LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070324\
Data File : VU059765.D
Acq On : 03 Jul 2024 02:20
Operator : MD/SY
Sample : P3121-19DL 20X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0BM6DL

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\SFAMUTR061724WMA.M
Title : TRACE VOA SFAM1.0

Signal : TIC: VU059765.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.358	14	21	36	rVB2	17897	21774	2.54%	0.329%
2	1.592	85	94	113	rVB	69220	89783	10.48%	1.355%
3	1.904	165	191	204	rBV	84943	167488	19.55%	2.528%
4	1.978	206	214	246	rVB	116051	225175	26.29%	3.398%
5	2.187	269	279	294	rVB2	51373	75606	8.83%	1.141%
6	2.554	381	393	413	rVB	107764	185411	21.65%	2.798%
7	3.033	529	542	548	rBV4	21396	44503	5.20%	0.672%
8	3.126	563	571	576	rBV3	5860	10002	1.17%	0.151%
9	3.174	577	586	606	rVB	16861	43118	5.03%	0.651%
10	3.345	626	639	657	rVB3	37959	83772	9.78%	1.264%
11	3.686	732	745	761	rBV5	12342	27165	3.17%	0.410%
12	4.518	986	1004	1023	rBV3	43941	107093	12.50%	1.616%
13	4.653	1023	1046	1082	rBV2	309384	856579	100.00%	12.927%
14	5.052	1157	1170	1184	rVV2	100373	225739	26.35%	3.407%
15	5.113	1184	1189	1204	rVB3	13505	26814	3.13%	0.405%
16	5.377	1256	1271	1285	rVV3	40377	96515	11.27%	1.457%
17	5.448	1285	1293	1312	rVB7	7039	19141	2.23%	0.289%
18	5.586	1319	1336	1341	rBV5	5258	10055	1.17%	0.152%
19	5.714	1358	1376	1403	rBV2	204880	535629	62.53%	8.084%
20	5.840	1404	1415	1424	rBV5	6098	10791	1.26%	0.163%
21	5.965	1444	1454	1470	rVB7	10914	28522	3.33%	0.430%
22	6.242	1527	1540	1572	rBV	193666	395698	46.20%	5.972%
23	6.537	1619	1632	1658	rBV5	42740	92877	10.84%	1.402%
24	6.682	1664	1677	1691	rBV	124014	246762	28.81%	3.724%
25	6.753	1691	1699	1715	rVB5	17416	37286	4.35%	0.563%
26	7.152	1813	1823	1829	rBV7	5968	11091	1.29%	0.167%
27	7.560	1935	1950	1972	rVB	55658	102615	11.98%	1.549%
28	7.891	2032	2053	2069	rBV	240142	426987	49.85%	6.444%
29	8.174	2127	2141	2155	rBV2	34224	60056	7.01%	0.906%
30	8.402	2204	2212	2225	rVB4	5280	8578	1.00%	0.129%
31	8.547	2246	2257	2270	rVB2	36485	62640	7.31%	0.945%
32	8.634	2272	2284	2313	rBV	240916	502405	58.65%	7.582%
33	9.412	2513	2526	2545	rBV	270757	463251	54.08%	6.991%
34	9.566	2563	2574	2588	rVB2	20132	32862	3.84%	0.496%
35	9.692	2603	2613	2625	rBV2	14134	25028	2.92%	0.378%
36	10.479	2850	2858	2866	rBV2	6777	9499	1.11%	0.143%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070324\
Data File : VU059765.D
Acq On : 03 Jul 2024 02:20
Operator : MD/SY
Sample : P3121-19DL 20X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0BM6DL

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\SFAMUTR061724WMA.M
Title : TRACE VOA SFAM1.0

