

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV020725\
 Data File : VV038655.D
 Acq On : 07 Feb 2025 19:04
 Operator : SY/MD
 Sample : Q1334-14
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 E29B5

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: VV038655.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.304	73	82	91	rBV2	225630	358385	2.29%	0.949%
2	1.378	94	105	109	rBV	260762	447412	2.86%	1.184%
3	1.410	109	115	144	rVB2	649369	1246148	7.96%	3.299%
4	1.558	157	161	171	rVB	145143	179735	1.15%	0.476%
5	2.101	322	330	345	rVB	242919	354166	2.26%	0.938%
6	4.288	996	1010	1029	rVB2	155366	385590	2.46%	1.021%
7	4.982	1212	1226	1262	rVB2	402756	1034075	6.61%	2.738%
8	5.590	1405	1415	1439	rVB	276243	595882	3.81%	1.578%
9	5.712	1442	1453	1471	rBV2	87926	196577	1.26%	0.520%
10	6.063	1543	1562	1589	rBV	203249	441119	2.82%	1.168%
11	6.960	1830	1841	1858	rBV	88745	177011	1.13%	0.469%
12	7.278	1930	1940	1953	rBV	399973	702396	4.49%	1.860%
13	7.349	1953	1962	1989	rVB	454435	815571	5.21%	2.159%
14	8.050	2169	2180	2219	rBV	429989	906580	5.79%	2.400%
15	8.796	2402	2412	2443	rBV	437859	754275	4.82%	1.997%
16	10.152	2820	2834	2849	rVB	153641	249591	1.60%	0.661%
17	11.181	3144	3154	3174	rVB	447247	698781	4.47%	1.850%
18	11.467	3231	3243	3261	rBV	438772	943798	6.03%	2.499%
19	11.554	3262	3270	3296	rVB	434596	786789	5.03%	2.083%
20	12.699	3610	3626	3647	rBV4	83429	246322	1.57%	0.652%
21	13.432	3848	3854	3865	rVB	126172	191092	1.22%	0.506%
22	13.818	3963	3974	4001	rBV	2109437	3335990	21.32%	8.832%
23	14.220	4091	4099	4118	rVB	142517	268372	1.72%	0.710%
24	14.499	4175	4186	4195	rBV2	163475	278326	1.78%	0.737%
25	14.863	4286	4299	4324	rBV	2076788	3507113	22.42%	9.285%
26	15.091	4361	4370	4386	rVB	478457	721022	4.61%	1.909%
27	15.612	4519	4532	4566	rBV	9245597	15645467	100.00%	41.420%
28	15.866	4602	4611	4637	rVB	1250054	2019138	12.91%	5.345%
29	16.040	4657	4665	4679	rVB3	168107	286036	1.83%	0.757%

