LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082021\
Data File : VX023864.D
Acq On : 20 Aug 2021 01:39
Operator : JC/MD
Sample : M3479-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 210818092-02-VOA

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 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_X\Method\82X081721W.M
Title : SW846 8260

Signal : TIC: VX023864.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	25	28	51	rVB	196477	475309	5.62%	1.201%
2	2.386	206	213	227	rBV2	98590	190494	2.25%	0.481%
3	2.977	297	310	326	rBV	3819685	8455623	100.00%	21.373%
4	4.611	559	578	609	rBV	2522384	8334900	98.57%	21.067%
5	5.013	632	644	664	rBV	1279523	3825439	45.24%	9.669%
6	5.397	695	707	723	rVB	97085	278016	3.29%	0.703%
7	5.562	723	734	748	rVB	151343	432255	5.11%	1.093%
8	5.964	790	800	808	rBV	104538	276192	3.27%	0.698%
9	6.092	808	821	830	rVV6	29561	135135	1.60%	0.342%
10	6.245	838	846	856	rVB2	69483	193875	2.29%	0.490%
11	6.769	922	932	944	rVB	247759	584920	6.92%	1.478%
12	8.653	1234	1241	1247	rBV	536317	835563	9.88%	2.112%
13	8.720	1247	1252	1261	rVB3	69122	119178	1.41%	0.301%
14	8.805	1261	1266	1272	rBV	85941	137309	1.62%	0.347%
15	9.378	1352	1360	1366	rBV	112488	173051	2.05%	0.437%
16	10.055	1460	1471	1476	rBV	547710	794266	9.39%	2.008%
17	10.305	1507	1512	1518	rVB	152877	223016	2.64%	0.564%
18	10.646	1563	1568	1580	rBV	82920	135062	1.60%	0.341%
19	11.085	1634	1640	1646	rBV	444236	598381	7.08%	1.512%
20	11.482	1699	1705	1707	rVV4	63930	112327	1.33%	0.284%
21	11.890	1770	1772	1777	rVB	87452	91403	1.08%	0.231%
22	11.951	1777	1782	1788	rBV2	106604	147641	1.75%	0.373%
23	12.024	1788	1794	1800	rBV	519144	703411	8.32%	1.778%
24	12.427	1854	1860	1864	rBV	133376	165880	1.96%	0.419%
25	12.524	1872	1876	1882	rBV3	93043	155292	1.84%	0.393%
26	12.579	1882	1885	1889	rVB	104847	127744	1.51%	0.323%
27	12.768	1908	1916	1921	rBV	440689	620932	7.34%	1.569%
28	12.908	1928	1939	1943	rBV	1073592	1433160	16.95%	3.622%
29	12.969	1943	1949	1958	rVB2	197720	411592	4.87%	1.040%
30	13.268	1995	1998	2001	rBV	89345	108862	1.29%	0.275%
31	13.384	2007	2017	2020	rBV2	58136	111934	1.32%	0.283%
32	13.426	2020	2024	2028	rVV2	71234	102748	1.22%	0.260%
33	13.475	2028	2032	2035	rVV2	259603	383091	4.53%	0.968%
34	13.512	2035	2038	2043	rVB	237381	306939	3.63%	0.776%
35	13.591	2046	2051	2060	rBV2	371739	522163	6.18%	1.320%
36	13.774	2077	2081	2088	rVB2	351133	472958	5.59%	1.195%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082021\
Data File : VX023864.D
Acq On : 20 Aug 2021 01:39
Operator : JC/MD
Sample : M3479-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 210818092-02-VOA

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 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_X\Method\82X081721W.M
Title : SW846 8260

