LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012425\
Data File : VU062998.D
Acq On : 24 Jan 2025 17:17
Operator : MD/SY
Sample : Q1174-10
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2940

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\SFAMUTR010225WMA.M
Title : TRACE VOA SFAM1.0

Signal : TIC: VU062998.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.319	3	9	29	rVB	378443	620444	11.24%	4.499%
2	1.431	31	44	61	rBV	180580	228504	4.14%	1.657%
3	1.567	68	86	94	rBV2	70469	95366	1.73%	0.692%
4	1.663	108	116	118	rBV	117834	130597	2.37%	0.947%
5	2.650	413	423	438	rVB	53187	86973	1.58%	0.631%
6	2.775	448	462	473	rBV2	35563	75672	1.37%	0.549%
7	3.139	563	575	593	rVB	101780	199144	3.61%	1.444%
8	3.962	814	831	849	rBV	82248	195015	3.53%	1.414%
9	5.113	1178	1189	1208	rVB	46617	105587	1.91%	0.766%
10	5.804	1385	1404	1414	rBV2	111040	281535	5.10%	2.042%
11	5.859	1415	1421	1440	rVB	69365	144359	2.62%	1.047%
12	6.335	1557	1569	1586	rBV	128347	234092	4.24%	1.698%
13	6.762	1689	1702	1716	rBV2	65740	127754	2.31%	0.926%
14	7.608	1953	1965	1979	rBV2	35721	63724	1.15%	0.462%
15	7.840	2023	2037	2055	rBV2	40970	97169	1.76%	0.705%
16	7.933	2055	2066	2077	rVV	137216	234609	4.25%	1.701%
17	8.004	2077	2088	2105	rVB	282583	472929	8.57%	3.430%
18	8.663	2279	2293	2329	rBV2	101547	237064	4.30%	1.719%
19	9.428	2520	2531	2549	rBV	167921	294771	5.34%	2.138%
20	9.579	2568	2578	2602	rVB	118611	205137	3.72%	1.488%
21	9.701	2603	2616	2632	rVB	181653	312630	5.67%	2.267%
22	10.113	2731	2744	2765	rVB5	174570	383565	6.95%	2.782%
23	10.753	2932	2943	2955	rBV	56498	92644	1.68%	0.672%
24	11.463	3149	3164	3185	rBV	44792	76479	1.39%	0.555%
25	11.807	3257	3271	3286	rVB	180705	298882	5.42%	2.167%
26	12.055	3338	3348	3378	rBV2	72714	222864	4.04%	1.616%
27	12.187	3378	3389	3407	rVB	147954	251298	4.55%	1.822%
28	12.698	3536	3548	3554	rBV7	29948	59236	1.07%	0.430%
29	12.746	3556	3563	3575	rVB6	33142	81013	1.47%	0.588%
30	13.929	3923	3931	3952	rVB4	25105	59099	1.07%	0.429%
31	14.408	4063	4080	4096	rBV	174950	296617	5.37%	2.151%
32	14.817	4194	4207	4216	rBV	48355	109270	1.98%	0.792%
33	15.473	4399	4411	4432	rBV	98423	201973	3.66%	1.465%
34	15.707	4476	4484	4497	rVB3	51138	79569	1.44%	0.577%
35	16.222	4632	4644	4691	rBV	3344239	5518557	100.00%	40.021%
36	16.479	4714	4724	4755	rVB	803432	1275925	23.12%	9.253%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012425\
Data File : VU062998.D
Acq On : 24 Jan 2025 17:17
Operator : MD/SY
Sample : Q1174-10
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2940

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\SFAMUTR010225WMA.M
Title : TRACE VOA SFAM1.0

37	16.650	4768	4777	4798	rVB	88373	178194	3.23%	1.292%
38	16.756	4803	4810	4836	rVB10	31746	84568	1.53%	0.613%
39	16.965	4867	4875	4884	rVB	50534	76455	1.39%	0.554%

