LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012725\
Data File : VU063052.D
Acq On : 28 Jan 2025 06:56
Operator : MD/SY
Sample : Q1195-17
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2968

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: VU063052.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.354	14	20	37	rVB3	29900	48194	1.86%	0.538%
2	1.531	64	75	79	rBV3	13114	29709	1.15%	0.332%
3	1.586	83	92	102	rVB2	99462	164367	6.35%	1.834%
4	1.901	183	190	199	rVB	37153	43855	1.69%	0.489%
5	2.557	382	394	410	rBV	139674	223402	8.63%	2.493%
6	3.570	696	709	728	rBV3	9850	26425	1.02%	0.295%
7	4.631	1023	1039	1076	rBV2	42880	161251	6.23%	1.799%
8	5.039	1152	1166	1192	rVB	116798	227787	8.80%	2.542%
9	5.711	1353	1375	1397	rBV3	145462	387194	14.95%	4.320%
10	6.235	1525	1538	1565	rVB	148126	286278	11.06%	3.194%
11	6.679	1660	1676	1691	rBV	150601	287812	11.12%	3.212%
12	7.557	1933	1949	1971	rBV	96944	178614	6.90%	1.993%
13	7.888	2037	2052	2070	rBV	358107	629303	24.30%	7.022%
14	8.171	2123	2140	2156	rBV	62625	115075	4.44%	1.284%
15	8.624	2269	2281	2315	rBV	413259	807441	31.18%	9.010%
16	9.405	2512	2524	2547	rBV	463098	783781	30.27%	8.746%
17	10.743	2930	2940	2955	rBB2	53128	84878	3.28%	0.947%
18	11.801	3257	3269	3290	rBV	197177	331031	12.78%	3.694%
19	12.048	3330	3346	3377	rBV	233933	490212	18.93%	5.470%
20	12.183	3377	3388	3405	rVB	165137	280411	10.83%	3.129%
21	14.019	3954	3959	3970	rVB3	21925	35990	1.39%	0.402%
22	14.119	3985	3990	3999	rVB	21146	28551	1.10%	0.319%
23	14.412	4072	4081	4106	rVB	84740	140773	5.44%	1.571%
24	15.100	4278	4295	4307	rVB2	36509	62482	2.41%	0.697%
25	15.476	4401	4412	4427	rBV2	56632	108441	4.19%	1.210%
26	15.711	4477	4485	4497	rVB4	34034	52569	2.03%	0.587%
27	16.225	4632	4645	4693	rBV	1416961	2589339	100.00%	28.893%
28	16.479	4715	4724	4754	rVB	185486	356625	13.77%	3.979%

