LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012925\
Data File : VU063087.D
Acq On : 29 Jan 2025 12:24
Operator : MD/SY
Sample : Q1191-06
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : A44W6

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: VU063087.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.595	77	95	107	rBV	19443	31063	1.35%	0.463%
2	2.557	383	394	405	rBV	43024	70194	3.05%	1.046%
3	2.737	436	450	475	rBV	81768	159582	6.93%	2.378%
4	4.605	1020	1031	1054	rBV	33182	81787	3.55%	1.219%
5	5.049	1155	1169	1190	rBV2	59376	132316	5.74%	1.971%
6	5.711	1356	1375	1397	rBV2	90285	243833	10.58%	3.633%
7	6.238	1526	1539	1559	rBV2	112940	219732	9.54%	3.274%
8	6.679	1662	1676	1694	rBV2	55136	109488	4.75%	1.631%
9	7.557	1938	1949	1968	rBV3	33340	61333	2.66%	0.914%
10	7.888	2040	2052	2070	rBV	121883	210704	9.14%	3.139%
11	8.171	2130	2140	2156	rBV2	21088	37399	1.62%	0.557%
12	8.621	2270	2280	2313	rBV2	112981	217515	9.44%	3.241%
13	9.405	2513	2524	2547	rBV	157026	271376	11.78%	4.043%
14	10.746	2929	2941	2959	rBB	53176	89148	3.87%	1.328%
15	11.804	3257	3270	3288	rBV	183939	306910	13.32%	4.573%
16	12.048	3333	3346	3377	rBV	652805	1171542	50.84%	17.455%
17	12.183	3378	3388	3407	rVB2	155200	273663	11.88%	4.077%
18	14.412	4070	4081	4095	rBV	112839	178167	7.73%	2.654%
19	15.100	4285	4295	4308	rBV2	42224	63661	2.76%	0.948%
20	15.476	4399	4412	4429	rBV	46113	89498	3.88%	1.333%
21	15.711	4474	4485	4496	rVB4	36774	57813	2.51%	0.861%
22	16.225	4629	4645	4681	rBV	1359536	2304295	100.00%	34.331%
23	16.482	4715	4725	4752	rVB2	189780	330890	14.36%	4.930%

