LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102722\
Data File : VU051555.D
Acq On : 27 Oct 2022 21:46
Operator : JC/MD
Sample : N5300-11DL 20X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHA74DL

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\SFAMUTR100722WMA.M
Title : TRACE VOA SFAM1.0

Signal : TIC: VU051555.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.462	31	38	52	rBV2	20512	50503	4.94%	0.495%
2	1.597	73	80	89	rBV	103198	130718	12.78%	1.282%
3	1.909	169	177	198	rVB2	89880	150273	14.69%	1.474%
4	2.375	312	322	335	rVB	137957	211242	20.66%	2.072%
5	2.562	368	380	395	rBV	144104	234763	22.96%	2.303%
6	3.044	516	530	540	rBV4	26929	61410	6.00%	0.602%
7	3.182	558	573	593	rVB	33060	76547	7.49%	0.751%
8	3.356	611	627	641	rVB3	21470	46926	4.59%	0.460%
9	3.694	719	732	748	rVB4	12115	26887	2.63%	0.264%
10	3.832	758	775	777	rBV	7591	13174	1.29%	0.129%
11	3.989	806	824	848	rBV2	224557	587619	57.46%	5.764%
12	4.526	975	991	1008	rBV3	45229	111139	10.87%	1.090%
13	4.620	1008	1020	1061	rVV	182065	456737	44.66%	4.480%
14	5.060	1142	1157	1181	rBV	177923	409298	40.02%	4.015%
15	5.385	1244	1258	1271	rVB4	7749	16532	1.62%	0.162%
16	5.491	1279	1291	1304	rVB6	12691	25992	2.54%	0.255%
17	5.722	1342	1363	1370	rBV2	310824	802131	78.44%	7.868%
18	5.771	1371	1378	1405	rVB	480183	969297	94.78%	9.508%
19	6.247	1511	1526	1550	rBV	289517	556833	54.45%	5.462%
20	6.690	1648	1664	1679	rBV	205638	405575	39.66%	3.978%
21	6.761	1680	1686	1697	rVB5	8889	16036	1.57%	0.157%
22	7.565	1924	1936	1956	rBV2	80540	143292	14.01%	1.406%
23	7.710	1968	1981	1993	rBV7	5716	10293	1.01%	0.101%
24	7.896	2018	2039	2055	rBV	314691	552179	53.99%	5.417%
25	7.967	2055	2061	2072	rVB	11235	20022	1.96%	0.196%
26	8.179	2113	2127	2141	rBV2	50861	85974	8.41%	0.843%
27	8.632	2253	2268	2300	rBV	555305	1022651	100.00%	10.032%
28	9.417	2499	2512	2516	rBV	441717	718142	70.22%	7.045%
29	9.574	2551	2561	2575	rVB4	5560	11506	1.13%	0.113%
30	9.690	2588	2597	2609	rBV2	7830	13306	1.30%	0.131%
31	10.105	2716	2726	2737	rBV6	7694	13742	1.34%	0.135%
32	10.481	2833	2843	2854	rBV	34313	52337	5.12%	0.513%
33	10.587	2866	2876	2881	rBV5	9869	16317	1.60%	0.160%
34	10.658	2889	2898	2908	rVB3	21653	36831	3.60%	0.361%
35	10.754	2908	2928	2943	rBV	186567	325996	31.88%	3.198%
36	10.889	2957	2970	2990	rBV5	73322	154538	15.11%	1.516%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102722\
Data File : VU051555.D
Acq On : 27 Oct 2022 21:46
Operator : JC/MD
Sample : N5300-11DL 20X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHA74DL

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\SFAMUTR100722WMA.M
Title : TRACE VOA SFAM1.0

37	11.028	2995	3013	3025	rBV3	36967	65251	6.38%	0.640%
38	11.291	3083	3095	3108	rBV3	23736	38058	3.72%	0.373%
39	11.639	3184	3203	3220	rVB3	8475	23157	2.26%	0.227%
40	11.809	3244	3256	3274	rBV	388097	674964	66.00%	6.621%
41	11.893	3274	3282	3299	rVB	15080	27738	2.71%	0.272%
42	12.092	3332	3344	3362	rVB3	48812	83296	8.15%	0.817%
43	12.192	3362	3375	3394	rBV	318753	542639	53.06%	5.323%
44	12.571	3484	3493	3501	rBV2	14094	20311	1.99%	0.199%
45	12.860	3564	3583	3603	rBV3	50858	91298	8.93%	0.896%
46	12.973	3610	3618	3624	rBV	8327	11092	1.08%	0.109%
47	13.944	3913	3920	3927	rBV8	9240	14501	1.42%	0.142%
48	13.992	3927	3935	3945	rVB5	17755	30230	2.96%	0.297%
49	15.076	4261	4272	4282	rBV6	21676	34935	3.42%	0.343%