37	10.750	2931	2942	2957	rBV	100677	164989	19.26%	2.490%
38	10.904	2977	2990	3002	rBV2	6612	11382	1.33%	0.172%
39	11.807	3259	3271	3289	rBV	251237	404992	47.28%	6.112%
40	12.090	3346	3359	3375	rBV3	28511	46107	5.38%	0.696%
41	12.187	3375	3389	3409	rBV	216494	366829	42.82%	5.536%
42	12.569	3498	3508	3514	rBV2	6168	9485	1.11%	0.143%
43	12.676	3530	3541	3554	rBV	53024	85321	9.96%	1.288%
44	12.968	3622	3632	3641	rBV3	17584	25843	3.02%	0.390%
45	13.286	3723	3731	3749	rVB	16794	27994	3.27%	0.422%
46	13.447	3765	3781	3796	rBV3	43190	71386	8.33%	1.077%
47	13.778	3876	3884	3893	rBV3	11170	17907	2.09%	0.270%
48	13.833	3893	3901	3910	rVV8	6171	9449	1.10%	0.143%
49	13.936	3927	3933	3942	rVB2	11104	16090	1.88%	0.243%

Sum of corrected areas: 6626084

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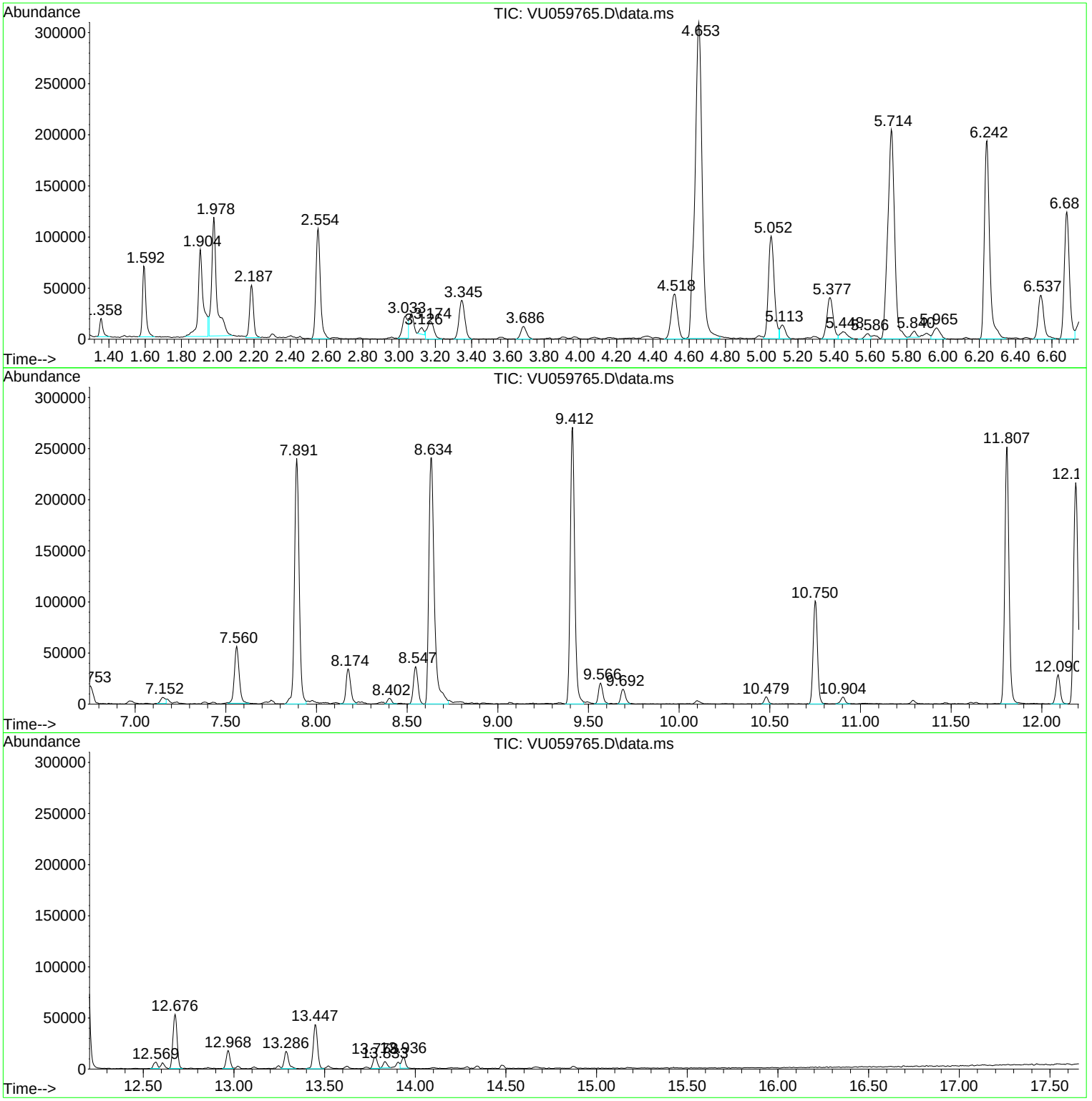
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0BM6DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.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\VU070324\
Data File : VU059765.D
Acq On : 03 Jul 2024 02:20
Operator : MD/SY
Sample : P3121-19DL 20X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0BM6DL

