

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122322\
 Data File : VU052546.D
 Acq On : 23 Dec 2022 18:42
 Operator : JC/MD
 Sample : N6171-19
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 GBQD5

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\SFAMUTR122022WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VU052546.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.395	3	17	57	rVB	6863964	14954478	100.00%	68.111%
2	1.970	179	196	216	rBV2	83812	191256	1.28%	0.871%
3	2.790	435	451	476	rVB2	186823	575408	3.85%	2.621%
4	3.822	761	772	794	rBV3	84857	223039	1.49%	1.016%
5	4.343	925	934	953	rVB3	64055	150509	1.01%	0.686%
6	4.652	1019	1030	1053	rVB	158680	334577	2.24%	1.524%
7	5.645	1327	1339	1365	rVB	367255	851857	5.70%	3.880%
8	6.546	1608	1619	1625	rBV3	73313	169877	1.14%	0.774%
9	6.616	1629	1641	1663	rVB5	258097	808399	5.41%	3.682%
10	6.951	1735	1745	1777	rVB	223257	426141	2.85%	1.941%
11	7.301	1841	1854	1885	rBV	141847	312389	2.09%	1.423%
12	8.272	2132	2156	2173	rBV	302983	560817	3.75%	2.554%
13	8.880	2326	2345	2363	rBV	250058	664759	4.45%	3.028%
14	9.603	2559	2570	2582	rBV	257551	442322	2.96%	2.015%
15	10.832	2941	2952	2969	rVB	105279	199792	1.34%	0.910%
16	11.857	3260	3271	3287	rBV	244849	421965	2.82%	1.922%
17	12.230	3374	3387	3405	rVB	287172	491559	3.29%	2.239%
18	15.751	4474	4482	4500	rBV2	104075	176905	1.18%	0.806%