Sum of corrected areas: 10194228

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102722\
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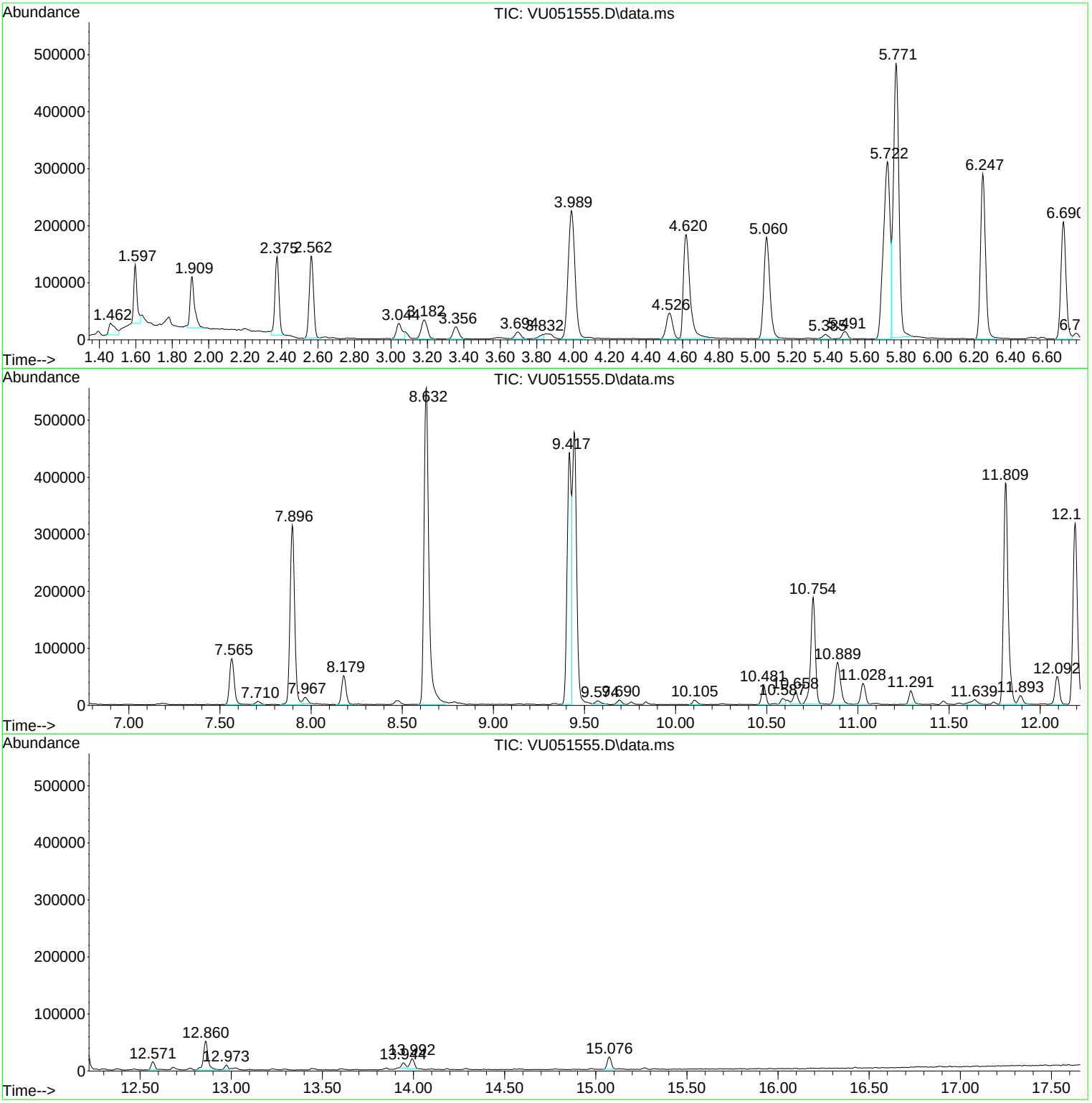
Operator : JC/MD
Sample : N5300-11DL 20X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHA74DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.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\VU102722\
Data File : VU051555.D
Acq On : 27 Oct 2022 21:46
Operator : JC/MD
Sample : N5300-11DL 20X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHA74DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.M
Quant Title : TRACE VOA SFAM1.0