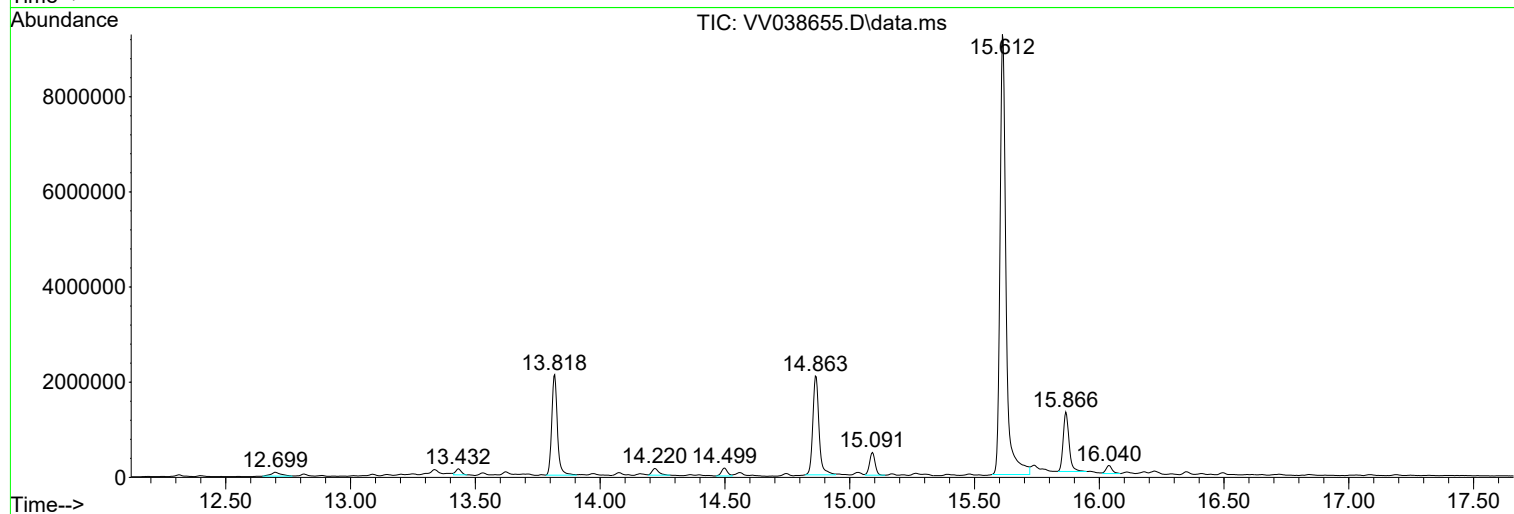
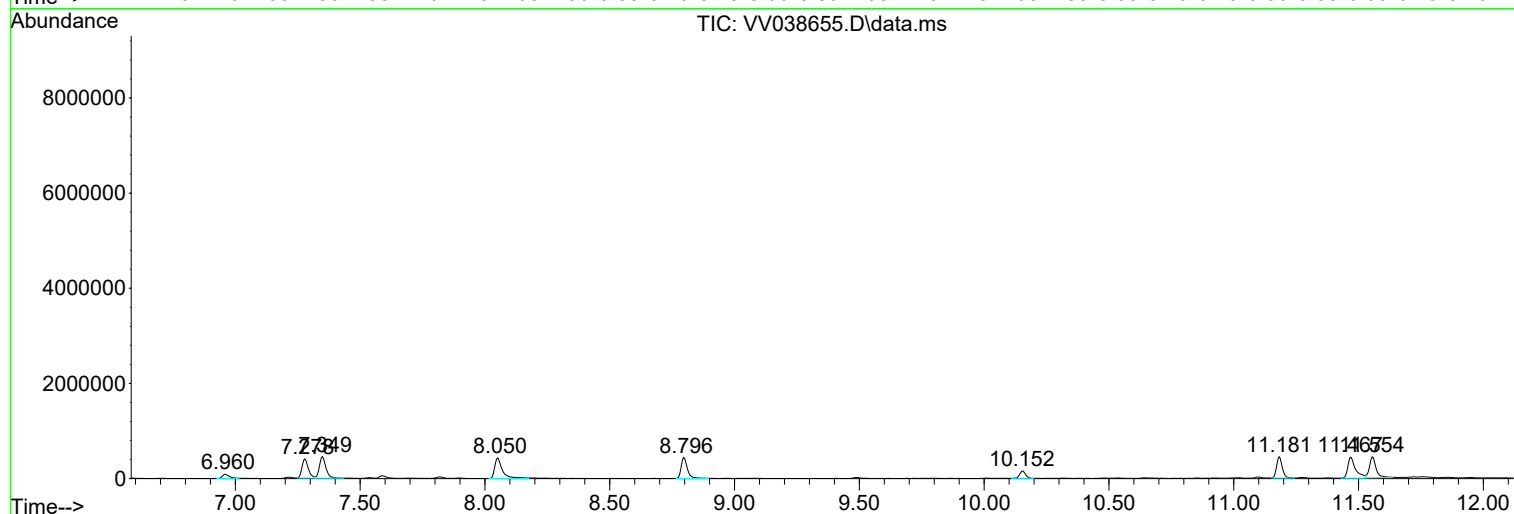
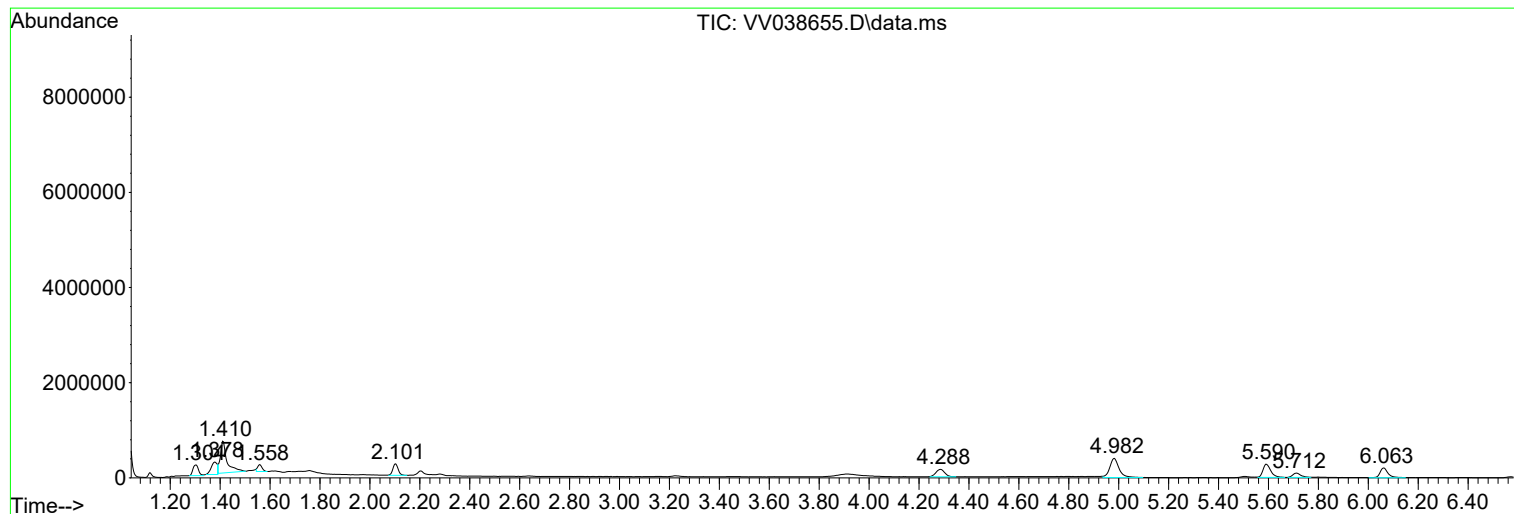
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR020625WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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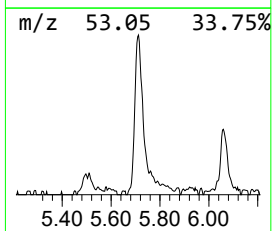
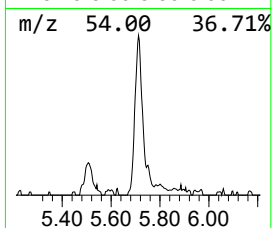
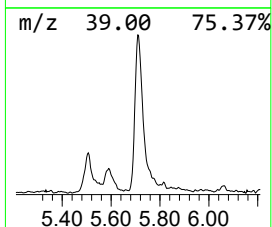
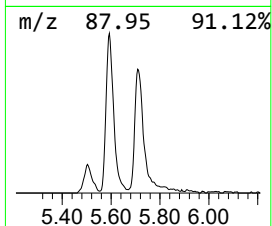
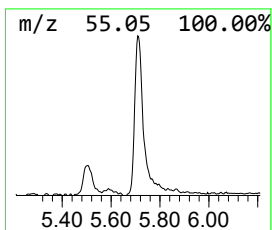
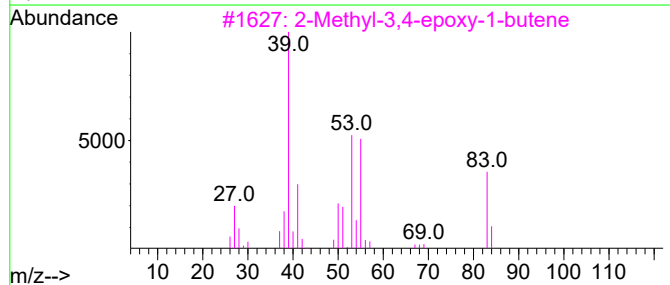
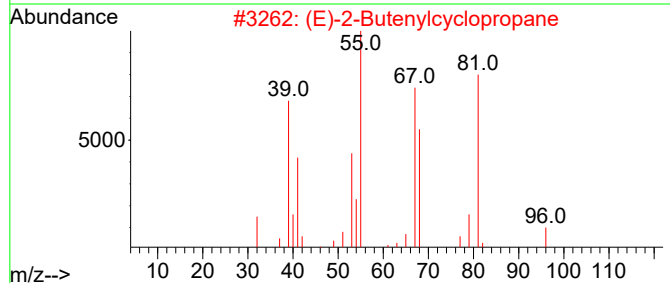
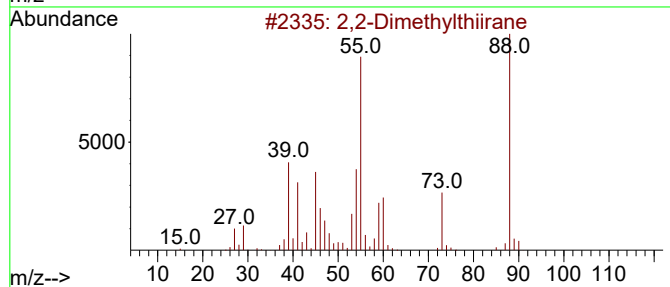
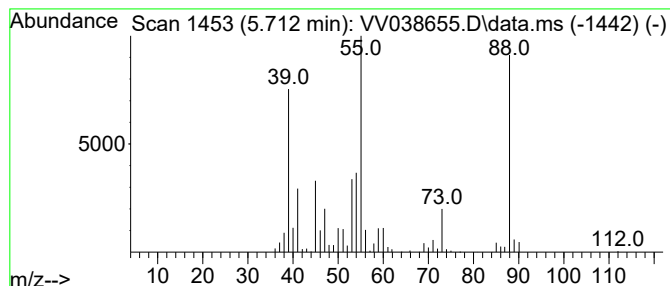
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR020625WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 2,2-Dimethylthiirane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.712	1.65 ug/L	196577	1,4-Difluorobenzene	5.590