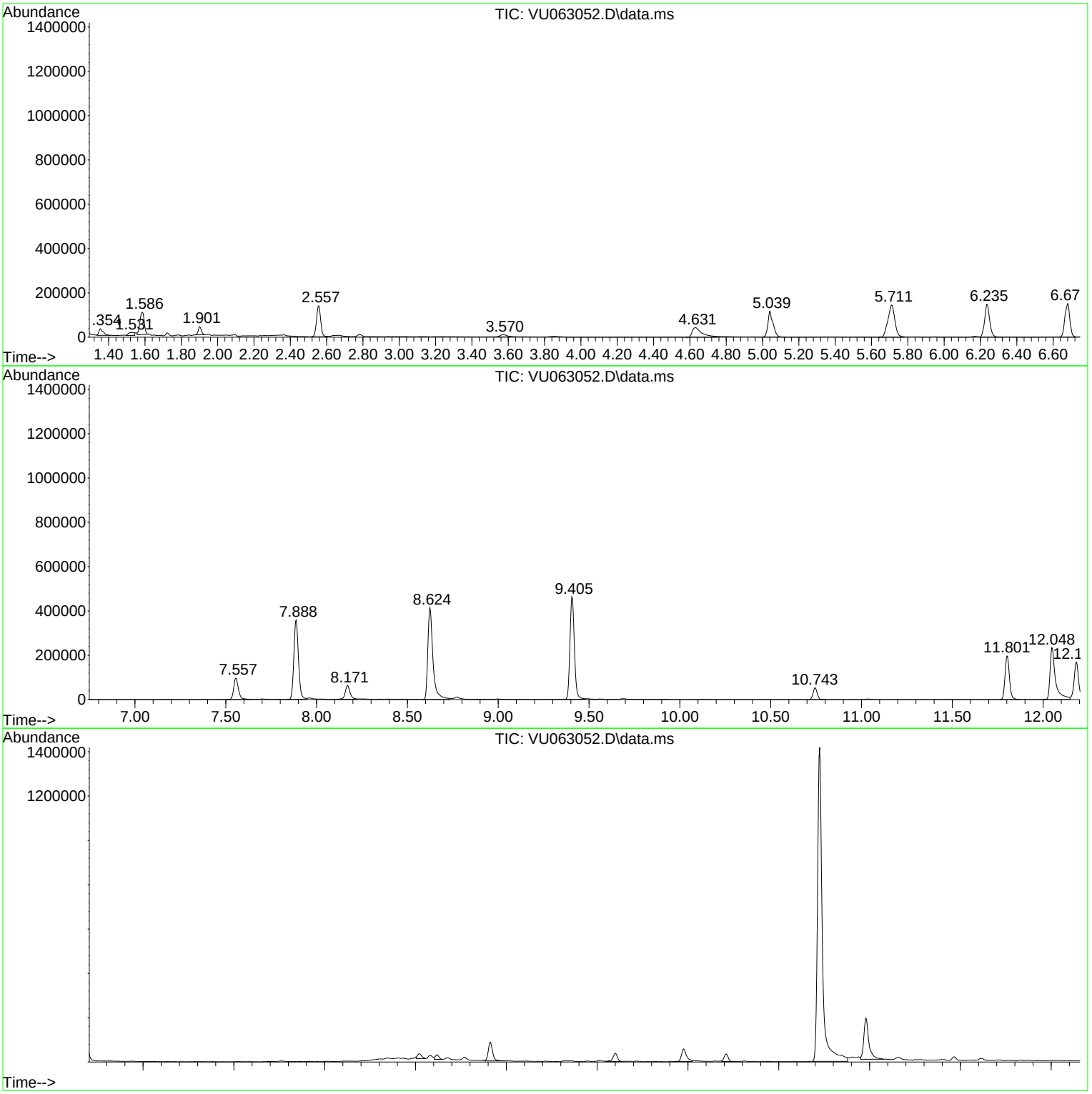
Sum of corrected areas: 8961790

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012725\
Data File : VU063052.D
Acq On : 28 Jan 2025 06:56
Operator : MD/SY
Sample : Q1195-17
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2968

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\VU012725\
Data File : VU063052.D
Acq On : 28 Jan 2025 06:56
Operator : MD/SY
Sample : Q1195-17
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2968

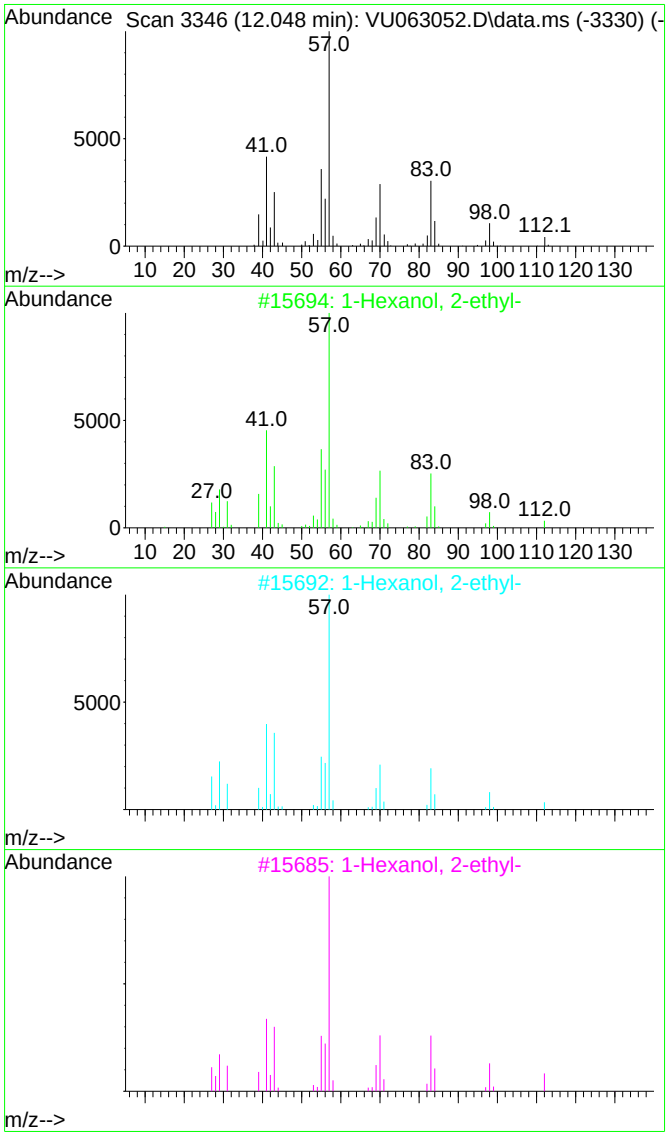
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012725WMA.M
Quant Title : TRACE VOA SFAM1.0

