LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012825\
Data File : VU063067.D
Acq On : 28 Jan 2025 15:08
Operator : MD/SY
Sample : Q1195-05
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2957

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: VU063067.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.522	57	72	75	rBV4	10044	18959	1.30%	0.311%
2	1.589	84	93	106	rVB2	33897	53245	3.64%	0.873%
3	1.904	182	191	200	rVB	21503	27478	1.88%	0.450%
4	2.554	380	393	407	rBV	57512	94076	6.43%	1.542%
5	4.615	1024	1034	1072	rBV	42664	119737	8.19%	1.962%
6	5.049	1154	1169	1186	rBV	78425	173077	11.84%	2.836%
7	5.711	1355	1375	1395	rBV3	133331	352074	24.08%	5.770%
8	6.235	1526	1538	1555	rBV	150315	287458	19.66%	4.711%
9	6.676	1661	1675	1695	rBV2	82871	163135	11.16%	2.673%
10	7.554	1938	1948	1969	rVB	46125	83912	5.74%	1.375%
11	7.885	2039	2051	2070	rBV	167018	299001	20.45%	4.900%
12	8.171	2129	2140	2159	rBV2	29625	53821	3.68%	0.882%
13	8.624	2268	2281	2314	rBV	163233	311373	21.29%	5.103%
14	9.406	2513	2524	2552	rBV	202856	350779	23.99%	5.749%
15	10.746	2930	2941	2961	rVB2	71147	117576	8.04%	1.927%
16	11.036	3019	3031	3044	rBV2	13200	21907	1.50%	0.359%
17	11.801	3258	3269	3287	rBV	222502	383358	26.22%	6.283%
18	12.049	3331	3346	3378	rBV	785793	1462249	100.00%	23.964%
19	12.184	3378	3388	3411	rVB	206746	365906	25.02%	5.997%
20	14.084	3973	3979	3987	rVB2	16126	21894	1.50%	0.359%
21	14.412	4071	4081	4100	rBV	115619	184881	12.64%	3.030%
22	15.103	4282	4296	4307	rBV	47306	74788	5.11%	1.226%
23	15.479	4403	4413	4425	rBV2	23077	43468	2.97%	0.712%
24	15.711	4474	4485	4501	rVB2	40388	61299	4.19%	1.005%
25	16.225	4633	4645	4670	rBV	471435	837657	57.29%	13.728%
26	16.482	4715	4725	4749	rVB2	77947	138864	9.50%	2.276%