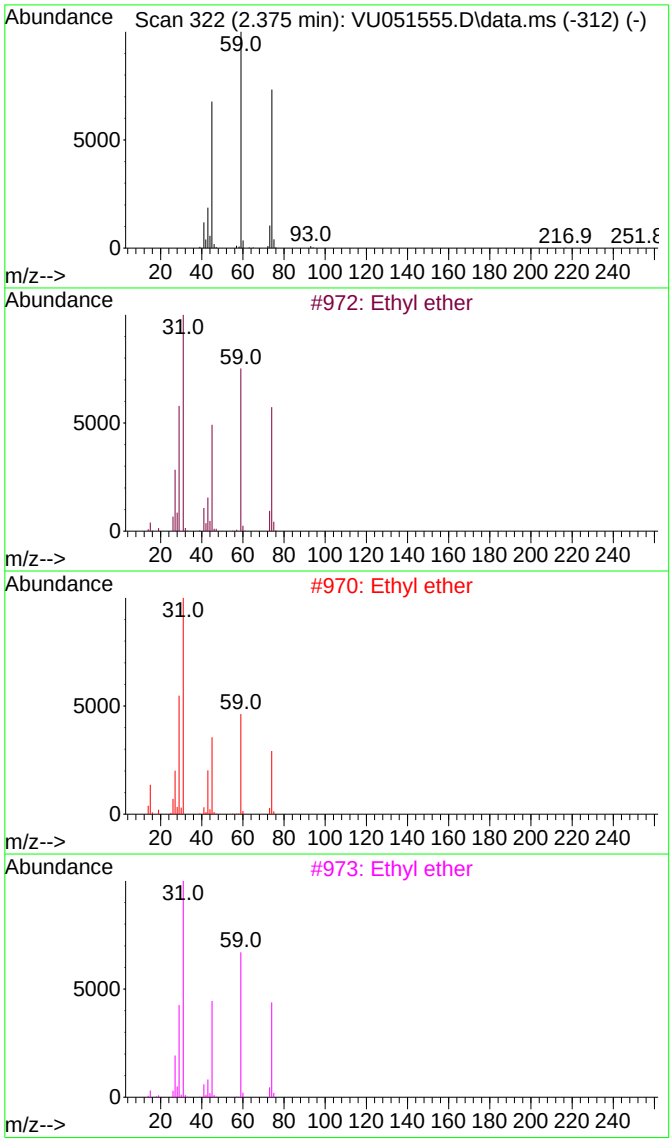
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

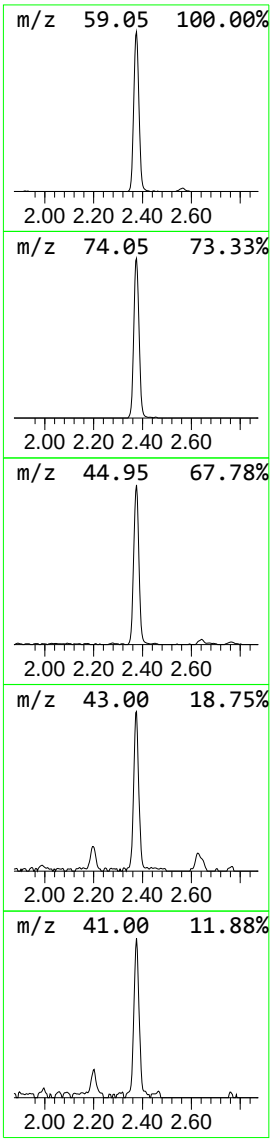
****

Peak Number 1 Ethyl ether Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.375	1.90 ug/L	211242	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl ether	74	C4H10O	000060-29-7	91
2	Ethyl ether	74	C4H10O	000060-29-7	90
3	Ethyl ether	74	C4H10O	000060-29-7	90
4	Ethyl ether	74	C4H10O	000060-29-7	59
5	Ethane, 1,2-diethoxy-	118	C6H14O2	000629-14-1	56