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,2-Dimethylthiirane	88	C4H8S	003772-13-2	86
2			(E)-2-Butenylcyclopropane	96	C7H12	076588-98-2	53
3			2-Methyl-3,4-epoxy-1-butene	84	C5H8O	1000432-31-7	50
4			Oxirane, ethenyl-	70	C4H6O	000930-22-3	47
5			3-Cyclobutene-1,2-dione, 3,4-dim...	110	C6H6O2	001121-15-9	40



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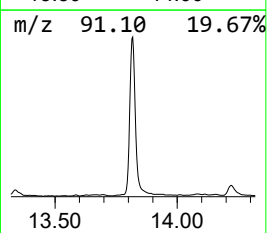
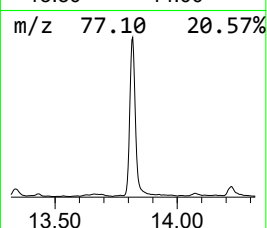
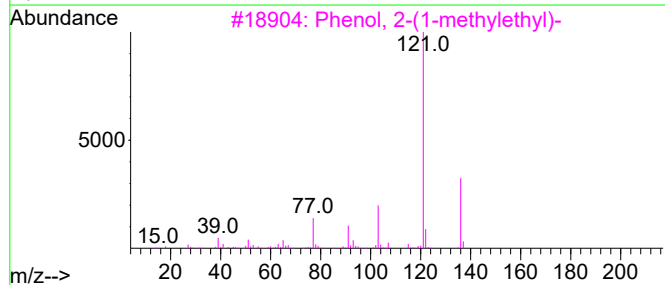
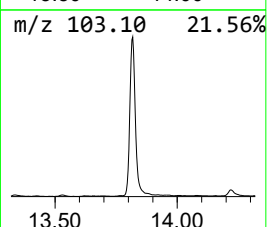
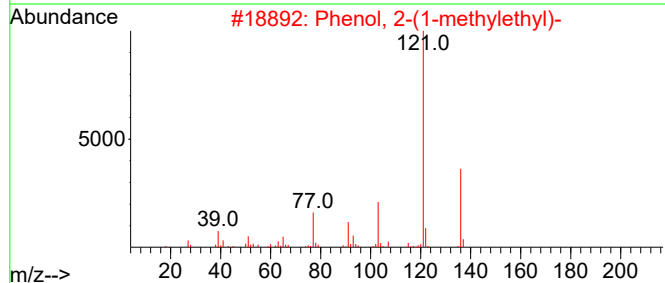
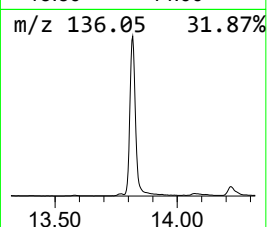
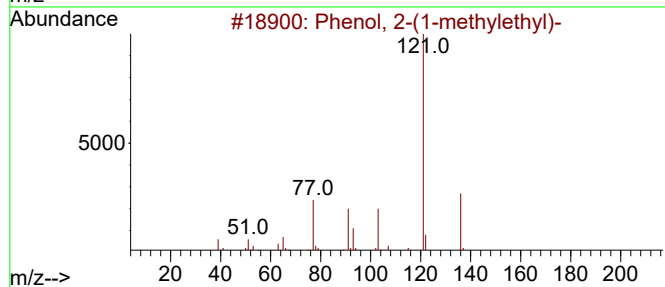
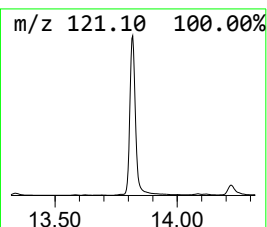
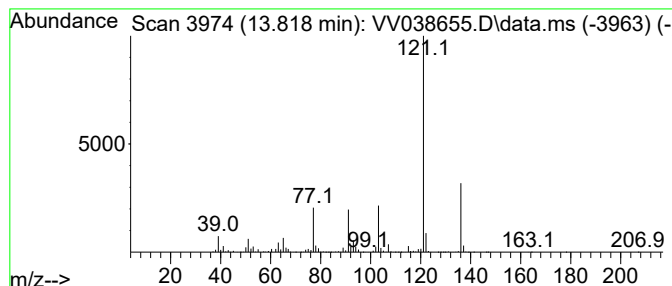
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR020625WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 8 Phenol, 2-(1-methylethyl)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.818	23.87 ug/L	3335990	1,4-Dichlorobenzene-d4	11.181