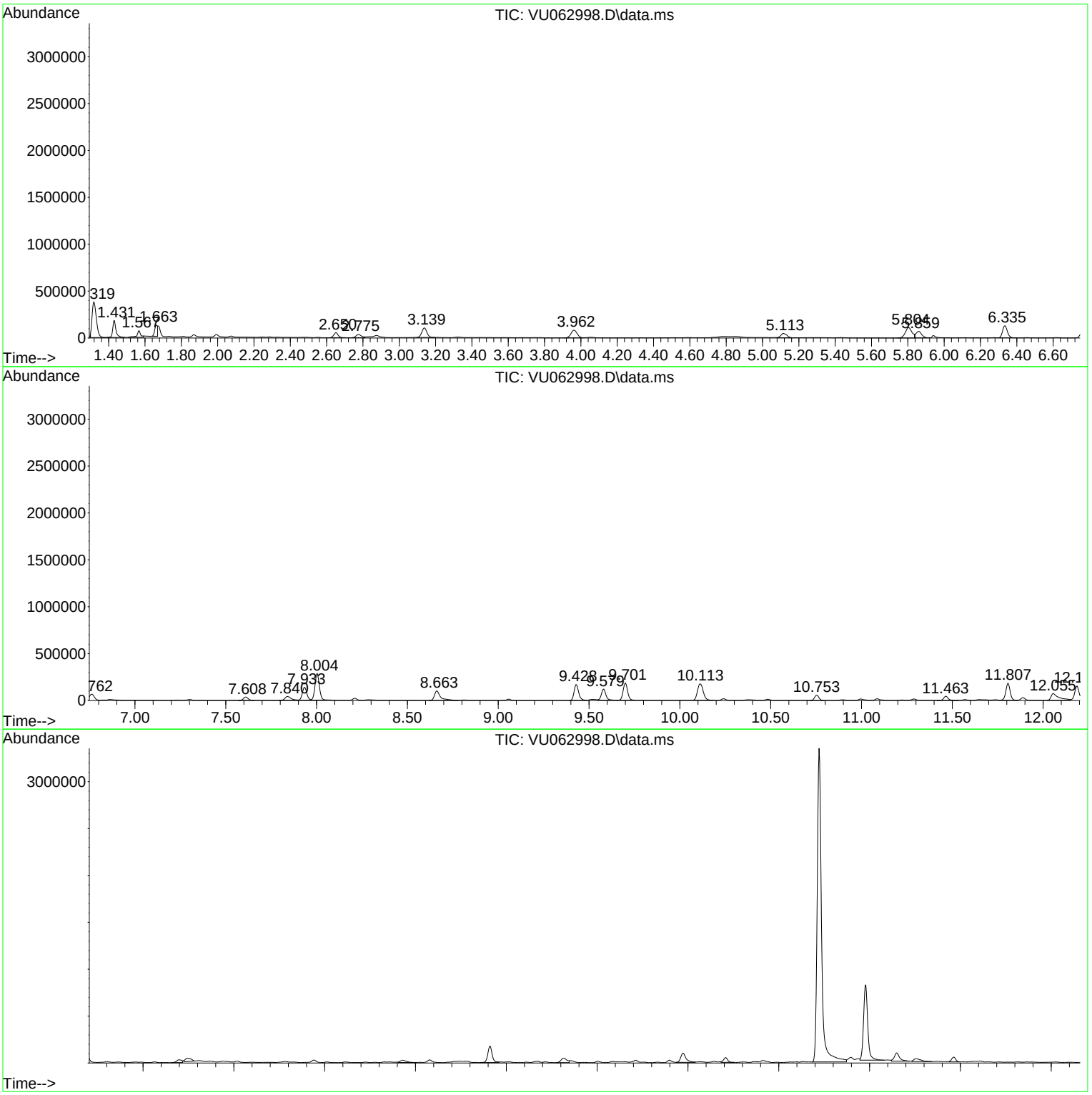
Sum of corrected areas: 13789283

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012425\
Data File : VU062998.D
Acq On : 24 Jan 2025 17:17
Operator : MD/SY
Sample : Q1174-10
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2940

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR010225WMA.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\VU012425\
Data File : VU062998.D
Acq On : 24 Jan 2025 17:17
Operator : MD/SY
Sample : Q1174-10
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2940

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR010225WMA.M
Quant Title : TRACE VOA SFAM1.0

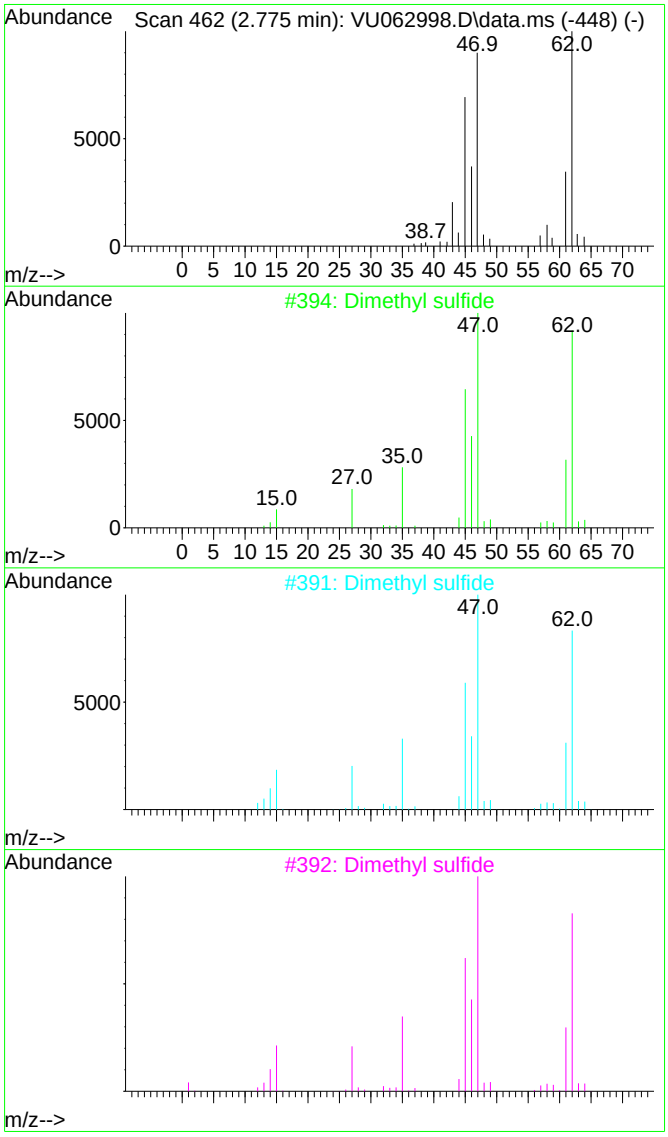
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

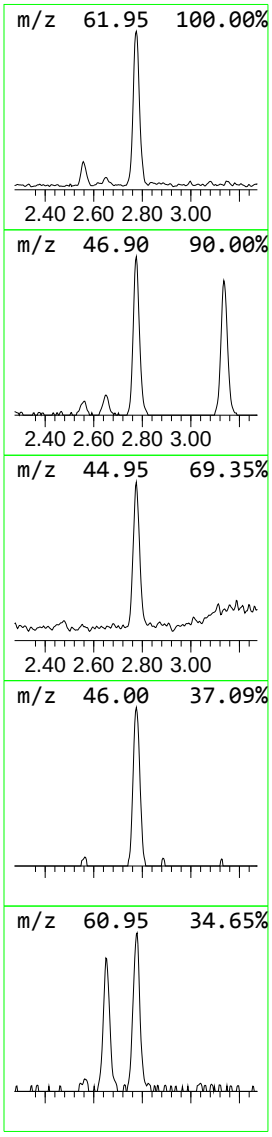
****

Peak Number 4 Dimethyl sulfide Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.775	1.62 ug/L	75672	1,4-Difluorobenzene	6.335

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl sulfide	62	C2H6S	000075-18-3	94
2	Dimethyl sulfide	62	C2H6S	000075-18-3	94
3	Dimethyl sulfide	62	C2H6S	000075-18-3	91
4	Dimethyl sulfide	62	C2H6S	000075-18-3	91
5	Dimethyl sulfide	62	C2H6S	000075-18-3	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012425\
Data File : VU062998.D
Acq On : 24 Jan 2025 17:17
Operator : MD/SY
Sample : Q1174-10
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2940