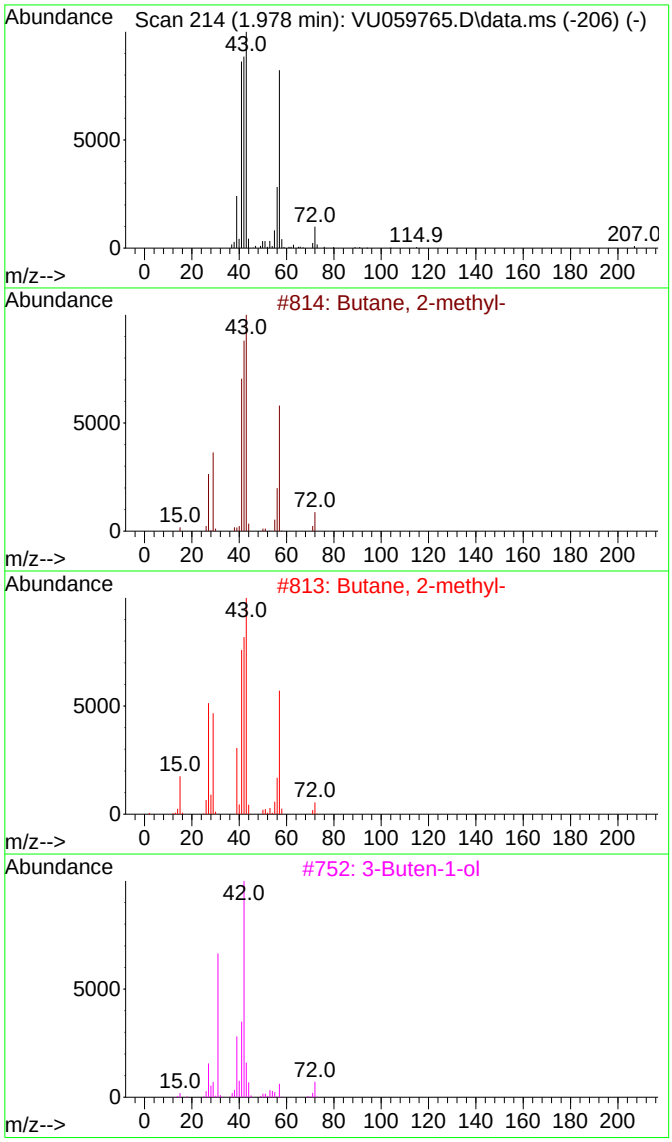
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

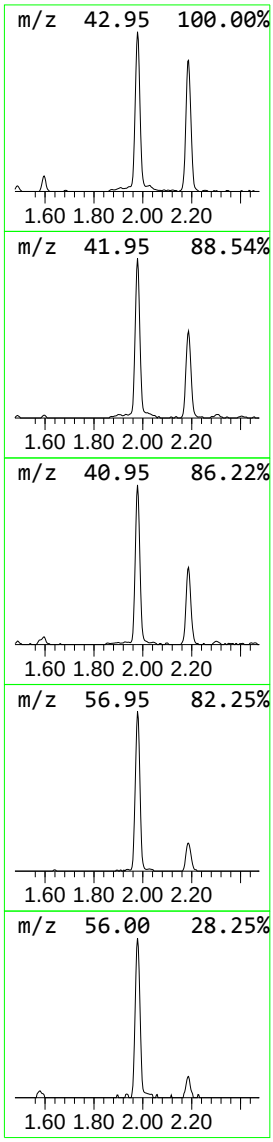
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.978	2.85 ug/L	225175	1,4-Difluorobenzene	6.242