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102722\
Data File : VU051555.D
Acq On : 27 Oct 2022 21:46
Operator : JC/MD
Sample : N5300-11DL 20X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHA74DL

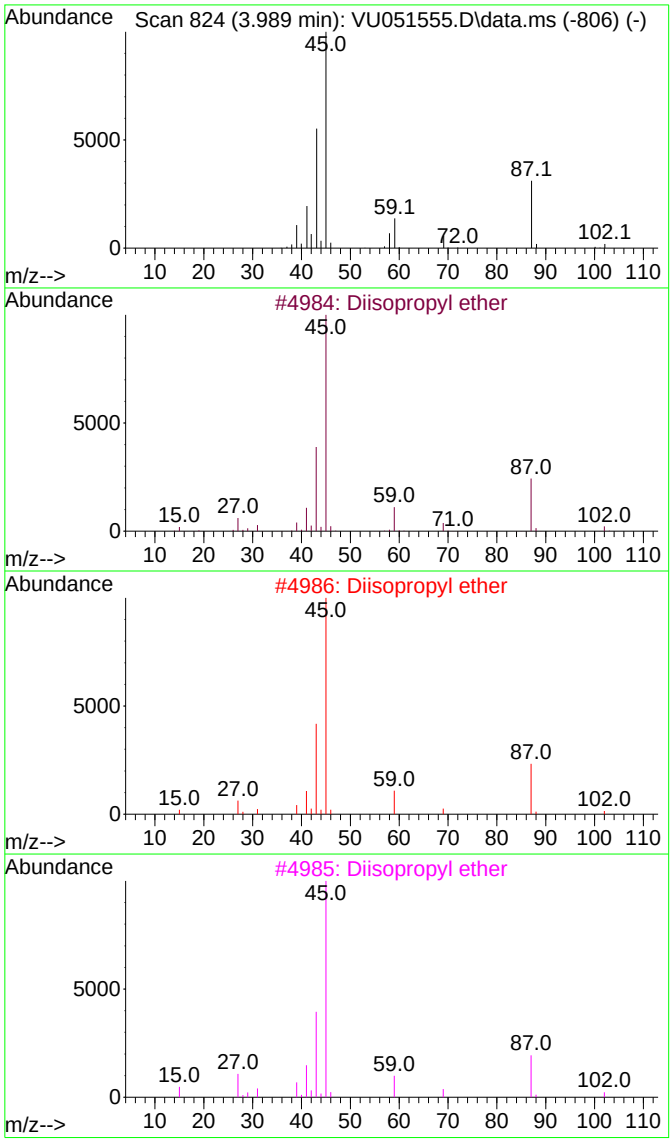
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.M
Quant Title : TRACE VOA SFAM1.0

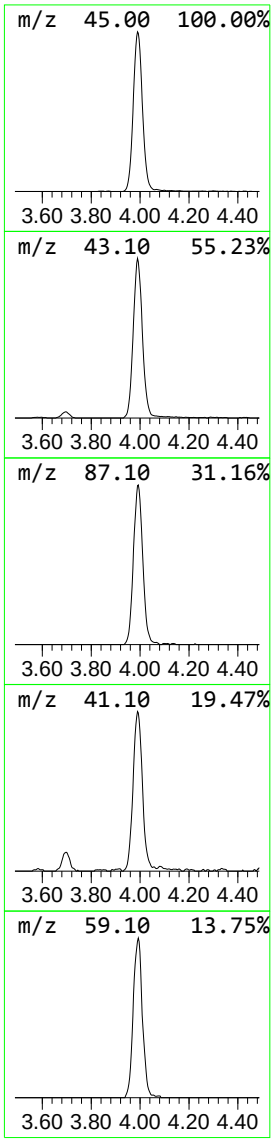
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Diisopropyl ether Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.989	5.28 ug/L	587619	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diisopropyl ether	102	C6H14O	000108-20-3	86
2	Diisopropyl ether	102	C6H14O	000108-20-3	86
3	Diisopropyl ether	102	C6H14O	000108-20-3	78
4	Diisopropyl ether	102	C6H14O	000108-20-3	78
5	Diisopropyl ether	102	C6H14O	000108-20-3	78





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102722\
Data File : VU051555.D
Acq On : 27 Oct 2022 21:46
Operator : JC/MD
Sample : N5300-11DL 20X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHA74DL