Sum of corrected areas: 6101972

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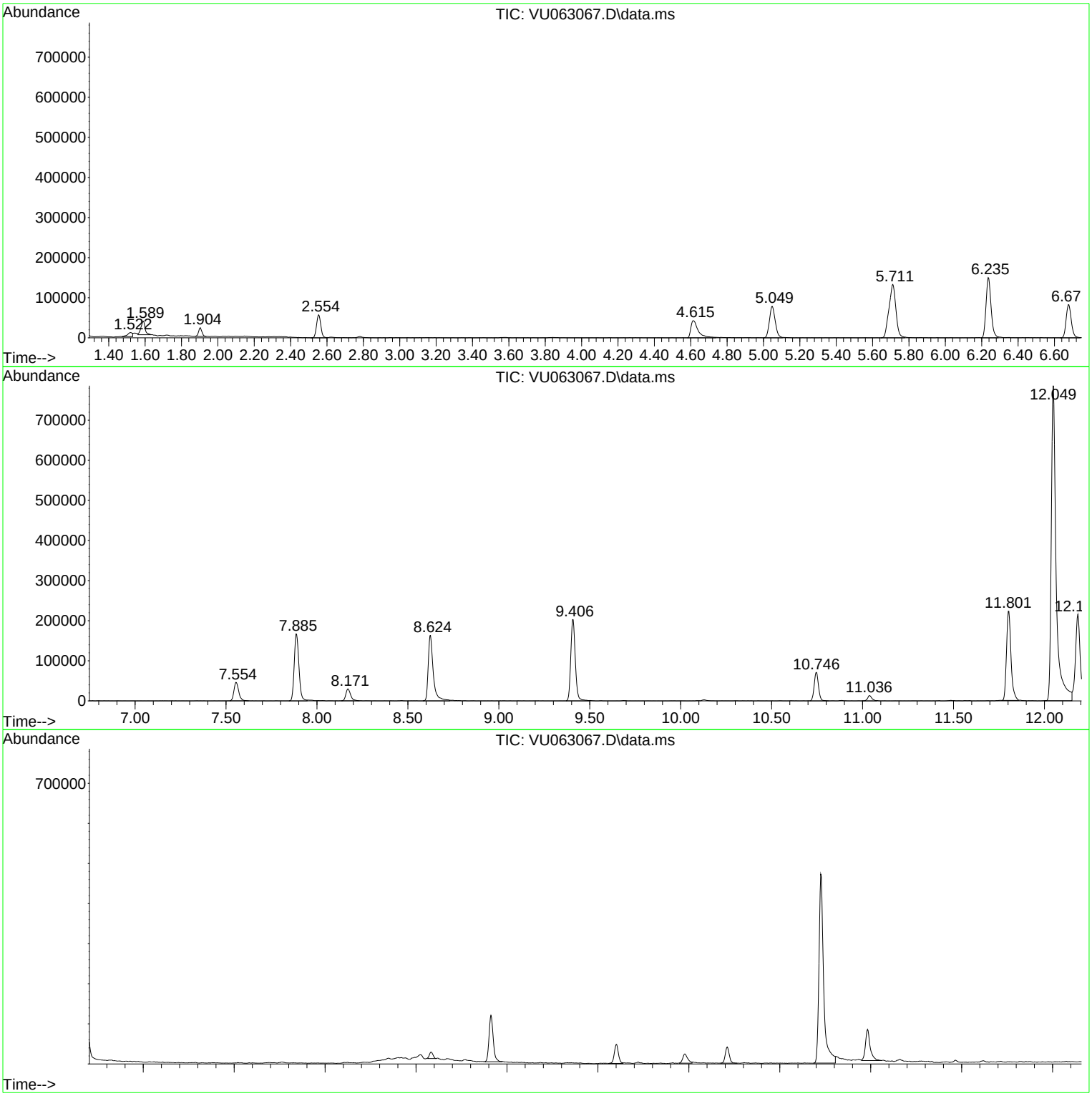
Sample : Q1195-05
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2957

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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Data File : VU063067.D
Acq On : 28 Jan 2025 15:08
Operator : MD/SY
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Misc : 25mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2957

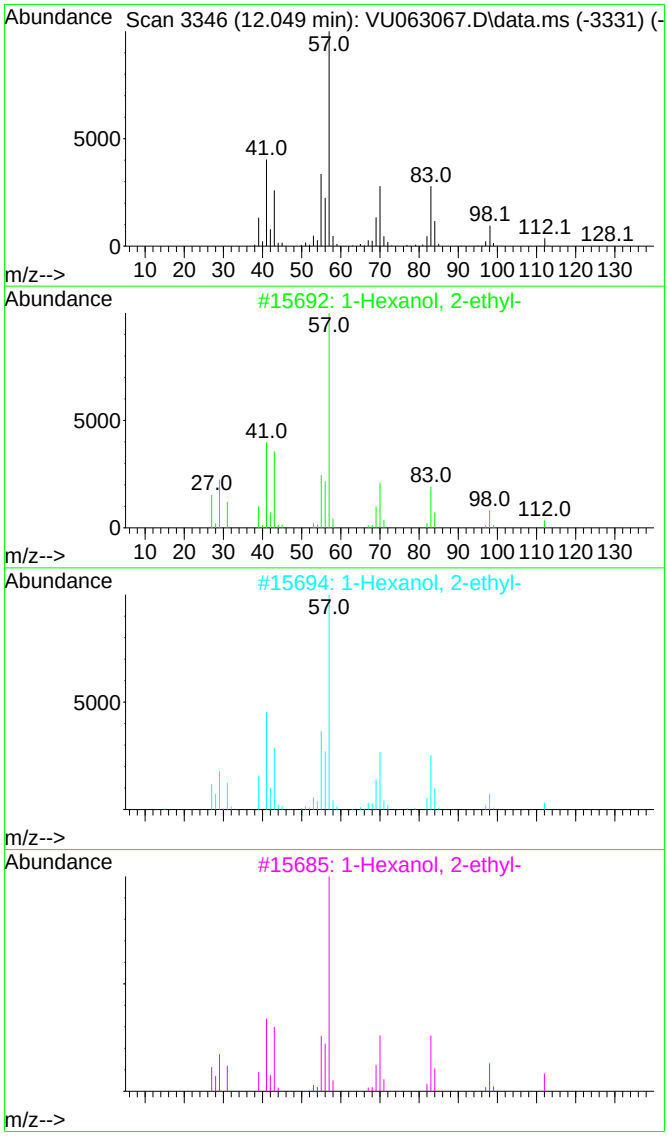
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012725WMA.M
Quant Title : TRACE VOA SFAM1.0

