LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020625\
Data File : VU063195.D
Acq On : 06 Feb 2025 14:57
Operator : MD/SY
Sample : Q1226-21DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DCZL6DL

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\SFAMUTR020425WMA.M
Title : TRACE VOA SFAM1.0

Signal : TIC: VU063195.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.477	48	58	80	rBV2	5853	14265	1.18%	0.239%
2	1.593	86	94	111	rVB	23903	29620	2.45%	0.497%
3	1.888	177	186	202	rVB	24087	32225	2.66%	0.541%
4	2.551	379	392	407	rBV	43596	71577	5.91%	1.201%
5	3.171	571	585	601	rVB	7049	15352	1.27%	0.258%
6	4.445	971	981	1001	rBV4	6223	18067	1.49%	0.303%
7	4.605	1019	1031	1067	rBV	51033	126708	10.46%	2.126%
8	5.046	1154	1168	1191	rBV2	47761	106669	8.81%	1.790%
9	5.711	1357	1375	1407	rBV2	93601	251762	20.79%	4.225%
10	6.236	1526	1538	1560	rBV	93193	179930	14.86%	3.019%
11	6.676	1661	1675	1695	rBV	61321	119878	9.90%	2.012%
12	7.557	1938	1949	1967	rBV	27737	49481	4.09%	0.830%
13	7.888	2039	2052	2069	rBV	106991	186355	15.39%	3.127%
14	8.171	2129	2140	2157	rBV	17339	28791	2.38%	0.483%
15	8.621	2270	2280	2308	rBV	177228	320672	26.48%	5.381%
16	9.406	2510	2524	2544	rBV	137676	230176	19.01%	3.863%
17	9.686	2596	2611	2624	rBV3	8870	18613	1.54%	0.312%
18	10.094	2728	2738	2751	rBV2	17515	27730	2.29%	0.465%
19	10.473	2846	2856	2874	rBV	29730	46917	3.87%	0.787%
20	10.743	2930	2940	2958	rVB	54091	87402	7.22%	1.467%
21	10.898	2977	2988	3004	rBV	53733	82082	6.78%	1.377%
22	10.988	3004	3016	3035	rVV	162163	345662	28.55%	5.801%
23	11.078	3035	3044	3060	rVB	70947	107689	8.89%	1.807%
24	11.280	3097	3107	3127	rVB	115107	177852	14.69%	2.985%
25	11.457	3152	3162	3180	rVB	209593	316936	26.18%	5.319%
26	11.547	3180	3190	3201	rBV	20539	32950	2.72%	0.553%
27	11.734	3238	3248	3256	rBV2	10643	14495	1.20%	0.243%
28	11.801	3256	3269	3282	rVV	138355	226506	18.71%	3.801%
29	11.885	3282	3295	3311	rVB	72698	121745	10.05%	2.043%
30	12.084	3346	3357	3375	rBV3	96268	171239	14.14%	2.874%
31	12.184	3375	3388	3408	rVB	138824	242660	20.04%	4.072%
32	12.290	3412	3421	3431	rVB	10939	15977	1.32%	0.268%
33	12.367	3435	3445	3458	rBV2	23063	35049	2.89%	0.588%
34	12.467	3460	3476	3497	rBV	708176	1210822	100.00%	20.319%
35	12.563	3497	3506	3513	rVB	21915	31047	2.56%	0.521%
36	12.634	3521	3528	3535	rBV3	19504	28687	2.37%	0.481%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020625\
Data File : VU063195.D
Acq On : 06 Feb 2025 14:57
Operator : MD/SY
Sample : Q1226-21DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DCZL6DL

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\SFAMUTR020425WMA.M
Title : TRACE VOA SFAM1.0

37	12.673	3535	3540	3558	rVB4	13707	28044	2.32%	0.471%
38	12.798	3570	3579	3589	rBV2	13629	21462	1.77%	0.360%
39	12.865	3589	3600	3612	rVB3	12173	22082	1.82%	0.371%
40	12.975	3625	3634	3641	rBV2	28737	49519	4.09%	0.831%
41	13.091	3660	3670	3681	rBV5	11203	17404	1.44%	0.292%
42	13.444	3770	3780	3786	rBV5	21288	34899	2.88%	0.586%
43	13.476	3786	3790	3803	rVB2	15450	22103	1.83%	0.371%
44	13.920	3917	3928	3934	rBV	123231	186830	15.43%	3.135%
45	13.962	3934	3941	3962	rVB4	109236	219892	18.16%	3.690%
46	14.312	4040	4050	4057	rBV3	11796	19456	1.61%	0.326%
47	14.357	4057	4064	4077	rVB3	8232	12960	1.07%	0.217%
48	14.695	4161	4169	4178	rBV3	10262	14673	1.21%	0.246%
49	15.171	4305	4317	4329	rBV	99192	168800	13.94%	2.833%
50	15.396	4375	4387	4410	rVB5	7346	17368	1.43%	0.291%