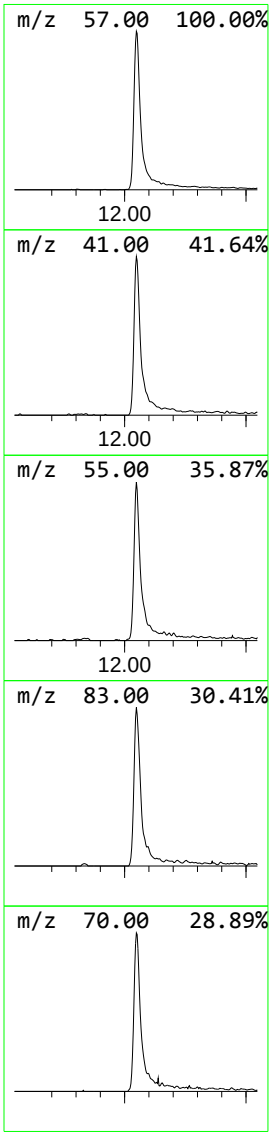
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.048	7.40 ug/L	490212	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	83
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\VU012725\
Data File : VU063052.D
Acq On : 28 Jan 2025 06:56
Operator : MD/SY
Sample : Q1195-17
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2968

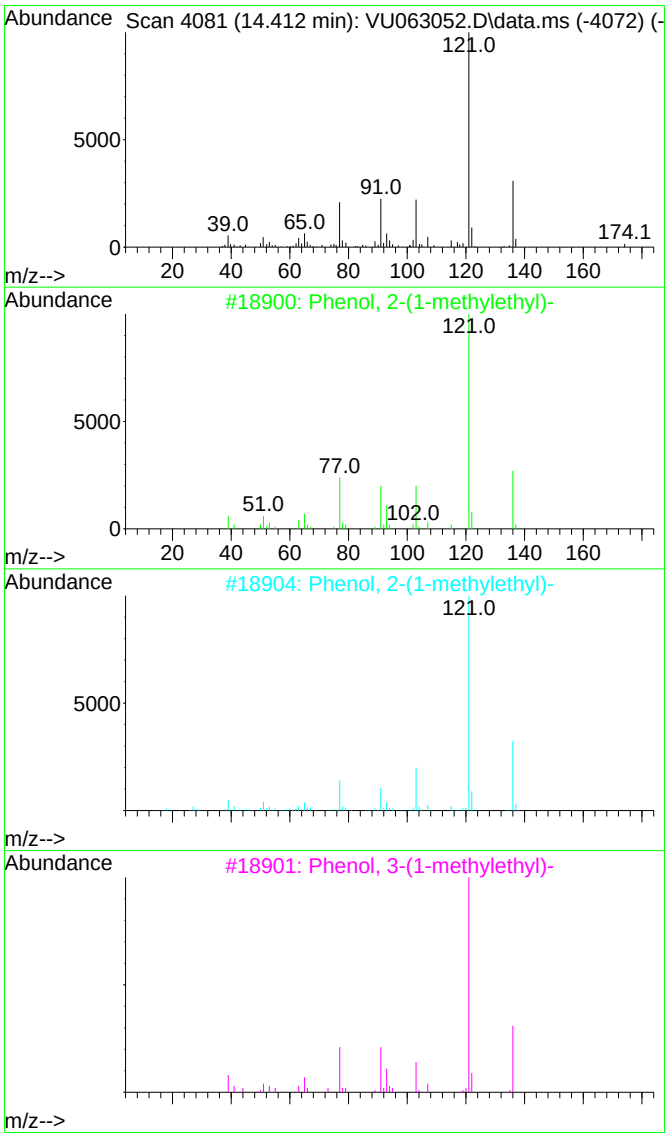
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012725WMA.M
Quant Title : TRACE VOA SFAM1.0