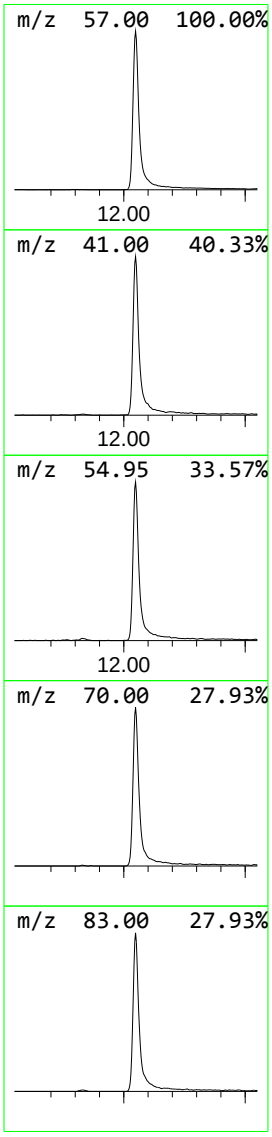
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.049	19.07 ug/L	1462250	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	90
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
4	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012825\
Data File : VU063067.D
Acq On : 28 Jan 2025 15:08
Operator : MD/SY
Sample : Q1195-05
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2957

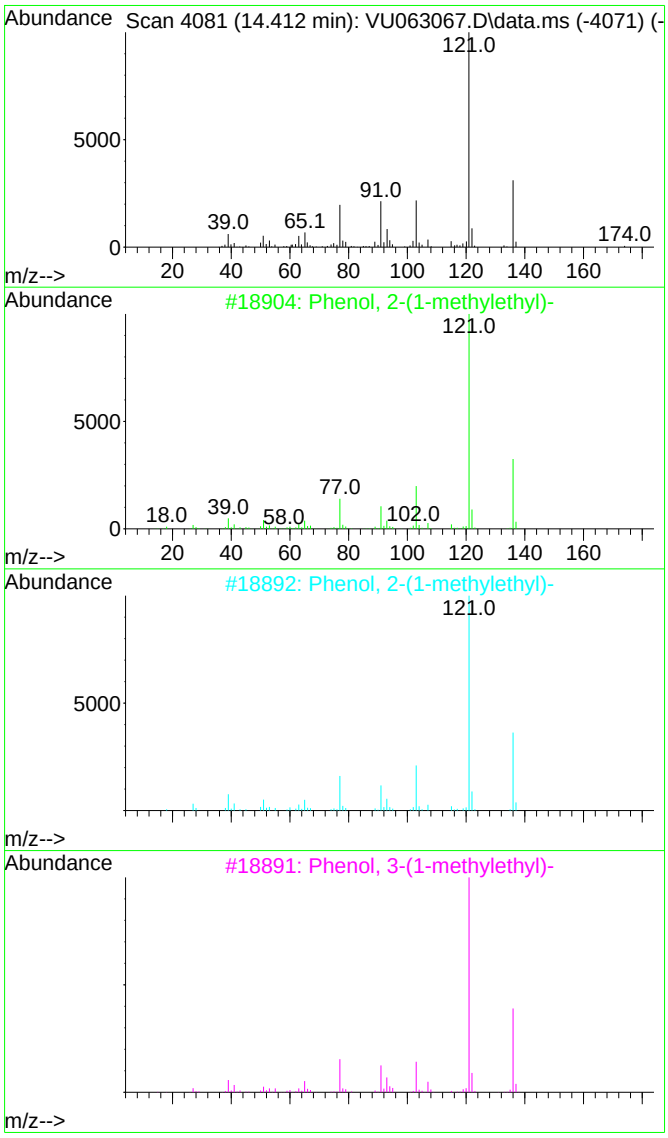
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012725WMA.M
Quant Title : TRACE VOA SFAM1.0