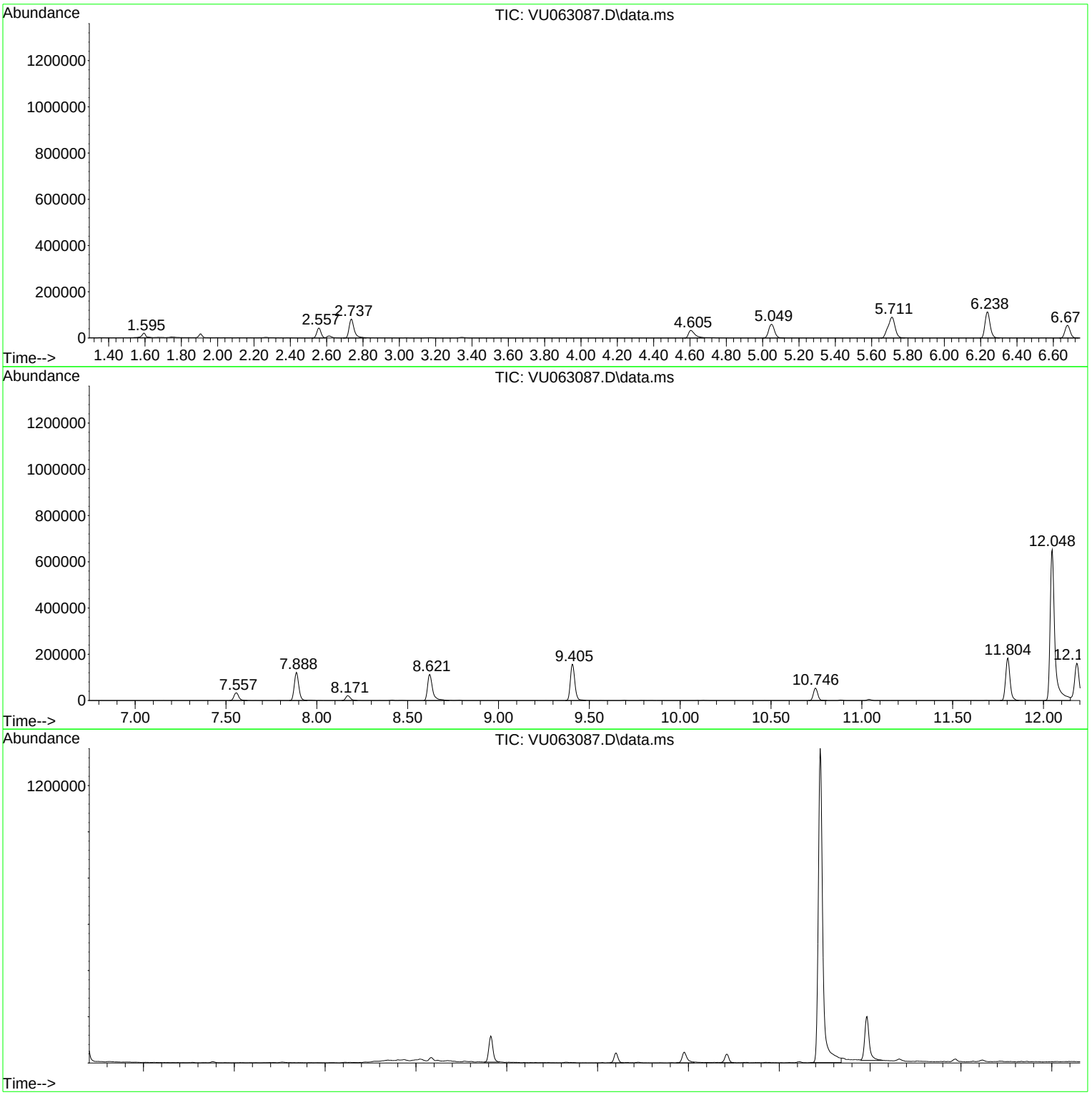
Sum of corrected areas: 6711909

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012925\
Data File : VU063087.D
Acq On : 29 Jan 2025 12:24
Operator : MD/SY
Sample : Q1191-06
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A44W6

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012925\
Data File : VU063087.D
Acq On : 29 Jan 2025 12:24
Operator : MD/SY
Sample : Q1191-06
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A44W6

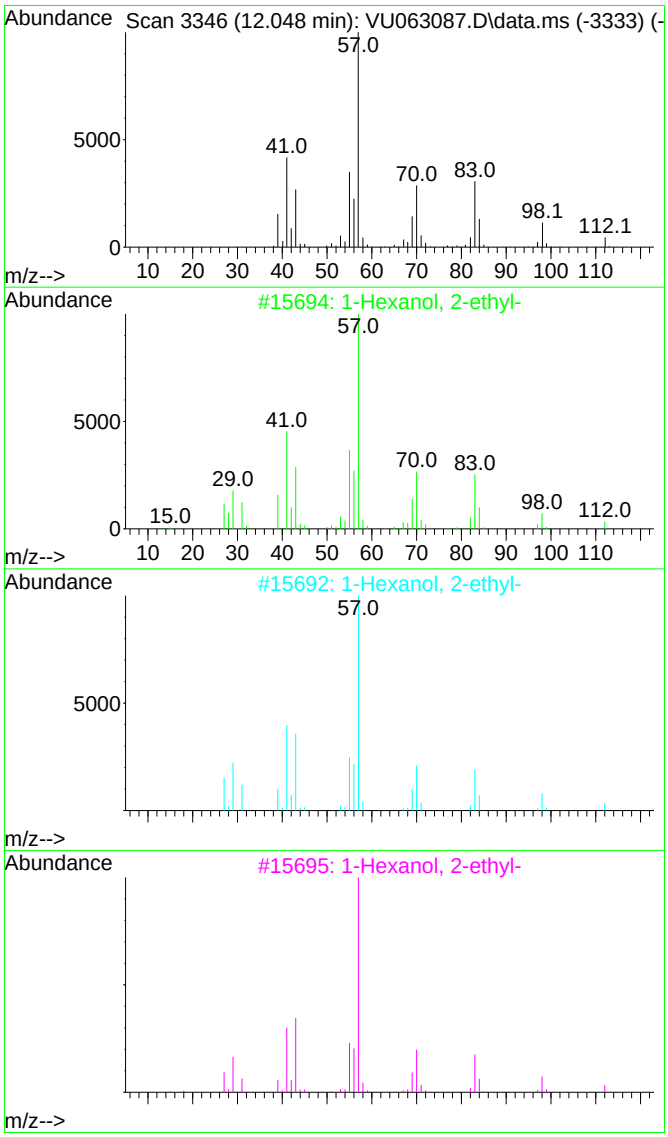
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012725WMA.M
Quant Title : TRACE VOA SFAM1.0