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	87
2	Butane, 2-methyl-	72	C5H12	000078-78-4	86
3	3-Buten-1-ol	72	C4H8O	000627-27-0	43
4	Pentane	72	C5H12	000109-66-0	42
5	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	36





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070324\
Data File : VU059765.D
Acq On : 03 Jul 2024 02:20
Operator : MD/SY
Sample : P3121-19DL 20X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0BM6DL

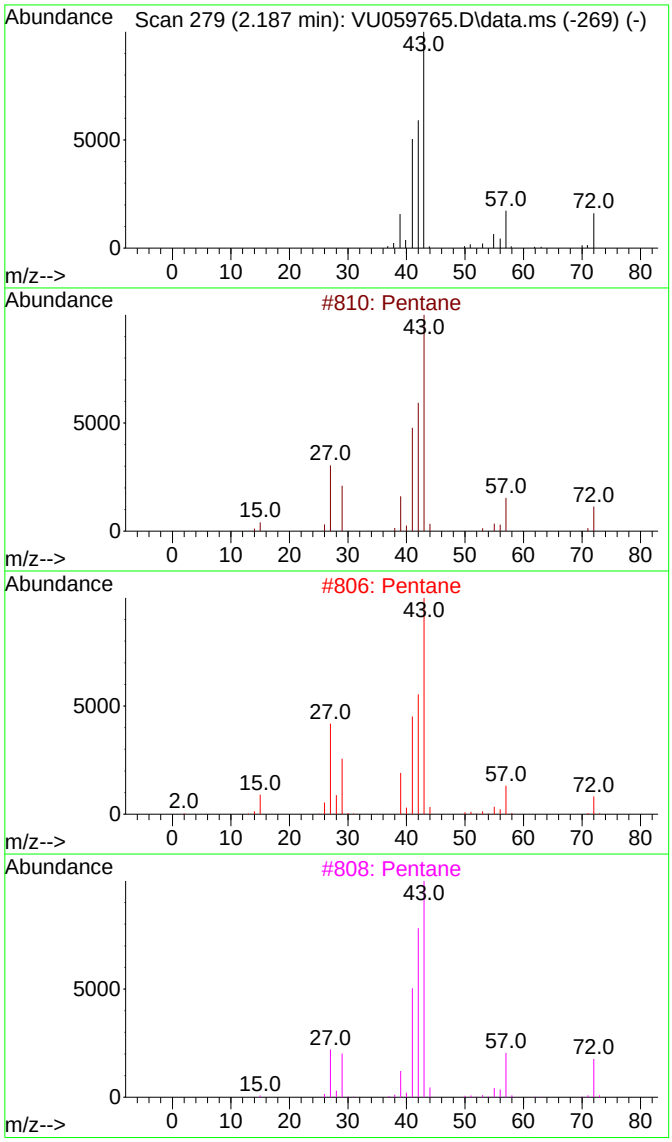
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

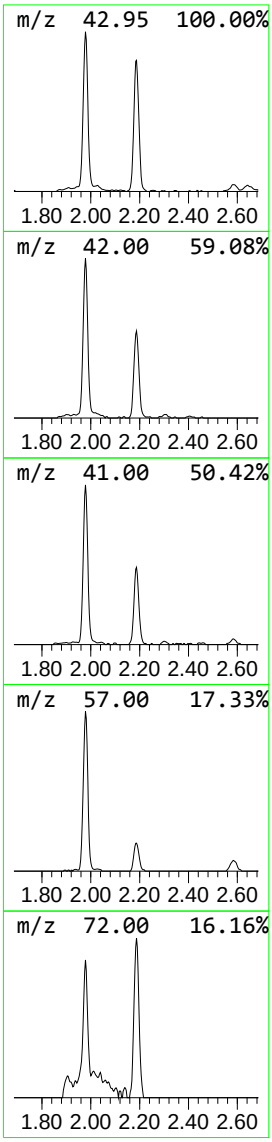
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.187	0.96 ug/L	75606	1,4-Difluorobenzene	6.242