37	13.847	2088	2093	2100	rBV6	46810	92355	1.09%	0.233%
38	13.926	2100	2106	2109	rBV3	59882	131872	1.56%	0.333%
39	14.237	2151	2157	2164	rBV4	44675	91673	1.08%	0.232%
40	14.316	2166	2170	2176	rVV4	65520	90634	1.07%	0.229%
41	14.414	2182	2186	2194	rBV3	51530	121701	1.44%	0.308%
42	14.609	2214	2218	2220	rBV3	73949	104360	1.23%	0.264%
43	14.640	2220	2223	2231	rVB	286765	386167	4.57%	0.976%
44	14.719	2231	2236	2240	rBV	436128	555332	6.57%	1.404%
45	14.761	2240	2243	2244	rVV	124145	146954	1.74%	0.371%
46	14.780	2244	2246	2253	rVB	247429	307775	3.64%	0.778%
47	15.213	2309	2317	2321	rBV2	117663	185800	2.20%	0.470%
48	15.359	2334	2341	2349	rBV	814307	1339220	15.84%	3.385%
49	15.487	2354	2362	2365	rBV2	894122	1569001	18.56%	3.966%
50	15.615	2378	2383	2387	rBV	116185	190314	2.25%	0.481%
51	15.713	2394	2399	2411	rVB8	60764	182655	2.16%	0.462%
52	15.841	2411	2420	2428	rBV3	39502	141028	1.67%	0.356%
53	15.932	2430	2435	2440	rVV4	66773	130704	1.55%	0.330%
54	16.097	2454	2462	2467	rBV6	65899	161460	1.91%	0.408%
55	16.188	2467	2477	2482	rBV4	209029	469228	5.55%	1.186%
56	16.334	2494	2501	2508	rVB	380398	710844	8.41%	1.797%
57	16.688	2550	2559	2568	rVB	107202	277902	3.29%	0.702%