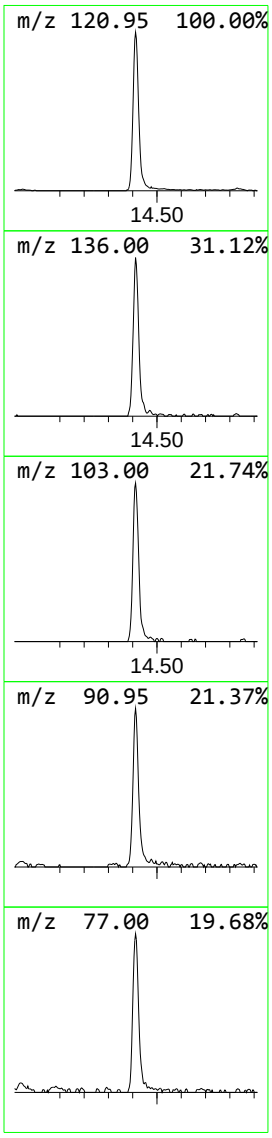
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.412	2.41 ug/L	184881	1,4-Dichlorobenzene-d4	11.804

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, 3-(1-methylethyl)-	136	C9H12O	000618-45-1	91
4	Phenol, 3-(1-methylethyl)-	136	C9H12O	000618-45-1	90
5	p-Cumenol	136	C9H12O	000099-89-8	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012825\
Data File : VU063067.D
Acq On : 28 Jan 2025 15:08
Operator : MD/SY
Sample : Q1195-05
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2957

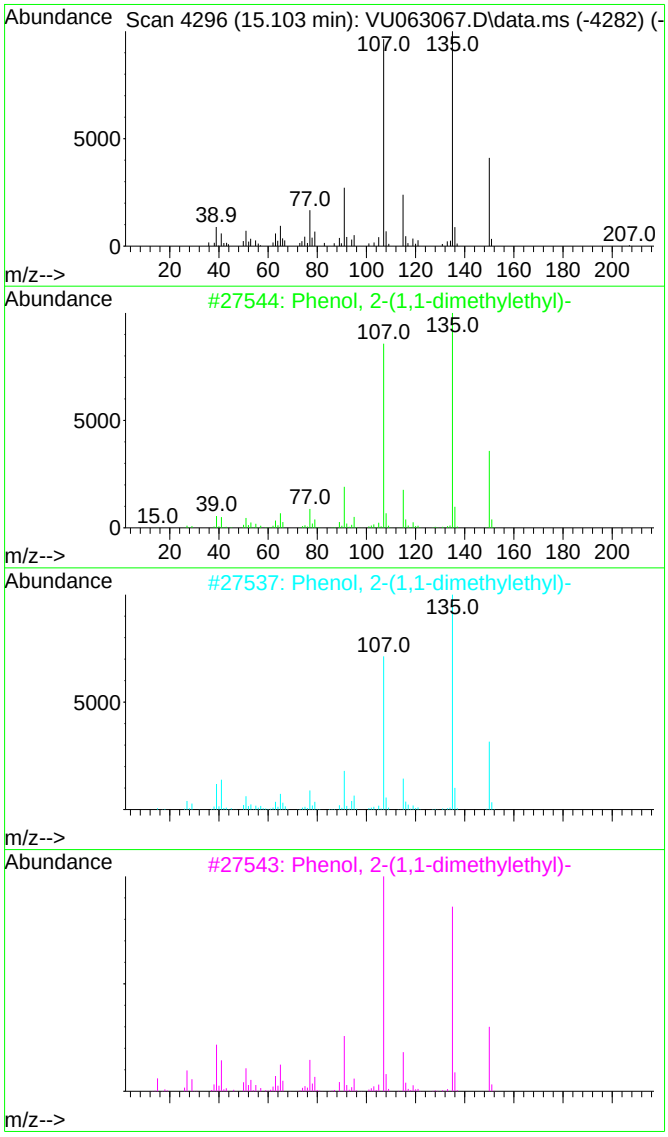
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012725WMA.M
Quant Title : TRACE VOA SFAM1.0