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	90
2	Pentane	72	C5H12	000109-66-0	86
3	Pentane	72	C5H12	000109-66-0	86
4	Pentane	72	C5H12	000109-66-0	86
5	Pentane	72	C5H12	000109-66-0	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070324\
Data File : VU059765.D
Acq On : 03 Jul 2024 02:20
Operator : MD/SY
Sample : P3121-19DL 20X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0BM6DL

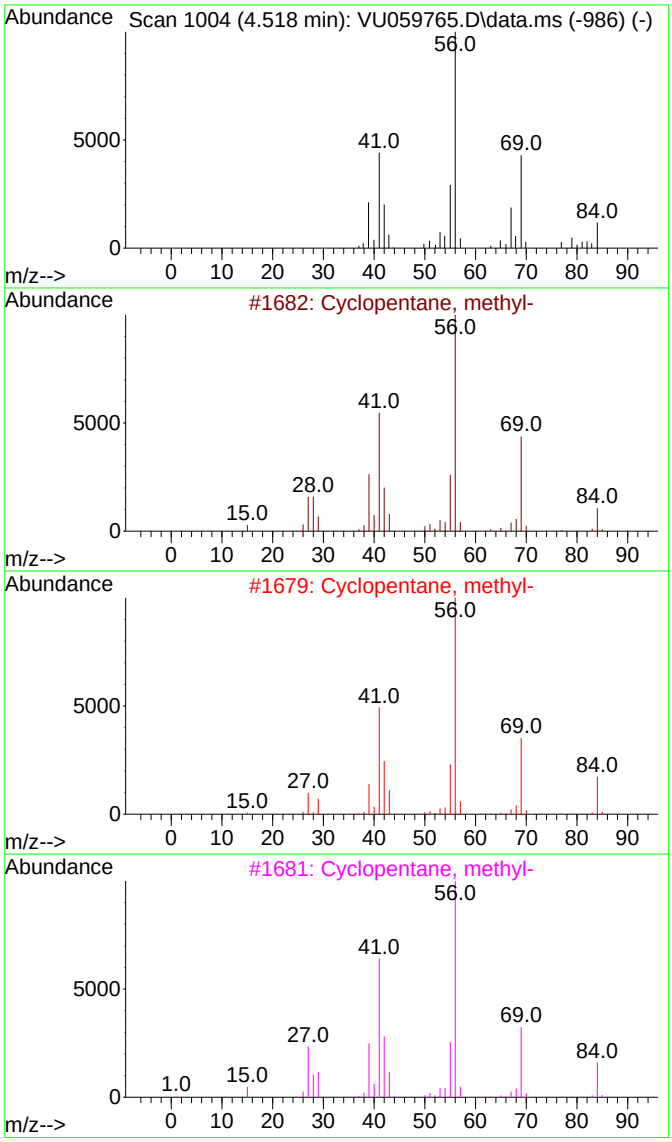
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

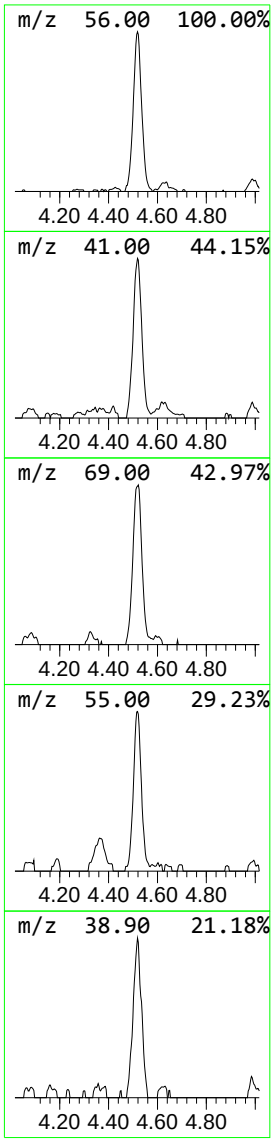
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (DEL) Alkane: Cyclic4.518 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.518	1.35 ug/L	107093	1,4-Difluorobenzene	6.242