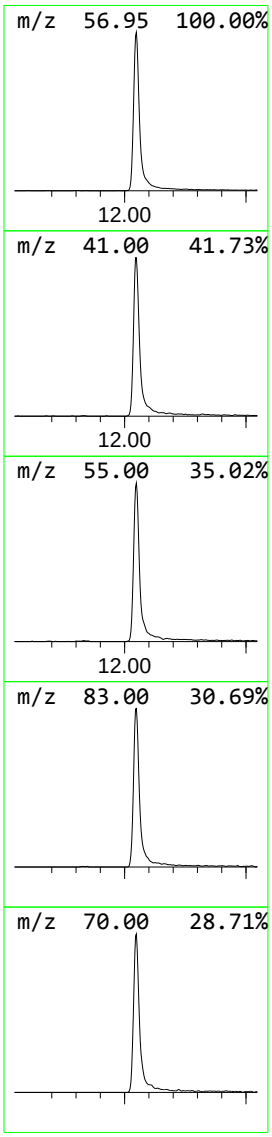
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.048	19.09 ug/L	1171540	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	83
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
4	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
5	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012925\
Data File : VU063087.D
Acq On : 29 Jan 2025 12:24
Operator : MD/SY
Sample : Q1191-06
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A44W6

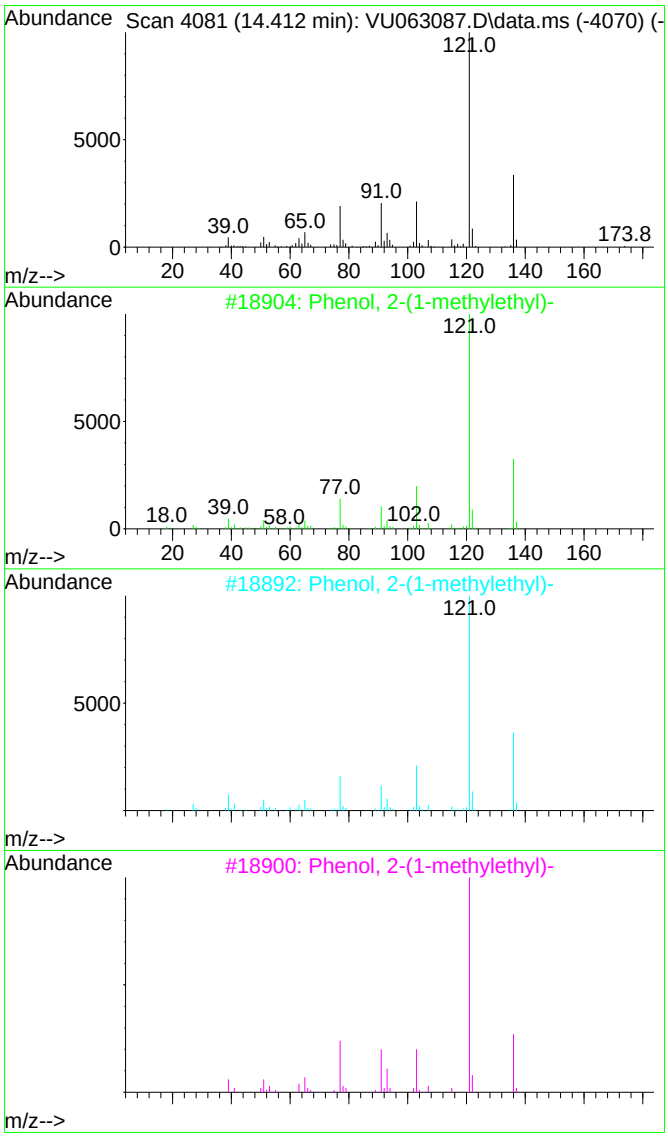
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012725WMA.M
Quant Title : TRACE VOA SFAM1.0

