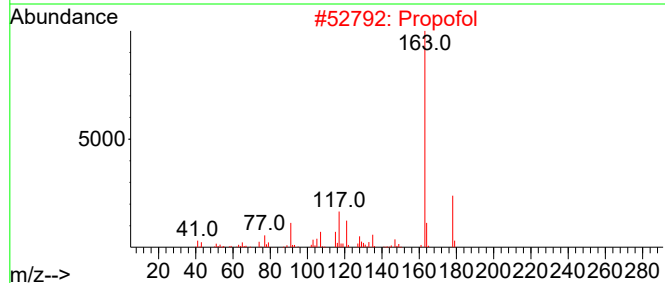
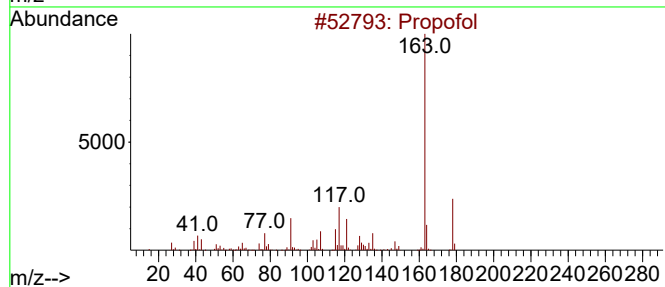
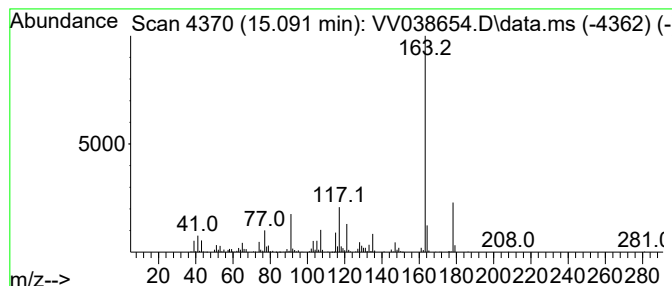
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 18 Propofol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.091	3.41 ug/L	485486	1,4-Dichlorobenzene-d4	11.178

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propofol	178	C12H18O	002078-54-8	97
2			Propofol	178	C12H18O	002078-54-8	96
3			Propofol	178	C12H18O	002078-54-8	95
4			Phenol, 2,4-bis(1-methylethyl)-	178	C12H18O	002934-05-6	95
5			Propofol	178	C12H18O	002078-54-8	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV020725\
Data File : VV038654.D
Acq On : 07 Feb 2025 18:39
Operator : SY/MD
Sample : Q1334-13
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
E29B4