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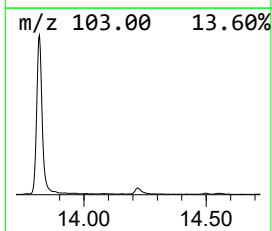
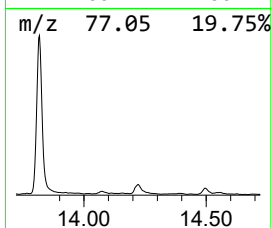
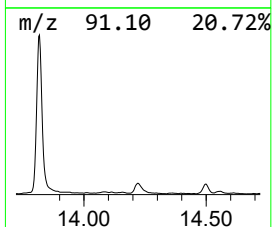
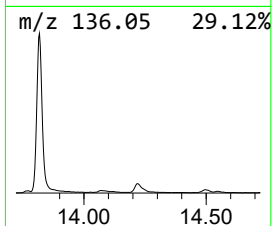
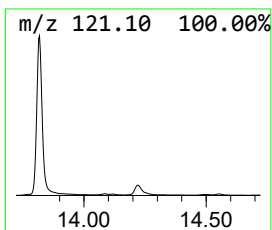
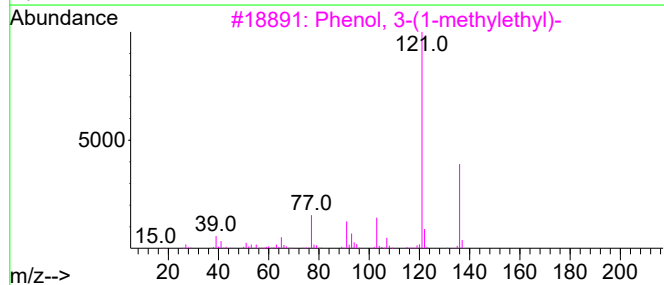
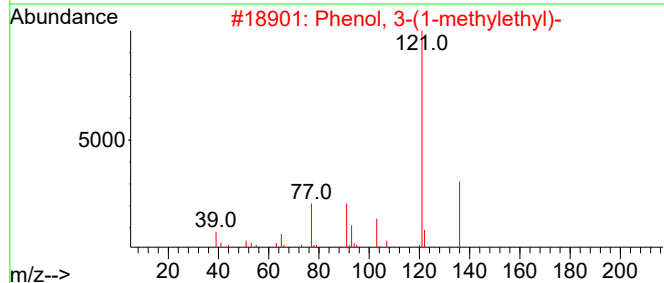
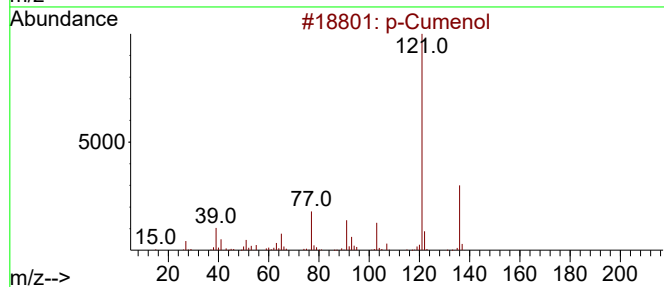
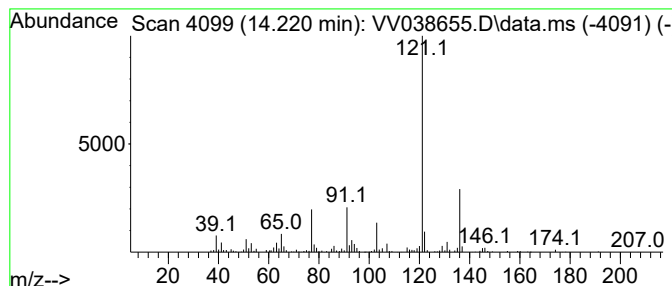
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR020625WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 9 p-Cumenol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.220	1.92 ug/L	268372	1,4-Dichlorobenzene-d4	11.181

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			p-Cumenol	136	C9H12O	000099-89-8	94
2			Phenol, 3-(1-methylethyl)-	136	C9H12O	000618-45-1	93
3			Phenol, 3-(1-methylethyl)-	136	C9H12O	000618-45-1	90
4			p-Cumenol	136	C9H12O	000099-89-8	87
5			Phenol, 2-ethyl-6-methyl-	136	C9H12O	001687-64-5	87