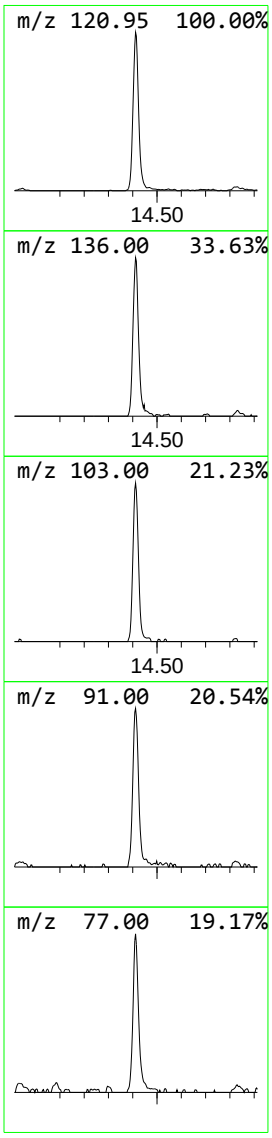
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Phenol, 2-(1-methylethyl)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.412	2.90 ug/L	178167	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	90
3	Phenol, 2-(1-methylethyl)-	136	C9H12O	000088-69-7	90
4	Phenol, 3-(1-methylethyl)-	136	C9H12O	000618-45-1	87
5	p-Cumenol	136	C9H12O	000099-89-8	87





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012925\
Data File : VU063087.D
Acq On : 29 Jan 2025 12:24
Operator : MD/SY
Sample : Q1191-06
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A44W6

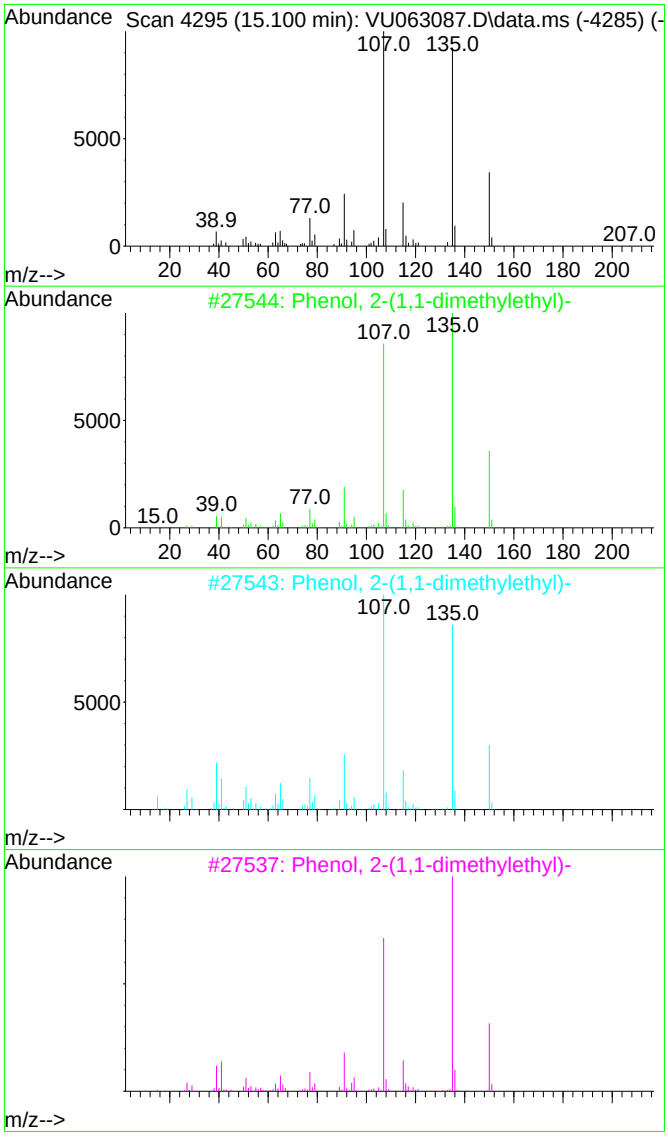
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012725WMA.M
Quant Title : TRACE VOA SFAM1.0