Sum of corrected areas: 39563040

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Acq On : 20 Aug 2021 01:39
Operator : JC/MD
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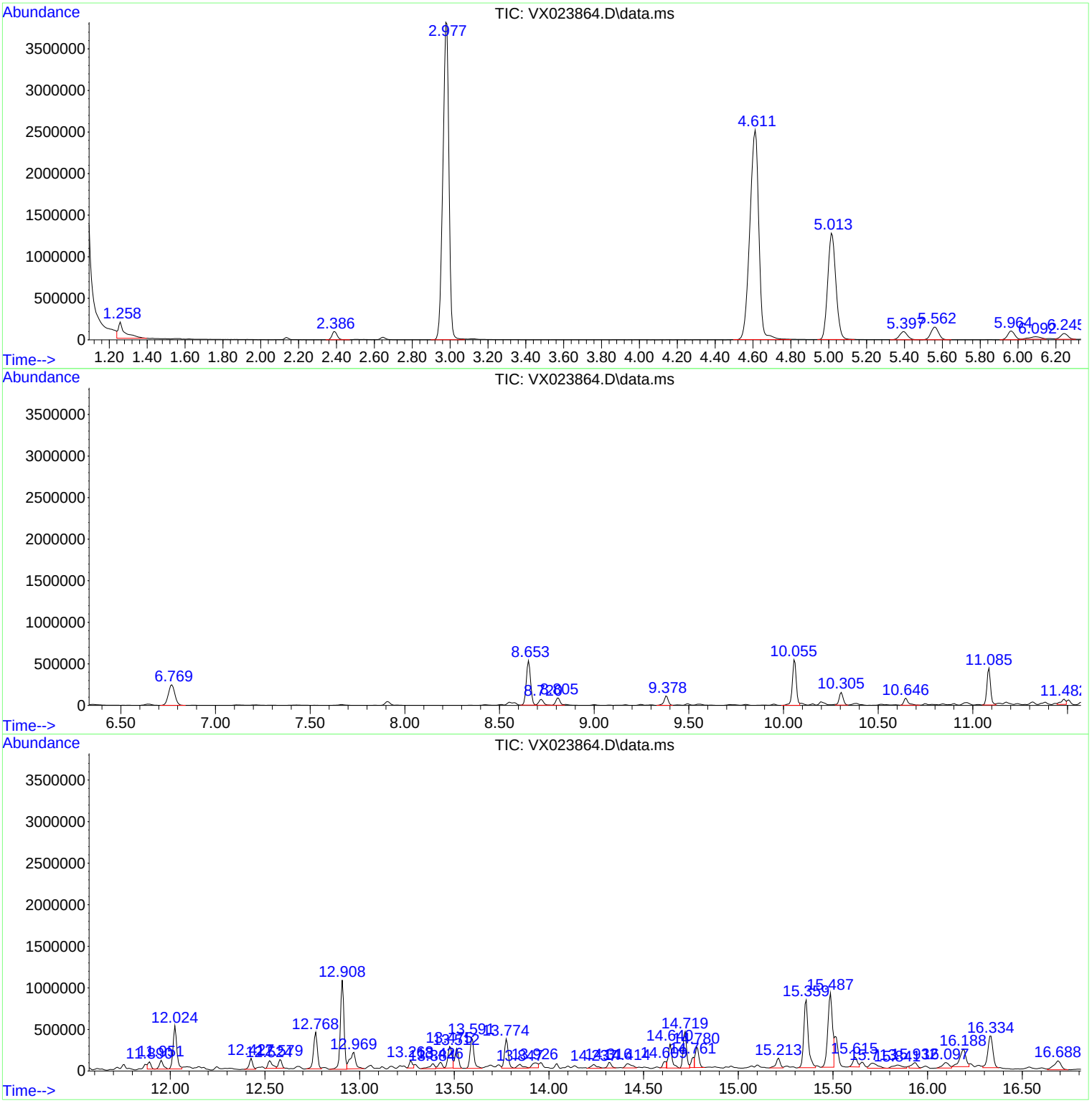
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
210818092-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082021\
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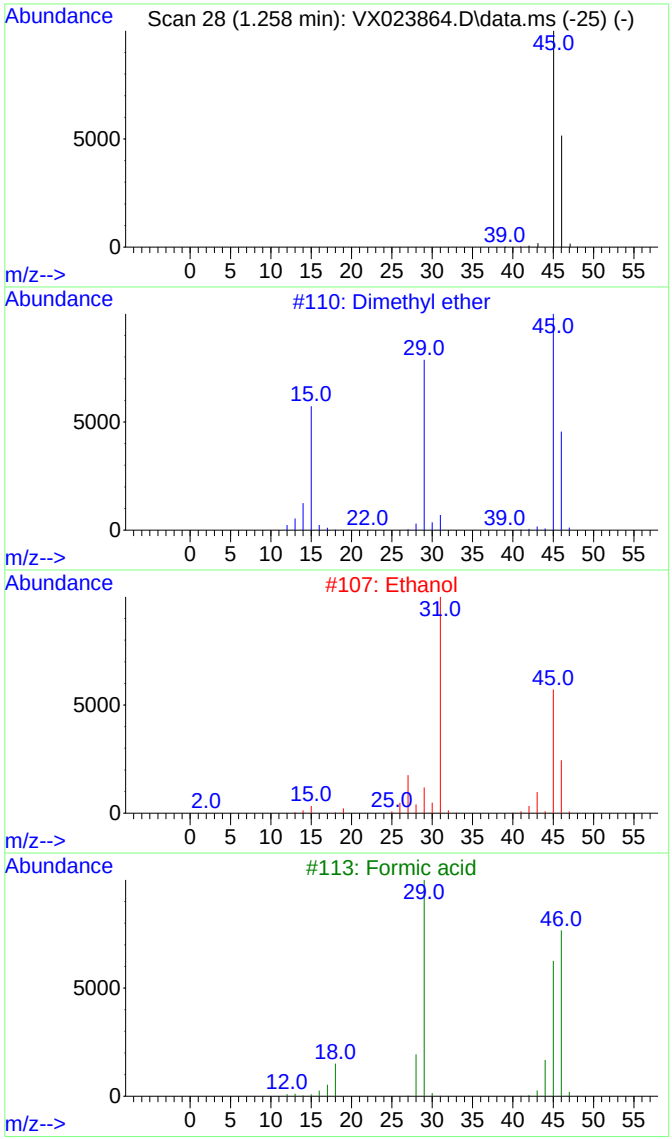
Quant Title : SW846 8260

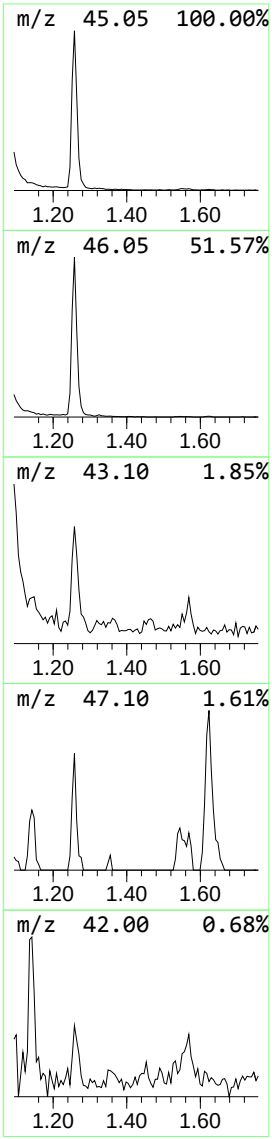
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Dimethyl ether Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.258	54.98 ug/l	475309	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl ether	46	C2H6O	000115-10-6	74
2	Ethanol	46	C2H6O	000064-17-5	7
3	Formic acid	46	CH2O2	000064-18-6	7
4	Ethene, fluoro-	46	C2H3F	000075-02-5	4
5	Hydrazine, methyl-	46	CH6N2	000060-34-4	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082021\
Data File : VX023864.D
Acq On : 20 Aug 2021 01:39
Operator : JC/MD
Sample : M3479-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
210818092-02-VOA

