LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122822\
Data File : VU052592.D
Acq On : 28 Dec 2022 16:38
Operator : JC/MD
Sample : N6171-18
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQD4

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: VU052592.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.514	28	54	94	rBV	6693377	15554686	100.00%	45.949%
2	2.993	504	514	536	rBV10	1829803	3333703	21.43%	9.848%
3	4.227	889	898	929	rBV10	1752337	2871126	18.46%	8.481%
4	6.185	1497	1507	1525	rVB	120750	227847	1.46%	0.673%
5	6.655	1631	1653	1657	rBV2	246393	539213	3.47%	1.593%
6	6.687	1658	1663	1683	rVB	324703	537837	3.46%	1.589%
7	7.009	1751	1763	1788	rVB	232352	408574	2.63%	1.207%
8	7.353	1857	1870	1887	rBV	141144	260863	1.68%	0.771%
9	8.304	2152	2166	2179	rBV	253003	426835	2.74%	1.261%
10	8.896	2329	2350	2366	rBV	270914	725905	4.67%	2.144%
11	9.037	2381	2394	2408	rBV	552343	997327	6.41%	2.946%
12	9.619	2561	2575	2587	rBV	282395	483905	3.11%	1.429%
13	10.446	2819	2832	2853	rBV2	194345	362831	2.33%	1.072%
14	10.838	2942	2954	2972	rVB	112190	211555	1.36%	0.625%
15	11.729	3213	3231	3260	rBV	899071	1430688	9.20%	4.226%
16	11.860	3260	3272	3286	rVV	327723	556900	3.58%	1.645%
17	11.938	3286	3296	3310	rVB	147343	241760	1.55%	0.714%
18	12.233	3375	3388	3400	rBV	272408	460305	2.96%	1.360%
19	12.709	3523	3536	3552	rBV	353631	607306	3.90%	1.794%
20	12.899	3583	3595	3620	rBV	893848	1358089	8.73%	4.012%
21	13.465	3759	3771	3783	rBV3	136740	241623	1.55%	0.714%
22	13.983	3926	3932	3949	rVB	137687	208057	1.34%	0.615%
23	15.410	4364	4376	4402	rBV	367750	612776	3.94%	1.810%
24	17.455	4999	5012	5052	rBV	578290	1192667	7.67%	3.523%

Sum of corrected areas: 33852378

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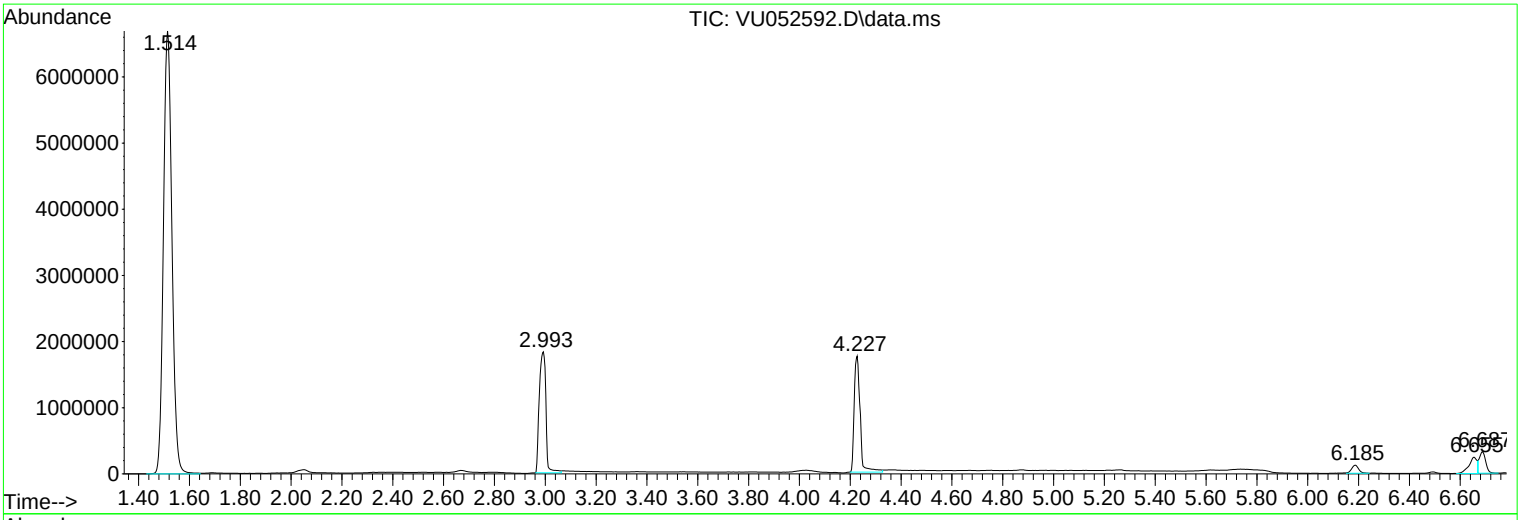
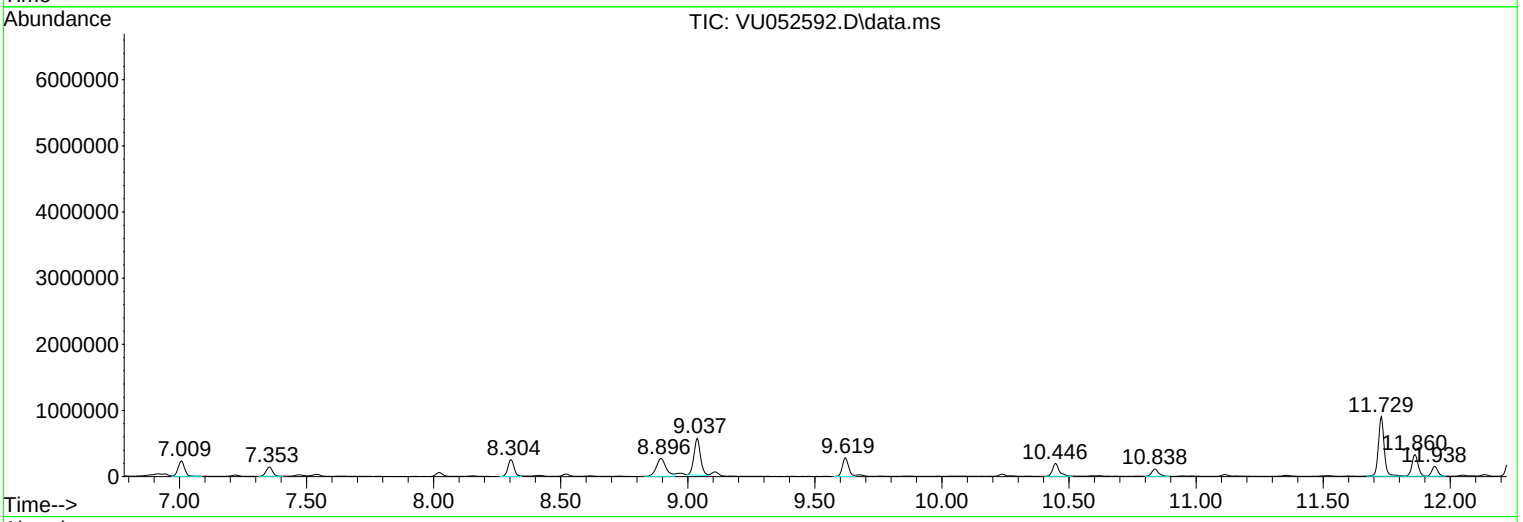
Sample : N6171-18
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