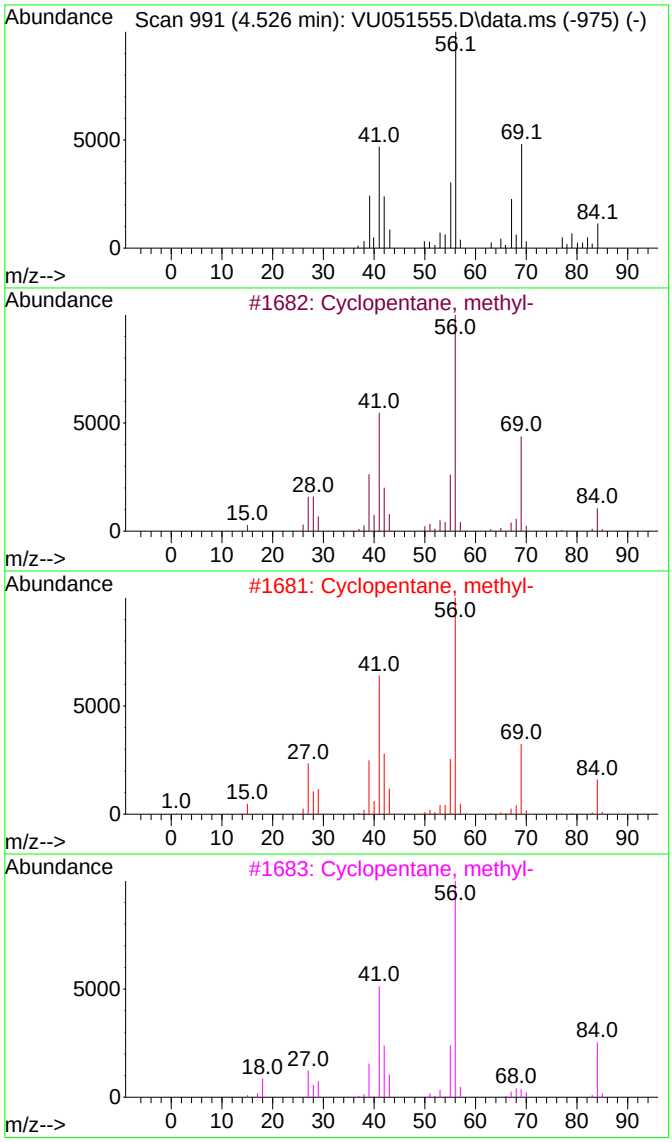
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.M
Quant Title : TRACE VOA SFAM1.0

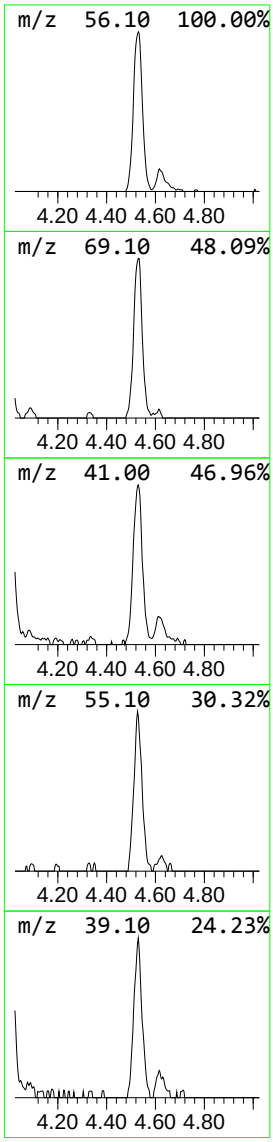
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (DEL) Alkane: Cyclic4.526 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.526	1.00 ug/L	111139	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	81
2	Cyclopentane, methyl-	84	C6H12	000096-37-7	64
3	Cyclopentane, methyl-	84	C6H12	000096-37-7	53
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	52
5	Cyclobutane, ethyl-	84	C6H12	004806-61-5	49





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102722\
Data File : VU051555.D
Acq On : 27 Oct 2022 21:46
Operator : JC/MD
Sample : N5300-11DL 20X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHA74DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.M
Quant Title : TRACE VOA SFAM1.0