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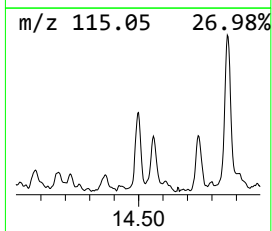
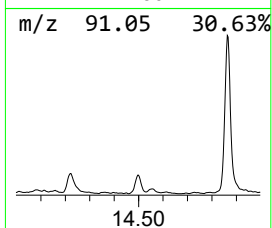
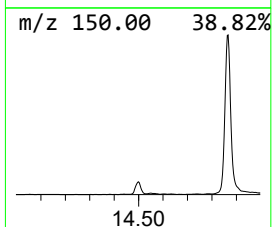
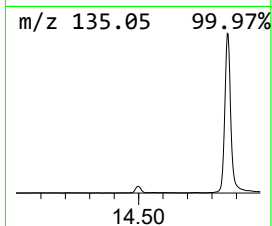
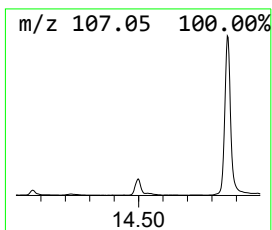
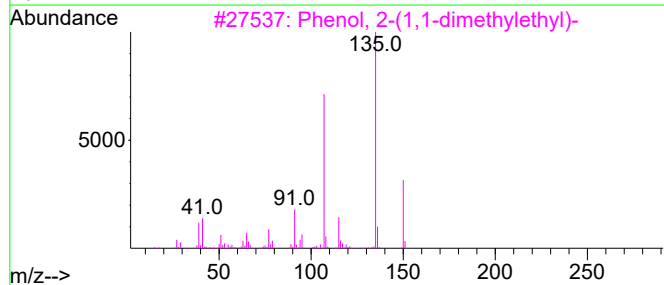
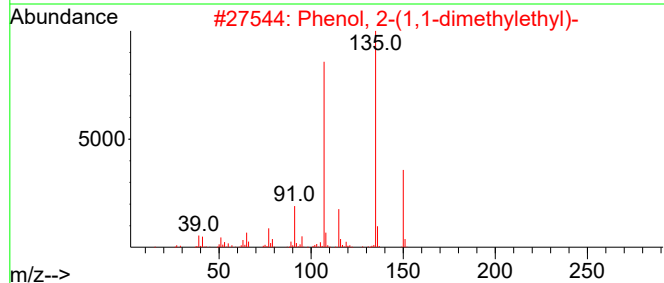
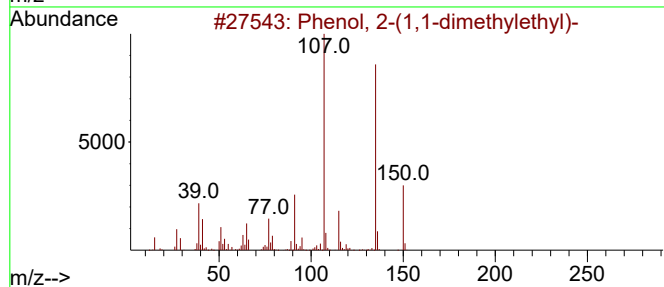
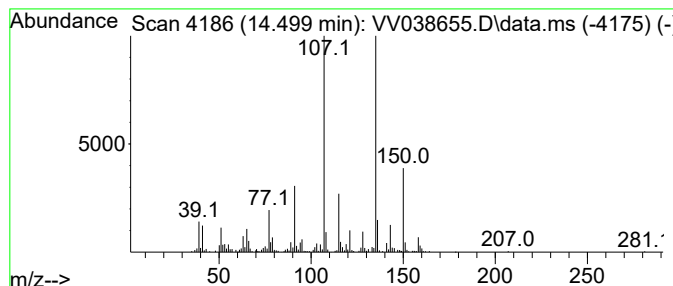
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Phenol, 2-(1,1-dimethylethyl)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.499	1.99 ug/L	278326	1,4-Dichlorobenzene-d4	11.181

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	94
2			Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	76
3			Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	68
4			Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	64
5			4-Hydroxy-2-methylacetophenone	150	C9H10O2	000875-59-2	53



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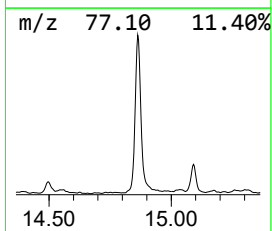
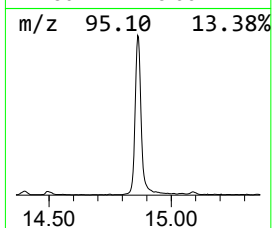
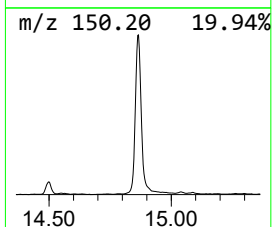
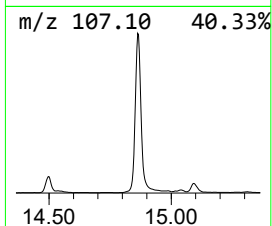
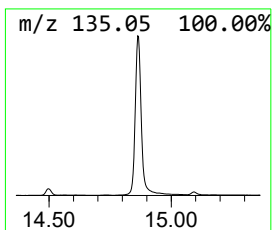
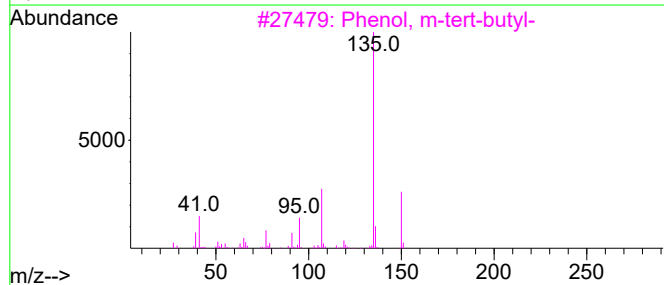
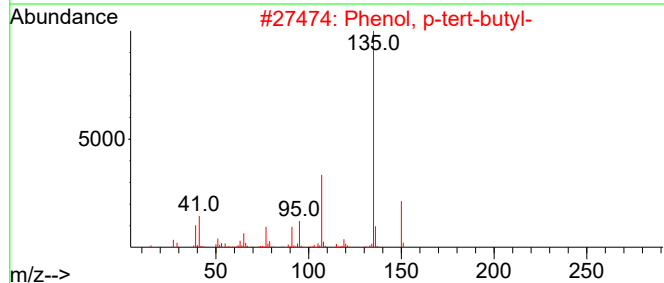
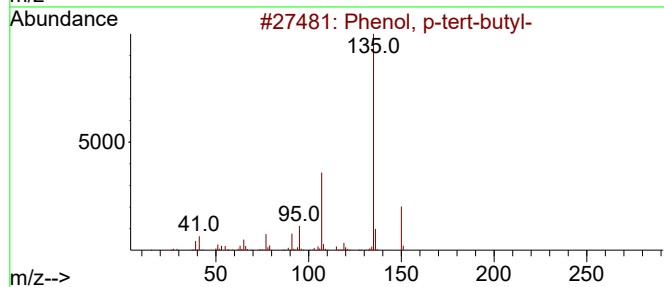
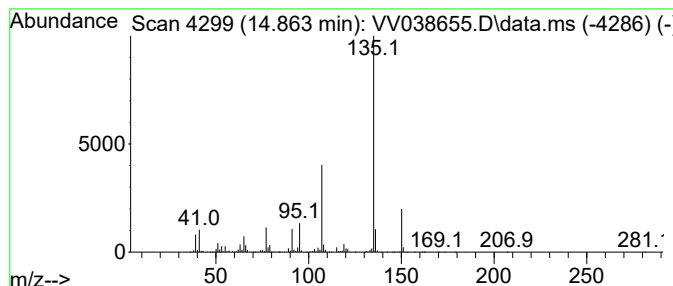
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Phenol, p-tert-butyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.863	25.09 ug/L	3507110	1,4-Dichlorobenzene-d4	11.181