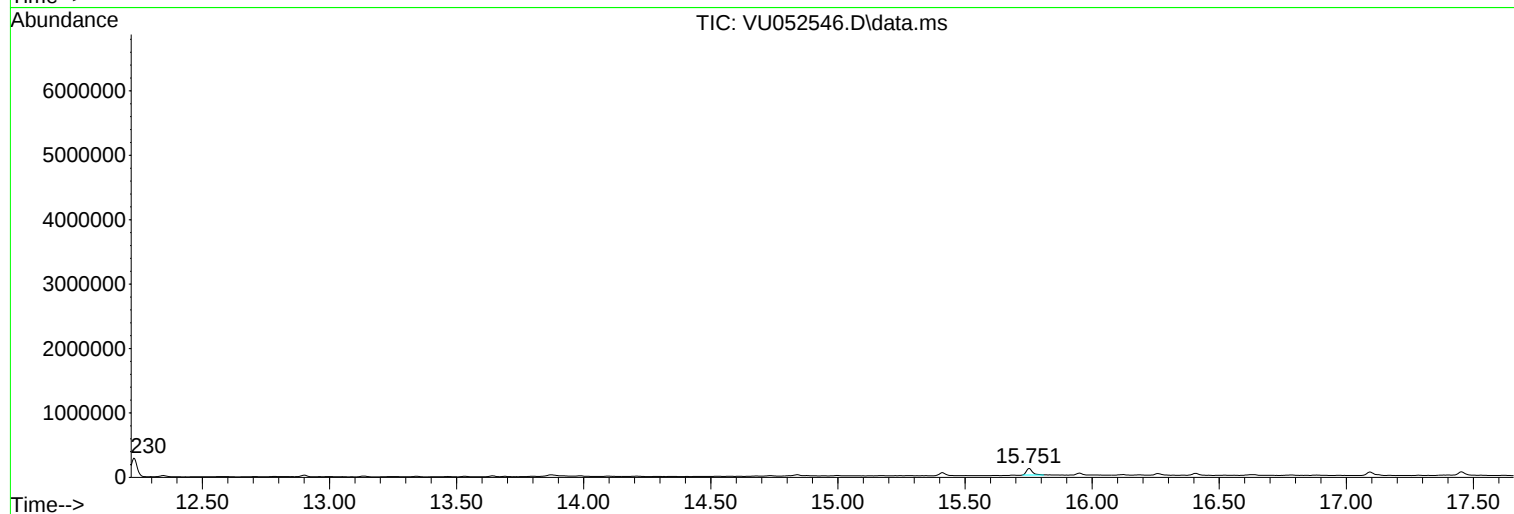
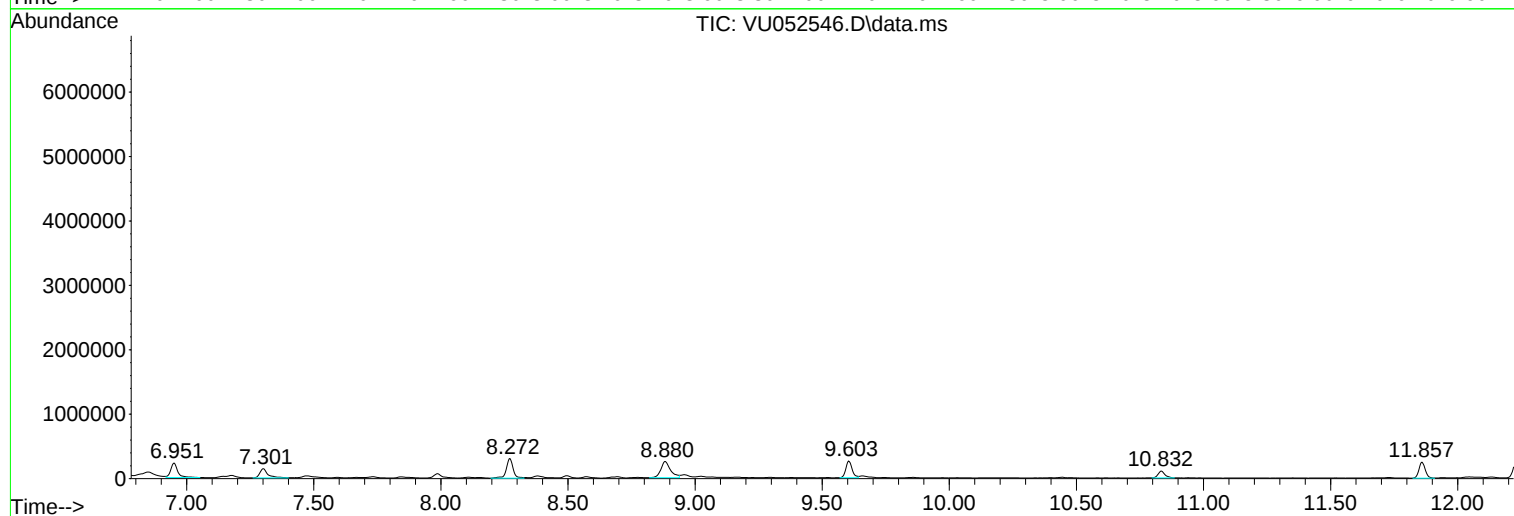