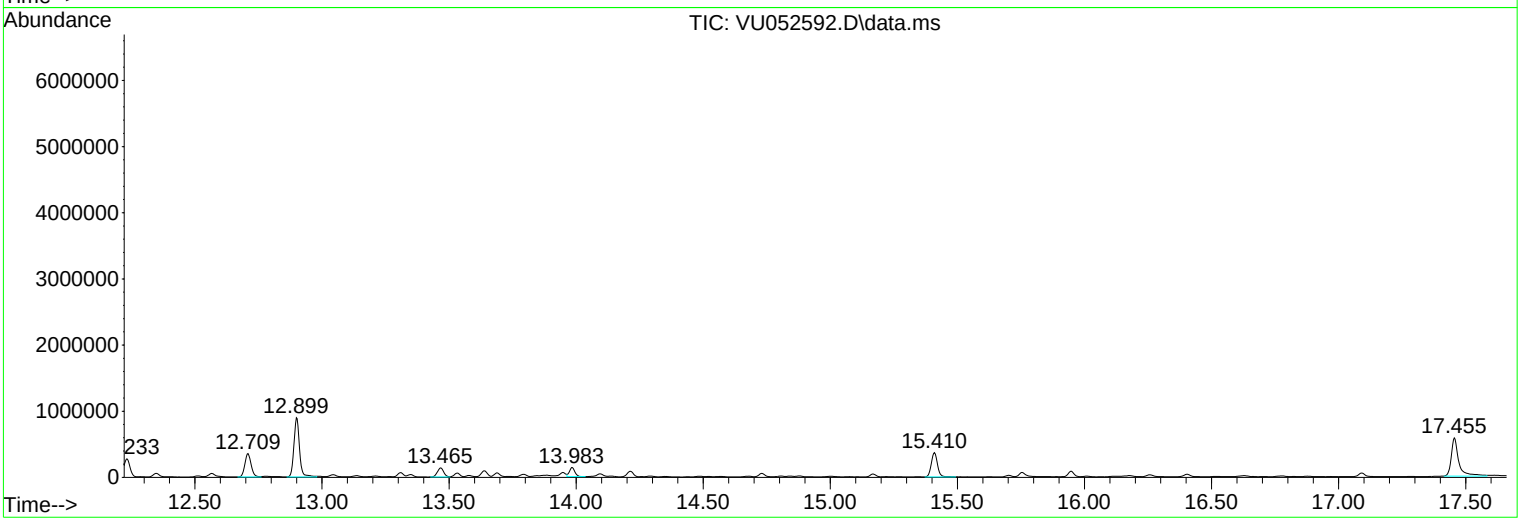
Instrument :
MSVOA_U
ClientSampleId :
GBQD4

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\VU122822\
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Instrument :
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GBQD4

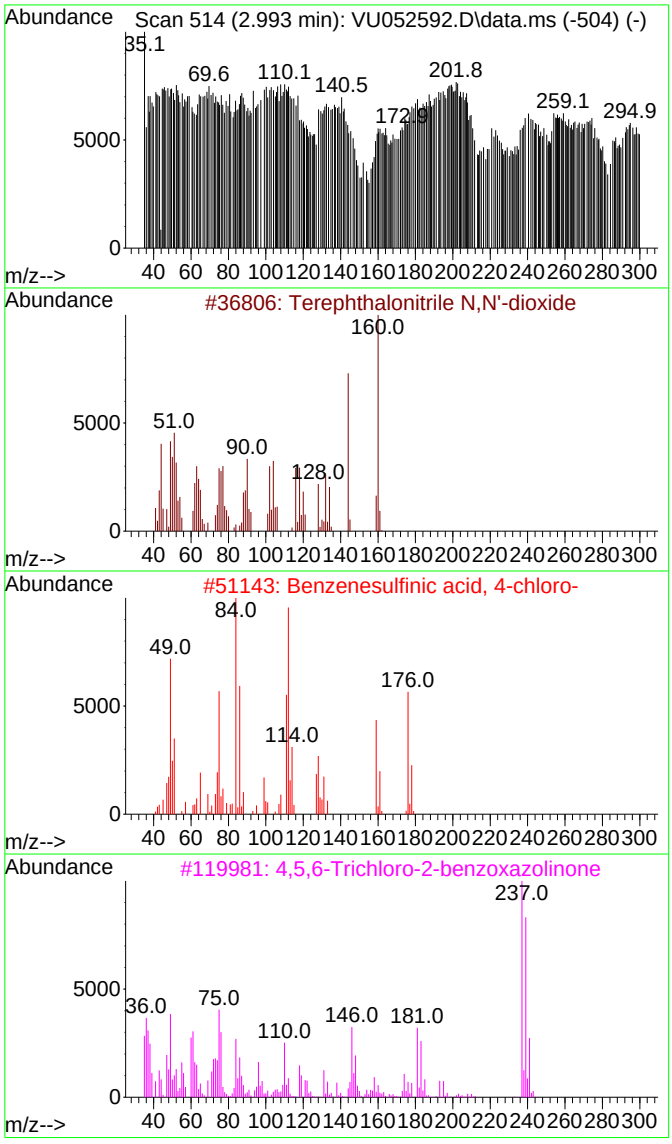
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

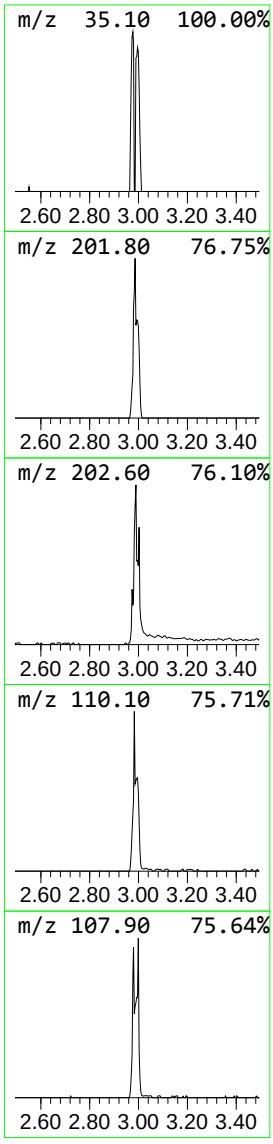
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Terephthalonitrile N,N'-dio... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.993	40.80 ug/L	3333700	1,4-Difluorobenzene	7.009