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	93
5			Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	93



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ClientSampleId :
E29B5

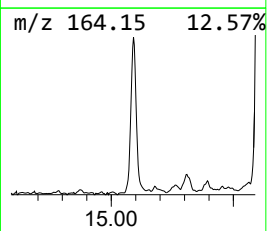
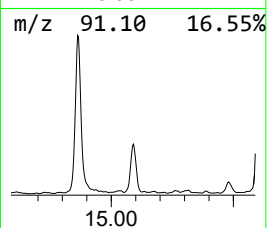
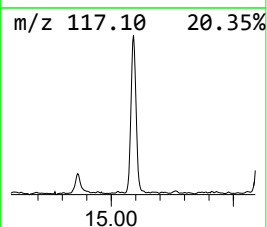
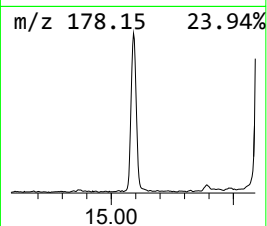
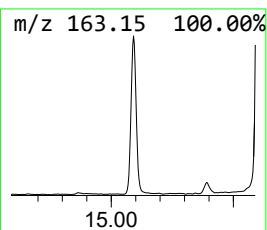
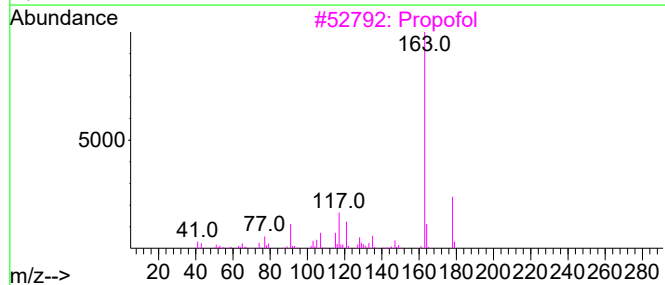
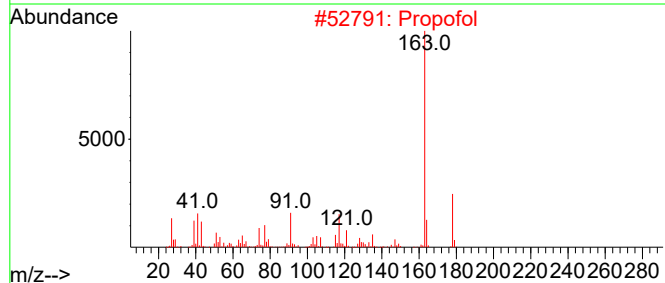
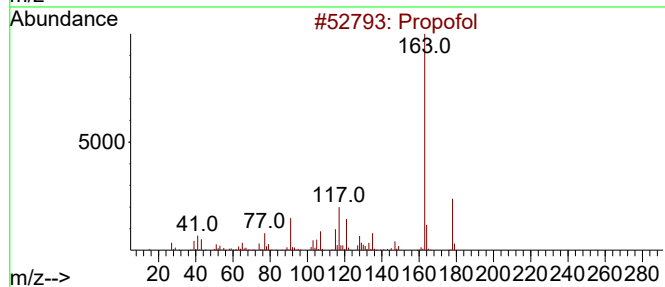
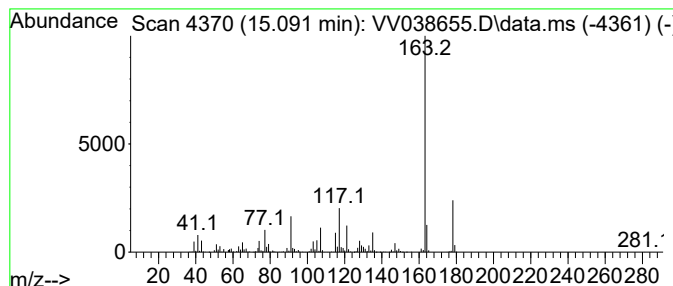
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 12 Propofol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.091	5.16 ug/L	721022	1,4-Dichlorobenzene-d4	11.181

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propofol			178	C12H18O	002078-54-8	97
2	Propofol			178	C12H18O	002078-54-8	97
3	Propofol			178	C12H18O	002078-54-8	96
4	Propofol			178	C12H18O	002078-54-8	95
5	Propofol			178	C12H18O	002078-54-8	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV020725\
Data File : VV038655.D
Acq On : 07 Feb 2025 19:04
Operator : SY/MD
Sample : Q1334-14
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
E29B5