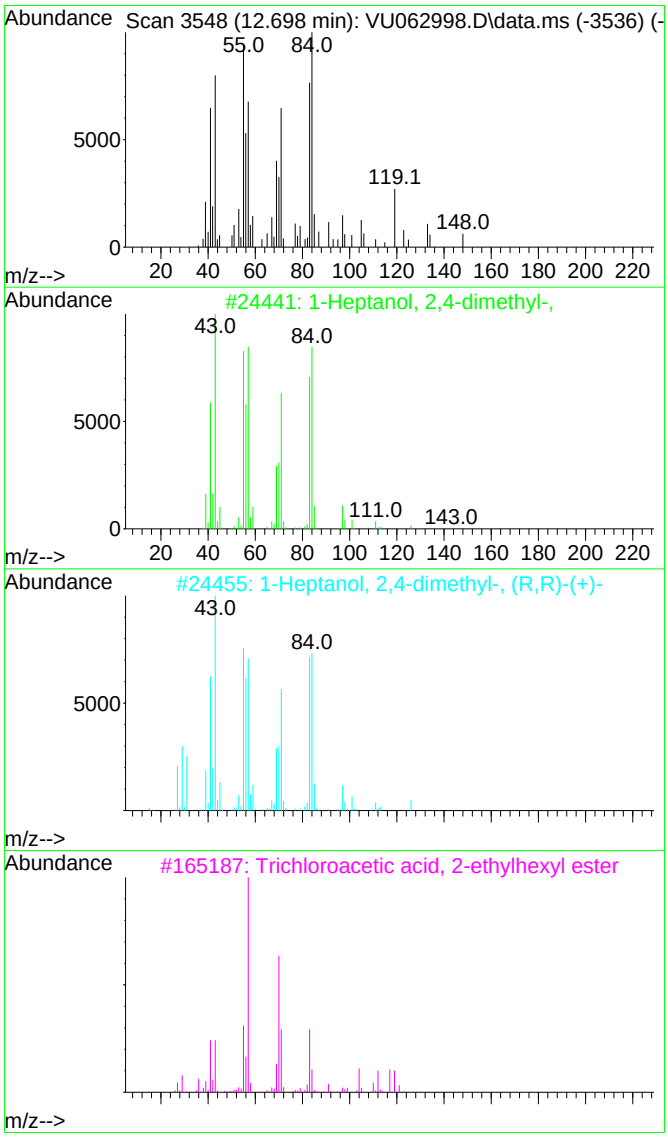
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR010225WMA.M
Quant Title : TRACE VOA SFAM1.0

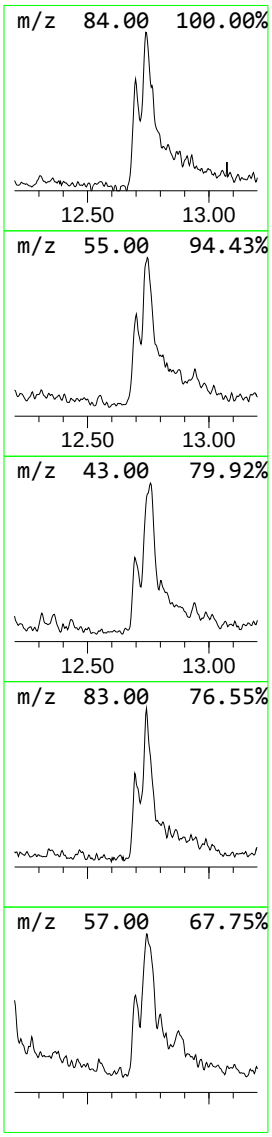
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1-Heptanol, 2,4-dimethyl-, Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.698	0.99 ug/L	59236	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptanol, 2,4-dimethyl-,	144	C9H20O	098982-97-9	90
2	1-Heptanol, 2,4-dimethyl-, (R,R)...	144	C9H20O	018450-73-2	59
3	Trichloroacetic acid, 2-ethylhex...	274	C10H17Cl3O2	016397-79-8	50
4	2-Pentenal, (E)-	84	C5H8O	001576-87-0	46
5	2H-Pyran, 3,4-dihydro-	84	C5H8O	000110-87-2	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012425\
Data File : VU062998.D
Acq On : 24 Jan 2025 17:17
Operator : MD/SY
Sample : Q1174-10
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2940

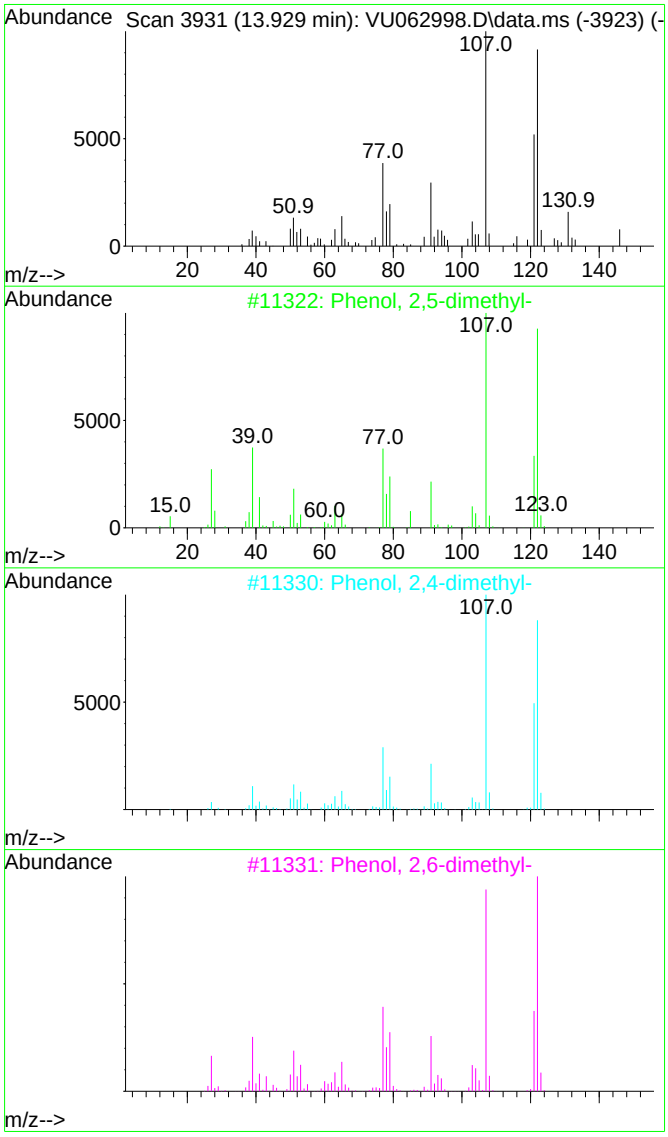
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR010225WMA.M
Quant Title : TRACE VOA SFAM1.0

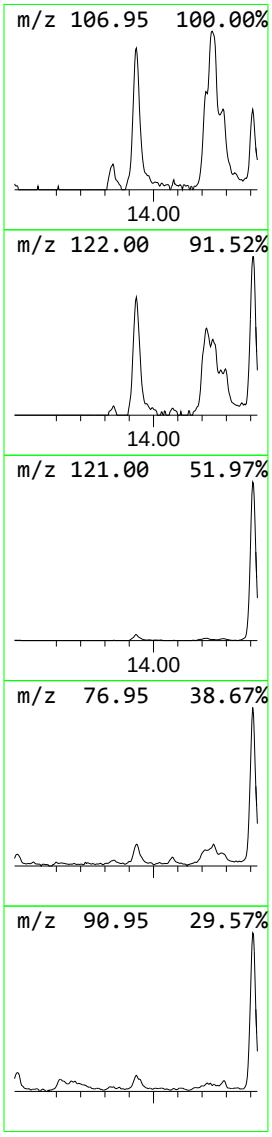
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Phenol, 2,5-dimethyl- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.929	0.99 ug/L	59099	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,5-dimethyl-	122	C8H10O	000095-87-4	93
2	Phenol, 2,4-dimethyl-	122	C8H10O	000105-67-9	93
3	Phenol, 2,6-dimethyl-	122	C8H10O	000576-26-1	91
4	Phenol, 2,6-dimethyl-	122	C8H10O	000576-26-1	91
5	Phenol, 2,3-dimethyl-	122	C8H10O	000526-75-0	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012425\
Data File : VU062998.D
Acq On : 24 Jan 2025 17:17
Operator : MD/SY
Sample : Q1174-10
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2940