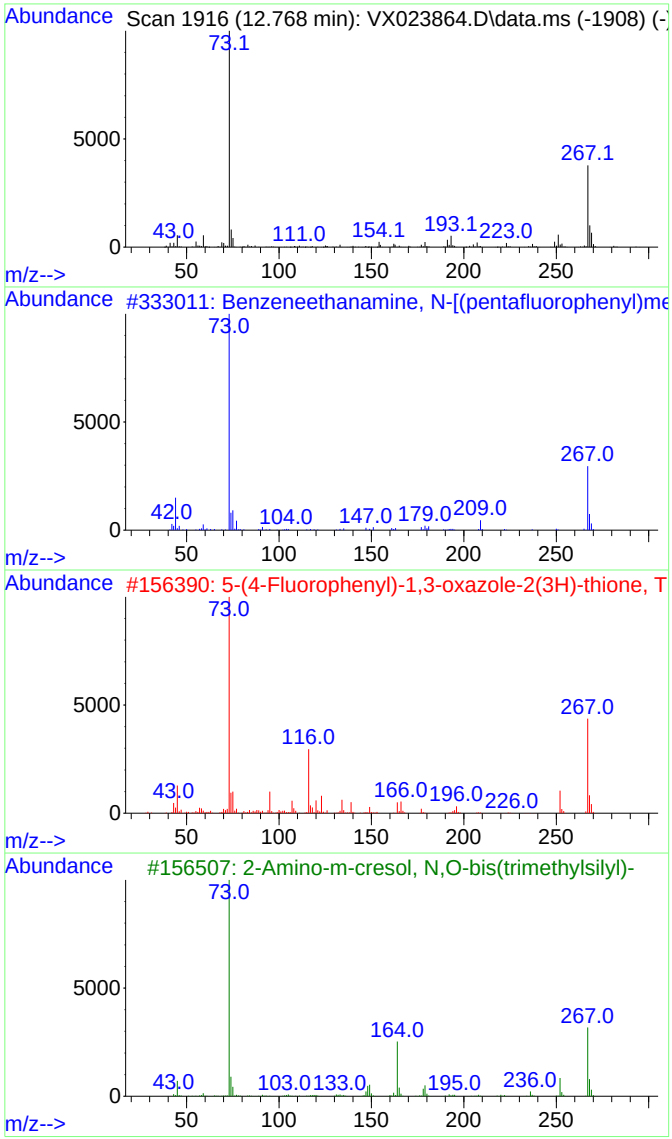
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

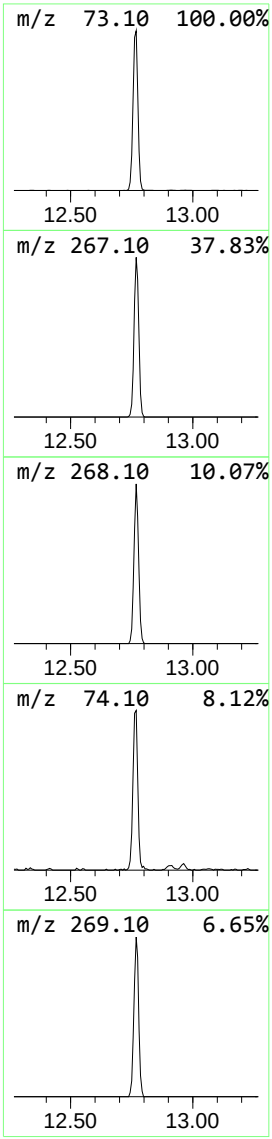
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzeneethanamine, N-[(pent... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.768	44.14 ug/l	620932	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneethanamine, N-[(pentafluo...	475	C21H26F5NO2Si2	055429-85-1	53
2	5-(4-Fluorophenyl)-1,3-oxazole-2...	267	C12H14FNOSSi	1000497-07-6	53
3	2-Amino-m-cresol, N,O-bis(trimet...	267	C13H25NOSi2	1000449-77-1	53
4	Tetrasiloxane, 1,1,3,3,5,5,7,7-o...	282	C8H26O3Si4	001000-05-1	50
5	Salicylic acid, 2TMS derivative	282	C13H22O3Si2	003789-85-3	39