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Terephthalonitrile N,N'-dioxide	160	C8H4N2O2	003729-34-8	95
2	Benzenesulfinic acid, 4-chloro-	176	C6H5ClO2S	000100-03-8	55
3	4,5,6-Trichloro-2-benzoxazolinone	237	C7H2Cl3NO2	050995-94-3	52
4	Benzene, 1-(difluoroisocyanatome...	214	C8H4F2N2O3	055669-96-0	46
5	Benzaldehyde, (1,4-dihydro-6-met...	228	C12H12N4O	058010-88-1	46





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122822\
Data File : VU052592.D
Acq On : 28 Dec 2022 16:38
Operator : JC/MD
Sample : N6171-18
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQD4

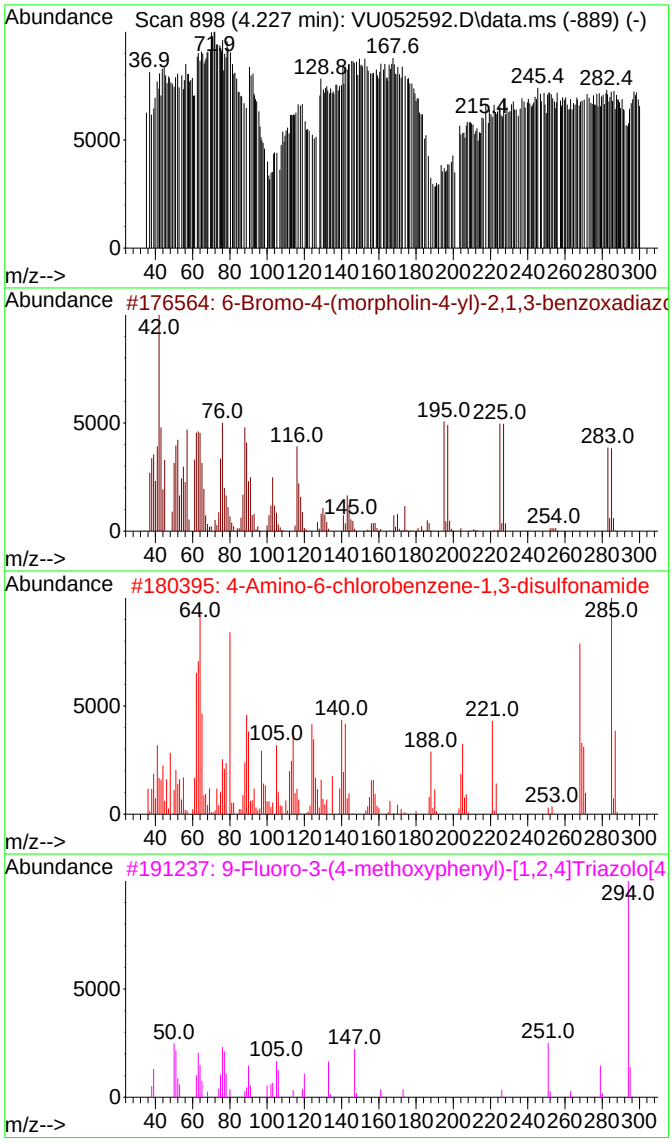
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

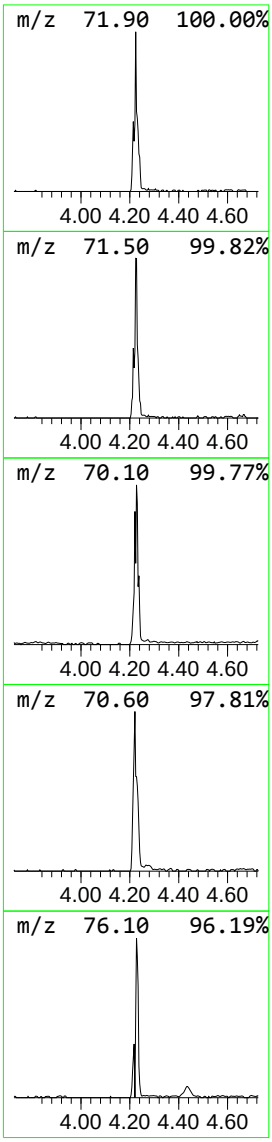
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 6-Bromo-4-(morpholin-4-yl)-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.227	35.14 ug/L	2871130	1,4-Difluorobenzene	7.009

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Bromo-4-(morpholin-4-yl)-2,1,3...	283	C10H10BrN3O2	1000389-05-2	84
2	4-Amino-6-chlorobenzene-1,3-disu...	285	C6H8ClN3O4S2	000121-30-2	74
3	9-Fluoro-3-(4-methoxyphenyl)-[1,...	294	C16H11FN4O	1000388-73-8	55
4	2(1H)-Quinoxalinone, 4-(2-chloro...	252	C12H13ClN2O2	1000362-81-0	55
5	[1,2,4]Triazolo[4,3-a]quinoxalin...	198	C11H10N4	1000362-67-9	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122822\
Data File : VU052592.D
Acq On : 28 Dec 2022 16:38
Operator : JC/MD
Sample : N6171-18
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQD4

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

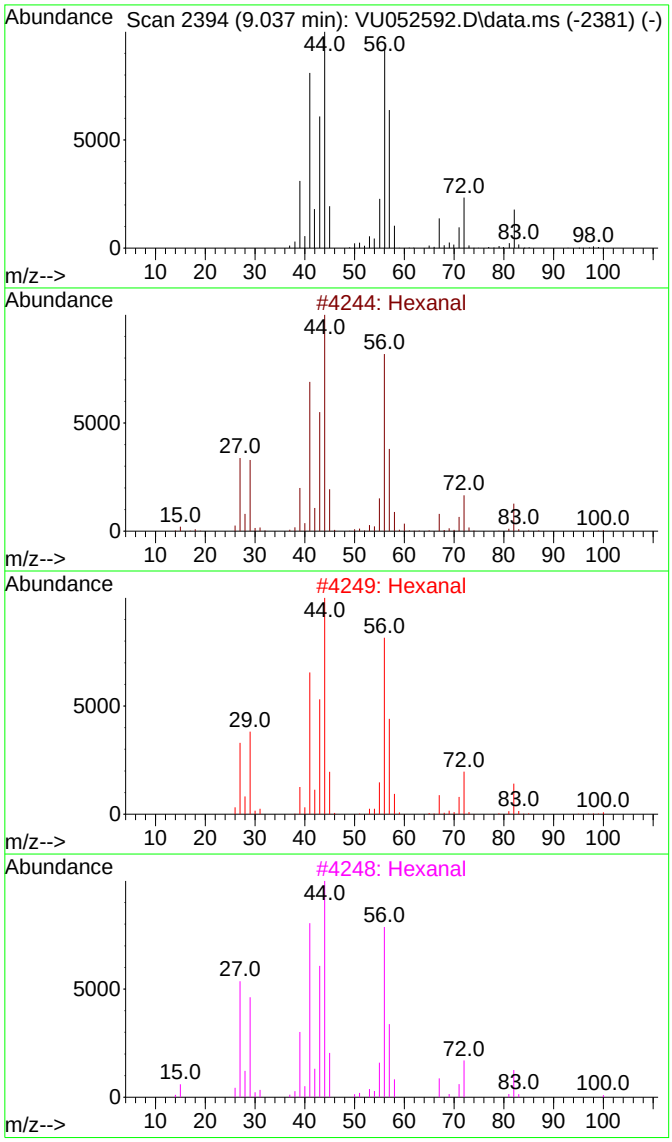
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