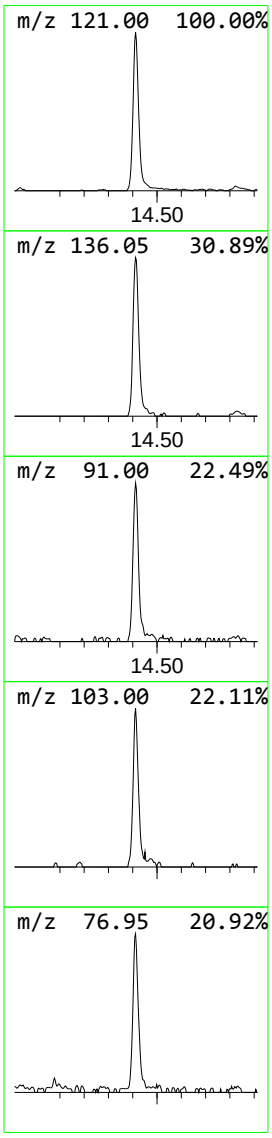
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Phenol, 2-(1-methylethyl)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.412	2.13 ug/L	140773	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	94
2	Phenol, 2-(1-methylethyl)-	136	C9H12O	000088-69-7	91
3	Phenol, 3-(1-methylethyl)-	136	C9H12O	000618-45-1	87
4	Phenol, 3-(1-methylethyl)-	136	C9H12O	000618-45-1	86
5	Phenol, 3-(1-methylethyl)-	136	C9H12O	000618-45-1	86





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012725\
Data File : VU063052.D
Acq On : 28 Jan 2025 06:56
Operator : MD/SY
Sample : Q1195-17
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2968

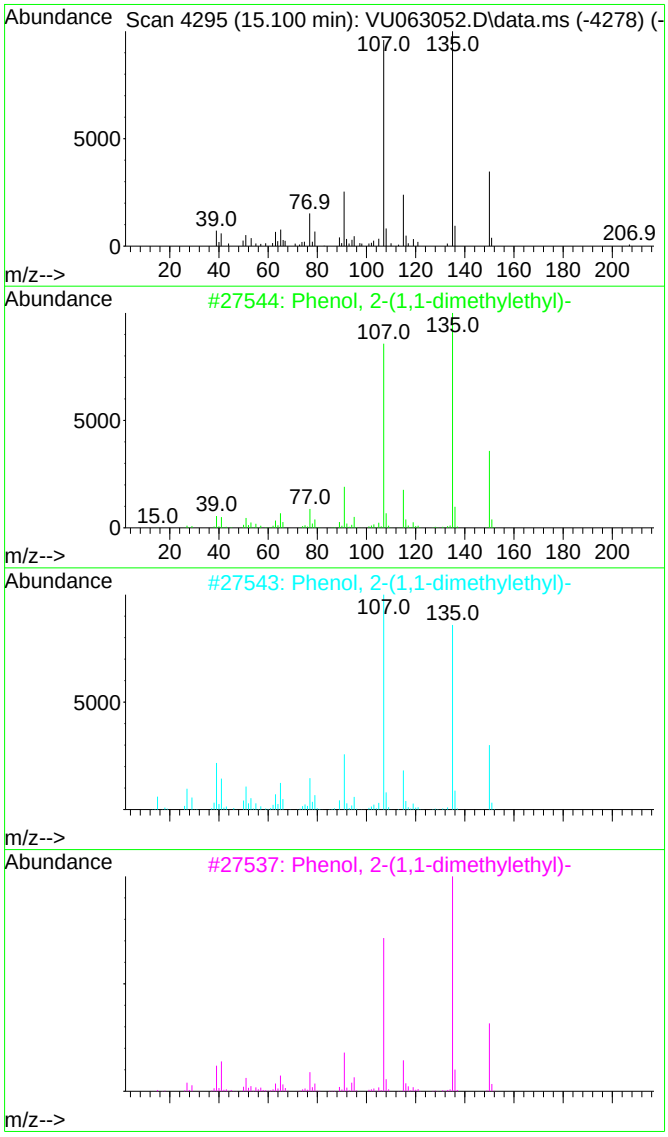
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012725WMA.M
Quant Title : TRACE VOA SFAM1.0