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082021\
Data File : VX023864.D
Acq On : 20 Aug 2021 01:39
Operator : JC/MD
Sample : M3479-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 210818092-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

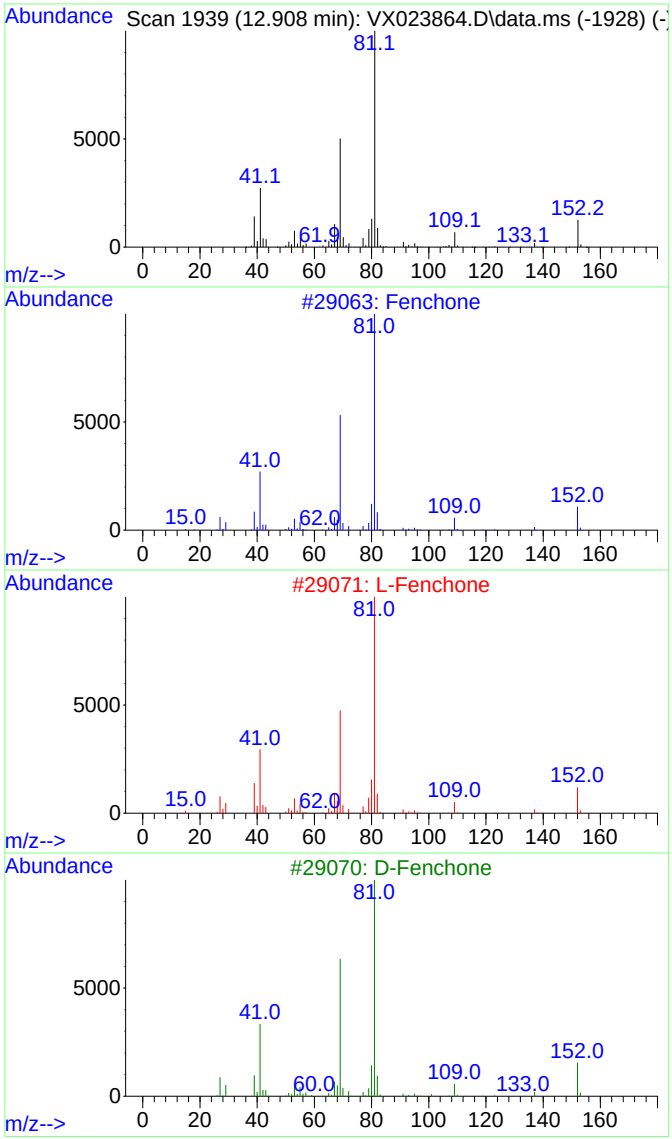
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

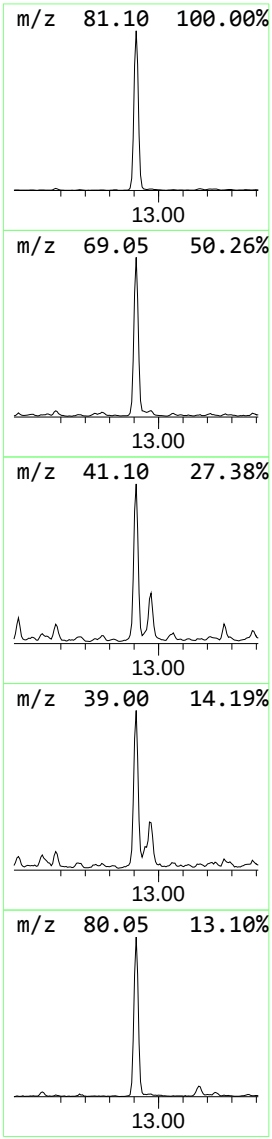
****

Peak Number 4 Fenchone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.908	101.87 ug/l	1433160	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fenchone	152	C10H16O	001195-79-5	95
2	L-Fenchone	152	C10H16O	007787-20-4	94
3	D-Fenchone	152	C10H16O	004695-62-9	94
4	2,4-Decadienal, (E,E)-	152	C10H16O	025152-84-5	59
5	Ethanone, 1-(2-methyl-2-cyclopen...	124	C8H12O	001767-84-6	42