Sum of corrected areas: 5959080

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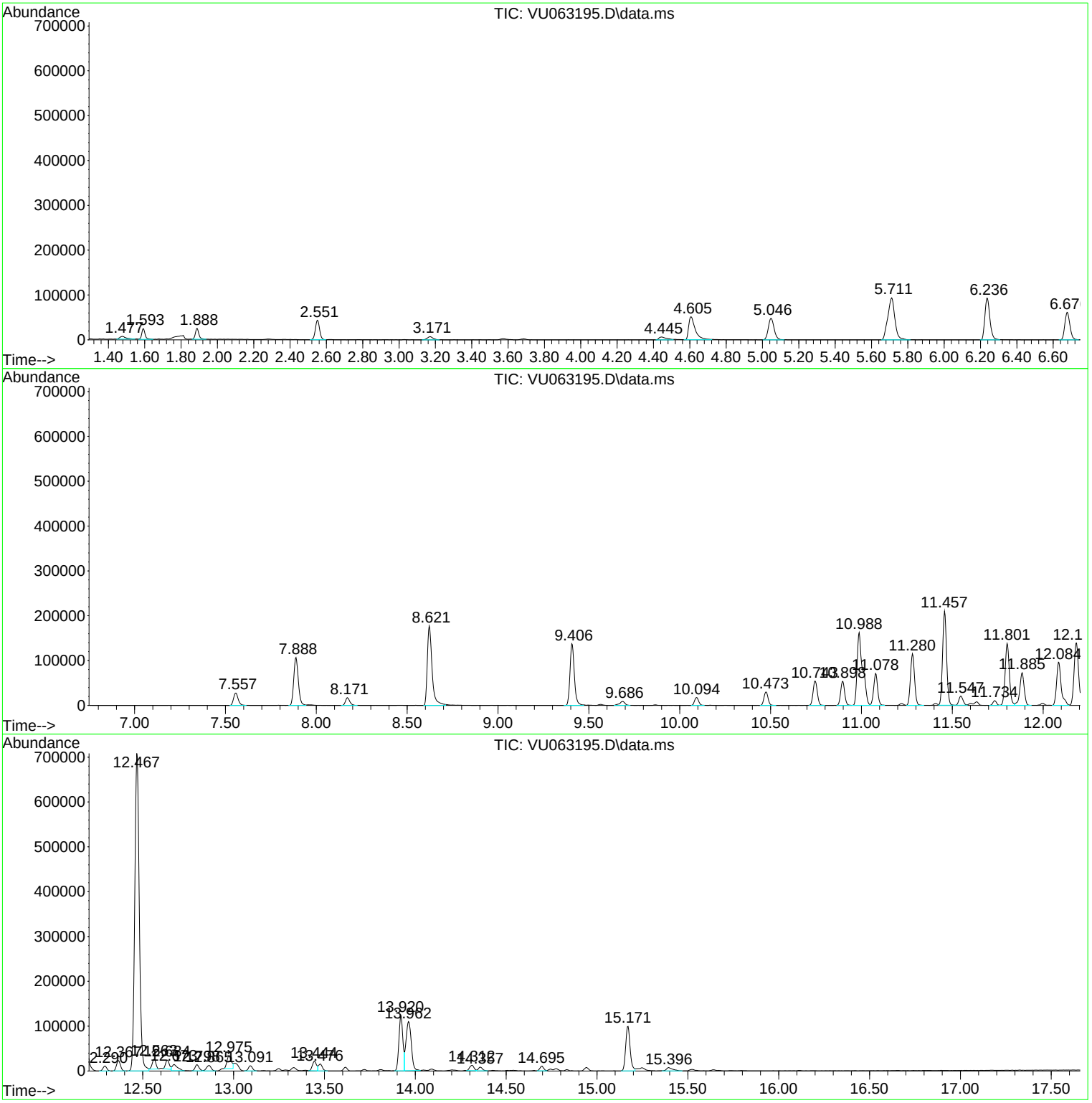
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DCZL6DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR020425WMA.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\VU020625\
Data File : VU063195.D
Acq On : 06 Feb 2025 14:57
Operator : MD/SY
Sample : Q1226-21DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
DCZL6DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR020425WMA.M
Quant Title : TRACE VOA SFAM1.0

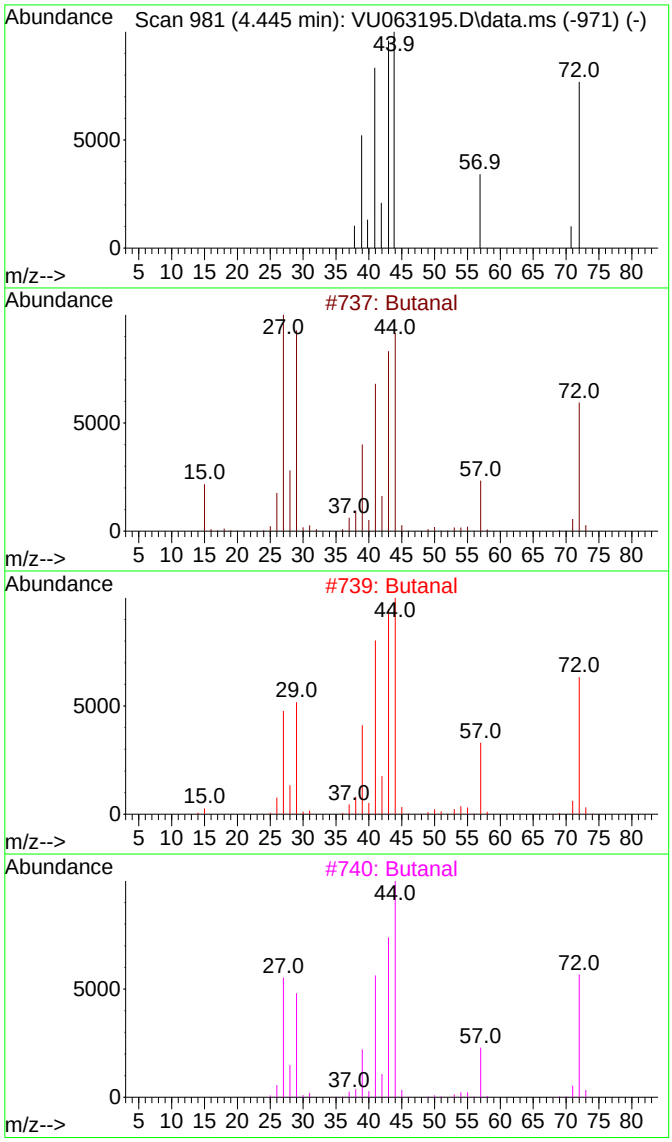
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

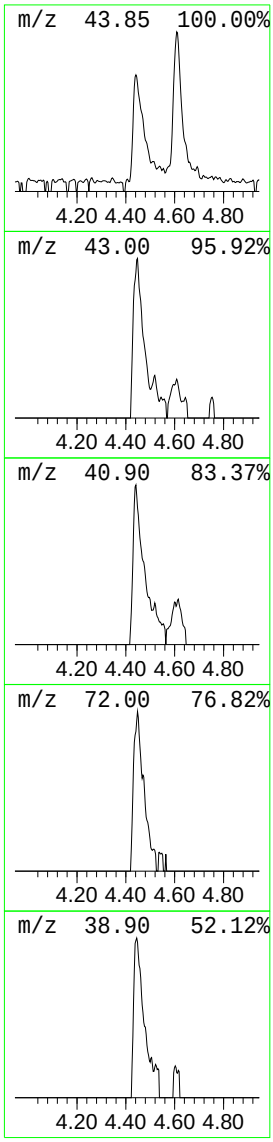
****

Peak Number 1 Butanal Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.445	0.50 ug/L	18067	1,4-Difluorobenzene	6.236