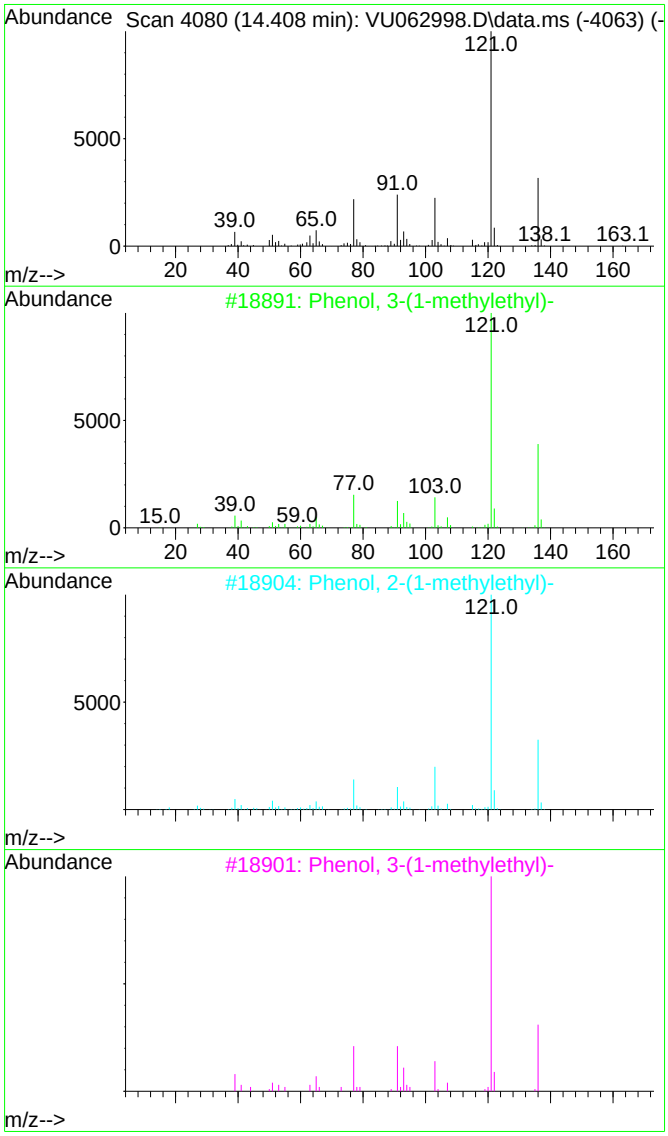
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR010225WMA.M
Quant Title : TRACE VOA SFAM1.0

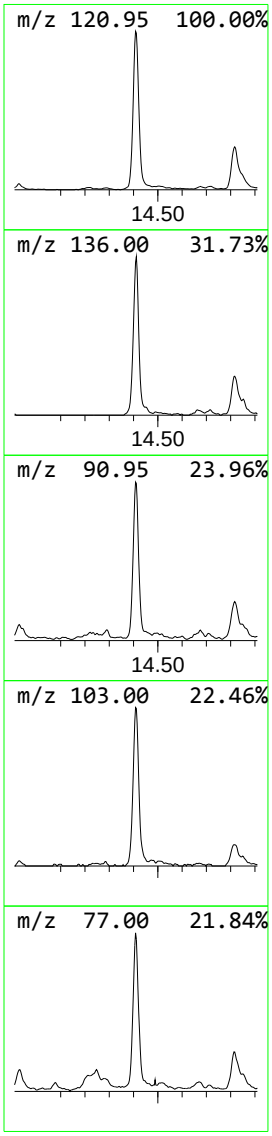
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Phenol, 3-(1-methylethyl)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.409	4.96 ug/L	296617	1,4-Dichlorobenzene-d4	11.807

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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012425\
Data File : VU062998.D
Acq On : 24 Jan 2025 17:17
Operator : MD/SY
Sample : Q1174-10
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2940

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR010225WMA.M
Quant Title : TRACE VOA SFAM1.0

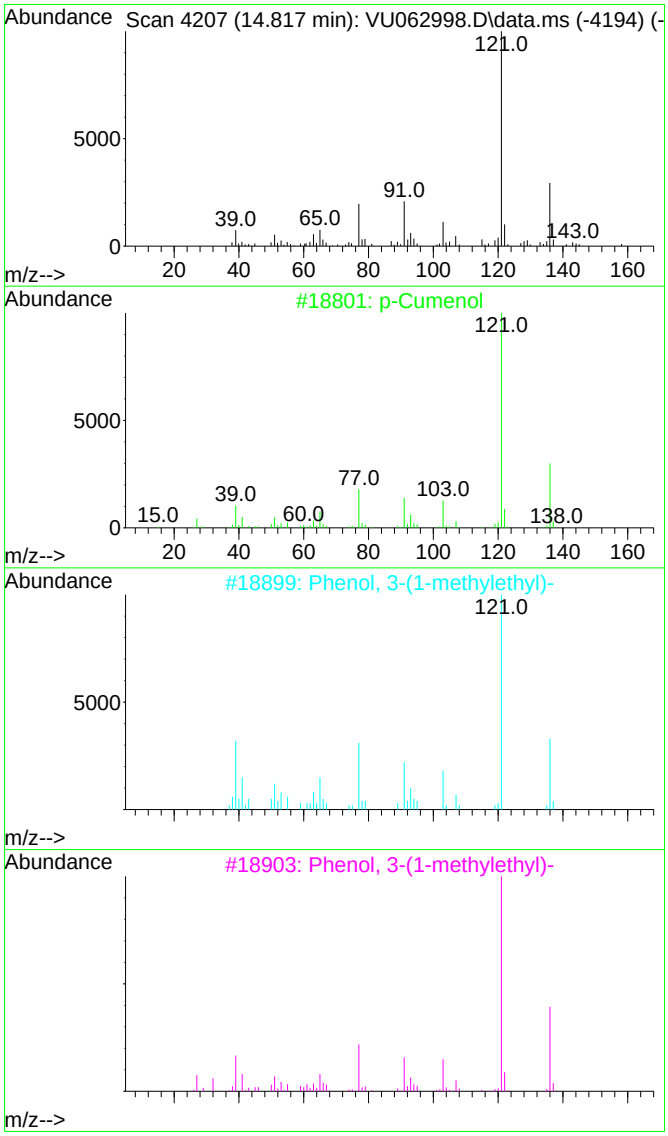
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