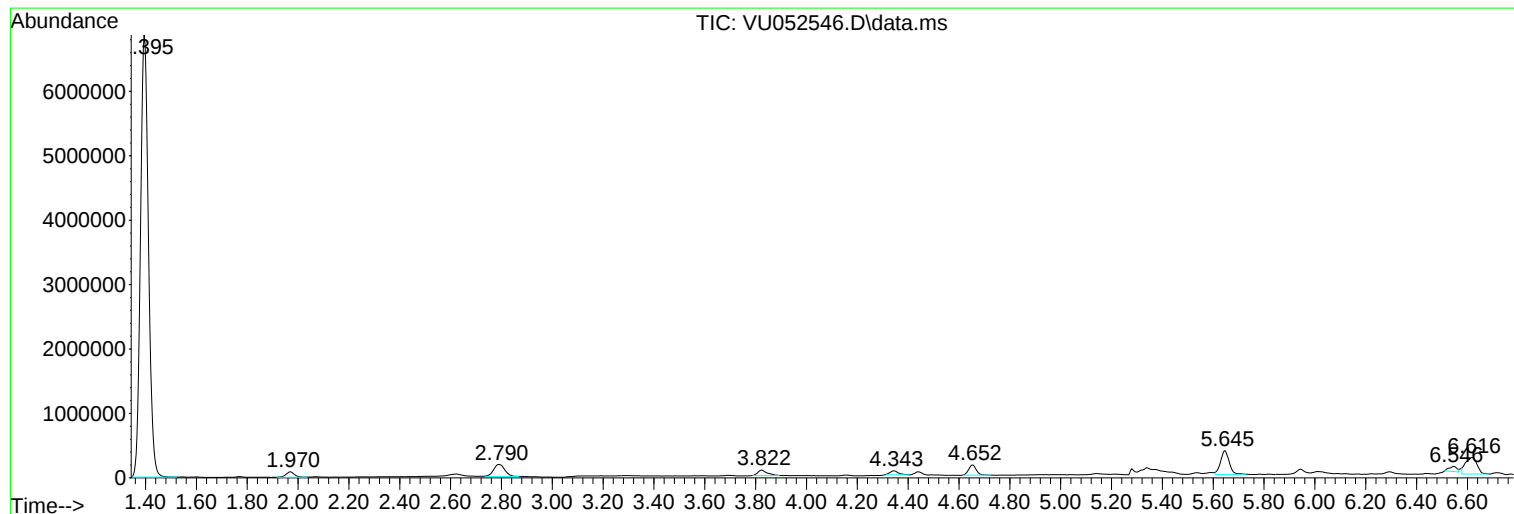
Sum of corrected areas: 21956049