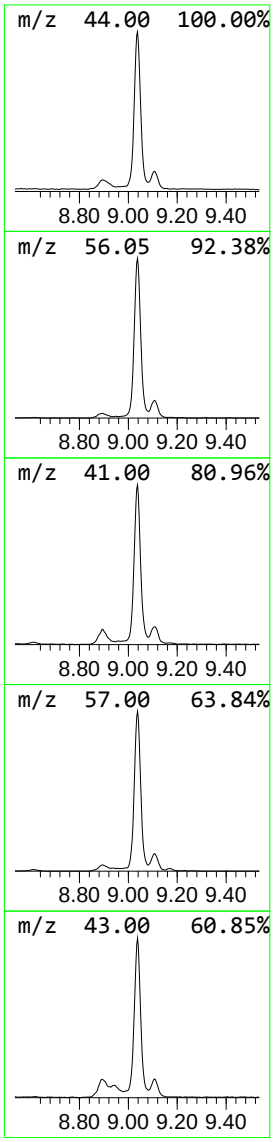
****

Peak Number 4 Hexanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.037	10.31 ug/L	997327	Chlorobenzene-d5	9.619

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal	100	C6H12O	000066-25-1	90
2	Hexanal	100	C6H12O	000066-25-1	90
3	Hexanal	100	C6H12O	000066-25-1	90
4	Hexanal	100	C6H12O	000066-25-1	83
5	Hexanal	100	C6H12O	000066-25-1	83





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122822\
Data File : VU052592.D
Acq On : 28 Dec 2022 16:38
Operator : JC/MD
Sample : N6171-18
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQD4

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

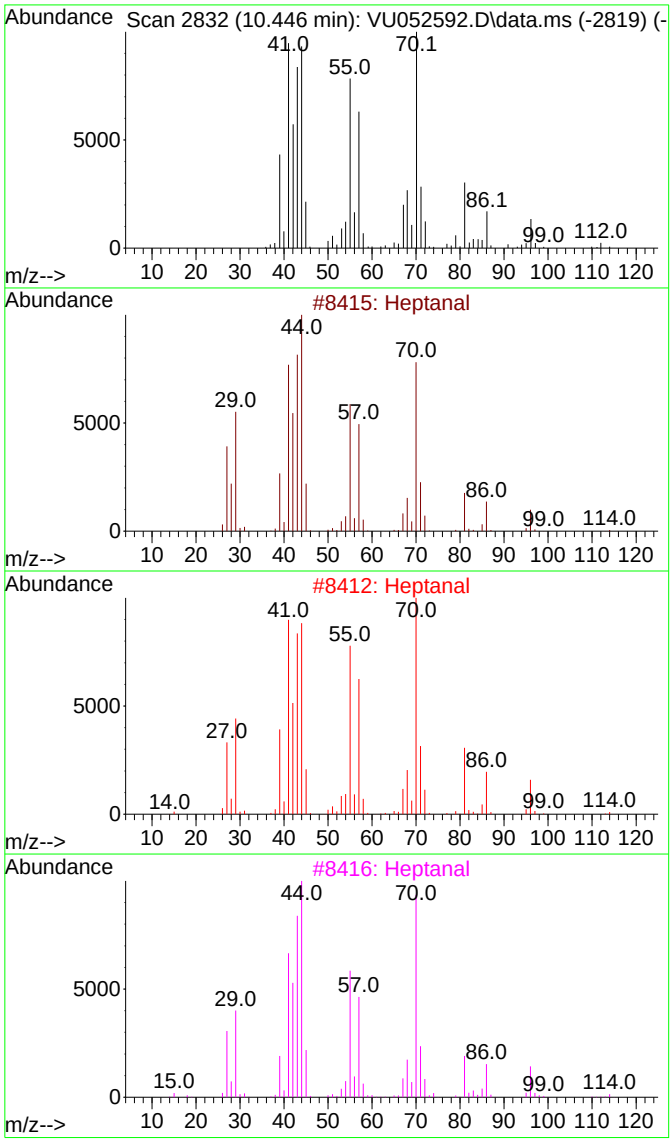
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

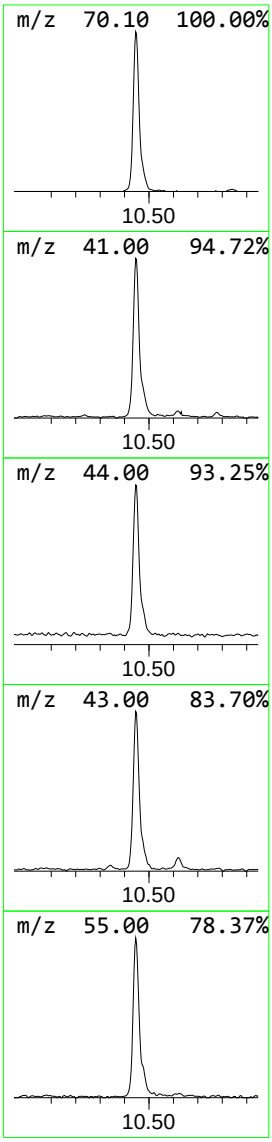
****

Peak Number 5 Heptanal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.446	3.75 ug/L	362831	Chlorobenzene-d5	9.619

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanal	114	C7H14O	000111-71-7	95
2	Heptanal	114	C7H14O	000111-71-7	86
3	Heptanal	114	C7H14O	000111-71-7	86
4	Heptanal	114	C7H14O	000111-71-7	76
5	Heptanal	114	C7H14O	000111-71-7	58





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122822\
Data File : VU052592.D
Acq On : 28 Dec 2022 16:38
Operator : JC/MD
Sample : N6171-18
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQD4