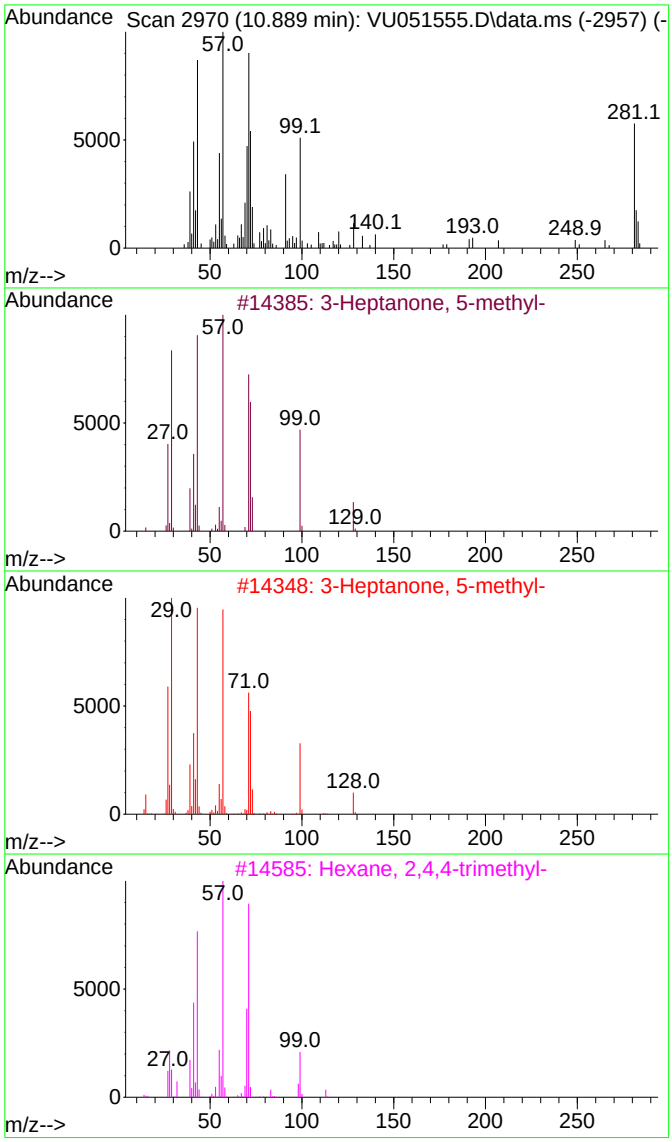
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

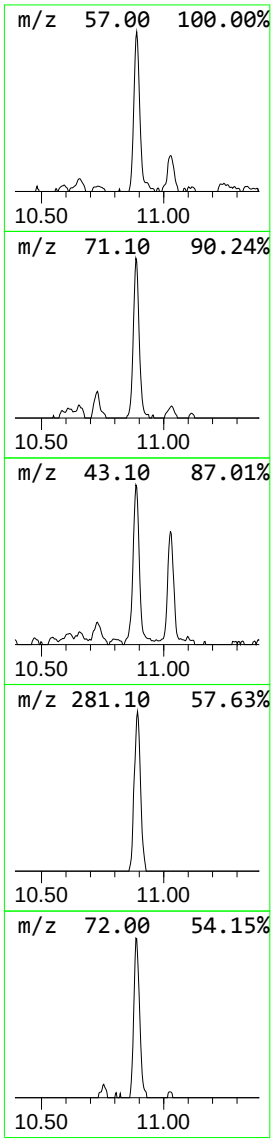
****

Peak Number 6 3-Heptanone, 5-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.890	1.14 ug/L	154538	1,4-Dichlorobenzene-d4	11.809

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Heptanone, 5-methyl-	128	C8H16O	000541-85-5	53
2	3-Heptanone, 5-methyl-	128	C8H16O	000541-85-5	49
3	Hexane, 2,4,4-trimethyl-	128	C9H20	016747-30-1	43
4	3-Heptanone, 6-methyl-	128	C8H16O	000624-42-0	38
5	Ethanone, 1-(2,2-dimethylcyclope...	140	C9H16O	003664-75-3	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102722\
Data File : VU051555.D
Acq On : 27 Oct 2022 21:46
Operator : JC/MD
Sample : N5300-11DL 20X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHA74DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.M
Quant Title : TRACE VOA SFAM1.0