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	87
2	Cyclopentane, methyl-	84	C6H12	000096-37-7	72
3	Cyclopentane, methyl-	84	C6H12	000096-37-7	72
4	Cyclopentane, methyl-	84	C6H12	000096-37-7	64
5	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	58





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070324\
Data File : VU059765.D
Acq On : 03 Jul 2024 02:20
Operator : MD/SY
Sample : P3121-19DL 20X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0BM6DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

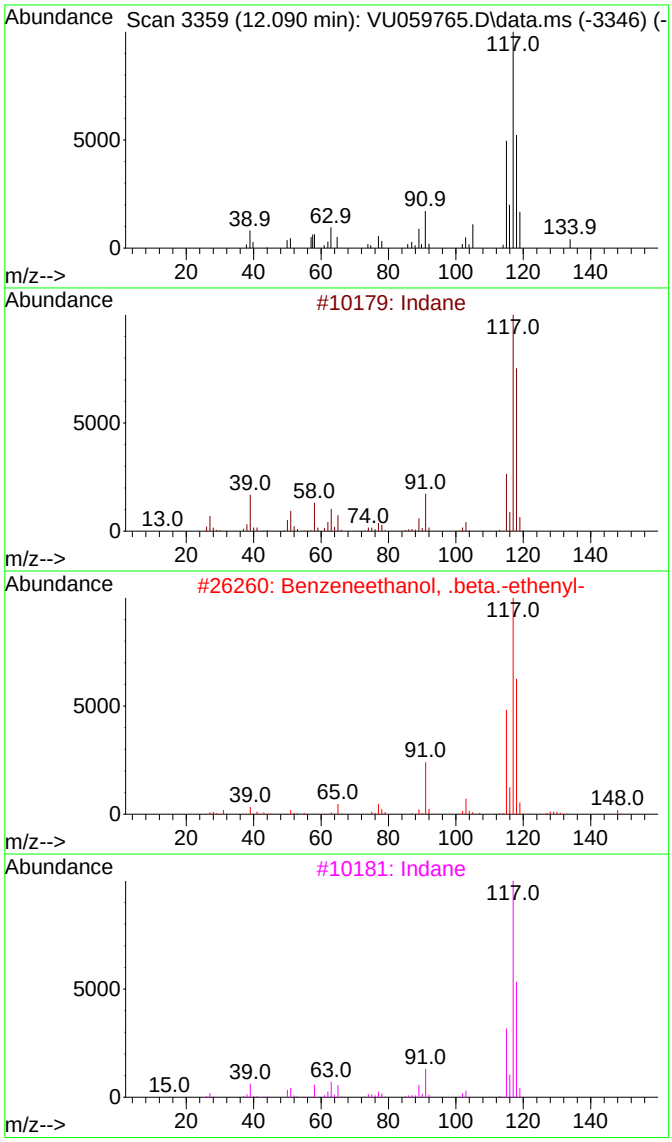
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

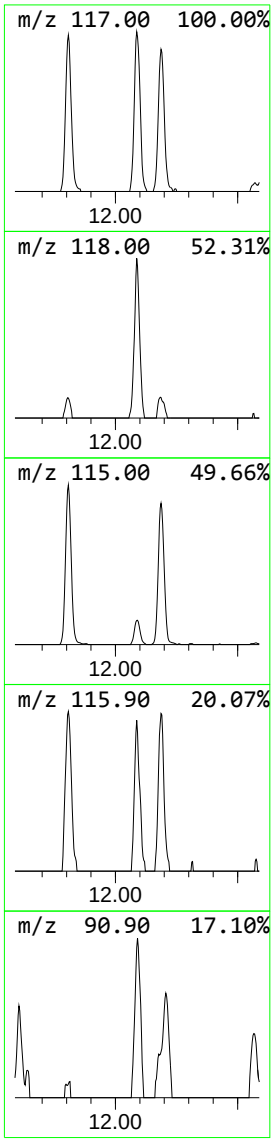
****

Peak Number 6 Indane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.090	0.57 ug/L	46107	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	64
2	Benzeneethanol, .beta.-ethenyl-	148	C10H12O	006052-63-7	64
3	Indane	118	C9H10	000496-11-7	64
4	Benzene, cyclopropyl-	118	C9H10	000873-49-4	53
5	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	53