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

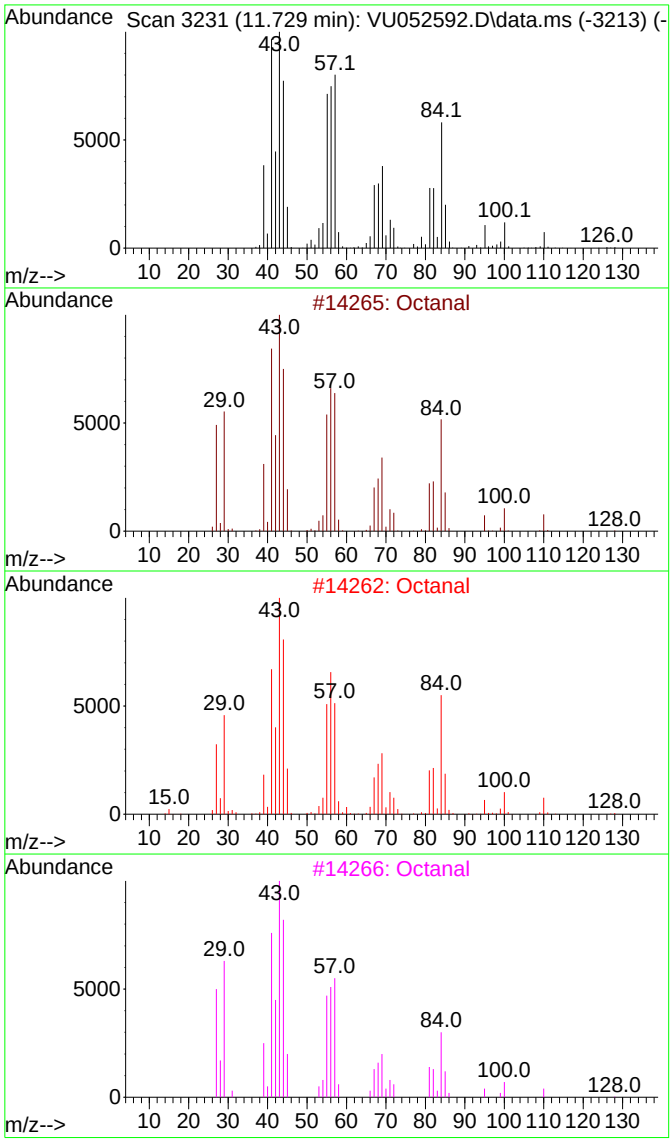
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

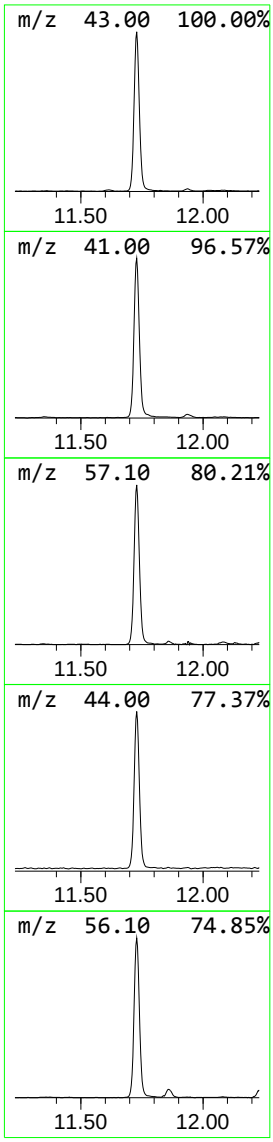
****

Peak Number 6 Octanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.729	12.85 ug/L	1430690	1,4-Dichlorobenzene-d4	11.860

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanal	128	C8H16O	000124-13-0	96
2	Octanal	128	C8H16O	000124-13-0	95
3	Octanal	128	C8H16O	000124-13-0	95
4	Octanal	128	C8H16O	000124-13-0	91
5	Octanal	128	C8H16O	000124-13-0	62





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122822\
Data File : VU052592.D
Acq On : 28 Dec 2022 16:38
Operator : JC/MD
Sample : N6171-18
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQD4

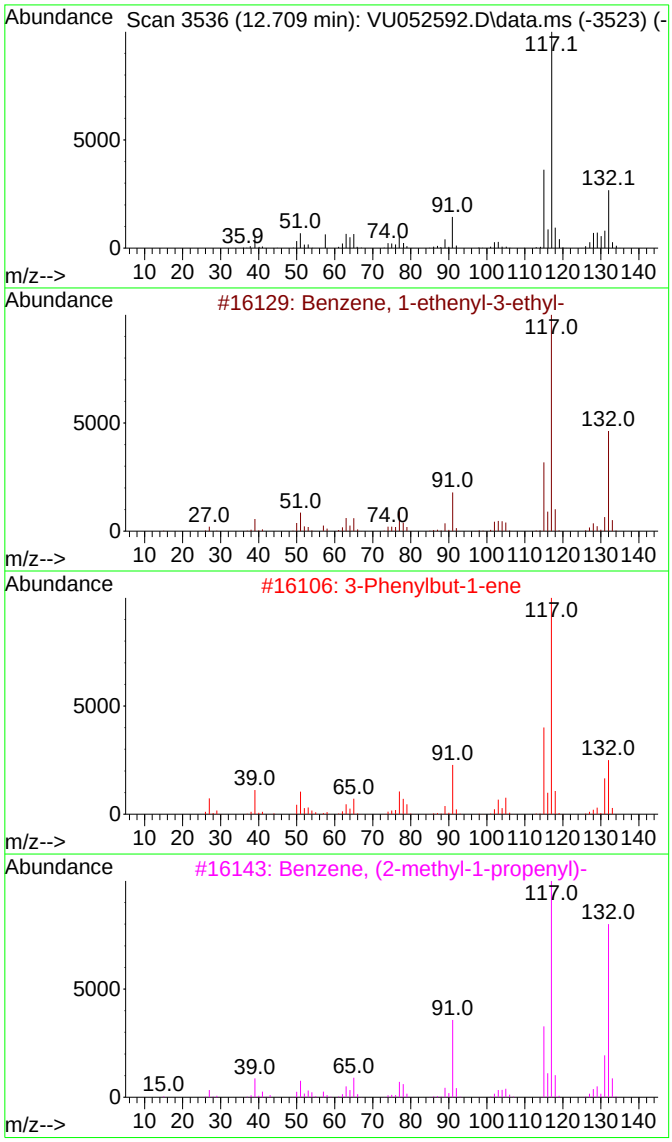
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

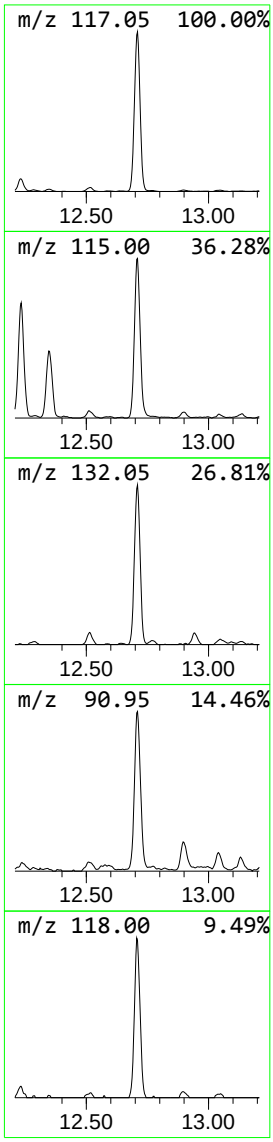
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.709	5.45 ug/L	607306	1,4-Dichlorobenzene-d4	11.860

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90
2	3-Phenylbut-1-ene	132	C10H12	000934-10-1	80
3	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	78
4	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	78
5	Indan, 1-methyl-	132	C10H12	000767-58-8	76