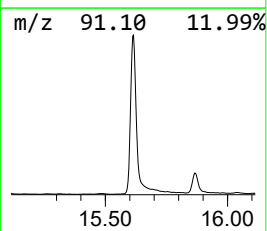
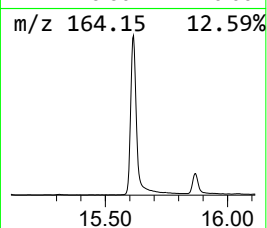
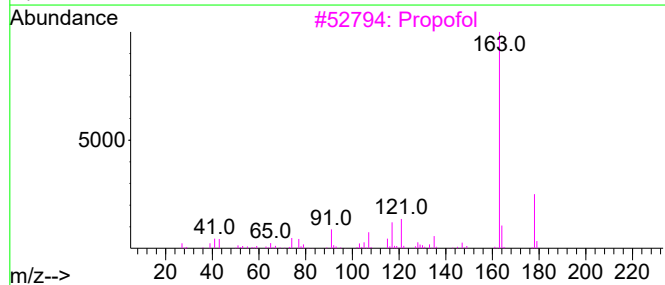
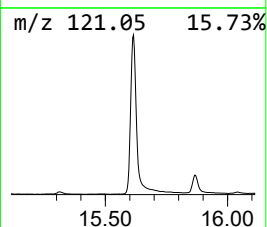
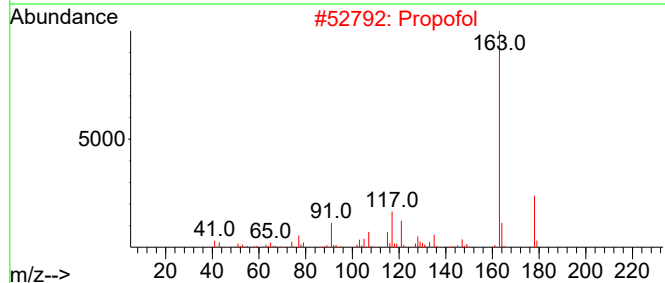
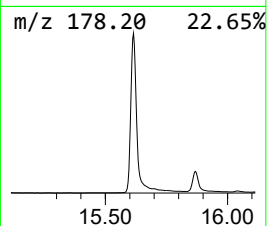
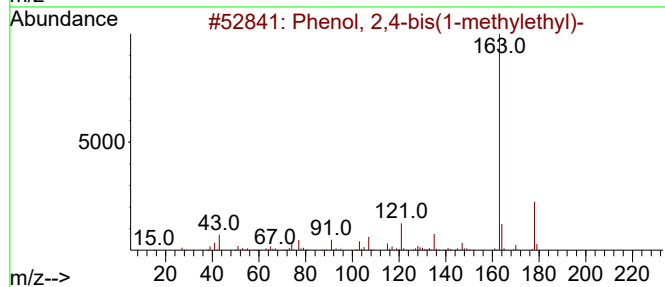
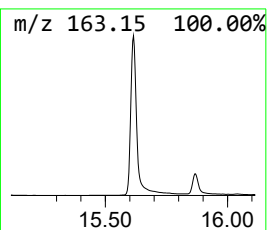
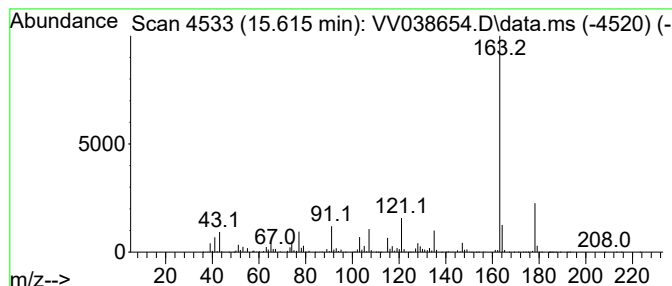
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 19 Phenol, 2,4-bis(1-methyleth... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	121.88 ug/L	17331700	1,4-Dichlorobenzene-d4	11.178

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,4-bis(1-methylethyl)-	178	C12H18O	002934-05-6	95
2			Propofol	178	C12H18O	002078-54-8	94
3			Propofol	178	C12H18O	002078-54-8	93
4			Phenol, 2,4-bis(1-methylethyl)-	178	C12H18O	002934-05-6	93
5			Propofol	178	C12H18O	002078-54-8	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV020725\
Data File : VV038654.D
Acq On : 07 Feb 2025 18:39
Operator : SY/MD
Sample : Q1334-13
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
E29B4