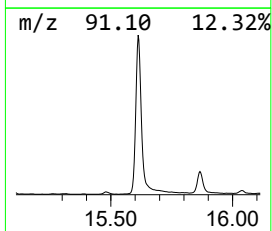
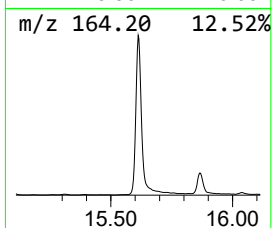
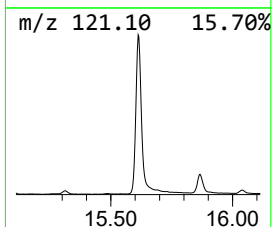
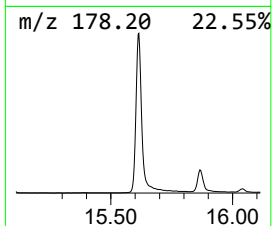
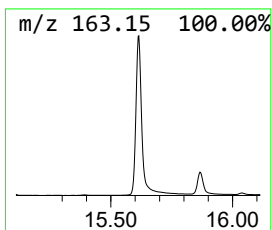
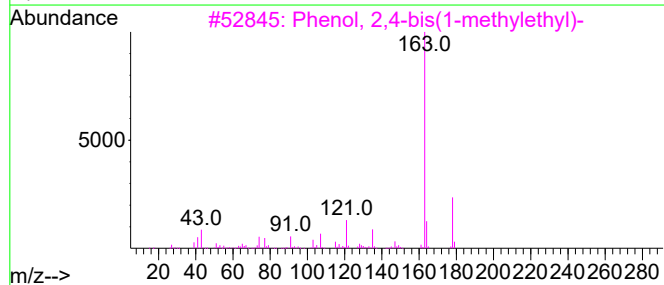
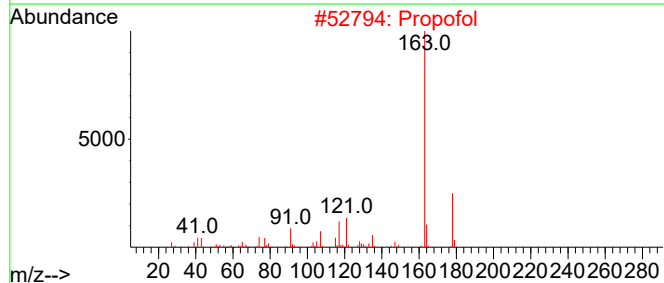
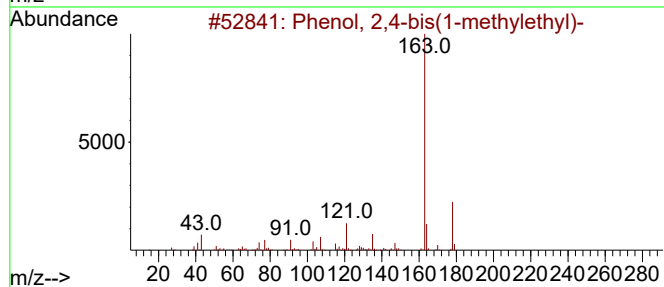
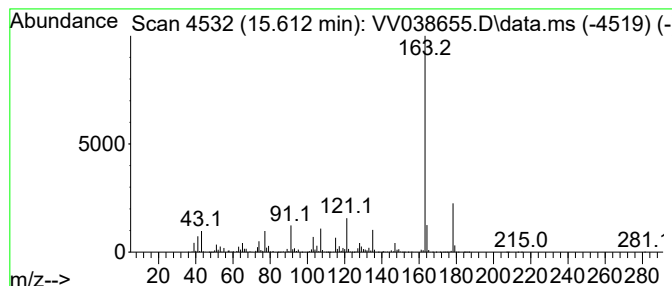
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 13 Phenol, 2,4-bis(1-methyleth... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.612	111.95 ug/L	15645500	1,4-Dichlorobenzene-d4	11.181

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	93
3			Phenol, 2,4-bis(1-methylethyl)-	178	C12H18O	002934-05-6	93
4			Propofol	178	C12H18O	002078-54-8	90
5			Propofol	178	C12H18O	002078-54-8	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV020725\
Data File : VV038655.D
Acq On : 07 Feb 2025 19:04
Operator : SY/MD
Sample : Q1334-14
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
E29B5

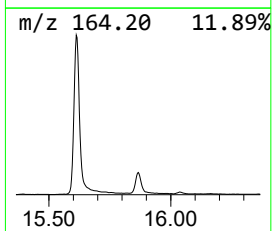
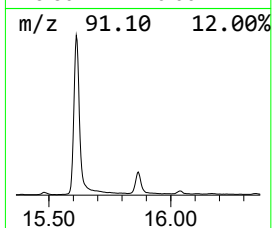
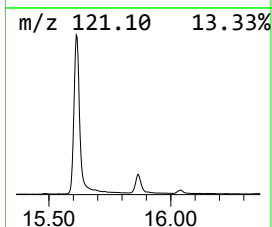
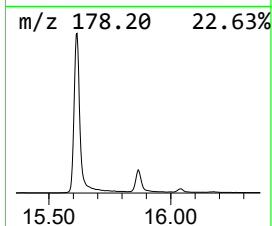
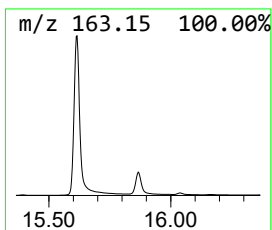
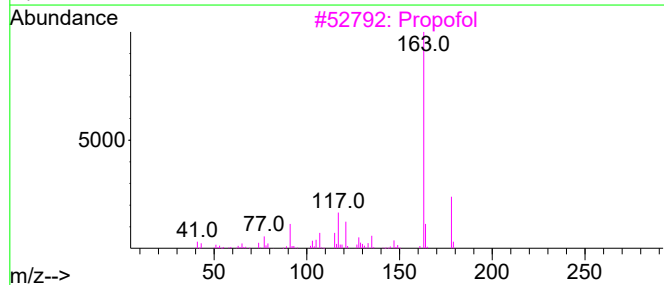
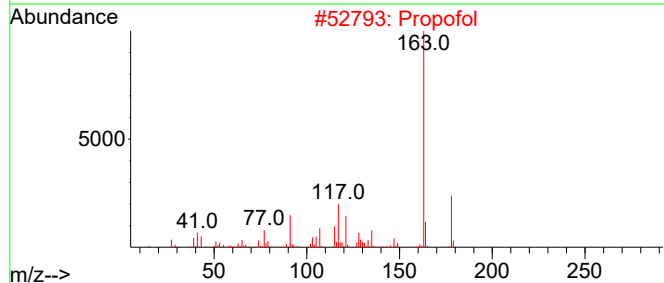
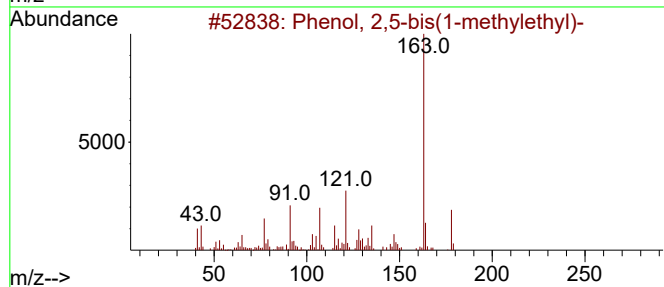
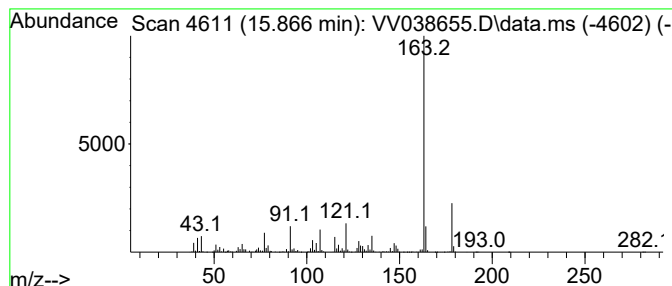
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 14 Phenol, 2,5-bis(1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.866	14.45 ug/L	2019140	1,4-Dichlorobenzene-d4	11.181