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122822\
Data File : VU052592.D
Acq On : 28 Dec 2022 16:38
Operator : JC/MD
Sample : N6171-18
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQD4

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

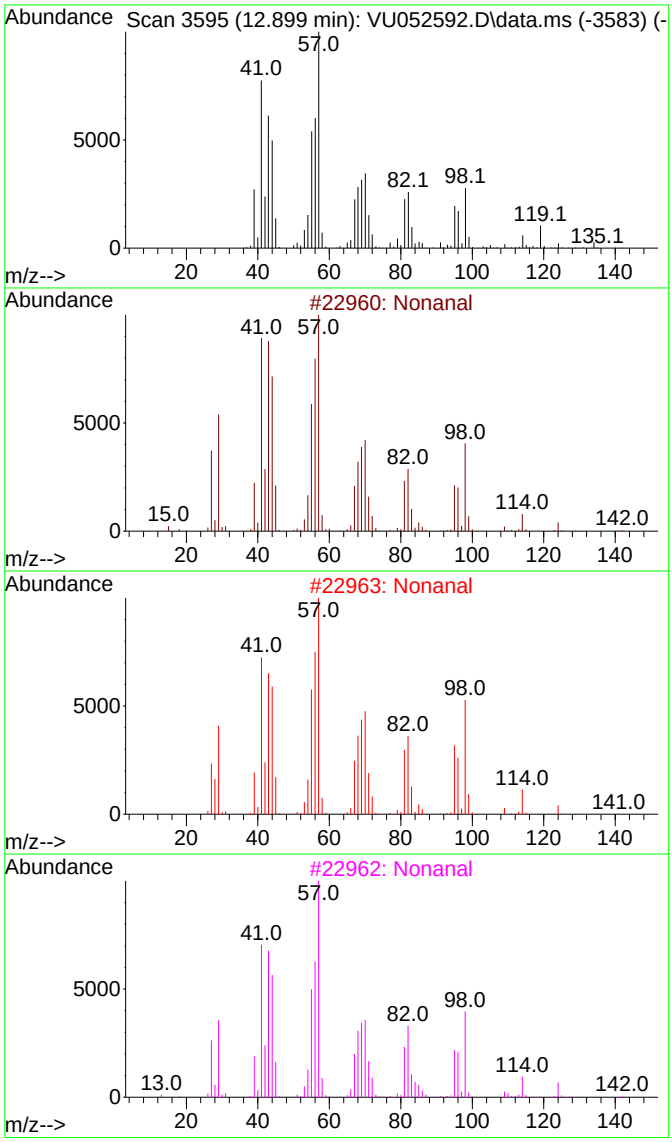
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

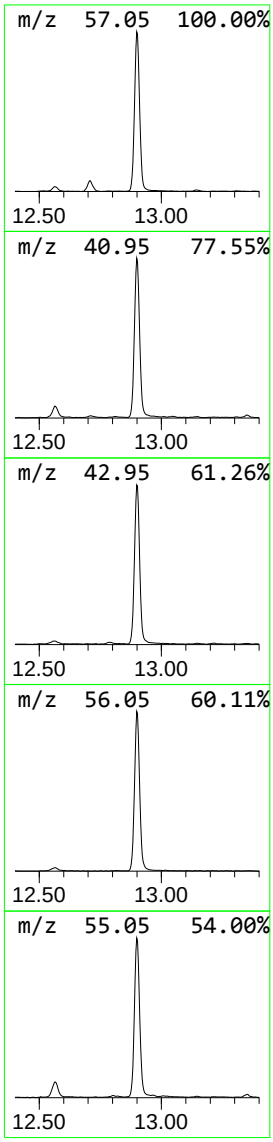
****

Peak Number 8 Nonanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.899	12.19 ug/L	1358090	1,4-Dichlorobenzene-d4	11.860

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanal	142	C9H18O	000124-19-6	90
2	Nonanal	142	C9H18O	000124-19-6	72
3	Nonanal	142	C9H18O	000124-19-6	64
4	Nonanal	142	C9H18O	000124-19-6	53
5	2-Heptene	98	C7H14	000592-77-8	30





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Instrument :
MSVOA_U
ClientSampleId :
GBQD4

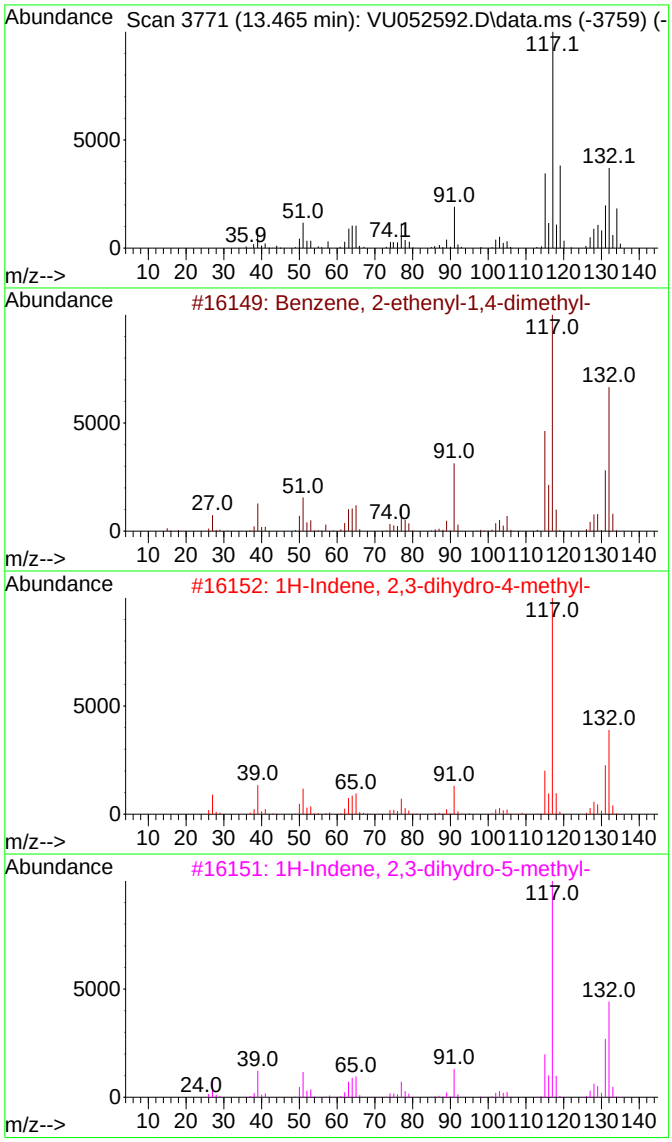
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