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ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0BM6DL

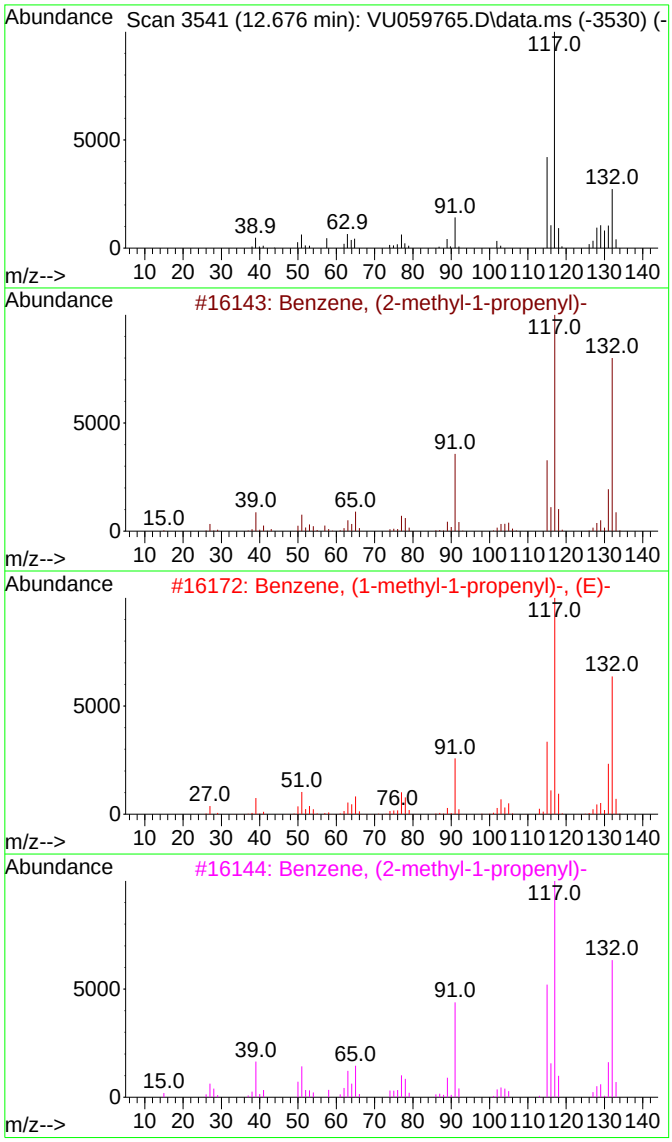
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

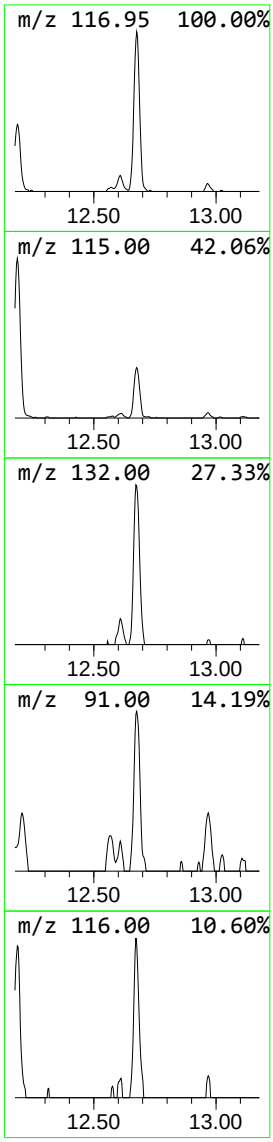
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, (2-methyl-1-propen... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.676	1.05 ug/L	85321	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	86
2	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	83
3	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	83
4	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	80
5	(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	80





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MSVOA_U
ClientSampleId :
C0BM6DL