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122322\
Data File : VU052546.D
Acq On : 23 Dec 2022 18:42
Operator : JC/MD
Sample : N6171-19
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQD5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.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\VU122322\
Data File : VU052546.D
Acq On : 23 Dec 2022 18:42
Operator : JC/MD
Sample : N6171-19
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQD5

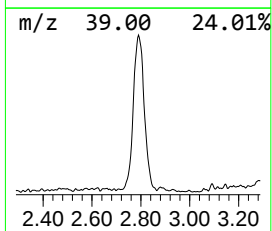
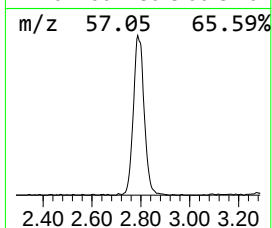
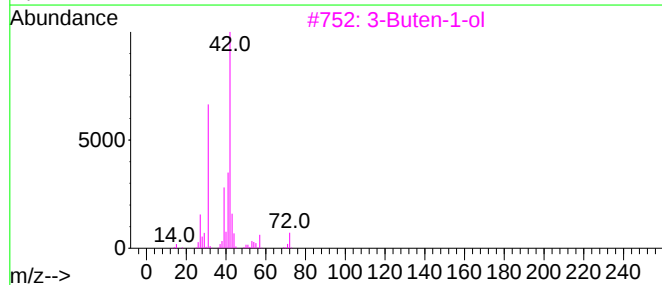
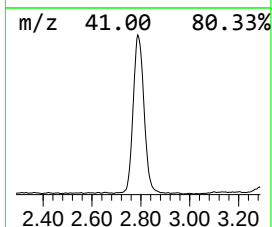
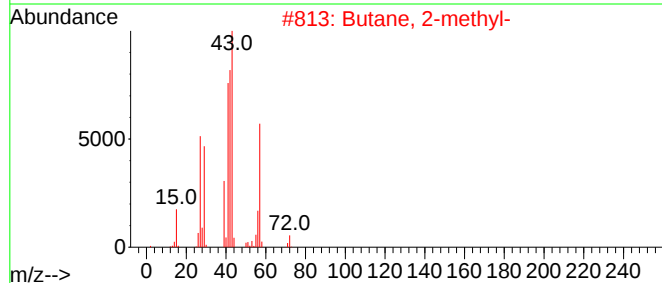
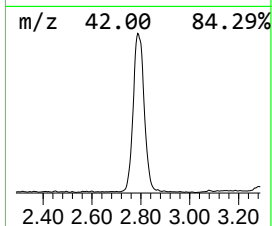
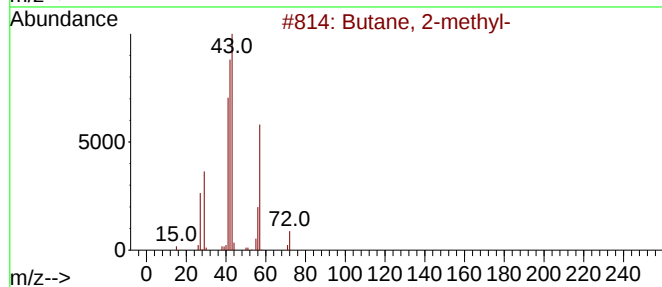
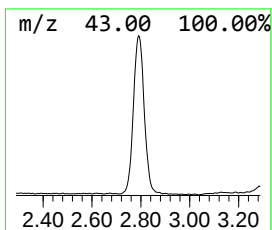
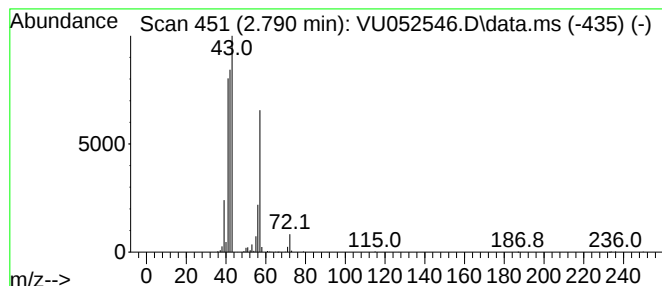
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.790	6.75 ug/L	575408	1,4-Difluorobenzene	6.951

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methyl-	72	C5H12	000078-78-4	90
2		Butane, 2-methyl-	72	C5H12	000078-78-4	90
3		3-Buten-1-ol	72	C4H8O	000627-27-0	47
4		Pentane	72	C5H12	000109-66-0	39
5		1-Butene	56	C4H8	000106-98-9	10



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122322\
Data File : VU052546.D
Acq On : 23 Dec 2022 18:42
Operator : JC/MD
Sample : N6171-19
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQD5