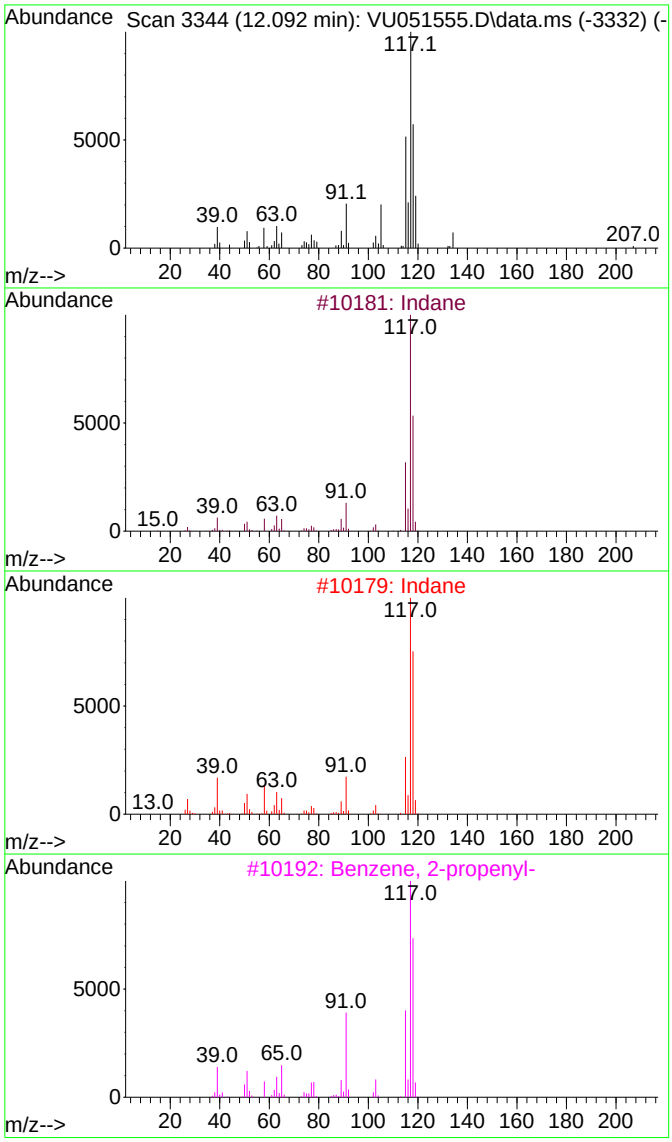
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

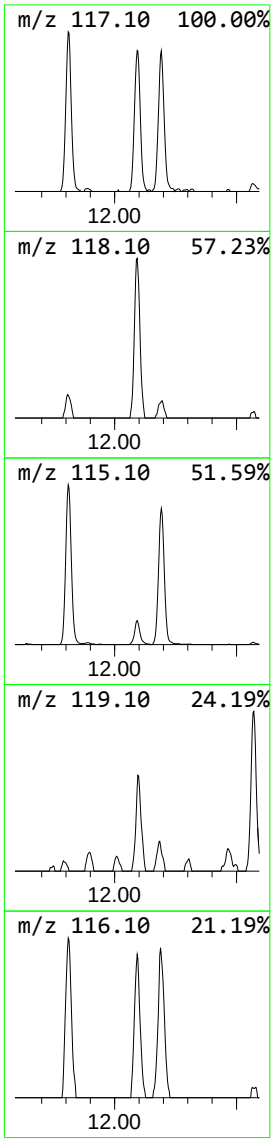
****

Peak Number 7 Indane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.092	0.62 ug/L	83296	1,4-Dichlorobenzene-d4	11.809

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	55
2	Indane	118	C9H10	000496-11-7	55
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	55
4	Indane	118	C9H10	000496-11-7	53
5	Benzene, cyclopropyl-	118	C9H10	000873-49-4	49





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Data File : VU051555.D
Acq On : 27 Oct 2022 21:46
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Sample : N5300-11DL 20X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHA74DL