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	91
2	Butanal	72	C4H8O	000123-72-8	91
3	Butanal	72	C4H8O	000123-72-8	72
4	Butanal	72	C4H8O	000123-72-8	72
5	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	17





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020625\
Data File : VU063195.D
Acq On : 06 Feb 2025 14:57
Operator : MD/SY
Sample : Q1226-21DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DCZL6DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR020425WMA.M
Quant Title : TRACE VOA SFAM1.0

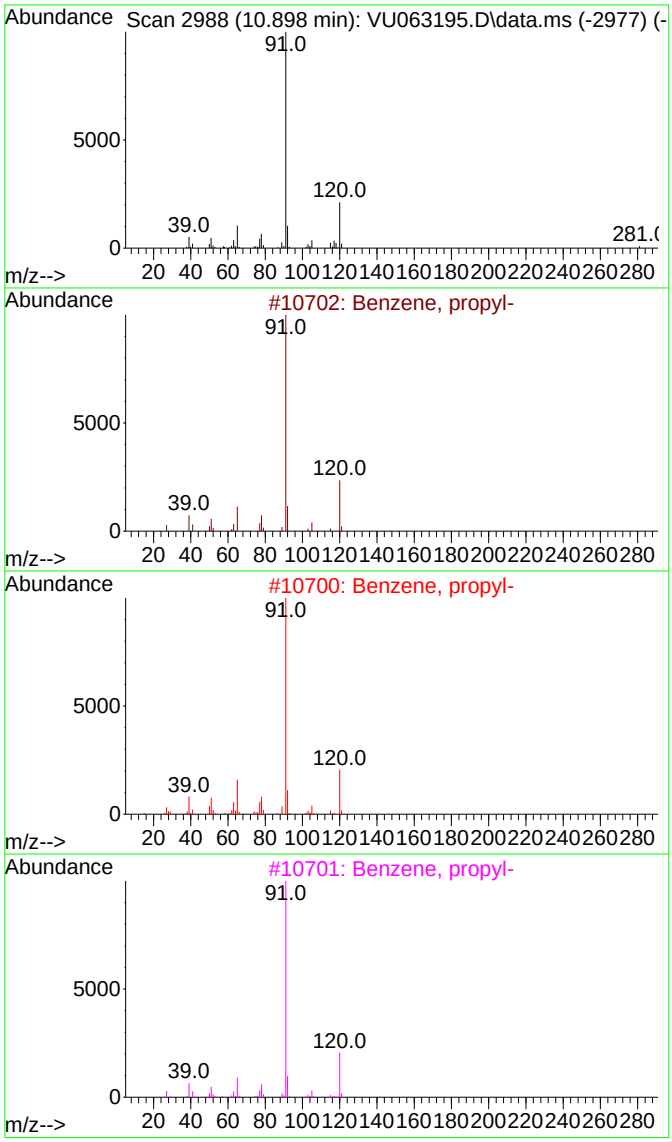
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

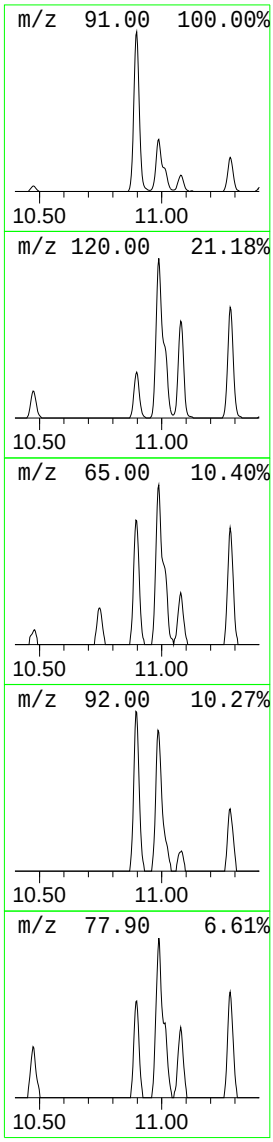
****

Peak Number 3 Benzene, propyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.898	1.81 ug/L	82082	1,4-Dichlorobenzene-d4	11.801

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, propyl-	120	C9H12	000103-65-1	93
2	Benzene, propyl-	120	C9H12	000103-65-1	93
3	Benzene, propyl-	120	C9H12	000103-65-1	87
4	Benzene, propyl-	120	C9H12	000103-65-1	83
5	Ethanol, 2-[(phenylmethyl)amino]-	151	C9H13NO	000104-63-2	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020625\
Data File : VU063195.D
Acq On : 06 Feb 2025 14:57
Operator : MD/SY
Sample : Q1226-21DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DCZL6DL

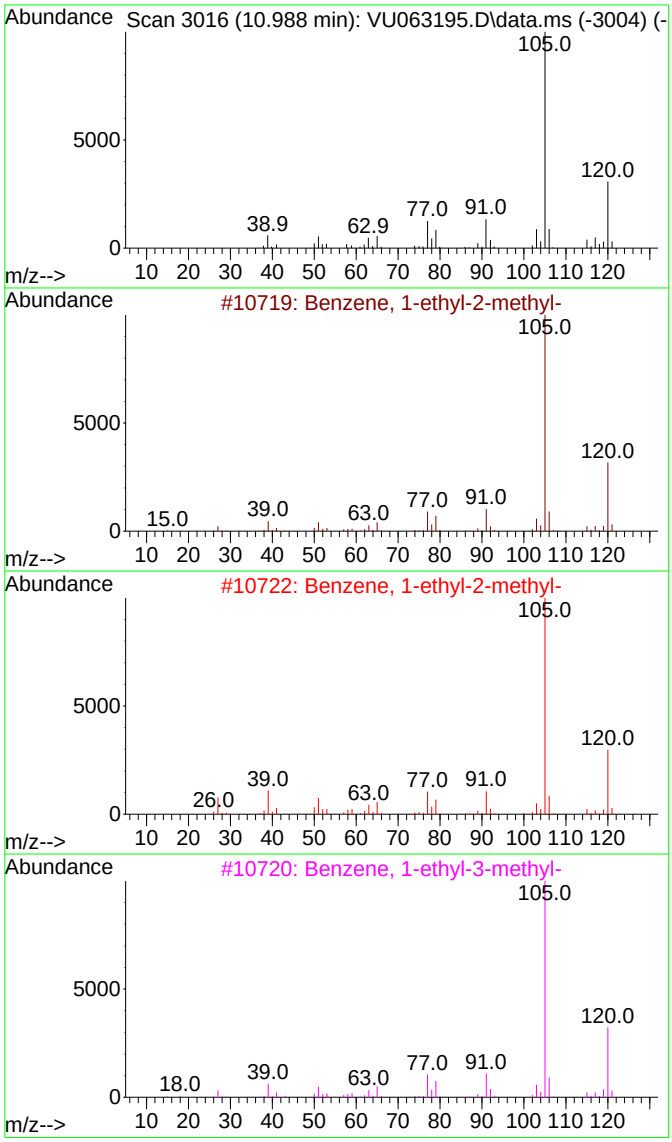
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR020425WMA.M
Quant Title : TRACE VOA SFAM1.0