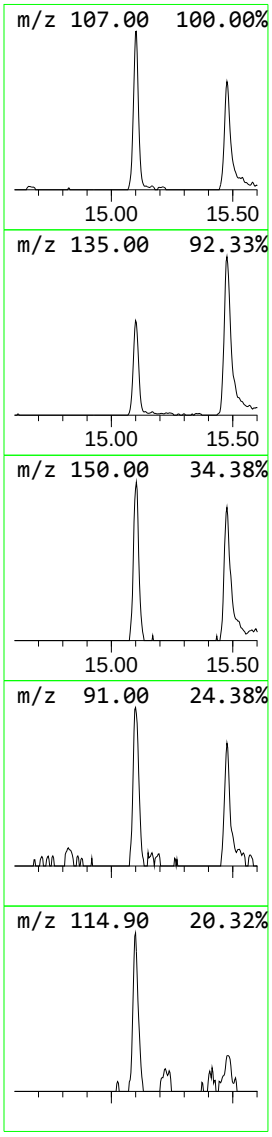
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Phenol, 2-(1,1-dimethylethyl)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.100	1.04 ug/L	63661	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	95
2	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	90
3	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	76
4	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	58
5	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	52





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012925\
Data File : VU063087.D
Acq On : 29 Jan 2025 12:24
Operator : MD/SY
Sample : Q1191-06
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A44W6

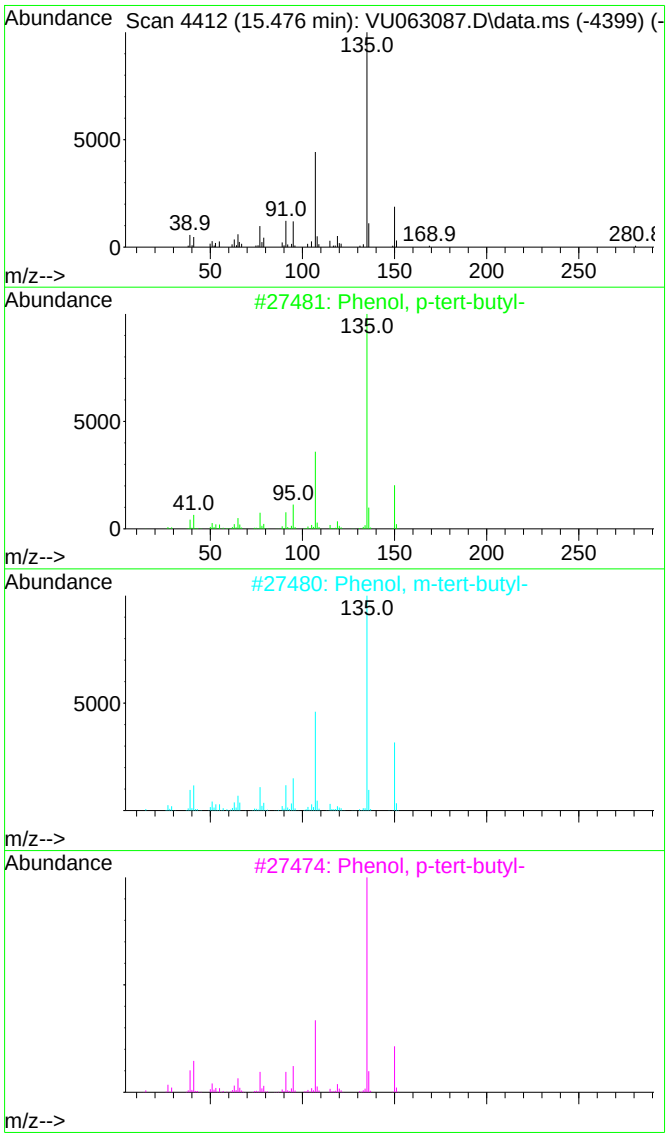
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012725WMA.M
Quant Title : TRACE VOA SFAM1.0

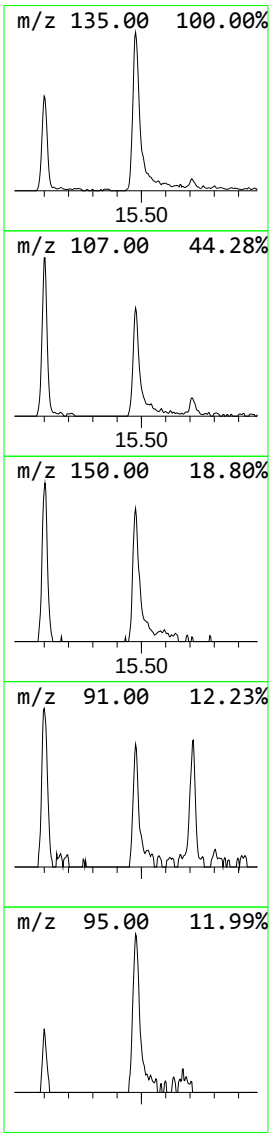
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Phenol, p-tert-butyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.476	1.46 ug/L	89498	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	97
2	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	91
3	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	87
4	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	87
5	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	87