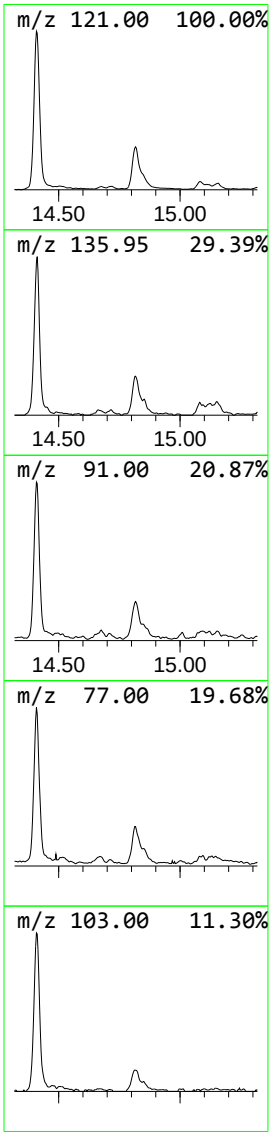
****

Peak Number 11 p-Cumenol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.817	1.83 ug/L	109270	1,4-Dichlorobenzene-d4	11.807

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	91
4	Phenol, 3-(1-methylethyl)-	136	C9H12O	000618-45-1	90
5	Phenol, 4-ethyl-3-methyl-	136	C9H12O	001123-94-0	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012425\
Data File : VU062998.D
Acq On : 24 Jan 2025 17:17
Operator : MD/SY
Sample : Q1174-10
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2940

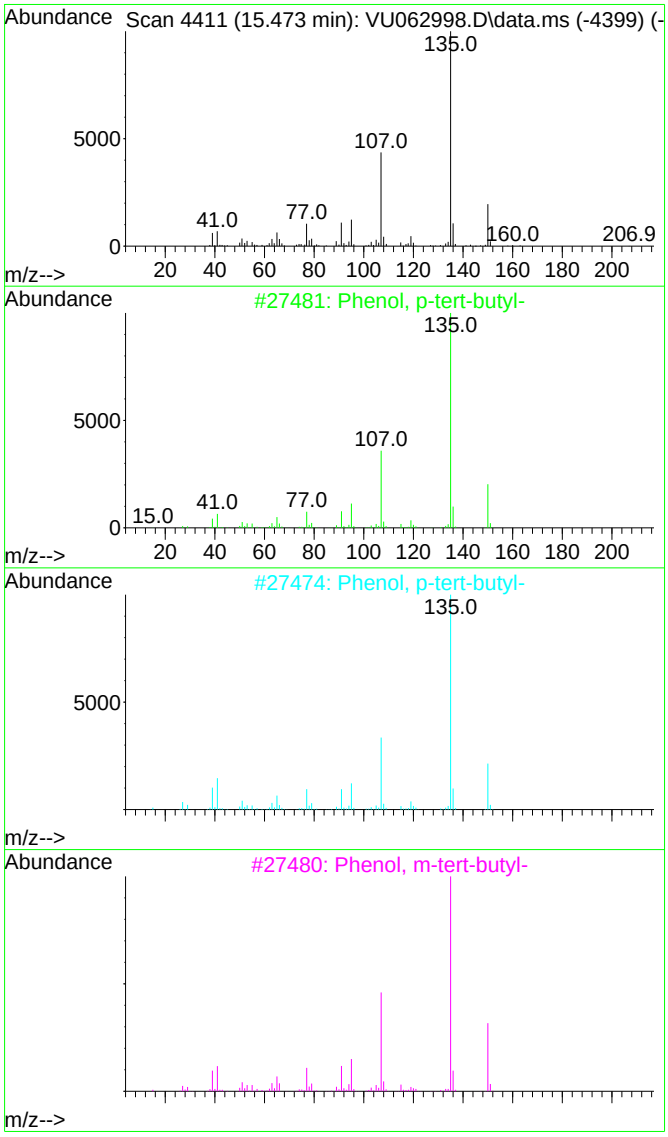
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR010225WMA.M
Quant Title : TRACE VOA SFAM1.0

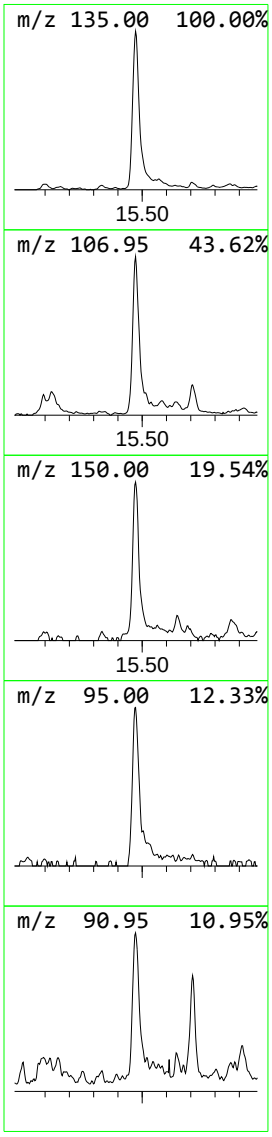
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Phenol, p-tert-butyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.473	3.38 ug/L	201973	1,4-Dichlorobenzene-d4	11.807

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	91
4	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	90
5	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	87





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012425\
Data File : VU062998.D
Acq On : 24 Jan 2025 17:17
Operator : MD/SY
Sample : Q1174-10
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2940