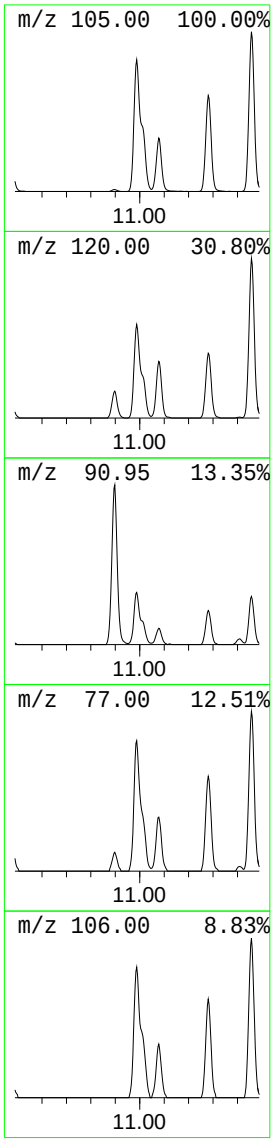
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 1-ethyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.988	7.63 ug/L	345662	1,4-Dichlorobenzene-d4	11.801

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
3	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020625\
Data File : VU063195.D
Acq On : 06 Feb 2025 14:57
Operator : MD/SY
Sample : Q1226-21DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DCZL6DL

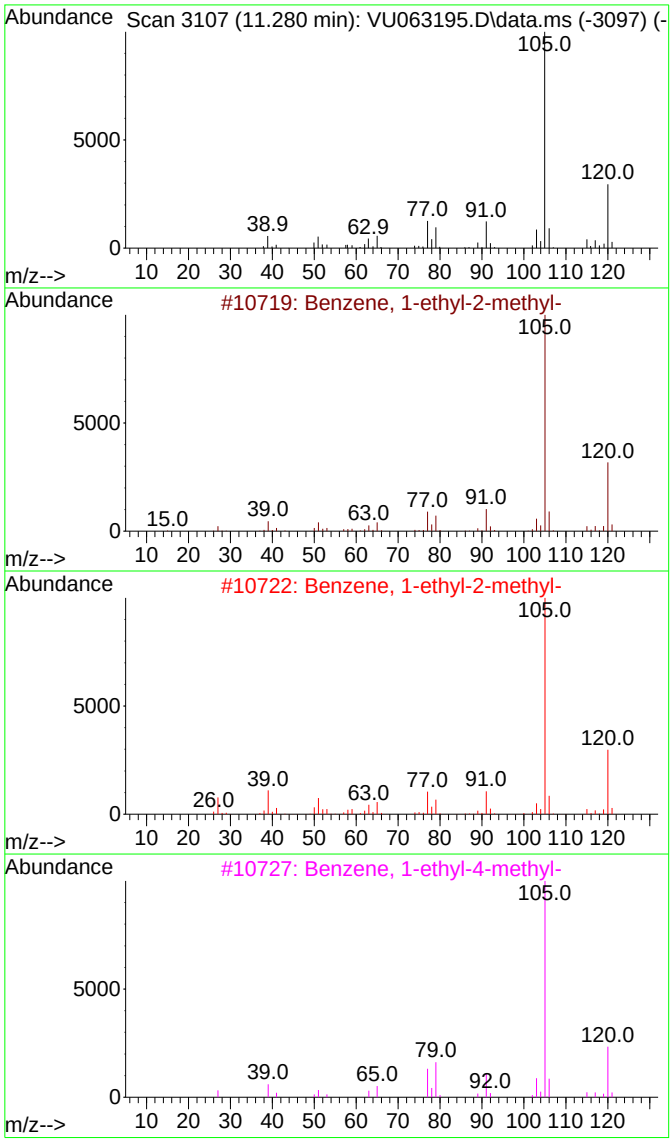
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR020425WMA.M
Quant Title : TRACE VOA SFAM1.0

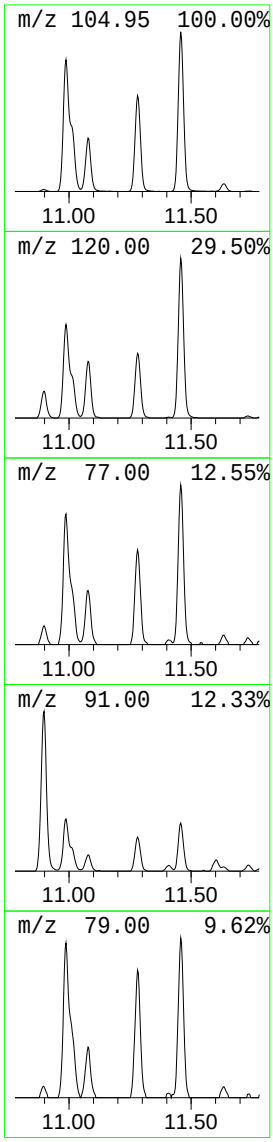
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1-ethyl-4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.280	3.93 ug/L	177852	1,4-Dichlorobenzene-d4	11.801

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020625\
Data File : VU063195.D
Acq On : 06 Feb 2025 14:57
Operator : MD/SY
Sample : Q1226-21DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DCZL6DL