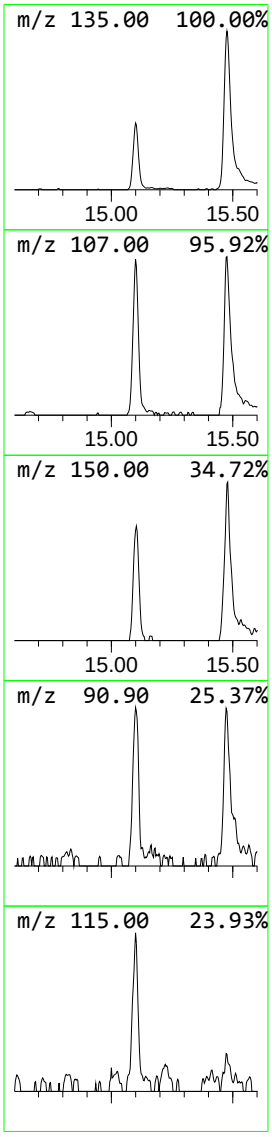
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Phenol, 2-(1,1-dimethylethyl)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.100	0.94 ug/L	62482	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	94
2	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	90
3	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	90
4	Ethanone, 2-ethoxy-1,2-diphenyl-	240	C16H16O2	000574-09-4	59
5	Benzaldehyde diethylacetal	180	C11H16O2	000774-48-1	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012725\
Data File : VU063052.D
Acq On : 28 Jan 2025 06:56
Operator : MD/SY
Sample : Q1195-17
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2968

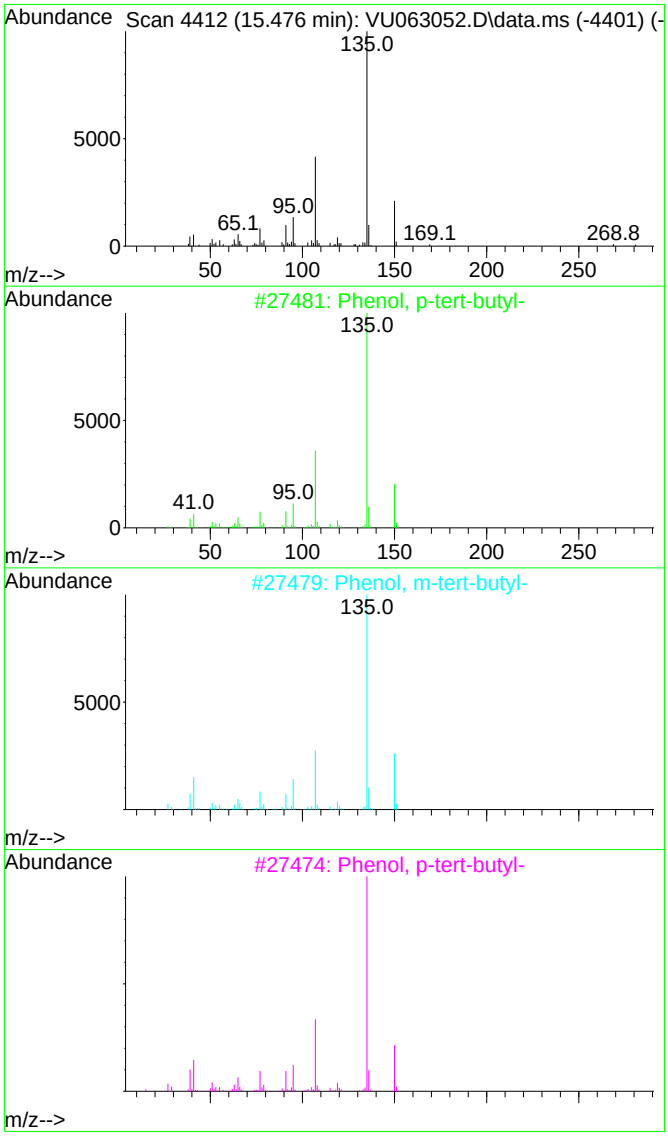
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012725WMA.M
Quant Title : TRACE VOA SFAM1.0

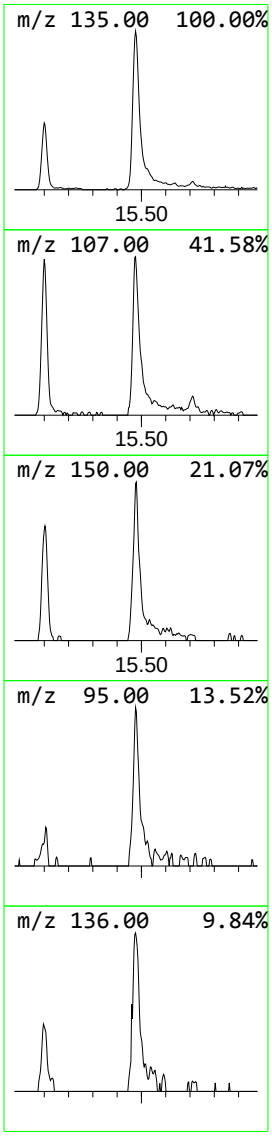
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Phenol, p-tert-butyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.476	1.64 ug/L	108441	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	96
2	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	94
3	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	94
4	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	94
5	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012725\
Data File : VU063052.D
Acq On : 28 Jan 2025 06:56
Operator : MD/SY
Sample : Q1195-17
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2968