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012925\
Data File : VU063087.D
Acq On : 29 Jan 2025 12:24
Operator : MD/SY
Sample : Q1191-06
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A44W6

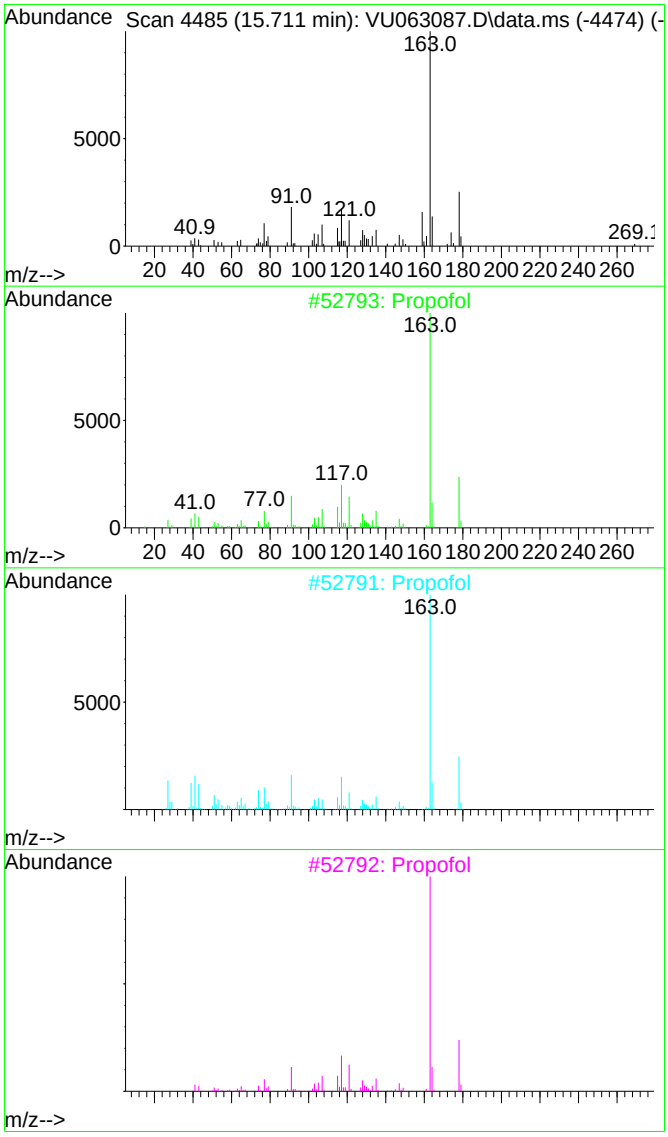
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012725WMA.M
Quant Title : TRACE VOA SFAM1.0

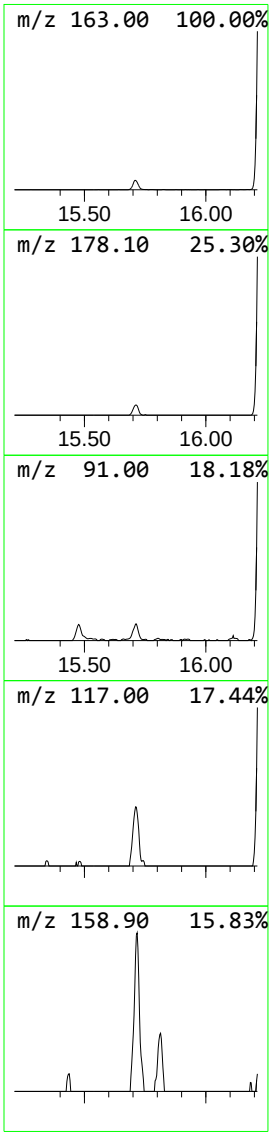
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Propofol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.711	0.94 ug/L	57813	1,4-Dichlorobenzene-d4	11.804

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	87
5	Propofol	178	C12H18O	002078-54-8	87





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012925\
Data File : VU063087.D
Acq On : 29 Jan 2025 12:24
Operator : MD/SY
Sample : Q1191-06
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A44W6