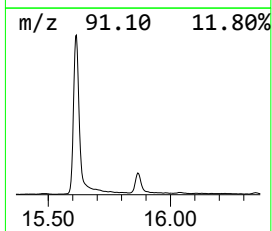
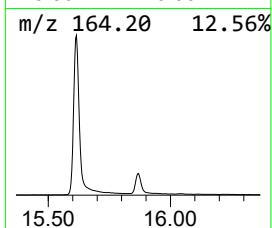
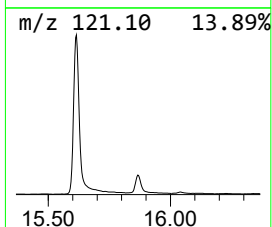
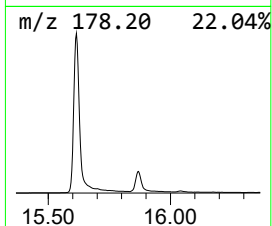
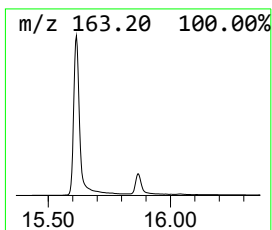
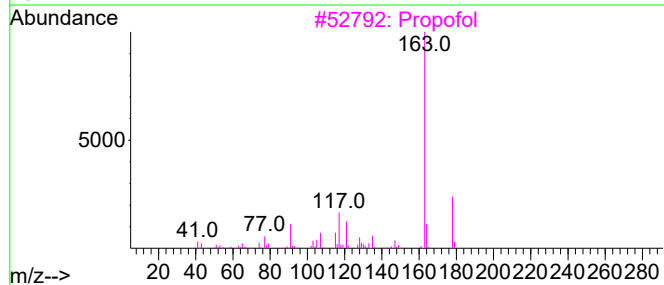
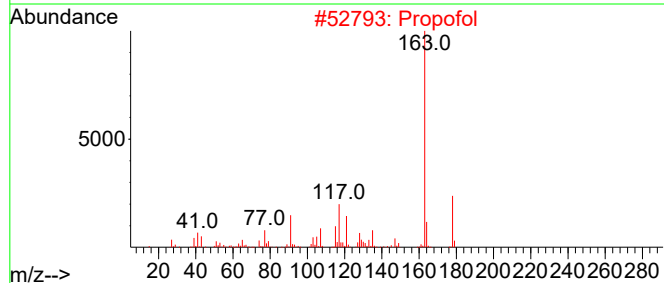
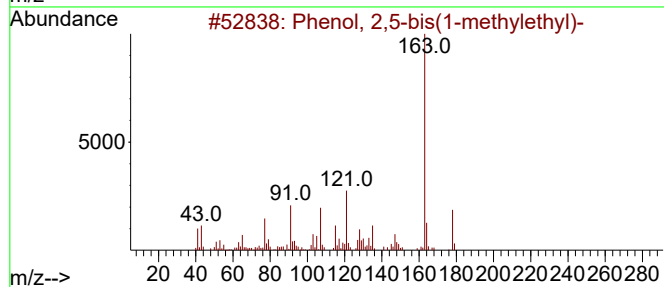
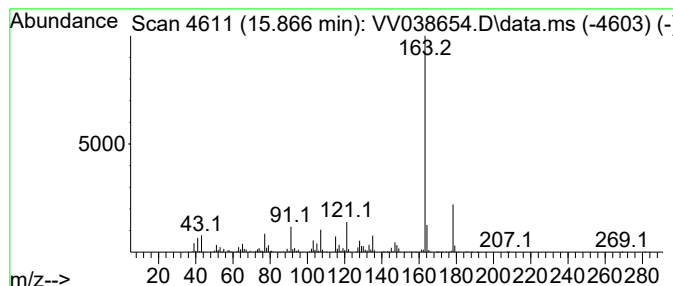
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 20 Phenol, 2,5-bis(1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.866	14.25 ug/L	2026730	1,4-Dichlorobenzene-d4	11.178

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	93
5			Phenol, 2,4-bis(1-methylethyl)-	178	C12H18O	002934-05-6	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV020725\
Data File : VV038654.D
Acq On : 07 Feb 2025 18:39
Operator : SY/MD
Sample : Q1334-13
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
E29B4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR020625WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.326	6.1	ug/L	731399	1	5.529	599083	5.0
2-Methyl-3-(met...	7.493	1.1	ug/L	201102	2	8.776	927040	5.0
3-(2-Methylprop...	11.095	1.4	ug/L	199088	3	11.178	711038	5.0
Phenol, 2-(1-me...	13.818	25.4	ug/L	3617340	3	11.178	711038	5.0
Phenol, 3-(1-me...	14.223	1.5	ug/L	207483	3	11.178	711038	5.0
Phenol, 2-(1,1-...	14.496	6.1	ug/L	863100	3	11.178	711038	5.0
Naphthalene, 2-...	14.561	2.3	ug/L	329147	3	11.178	711038	5.0
Naphthalene, 1-...	14.747	1.3	ug/L	180477	3	11.178	711038	5.0
Phenol, p-tert-...	14.866	13.4	ug/L	1908540	3	11.178	711038	5.0
Propofol	15.091	3.4	ug/L	485486	3	11.178	711038	5.0
Phenol, 2,4-bis...	15.615	121.9	ug/L	17331700	3	11.178	711038	5.0
Phenol, 2,5-bis...	15.866	14.3	ug/L	2026730	3	11.178	711038	5.0