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

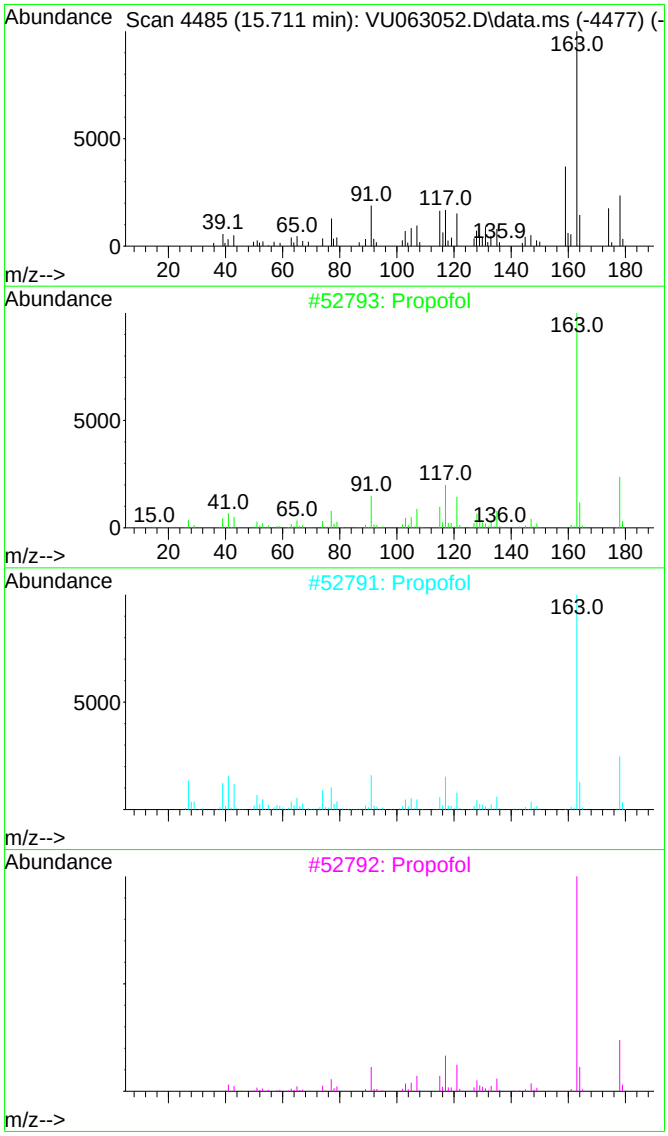
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

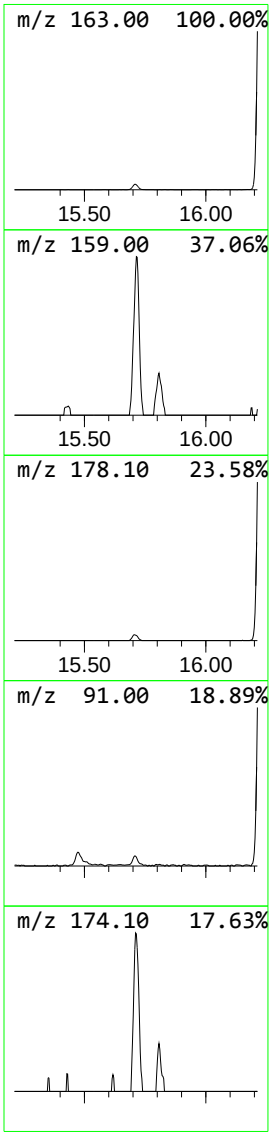
****

Peak Number 9 Propofol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.711	0.79 ug/L	52569	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	96
3	Propofol	178	C12H18O	002078-54-8	95
4	Propofol	178	C12H18O	002078-54-8	76
5	Phenol, 2-(1,1-dimethylethyl)-4-...	178	C12H18O	000096-70-8	70