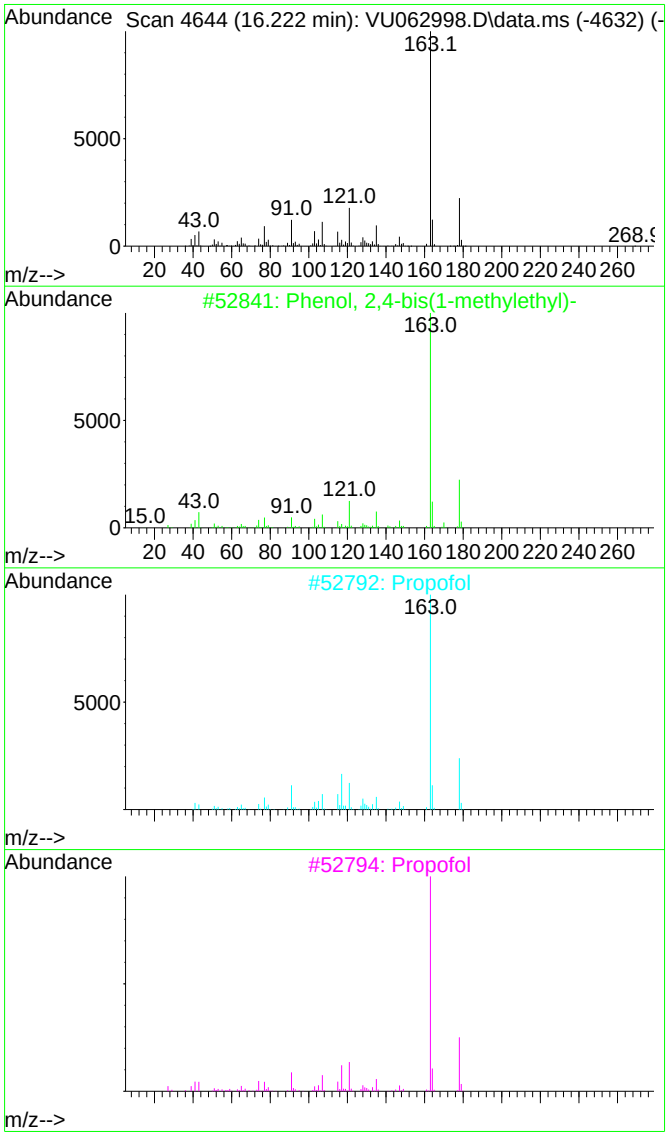
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR010225WMA.M
Quant Title : TRACE VOA SFAM1.0

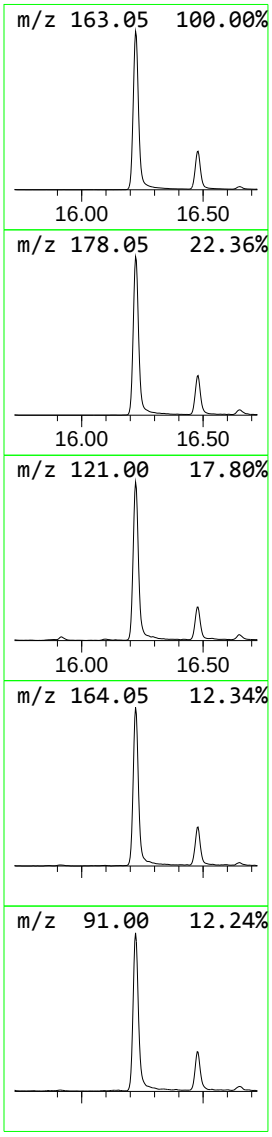
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.222	92.32 ug/L	5518560	1,4-Dichlorobenzene-d4	11.807

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	Propofol	178	C12H18O	002078-54-8	91
5	Propofol	178	C12H18O	002078-54-8	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012425\
Data File : VU062998.D
Acq On : 24 Jan 2025 17:17
Operator : MD/SY
Sample : Q1174-10
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2940

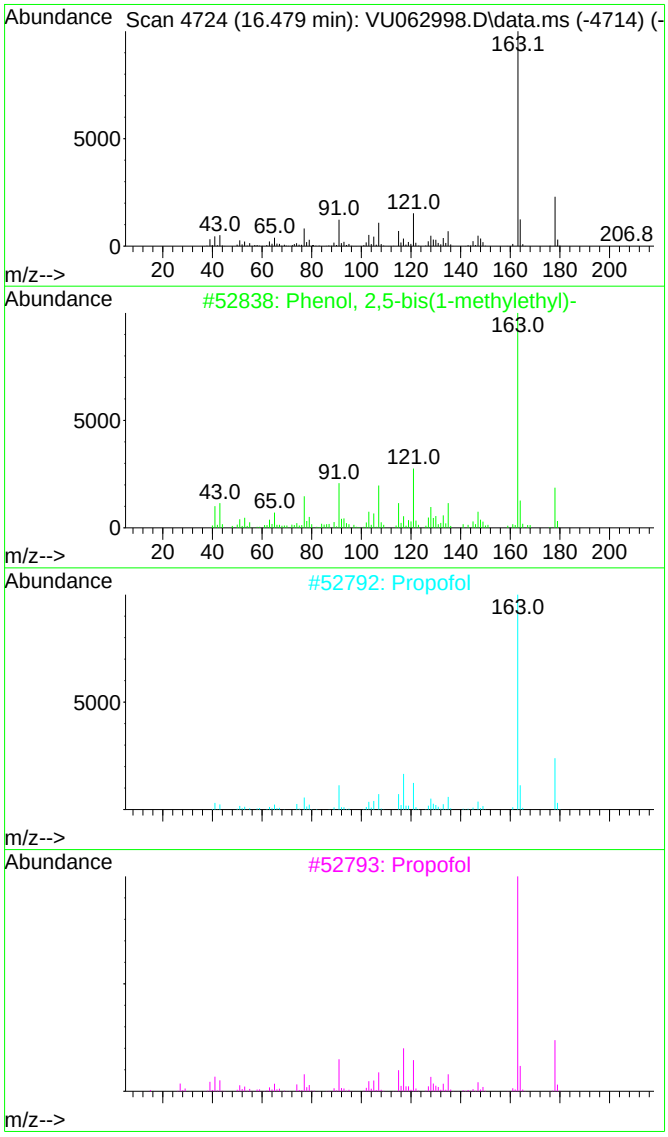
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR010225WMA.M
Quant Title : TRACE VOA SFAM1.0

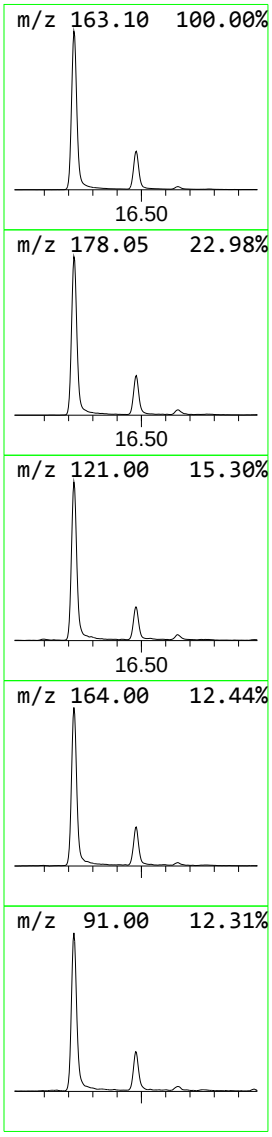
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 Phenol, 2,5-bis(1-methyleth... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.479	21.34 ug/L	1275930	1,4-Dichlorobenzene-d4	11.807

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	Phenol, 2,4-bis(1-methylethyl)-	178	C12H18O	002934-05-6	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012425\
Data File : VU062998.D
Acq On : 24 Jan 2025 17:17
Operator : MD/SY
Sample : Q1174-10
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2940