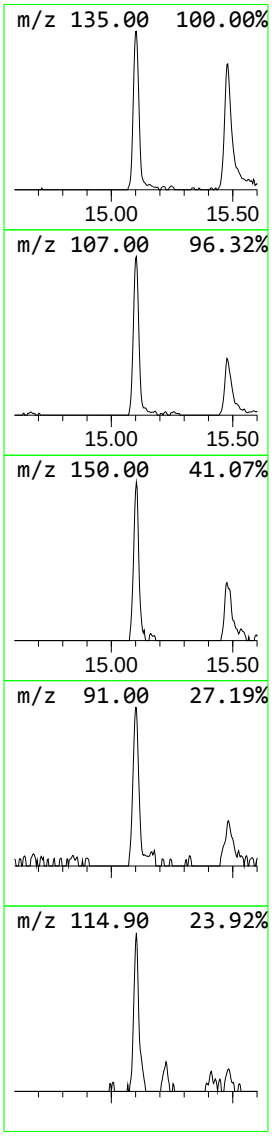
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Phenol, 2-(1,1-dimethylethyl)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.103	0.98 ug/L	74788	1,4-Dichlorobenzene-d4	11.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	93
2	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	87
3	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	87
4	1,5,6,7-Tetrahydro-4-indolone	135	C8H9NO	013754-86-4	52
5	4-Hydroxy-2-methylacetophenone	150	C9H10O2	000875-59-2	49





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Data File : VU063067.D
Acq On : 28 Jan 2025 15:08
Operator : MD/SY
Sample : Q1195-05
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2957

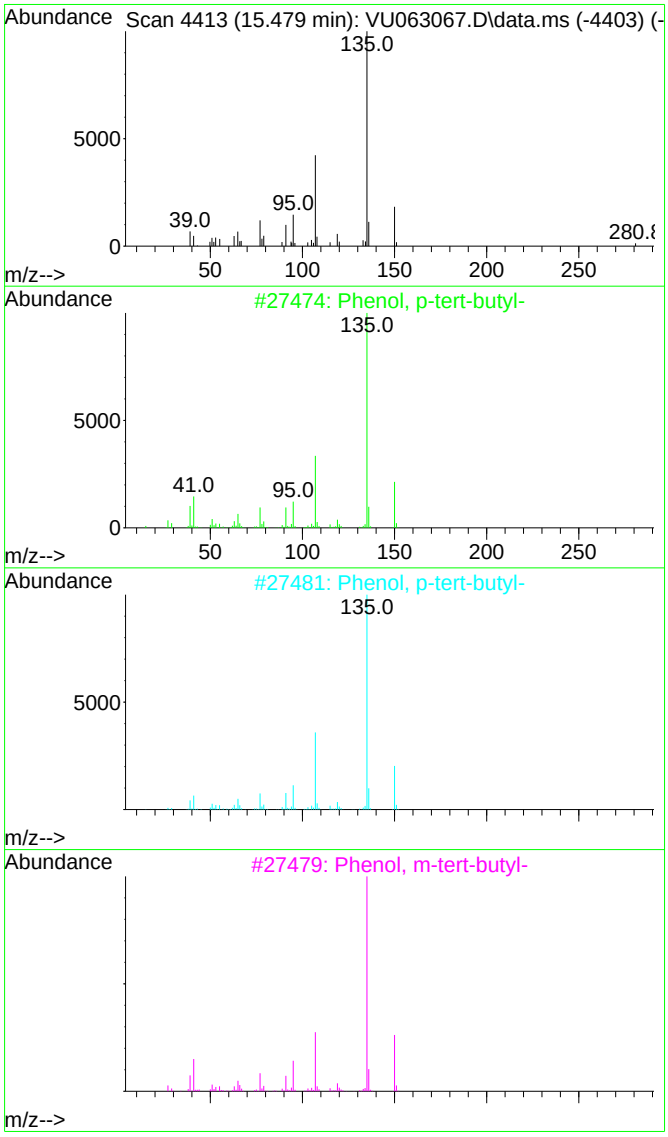
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012725WMA.M
Quant Title : TRACE VOA SFAM1.0

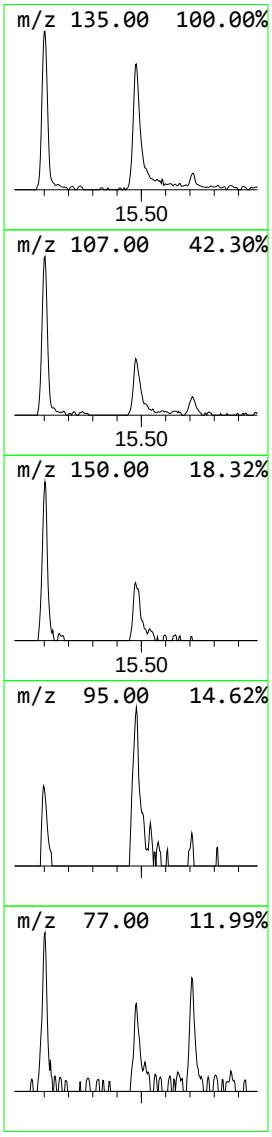
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Phenol, p-tert-butyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.479	0.57 ug/L	43468	1,4-Dichlorobenzene-d4	11.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	95
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	94
3	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	91
4	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	91
5	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012825\
Data File : VU063067.D
Acq On : 28 Jan 2025 15:08
Operator : MD/SY
Sample : Q1195-05
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2957