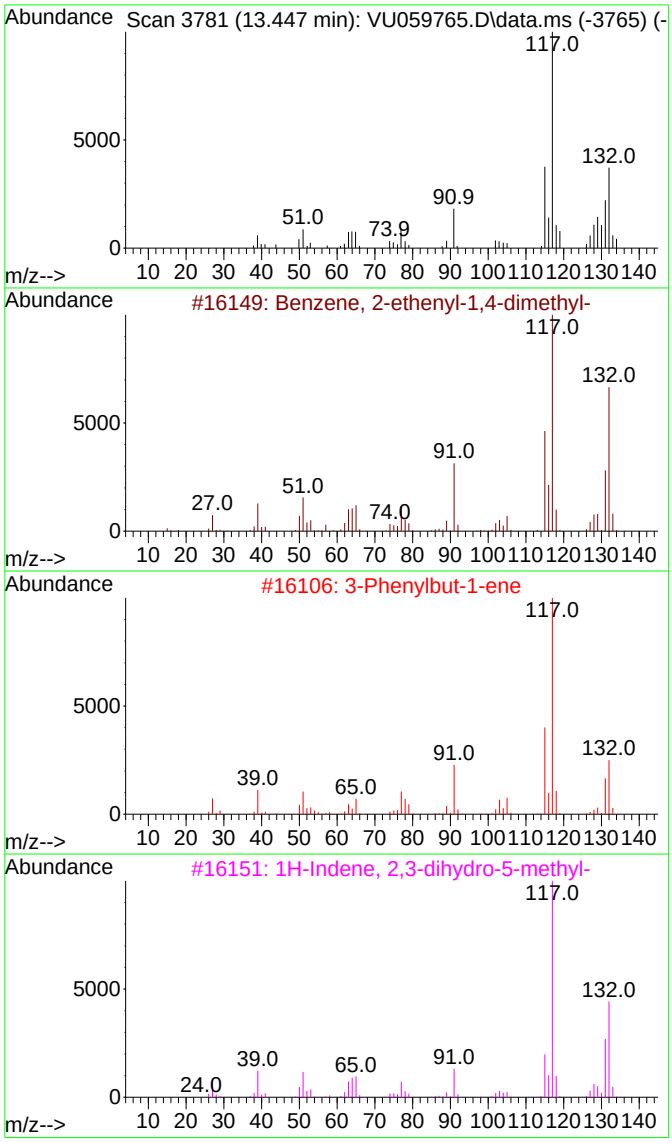
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

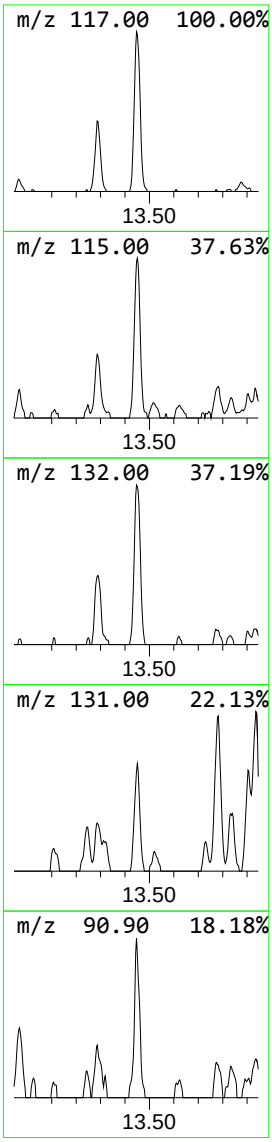
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.447	0.88 ug/L	71386	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	93
2	3-Phenylbut-1-ene	132	C10H12	000934-10-1	83
3	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	81
4	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	81
5	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	76





Tentatively Identified Compound (LSC) summary

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Data File : VU059765.D
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Instrument :
MSVOA_U
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C0BM6DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.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
(DEL) Alkane: S...	1.978	2.9	ug/L	225175	1	6.242	395698	5.0
(DEL) Alkane: S...	2.187	1.0	ug/L	75606	1	6.242	395698	5.0
(DEL) Alkane: C...	4.518	1.4	ug/L	107093	1	6.242	395698	5.0
Indane	12.090	0.6	ug/L	46107	3	11.807	404992	5.0
Benzene, (2-met...	12.676	1.1	ug/L	85321	3	11.807	404992	5.0
Benzene, 2-ethe...	13.447	0.9	ug/L	71386	3	11.807	404992	5.0