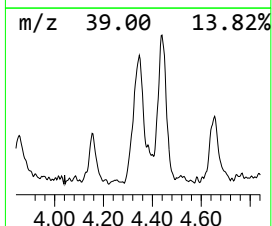
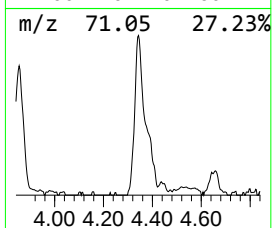
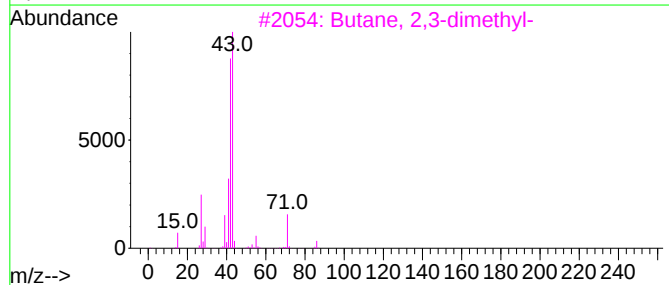
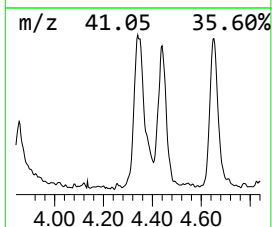
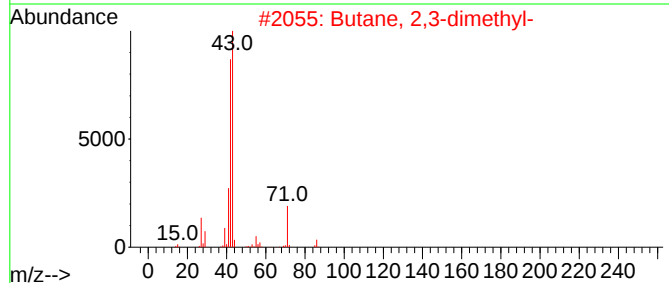
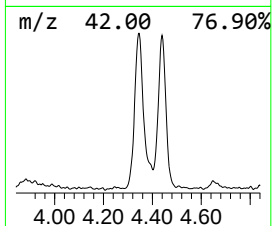
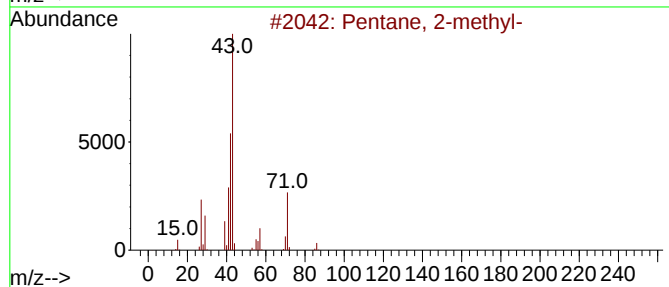
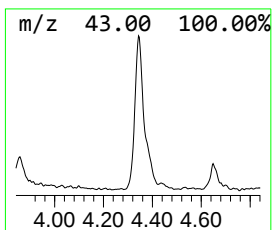
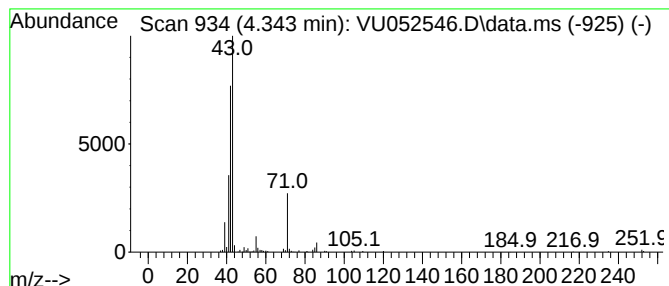
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.343	1.77 ug/L	150509	1,4-Difluorobenzene	6.951

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-methyl-	86	C6H14	000107-83-5	78
2			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	78
3			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	72
4			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	64
5			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122322\
Data File : VU052546.D
Acq On : 23 Dec 2022 18:42
Operator : JC/MD
Sample : N6171-19
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQD5