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

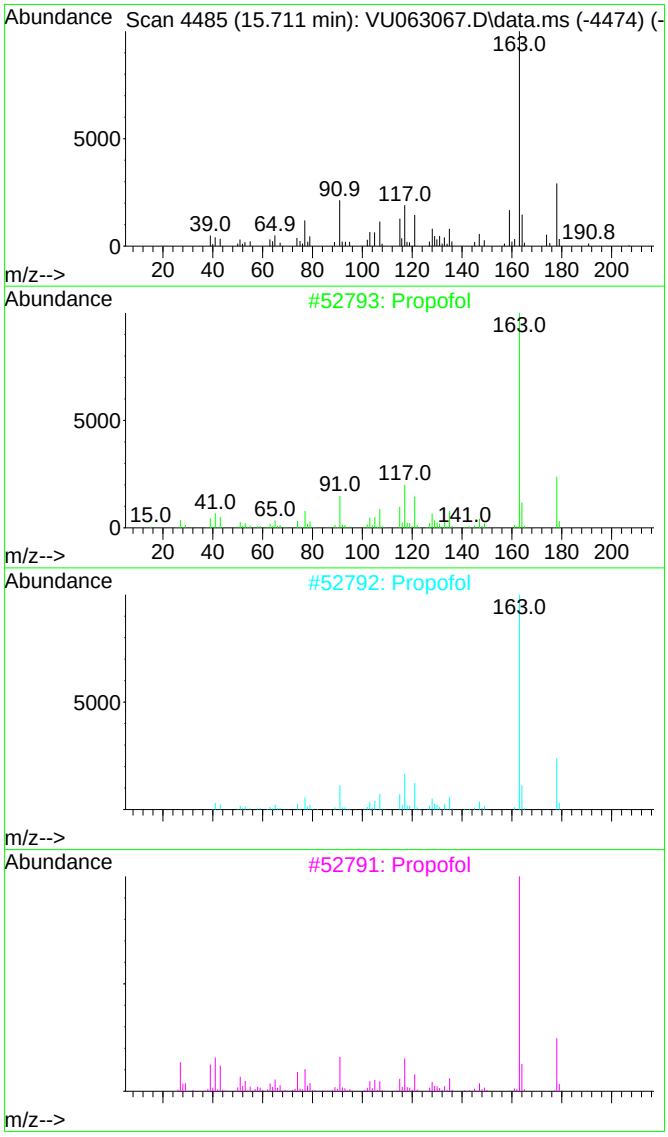
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

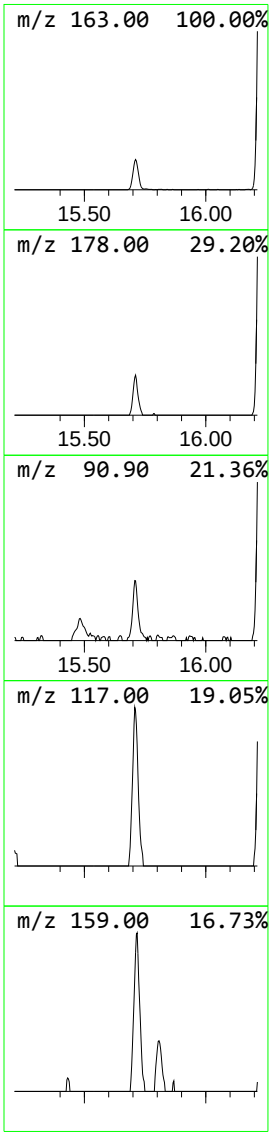
****

Peak Number 6 Propofol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.711	0.80 ug/L	61299	1,4-Dichlorobenzene-d4	11.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propofol	178	C12H18O	002078-54-8	96
2	Propofol	178	C12H18O	002078-54-8	95
3	Propofol	178	C12H18O	002078-54-8	94
4	Propofol	178	C12H18O	002078-54-8	87
5	Propofol	178	C12H18O	002078-54-8	87