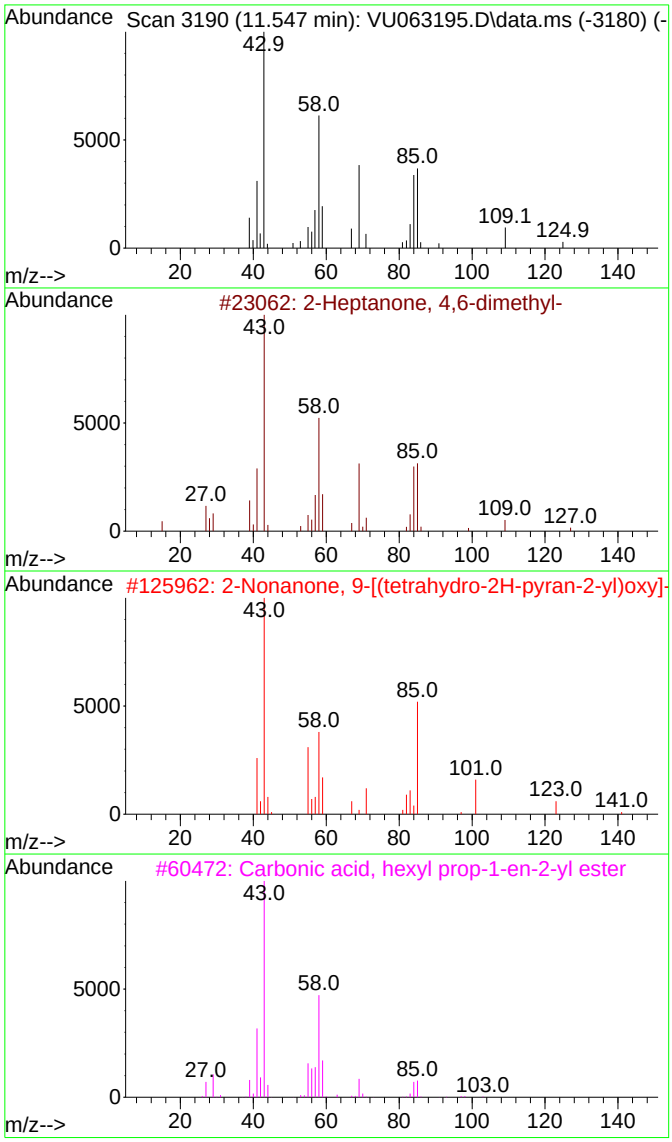
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR020425WMA.M
Quant Title : TRACE VOA SFAM1.0

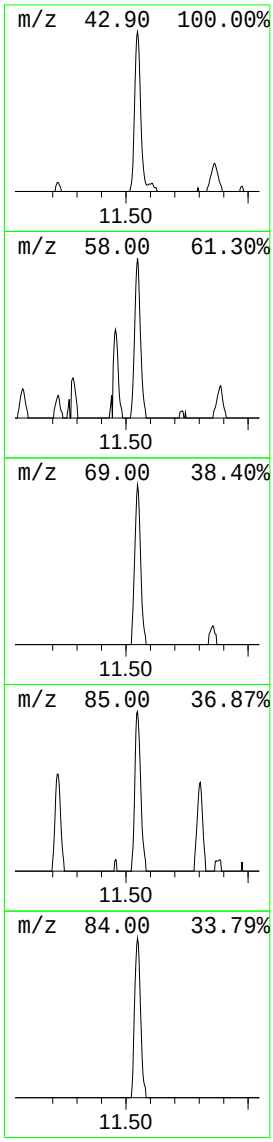
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2-Heptanone, 4,6-dimethyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.547	0.73 ug/L	32950	1,4-Dichlorobenzene-d4	11.801

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone, 4,6-dimethyl-	142	C9H18O	019549-80-5	90
2	2-Nonanone, 9-[(tetrahydro-2H-py...	242	C14H26O3	054699-41-1	50
3	Carbonic acid, hexyl prop-1-en-2...	186	C10H18O3	1000382-54-2	42
4	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	37
5	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	37





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Acq On : 06 Feb 2025 14:57
Operator : MD/SY
Sample : Q1226-21DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DCZL6DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR020425WMA.M
Quant Title : TRACE VOA SFAM1.0

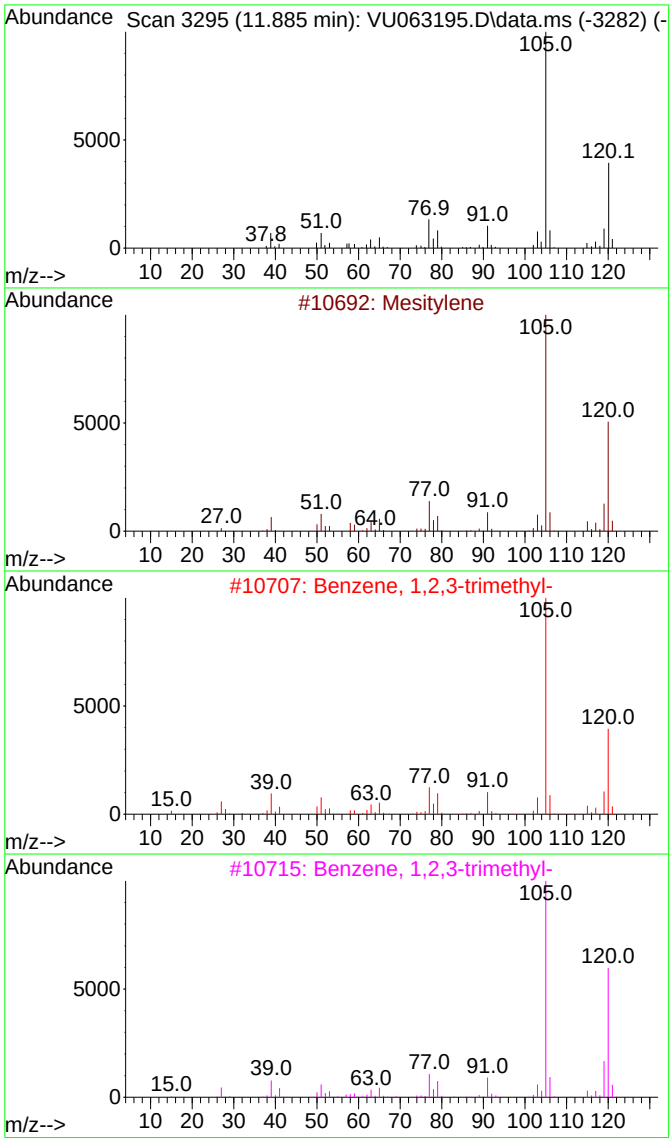
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