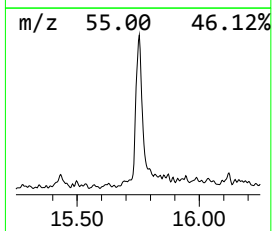
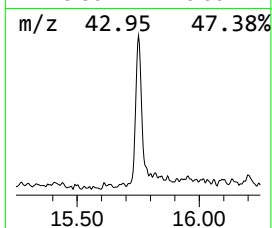
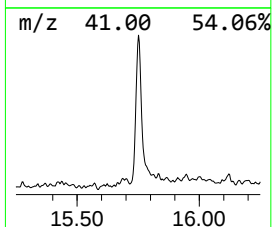
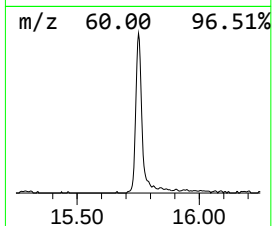
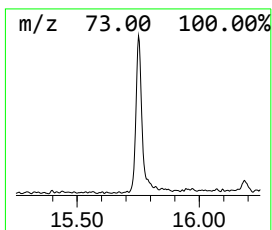
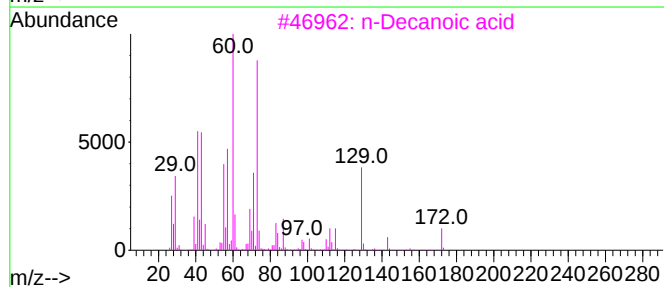
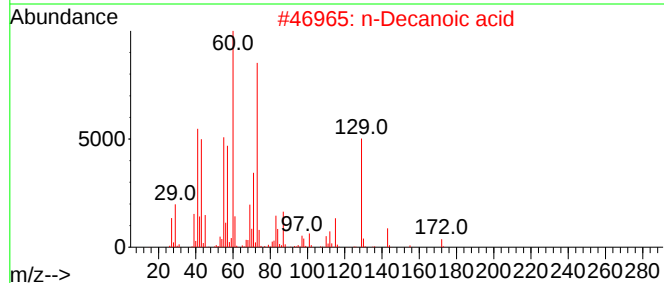
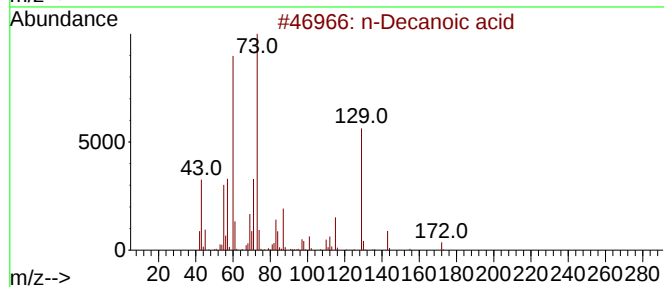
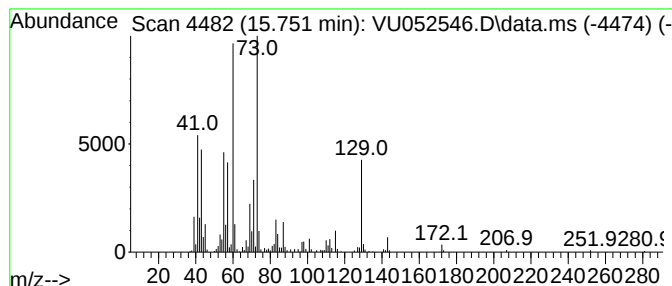
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 n-Decanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.751	2.10 ug/L	176905	1,4-Dichlorobenzene-d4	11.861

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Decanoic acid	172	C10H20O2	000334-48-5	97
2			n-Decanoic acid	172	C10H20O2	000334-48-5	97
3			n-Decanoic acid	172	C10H20O2	000334-48-5	78
4			n-Decanoic acid	172	C10H20O2	000334-48-5	76
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122322\
Data File : VU052546.D
Acq On : 23 Dec 2022 18:42
Operator : JC/MD
Sample : N6171-19
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQD5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	2.790	6.8	ug/L	575408	1	6.951	426141	5.0
(DEL) Alkane: S...	4.343	1.8	ug/L	150509	1	6.951	426141	5.0
n-Decanoic acid	15.751	2.1	ug/L	176905	3	11.861	421965	5.0