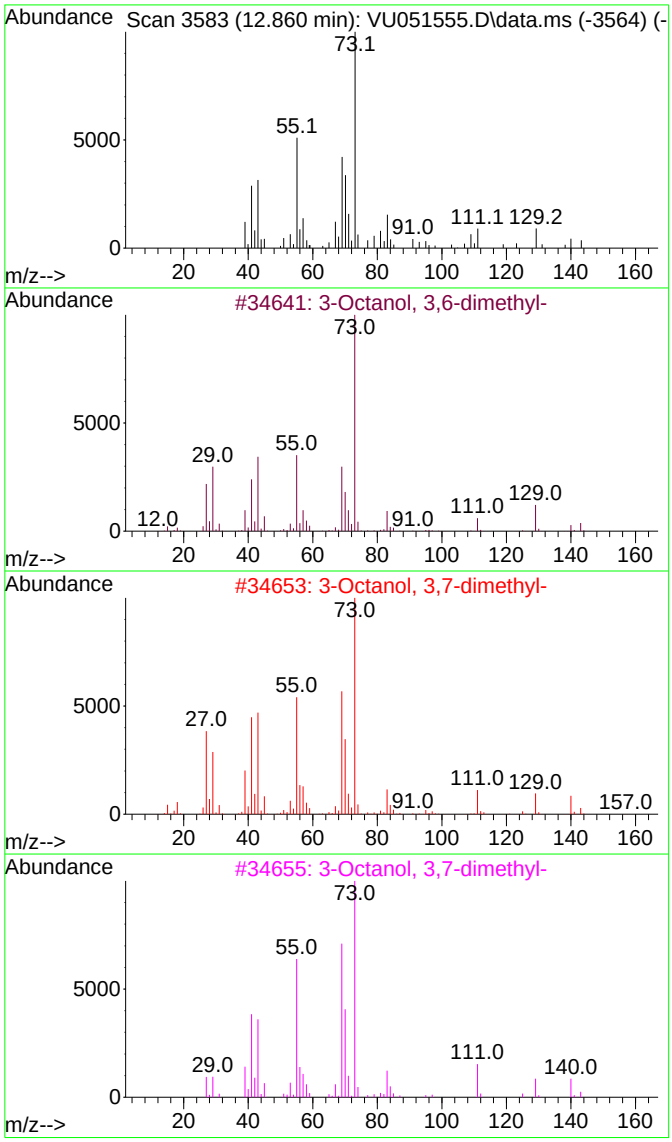
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.M
Quant Title : TRACE VOA SFAM1.0

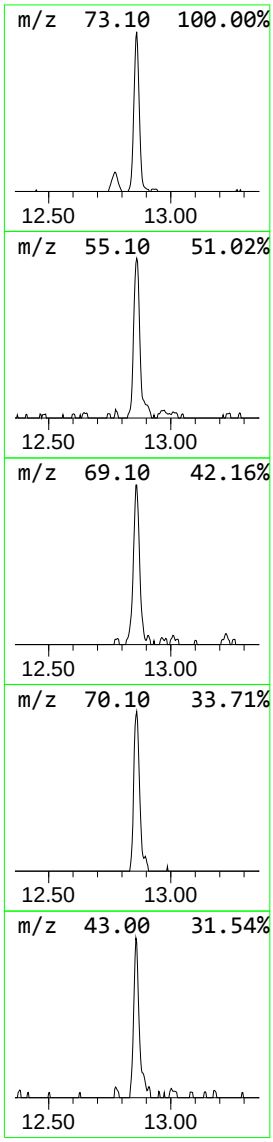
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 3-Octanol, 3,6-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.861	0.68 ug/L	91298	1,4-Dichlorobenzene-d4	11.809

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octanol, 3,6-dimethyl-	158	C10H22O	000151-19-9	59
2	3-Octanol, 3,7-dimethyl-	158	C10H22O	000078-69-3	50
3	3-Octanol, 3,7-dimethyl-	158	C10H22O	000078-69-3	50
4	3-Octanol, 3,7-dimethyl-	158	C10H22O	000078-69-3	47
5	4-Nonene, 3-methyl-, (Z)-	140	C10H20	063830-69-3	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102722\
Data File : VU051555.D
Acq On : 27 Oct 2022 21:46
Operator : JC/MD
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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHA74DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.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
Ethyl ether	2.375	1.9	ug/L	211242	1	6.247	556833	5.0
Diisopropyl ether	3.989	5.3	ug/L	587619	1	6.247	556833	5.0
(DEL) Alkane: C...	4.526	1.0	ug/L	111139	1	6.247	556833	5.0
3-Heptanone, 5-...	10.890	1.1	ug/L	154538	3	11.809	674964	5.0
Indane	12.092	0.6	ug/L	83296	3	11.809	674964	5.0
3-Octanol, 3,6-...	12.861	0.7	ug/L	91298	3	11.809	674964	5.0