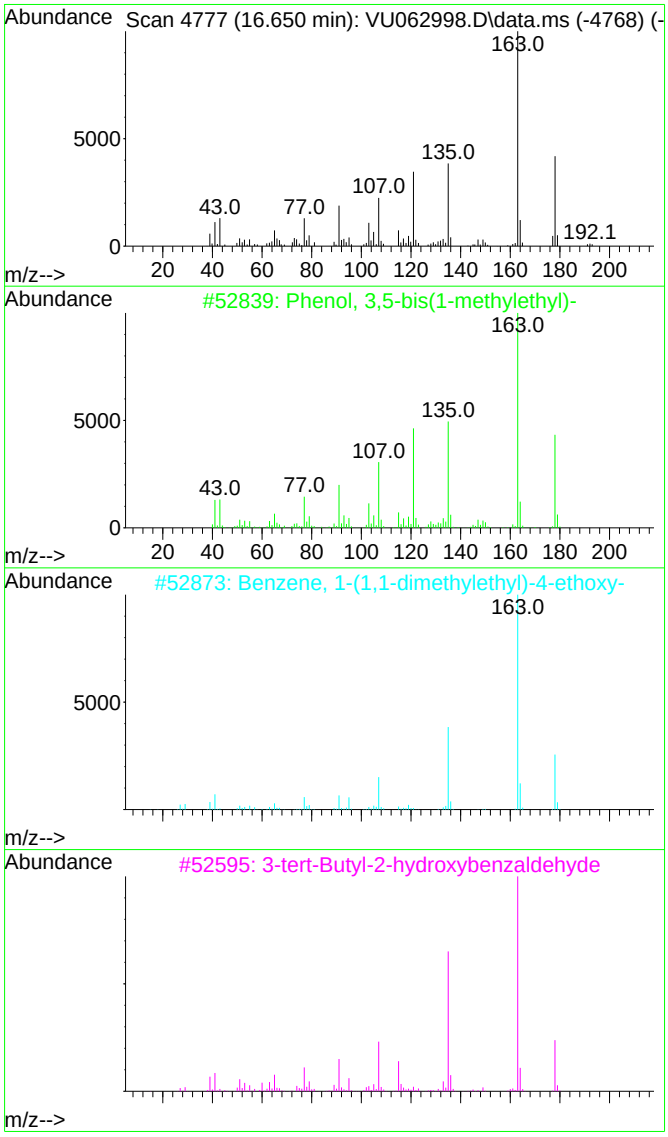
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR010225WMA.M
Quant Title : TRACE VOA SFAM1.0

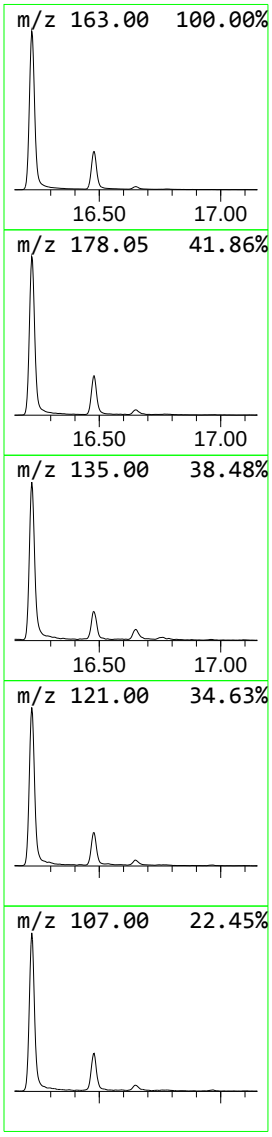
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 Phenol, 3,5-bis(1-methyleth... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.650	2.98 ug/L	178194	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 3,5-bis(1-methylethyl)-	178	C12H18O	026886-05-5	96
2	Benzene, 1-(1,1-dimethylethyl)-4...	178	C12H18O	017269-94-2	90
3	3-tert-Butyl-2-hydroxybenzaldehyde	178	C11H14O2	024623-65-2	86
4	5'-Hydroxy-2',3',4'-trimethylace...	178	C11H14O2	013667-28-2	83
5	6-tert-Butyl-2,4-dimethylphenol	178	C12H18O	001879-09-0	81





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012425\
Data File : VU062998.D
Acq On : 24 Jan 2025 17:17
Operator : MD/SY
Sample : Q1174-10
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2940

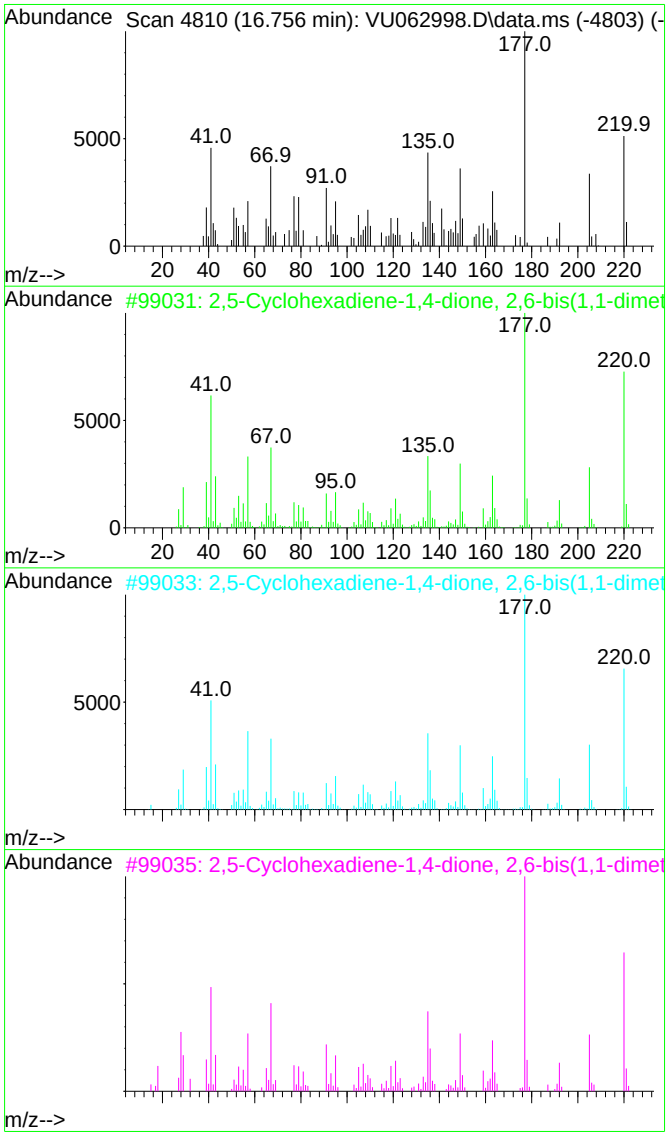
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR010225WMA.M
Quant Title : TRACE VOA SFAM1.0