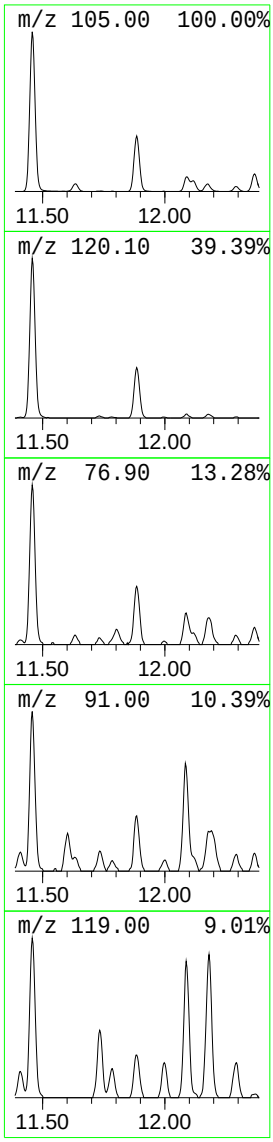
****

Peak Number 7 Benzene, 1,2,3-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.885	2.69 ug/L	121745	1,4-Dichlorobenzene-d4	11.801

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Mesitylene	120	C9H12	000108-67-8	97
2	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	94
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020625\
Data File : VU063195.D
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Operator : MD/SY
Sample : Q1226-21DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DCZL6DL

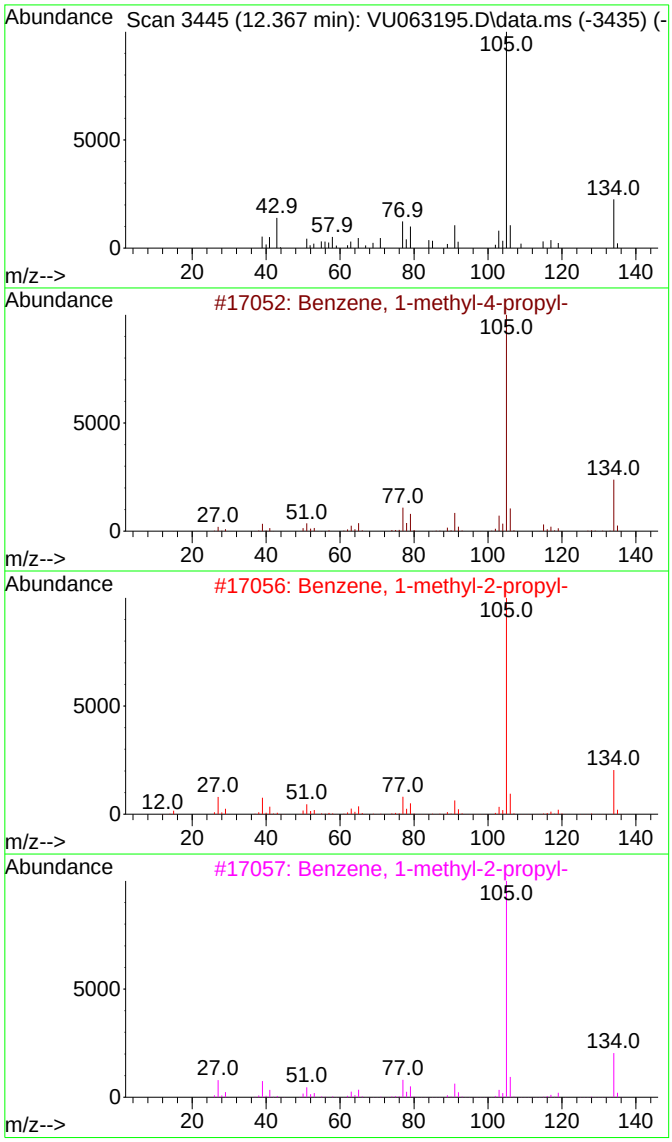
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR020425WMA.M
Quant Title : TRACE VOA SFAM1.0

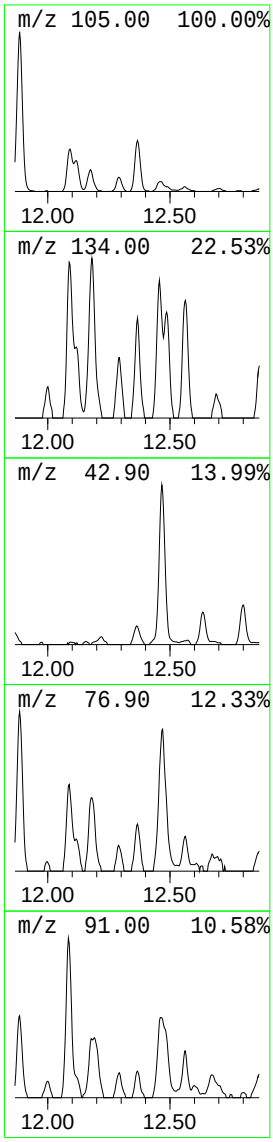
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1-methyl-4-propyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.367	0.77 ug/L	35049	1,4-Dichlorobenzene-d4	11.801

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-4-propyl-	134	C10H14	001074-55-1	94
2	Benzene, 1-methyl-2-propyl-	134	C10H14	001074-17-5	87
3	Benzene, 1-methyl-2-propyl-	134	C10H14	001074-17-5	87
4	Benzene, 1-methyl-2-propyl-	134	C10H14	001074-17-5	87
5	Benzene, 1-methyl-3-propyl-	134	C10H14	001074-43-7	87





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020625\
Data File : VU063195.D
Acq On : 06 Feb 2025 14:57
Operator : MD/SY
Sample : Q1226-21DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DCZL6DL