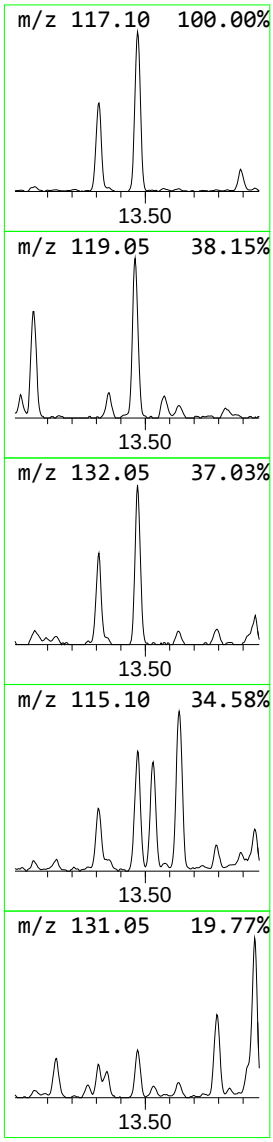
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.465	2.17 ug/L	241623	1,4-Dichlorobenzene-d4	11.860

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	91
2	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	76
3	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	70
4	3-Phenylbut-1-ene	132	C10H12	000934-10-1	70
5	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	70





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Data File : VU052592.D
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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQD4

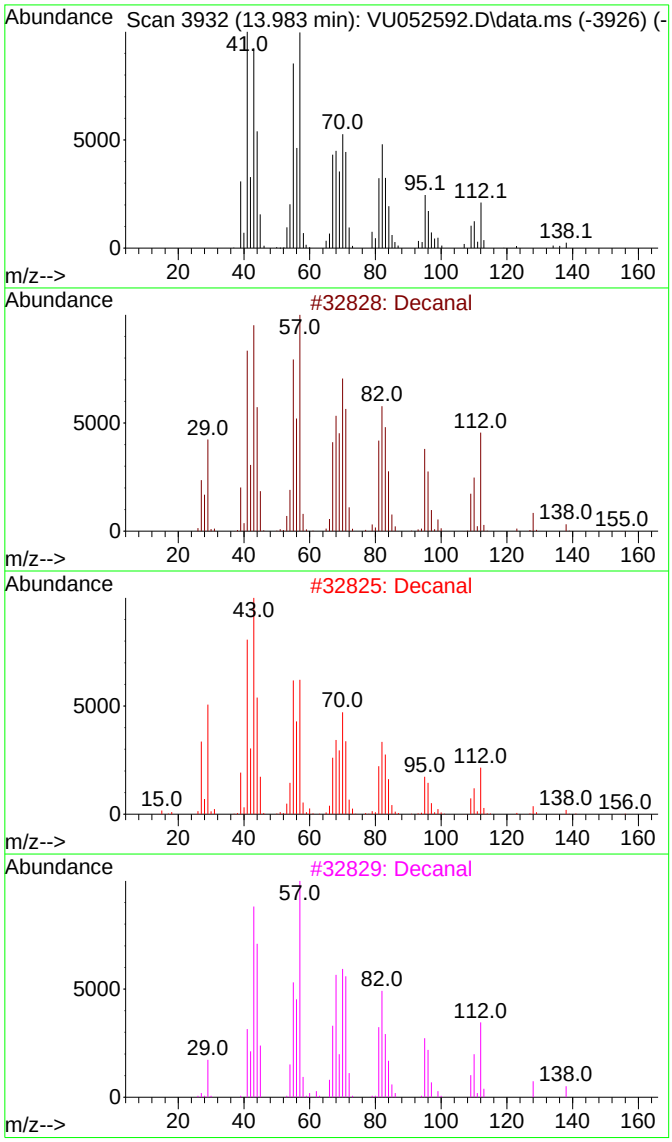
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

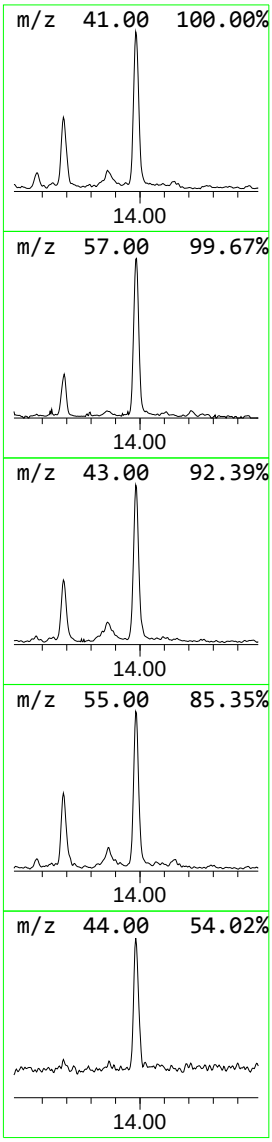
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Decanal Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.983	1.87 ug/L	208057	1,4-Dichlorobenzene-d4	11.860

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decanal	156	C10H20O	000112-31-2	91
2	Decanal	156	C10H20O	000112-31-2	91
3	Decanal	156	C10H20O	000112-31-2	83
4	Decanal	156	C10H20O	000112-31-2	80
5	Decanal	156	C10H20O	000112-31-2	80





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Data File : VU052592.D
Acq On : 28 Dec 2022 16:38
Operator : JC/MD
Sample : N6171-18
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQD4

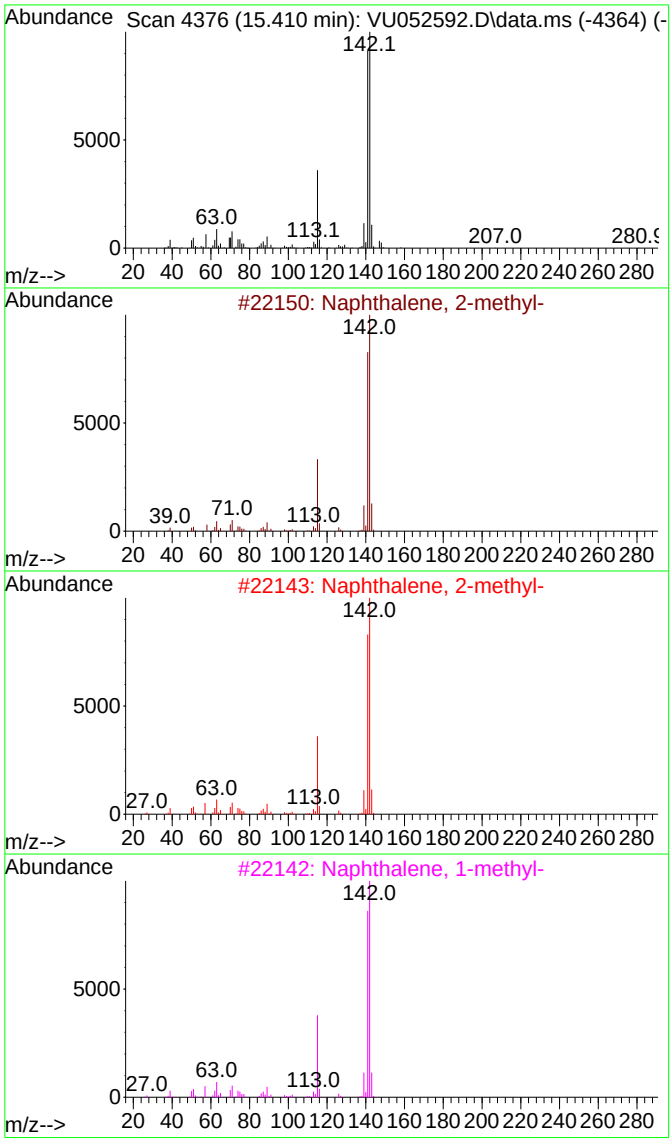
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