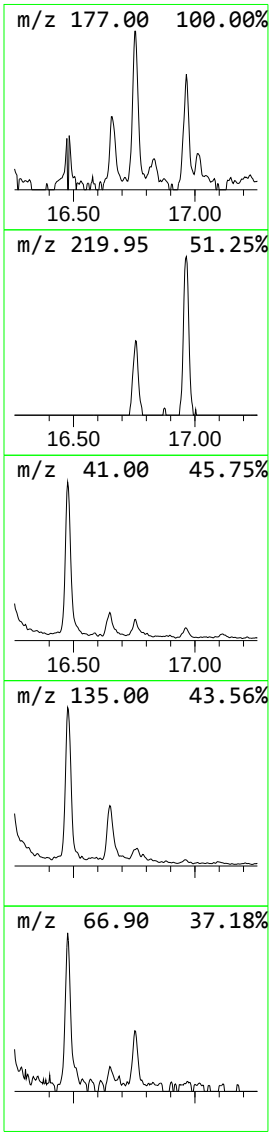
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 17 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.756	1.41 ug/L	84568	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	94
2	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	94
3	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	94
4	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	93
5	2-Hydroxy-4-methoxy-5-(2-methylb...	220	C13H16O3	2108511-28-8	55





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012425\
Data File : VU062998.D
Acq On : 24 Jan 2025 17:17
Operator : MD/SY
Sample : Q1174-10
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2940

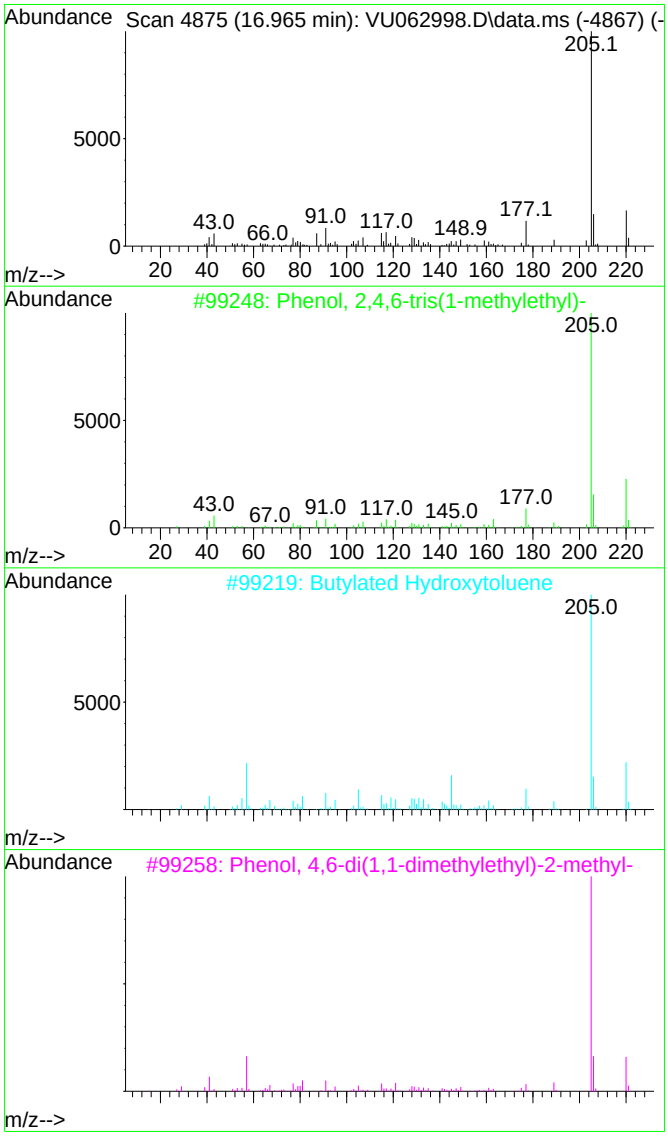
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR010225WMA.M
Quant Title : TRACE VOA SFAM1.0

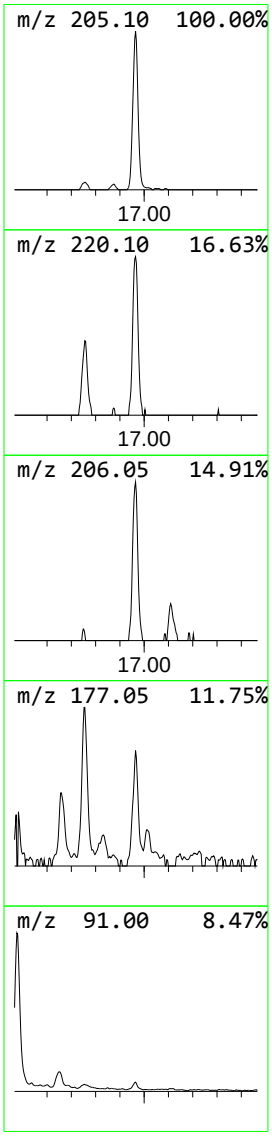
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 18 Phenol, 2,4,6-tris(1-methyl... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.965	1.28 ug/L	76455	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,4,6-tris(1-methylethyl)-	220	C15H24O	002934-07-8	93
2	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	90
3	Phenol, 4,6-di(1,1-dimethylethyl...	220	C15H24O	000616-55-7	81
4	Phenol, 4,6-di(1,1-dimethylethyl...	220	C15H24O	000616-55-7	74
5	Phenol, 2,6-bis(1,1-dimethylethy...	277	C17H27NO2	001918-11-2	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012425\
Data File : VU062998.D
Acq On : 24 Jan 2025 17:17
Operator : MD/SY
Sample : Q1174-10
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2940

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR010225WMA.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
Dimethyl sulfide	2.775	1.6	ug/L	75672	1	6.335	234092	5.0
1-Heptanol, 2,4...	12.698	1.0	ug/L	59236	3	11.807	298882	5.0
Phenol, 2,5-dim...	13.929	1.0	ug/L	59099	3	11.807	298882	5.0
Phenol, 3-(1-me...	14.409	5.0	ug/L	296617	3	11.807	298882	5.0
p-Cumenol	14.817	1.8	ug/L	109270	3	11.807	298882	5.0
Phenol, p-tert-...	15.473	3.4	ug/L	201973	3	11.807	298882	5.0
Phenol, 2,4-bis...	16.222	92.3	ug/L	5518560	3	11.807	298882	5.0
Phenol, 2,5-bis...	16.479	21.3	ug/L	1275930	3	11.807	298882	5.0
Phenol, 3,5-bis...	16.650	3.0	ug/L	178194	3	11.807	298882	5.0
2,5-Cyclohexadi...	16.756	1.4	ug/L	84568	3	11.807	298882	5.0
Phenol, 2,4,6-t...	16.965	1.3	ug/L	76455	3	11.807	298882	5.0