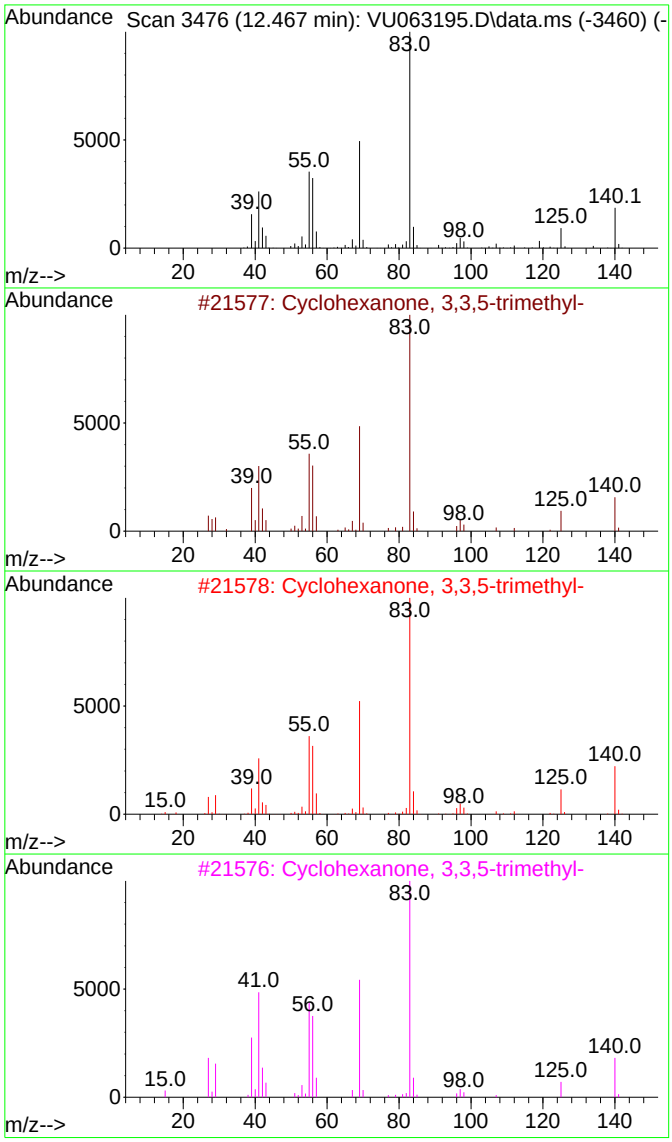
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR020425WMA.M
Quant Title : TRACE VOA SFAM1.0

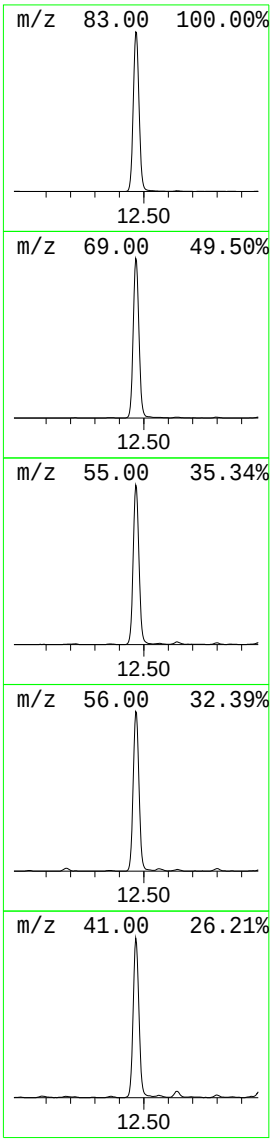
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Cyclohexanone, 3,3,5-trimet... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.467	26.73 ug/L	1210820	1,4-Dichlorobenzene-d4	11.801

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	97
2	Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	96
3	Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	95
4	Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	91
5	2,4,6-Trimethyl-3-heptene	140	C10H20	1000113-56-9	53





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Data File : VU063195.D
Acq On : 06 Feb 2025 14:57
Operator : MD/SY
Sample : Q1226-21DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DCZL6DL

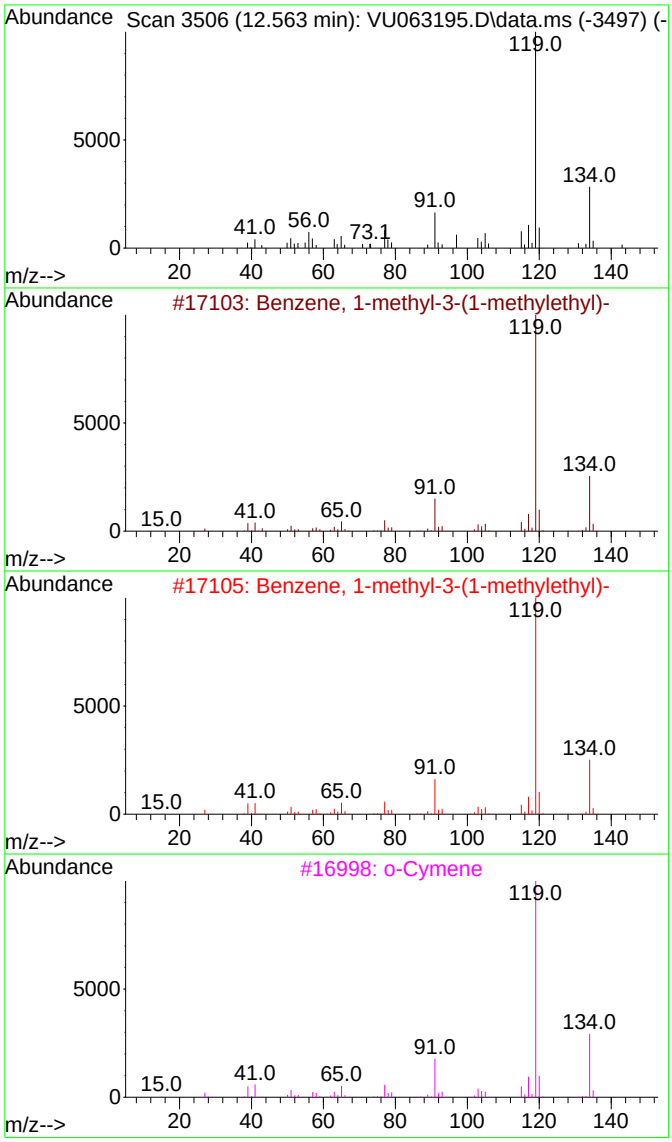
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR020425WMA.M
Quant Title : TRACE VOA SFAM1.0