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012825\
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Sample : Q1195-05
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2957

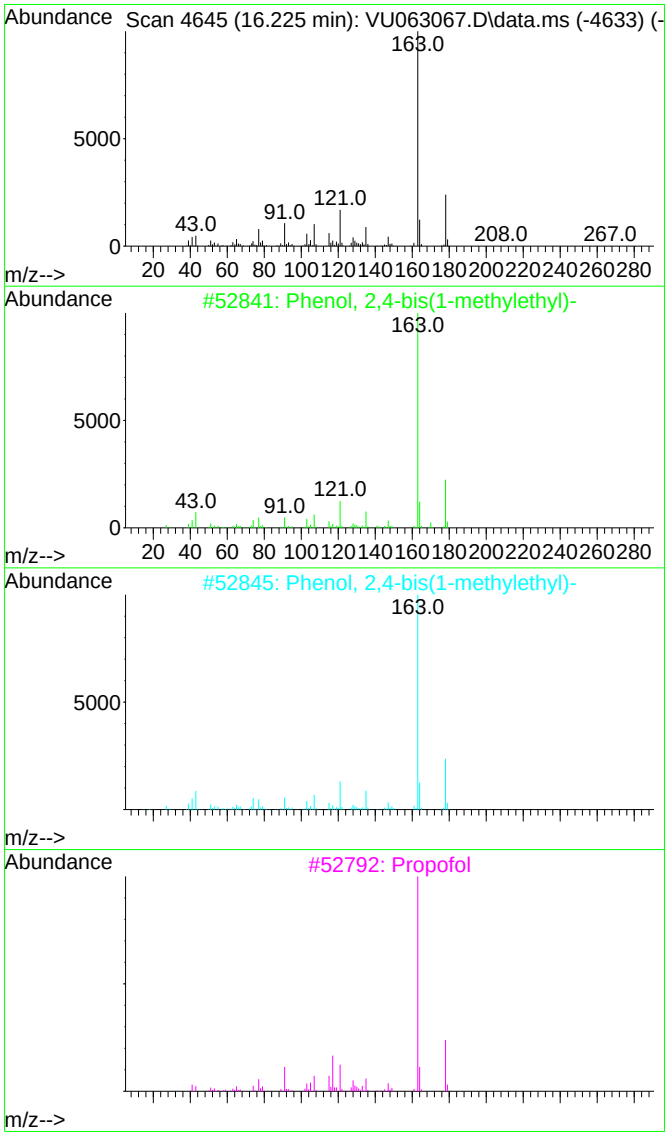
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012725WMA.M
Quant Title : TRACE VOA SFAM1.0

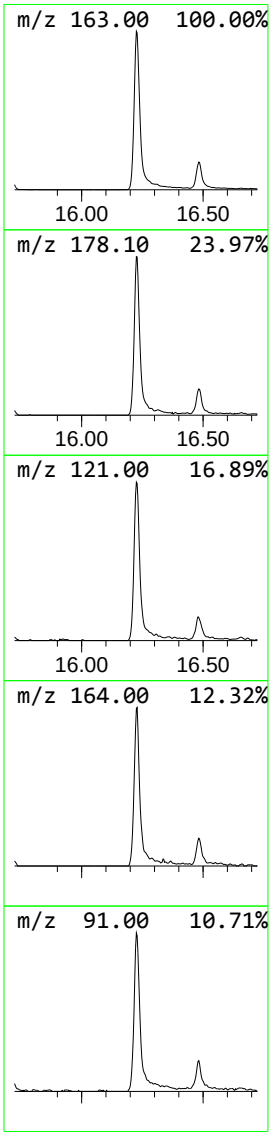
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Phenol, 2,4-bis(1-methyleth... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.225	10.93 ug/L	837657	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	95
2	Phenol, 2,4-bis(1-methylethyl)-	178	C12H18O	002934-05-6	94
3	Propofol	178	C12H18O	002078-54-8	94
4	Propofol	178	C12H18O	002078-54-8	93
5	Propofol	178	C12H18O	002078-54-8	90