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 : VV038655.D
Acq On : 07 Feb 2025 19:04
Operator : SY/MD
Sample : Q1334-14
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
E29B5

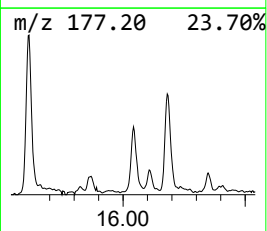
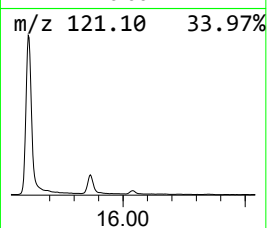
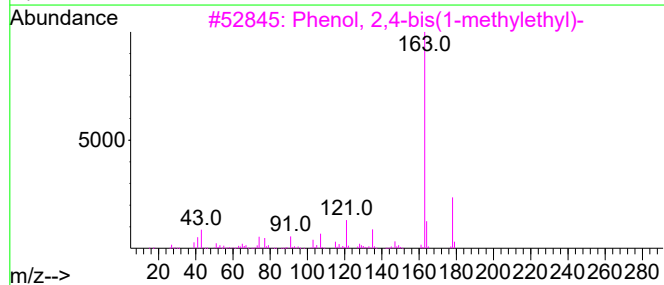
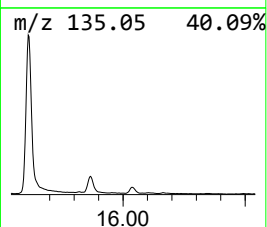
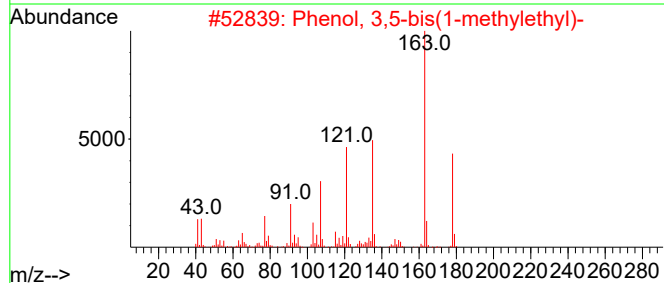
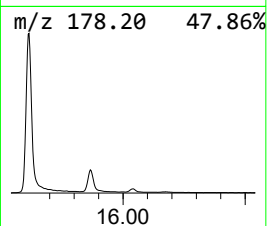
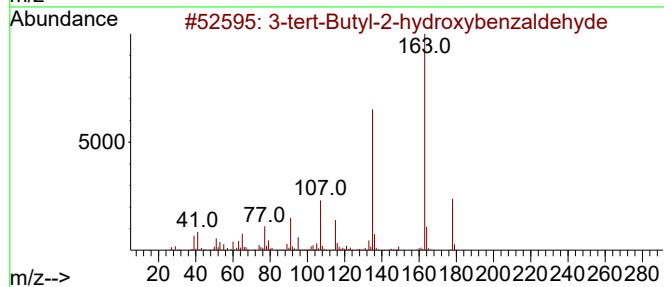
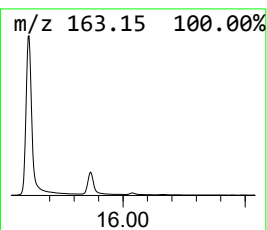
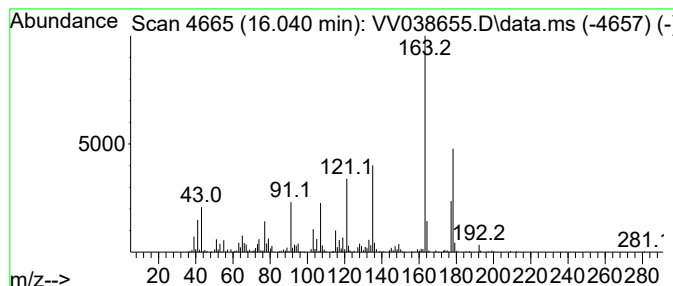
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 15 3-tert-Butyl-2-hydroxybenza... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.040	2.05 ug/L	286036	1,4-Dichlorobenzene-d4	11.181

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-tert-Butyl-2-hydroxybenzaldehyde	178	C11H14O2	024623-65-2	87
2		Phenol, 3,5-bis(1-methylethyl)-	178	C12H18O	026886-05-5	83
3		Phenol, 2,4-bis(1-methylethyl)-	178	C12H18O	002934-05-6	70
4		6-tert-Butyl-2,4-dimethylphenol	178	C12H18O	001879-09-0	68
5		Propofol	178	C12H18O	002078-54-8	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV020725\
Data File : VV038655.D
Acq On : 07 Feb 2025 19:04
Operator : SY/MD
Sample : Q1334-14
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
E29B5

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
2,2-Dimethylthi...	5.712	1.6	ug/L	196577	1	5.590	595882	5.0
Phenol, 2-(1-me...	13.818	23.9	ug/L	3335990	3	11.181	698781	5.0
p-Cumenol	14.220	1.9	ug/L	268372	3	11.181	698781	5.0
Phenol, 2-(1,1-...	14.499	2.0	ug/L	278326	3	11.181	698781	5.0
Phenol, p-tert-...	14.863	25.1	ug/L	3507110	3	11.181	698781	5.0
Propofol	15.091	5.2	ug/L	721022	3	11.181	698781	5.0
Phenol, 2,4-bis...	15.612	112.0	ug/L	15645500	3	11.181	698781	5.0
Phenol, 2,5-bis...	15.866	14.4	ug/L	2019140	3	11.181	698781	5.0
3-tert-Butyl-2-...	16.040	2.0	ug/L	286036	3	11.181	698781	5.0