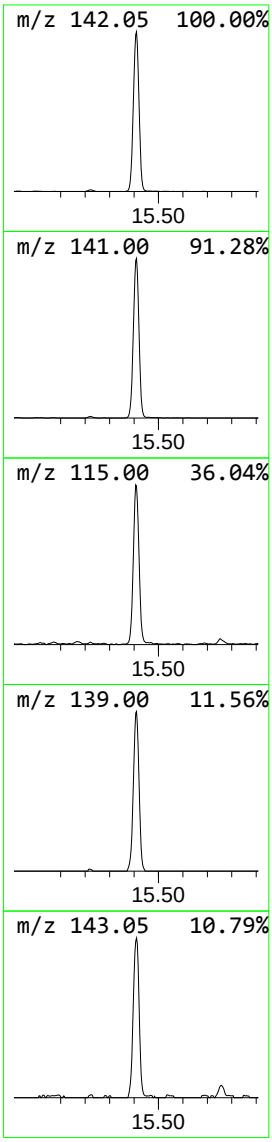
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Naphthalene, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.410	5.50 ug/L	612776	1,4-Dichlorobenzene-d4	11.860

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
4	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	95
5	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	94





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122822\
Data File : VU052592.D
Acq On : 28 Dec 2022 16:38
Operator : JC/MD
Sample : N6171-18
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQD4

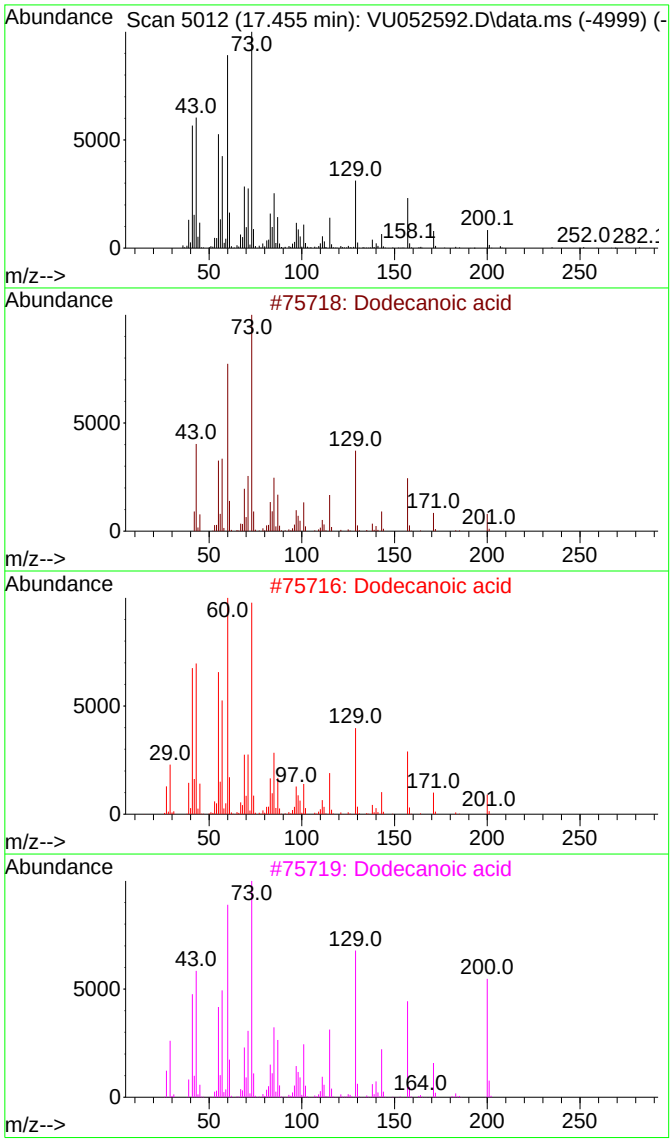
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

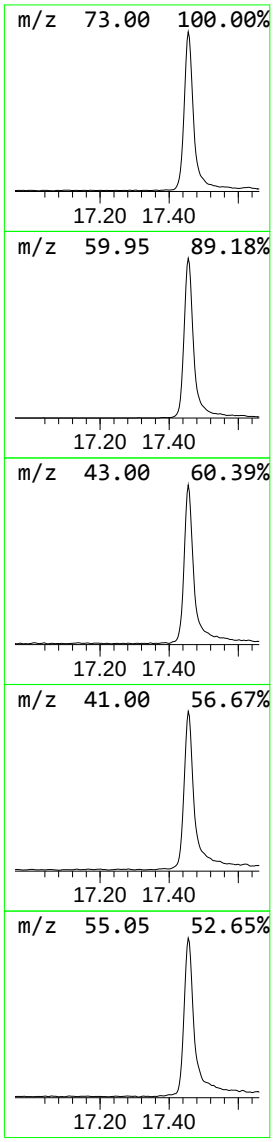
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Dodecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.455	10.71 ug/L	1192670	1,4-Dichlorobenzene-d4	11.860

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	98
2	Dodecanoic acid	200	C12H24O2	000143-07-7	98
3	Dodecanoic acid	200	C12H24O2	000143-07-7	95
4	Dodecanoic acid	200	C12H24O2	000143-07-7	93
5	Dodecanoic acid	200	C12H24O2	000143-07-7	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122822\
Data File : VU052592.D
Acq On : 28 Dec 2022 16:38
Operator : JC/MD
Sample : N6171-18
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQD4

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Terephthalonitr...	2.993	40.8	ug/L	3333700	1	7.009	408574	5.0
6-Bromo-4-(morp...	4.227	35.1	ug/L	2871130	1	7.009	408574	5.0
Hexanal	9.037	10.3	ug/L	997327	2	9.619	483905	5.0
Heptanal	10.446	3.8	ug/L	362831	2	9.619	483905	5.0
Octanal	11.729	12.9	ug/L	1430690	3	11.860	556900	5.0
Benzene, 1-ethe...	12.709	5.5	ug/L	607306	3	11.860	556900	5.0
Nonanal	12.899	12.2	ug/L	1358090	3	11.860	556900	5.0
Benzene, 2-ethe...	13.465	2.2	ug/L	241623	3	11.860	556900	5.0
Decanal	13.983	1.9	ug/L	208057	3	11.860	556900	5.0
Naphthalene, 2-...	15.410	5.5	ug/L	612776	3	11.860	556900	5.0
Dodecanoic acid	17.455	10.7	ug/L	1192670	3	11.860	556900	5.0