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012725\
Data File : VU063052.D
Acq On : 28 Jan 2025 06:56
Operator : MD/SY
Sample : Q1195-17
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2968

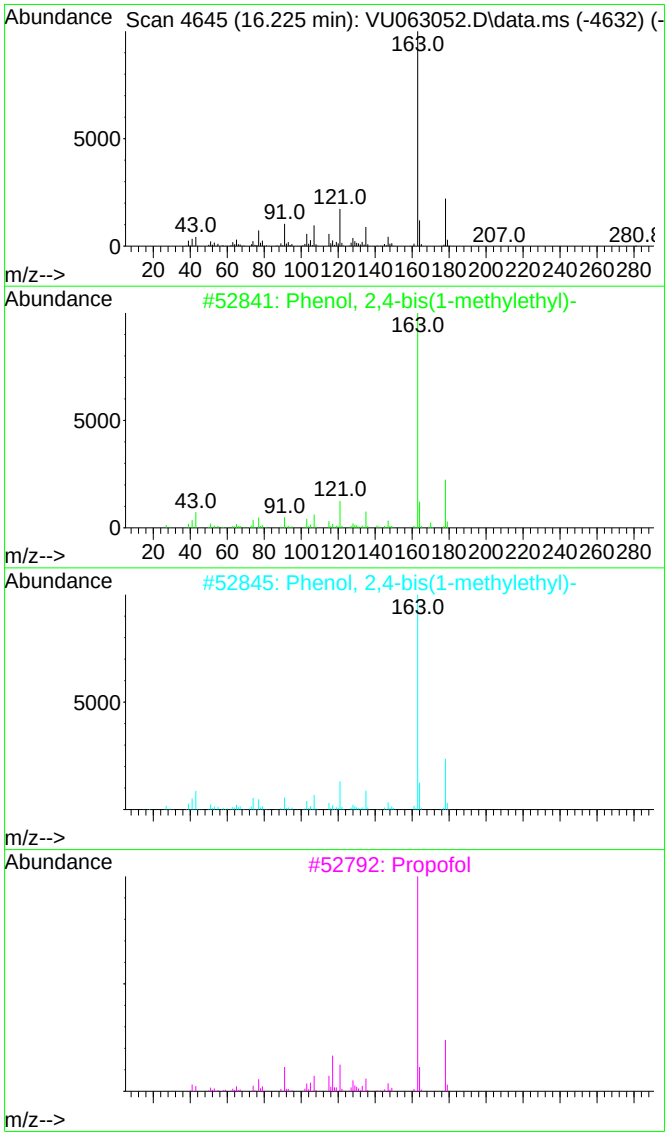
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012725WMA.M
Quant Title : TRACE VOA SFAM1.0

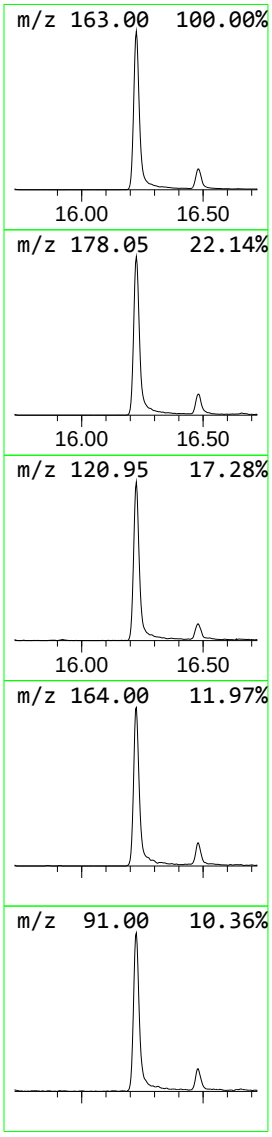
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Phenol, 2,4-bis(1-methyleth... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.225	39.11 ug/L	2589340	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	97
2	Phenol, 2,4-bis(1-methylethyl)-	178	C12H18O	002934-05-6	95
3	Propofol	178	C12H18O	002078-54-8	94
4	Propofol	178	C12H18O	002078-54-8	93
5	Propofol	178	C12H18O	002078-54-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012725\
Data File : VU063052.D
Acq On : 28 Jan 2025 06:56
Operator : MD/SY
Sample : Q1195-17
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2968