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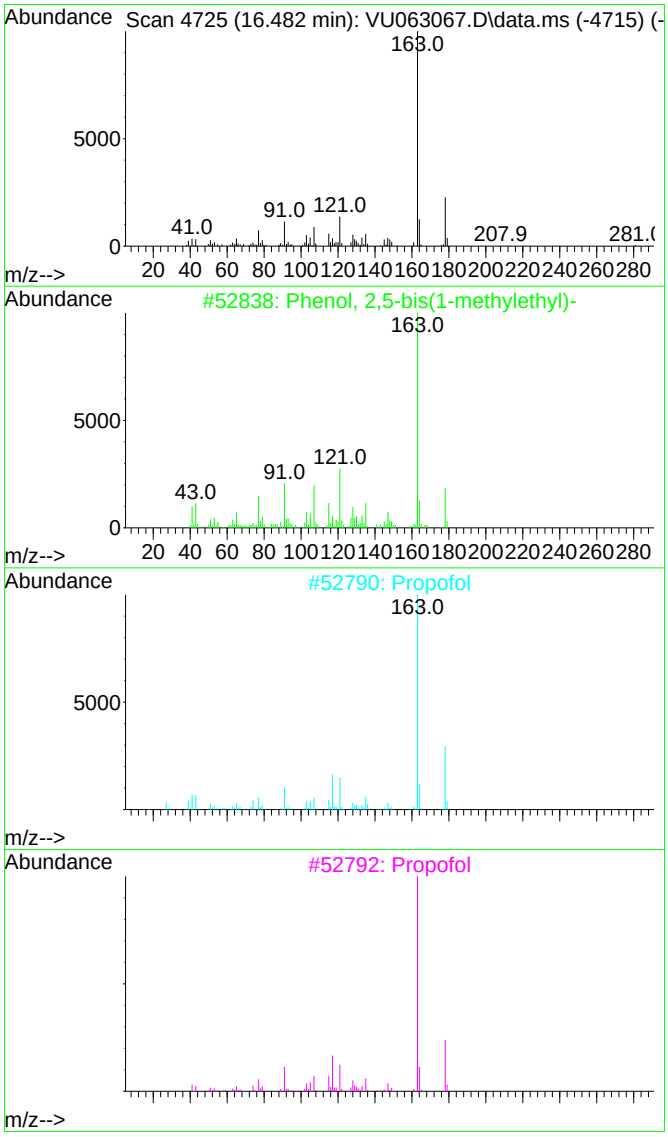
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012725WMA.M
Quant Title : TRACE VOA SFAM1.0

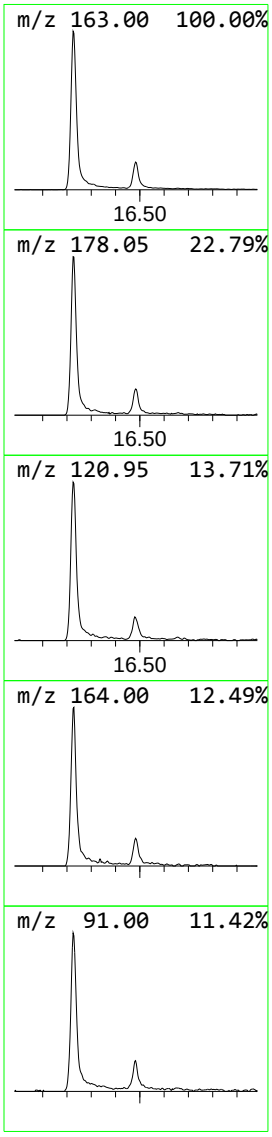
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Phenol, 2,5-bis(1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.483	1.81 ug/L	138864	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	94
5	Propofol	178	C12H18O	002078-54-8	94





Tentatively Identified Compound (LSC) summary

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Quant Title : TRACE VOA SFAM1.0

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
1-Hexanol, 2-et...	12.049	19.1	ug/L	1462250	3	11.804	383358	5.0
Phenol, 2-(1-me...	14.412	2.4	ug/L	184881	3	11.804	383358	5.0
Phenol, 2-(1,1-...	15.103	1.0	ug/L	74788	3	11.804	383358	5.0
Phenol, p-tert-...	15.479	0.6	ug/L	43468	3	11.804	383358	5.0
Propofol	15.711	0.8	ug/L	61299	3	11.804	383358	5.0
Phenol, 2,4-bis...	16.225	10.9	ug/L	837657	3	11.804	383358	5.0
Phenol, 2,5-bis...	16.483	1.8	ug/L	138864	3	11.804	383358	5.0