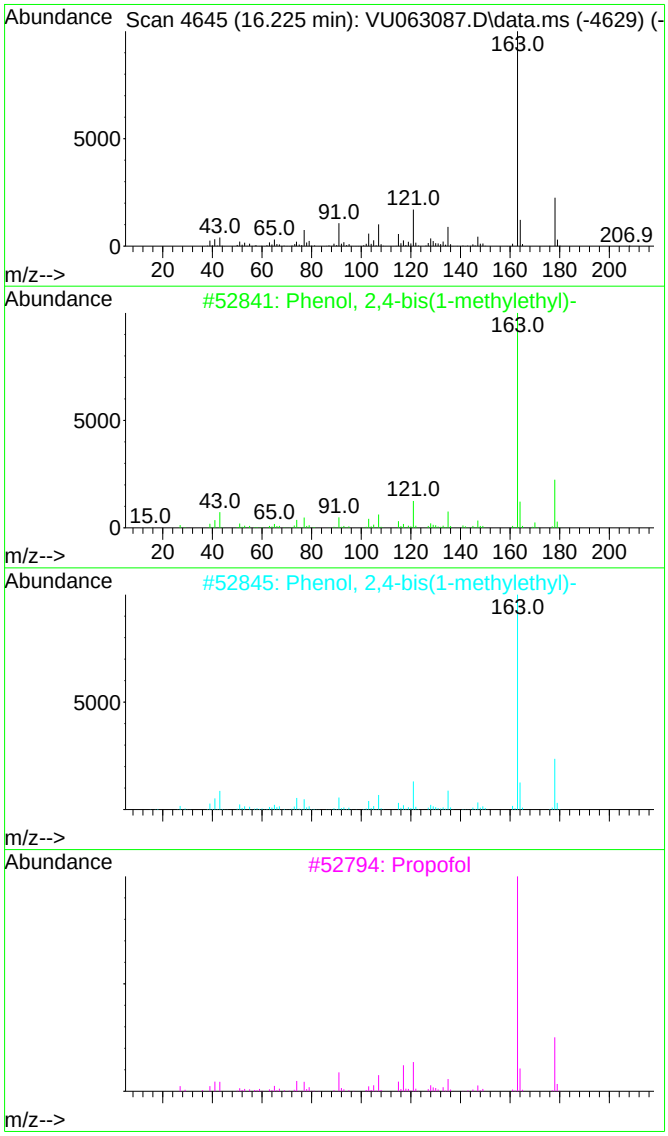
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012725WMA.M
Quant Title : TRACE VOA SFAM1.0

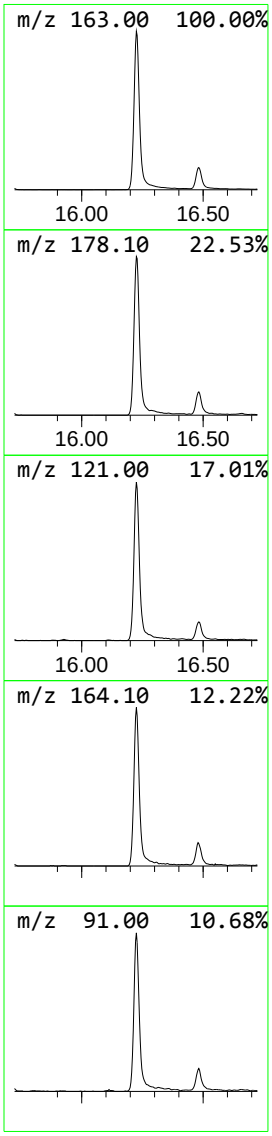
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.225	37.54 ug/L	2304300	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	93
3	Propofol	178	C12H18O	002078-54-8	93
4	Propofol	178	C12H18O	002078-54-8	90
5	Benzenemethanol, 4-(1,1-dimethyl...	178	C12H18O	034386-42-0	80





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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A44W6