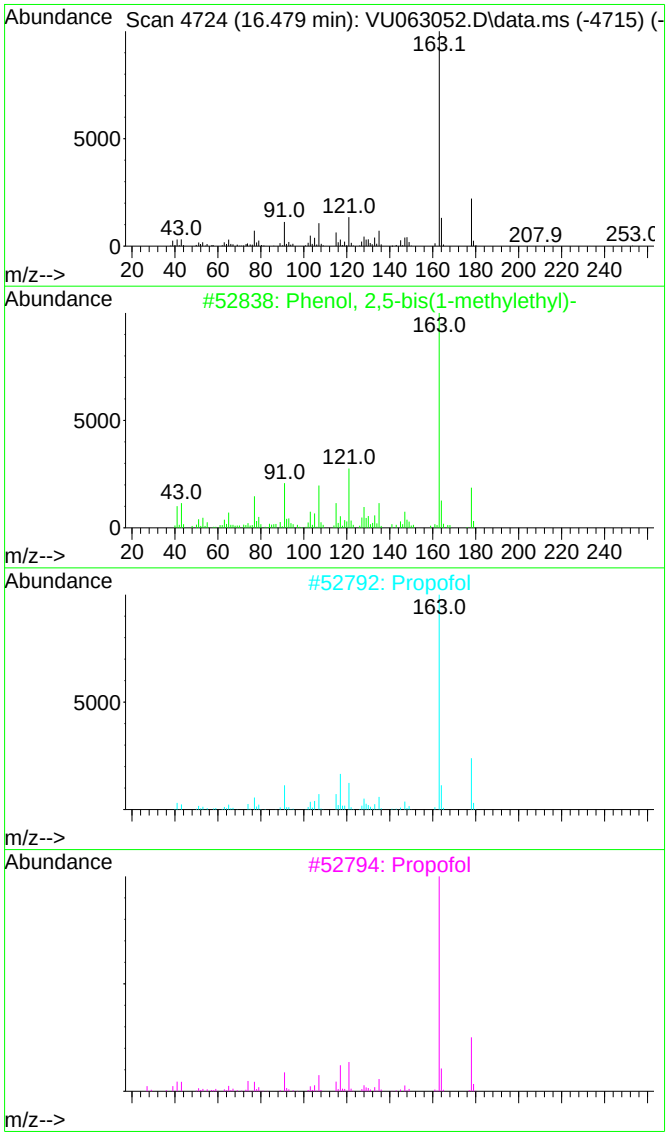
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012725WMA.M
Quant Title : TRACE VOA SFAM1.0

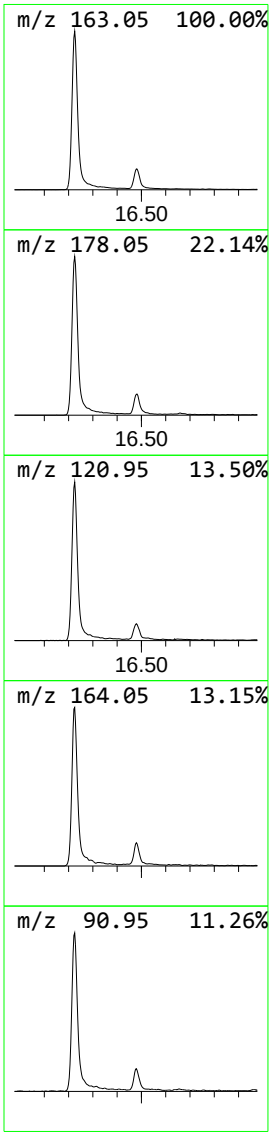
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Phenol, 2,5-bis(1-methyleth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.479	5.39 ug/L	356625	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	91
4	Phenol, 2,4-bis(1-methylethyl)-	178	C12H18O	002934-05-6	90
5	Phenol, 2,4-bis(1-methylethyl)-	178	C12H18O	002934-05-6	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012725\
Data File : VU063052.D
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Misc : 25mL/MSVOA_U/WATER
ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2968

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	7.4	ug/L	490212	3	11.804	331031	5.0
Phenol, 2-(1-me...	14.412	2.1	ug/L	140773	3	11.804	331031	5.0
Phenol, 2-(1,1-...	15.100	0.9	ug/L	62482	3	11.804	331031	5.0
Phenol, p-tert-...	15.476	1.6	ug/L	108441	3	11.804	331031	5.0
Propofol	15.711	0.8	ug/L	52569	3	11.804	331031	5.0
Phenol, 2,4-bis...	16.225	39.1	ug/L	2589340	3	11.804	331031	5.0
Phenol, 2,5-bis...	16.479	5.4	ug/L	356625	3	11.804	331031	5.0