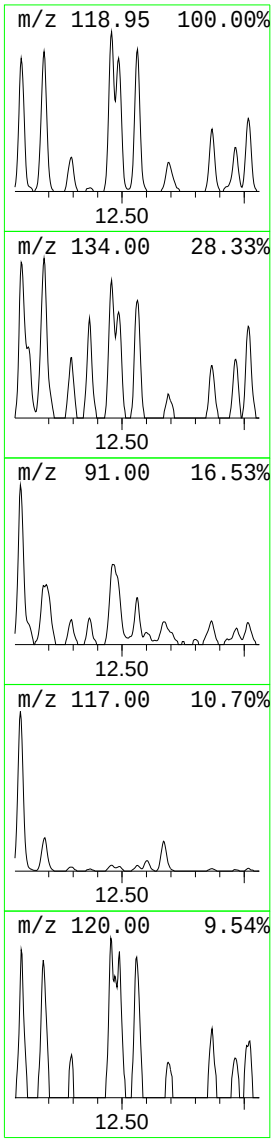
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Benzene, 1-methyl-3-(1-meth... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.563	0.69 ug/L	31047	1,4-Dichlorobenzene-d4	11.801

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
2	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
3	o-Cymene	134	C10H14	000527-84-4	95
4	p-Cymene	134	C10H14	000099-87-6	94
5	o-Cymene	134	C10H14	000527-84-4	94





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020625\
Data File : VU063195.D
Acq On : 06 Feb 2025 14:57
Operator : MD/SY
Sample : Q1226-21DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DCZL6DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR020425WMA.M
Quant Title : TRACE VOA SFAM1.0

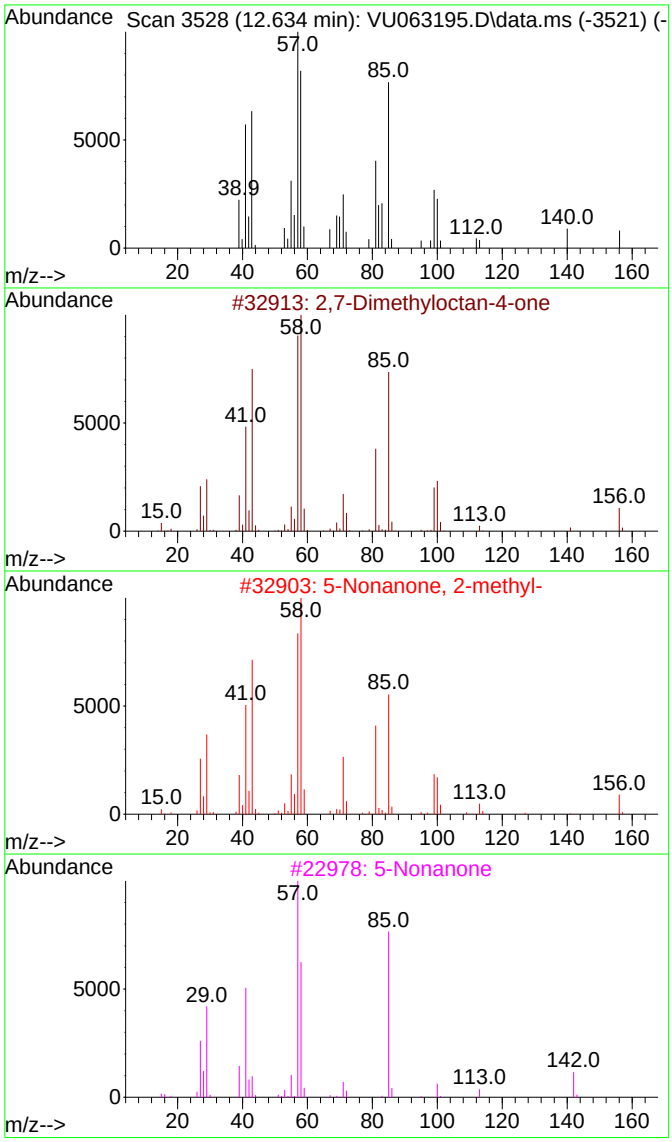
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

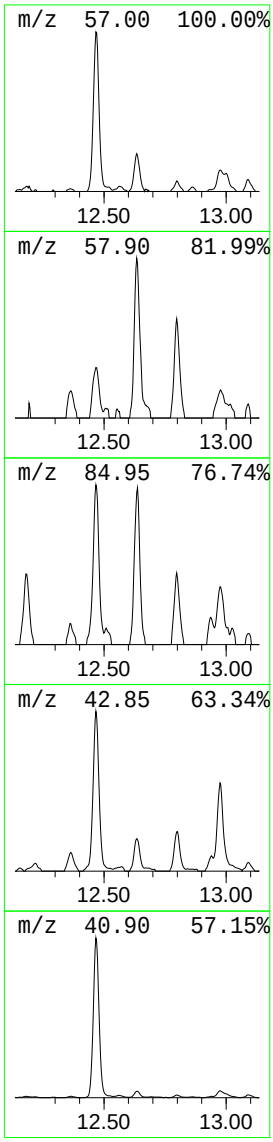
****

Peak Number 12 2,7-Dimethyloctan-4-one Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.634	0.63 ug/L	28687	1,4-Dichlorobenzene-d4	11.801

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,7-Dimethyloctan-4-one	156	C10H20O	059387-92-7	95
2	5-Nonanone, 2-methyl-	156	C10H20O	022287-02-1	53
3	5-Nonanone	142	C9H18O	000502-56-7	50
4	5-Nonanone	142	C9H18O	000502-56-7	50
5	1-Phospha-1-butyne, 3,3-dimethyl-	100	C5H9P	078129-68-7	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020625\
Data File : VU063195.D
Acq On : 06 Feb 2025 14:57
Operator : MD/SY
Sample : Q1226-21DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DCZL6DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR020425WMA.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
Butanal	4.445	0.5	ug/L	18067	1	6.236	179930	5.0
Benzene, propyl-	10.898	1.8	ug/L	82082	3	11.801	226506	5.0
Benzene, 1-ethy...	10.988	7.6	ug/L	345662	3	11.801	226506	5.0
Benzene, 1-ethy...	11.280	3.9	ug/L	177852	3	11.801	226506	5.0
2-Heptanone, 4,...	11.547	0.7	ug/L	32950	3	11.801	226506	5.0
Benzene, 1,2,3-...	11.885	2.7	ug/L	121745	3	11.801	226506	5.0
Benzene, 1-meth...	12.367	0.8	ug/L	35049	3	11.801	226506	5.0
Cyclohexanone, ...	12.467	26.7	ug/L	1210820	3	11.801	226506	5.0
Benzene, 1-meth...	12.563	0.7	ug/L	31047	3	11.801	226506	5.0
2,7-Dimethyloct...	12.634	0.6	ug/L	28687	3	11.801	226506	5.0