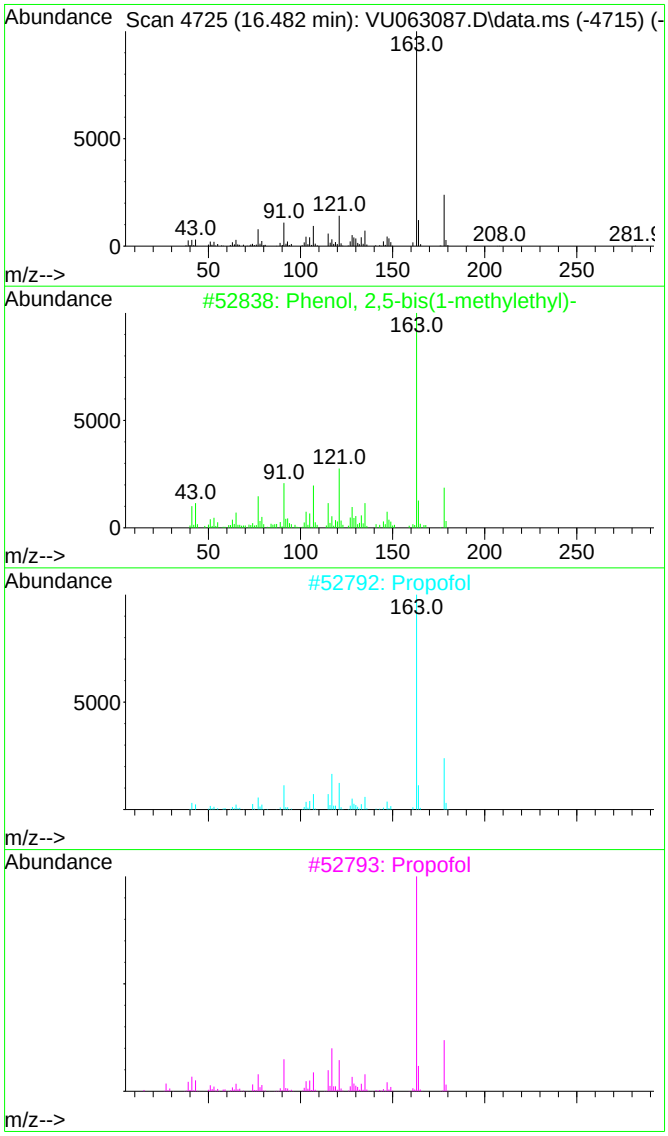
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012725WMA.M
Quant Title : TRACE VOA SFAM1.0

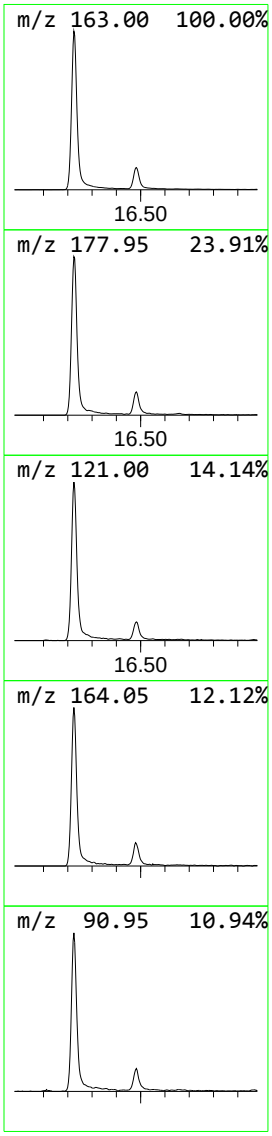
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Phenol, 2,5-bis(1-methyleth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.482	5.39 ug/L	330890	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	Phenol, 2,4-bis(1-methylethyl)-	178	C12H18O	002934-05-6	93
5	Propofol	178	C12H18O	002078-54-8	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012925\
Data File : VU063087.D
Acq On : 29 Jan 2025 12:24
Operator : MD/SY
Sample : Q1191-06
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A44W6

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
1-Hexanol, 2-et...	12.048	19.1	ug/L	1171540	3	11.804	306910	5.0
Phenol, 2-(1-me...	14.412	2.9	ug/L	178167	3	11.804	306910	5.0
Phenol, 2-(1,1-...	15.100	1.0	ug/L	63661	3	11.804	306910	5.0
Phenol, p-tert-...	15.476	1.5	ug/L	89498	3	11.804	306910	5.0
Propofol	15.711	0.9	ug/L	57813	3	11.804	306910	5.0
Phenol, 2,4-bis...	16.225	37.5	ug/L	2304300	3	11.804	306910	5.0
Phenol, 2,5-bis...	16.482	5.4	ug/L	330890	3	11.804	306910	5.0