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082021\
Data File : VX023864.D
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Sample : M3479-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
210818092-02-VOA

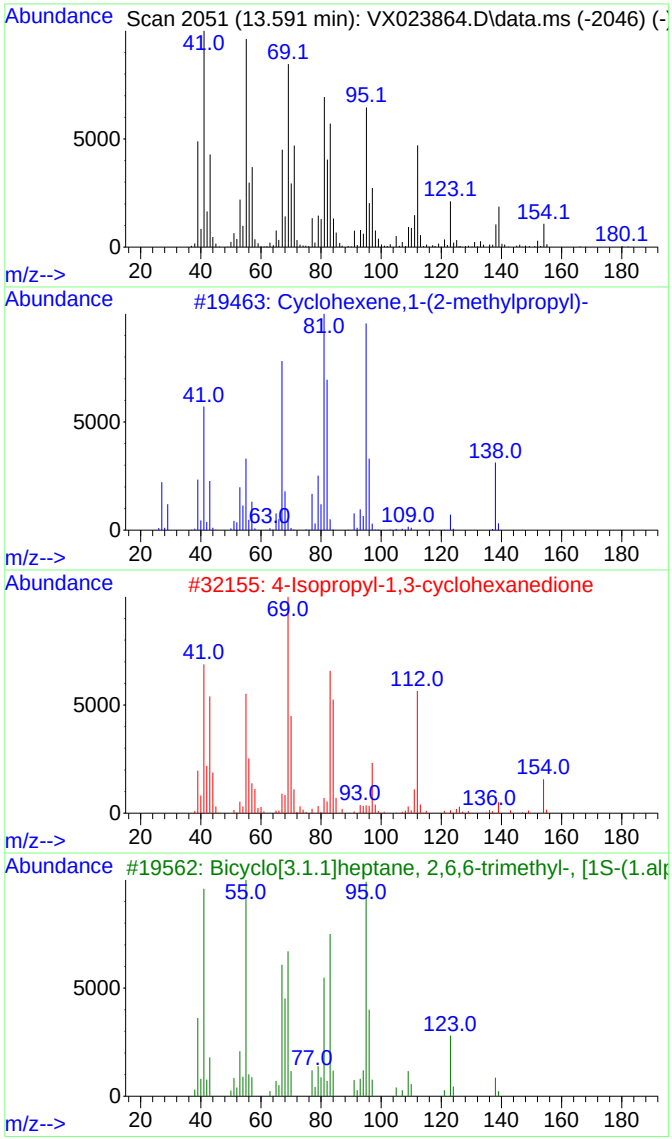
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

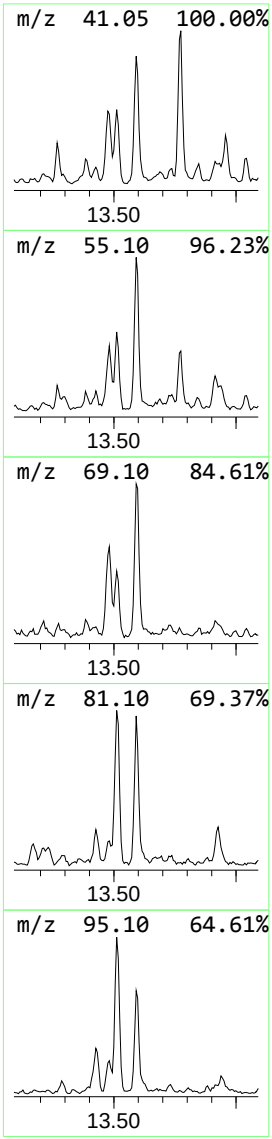
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclohexene,1-(2-methylprop... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.591	37.12 ug/l	522163	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene,1-(2-methylpropyl)-	138	C10H18	003983-03-7	72
2	4-Isopropyl-1,3-cyclohexanedione	154	C9H14O2	062831-62-3	46
3	Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	004755-33-3	42
4	1,6-Octadiene, 5,7-dimethyl-, (R)-	138	C10H18	085006-04-8	38
5	Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	004863-59-6	38





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ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 210818092-02-VOA

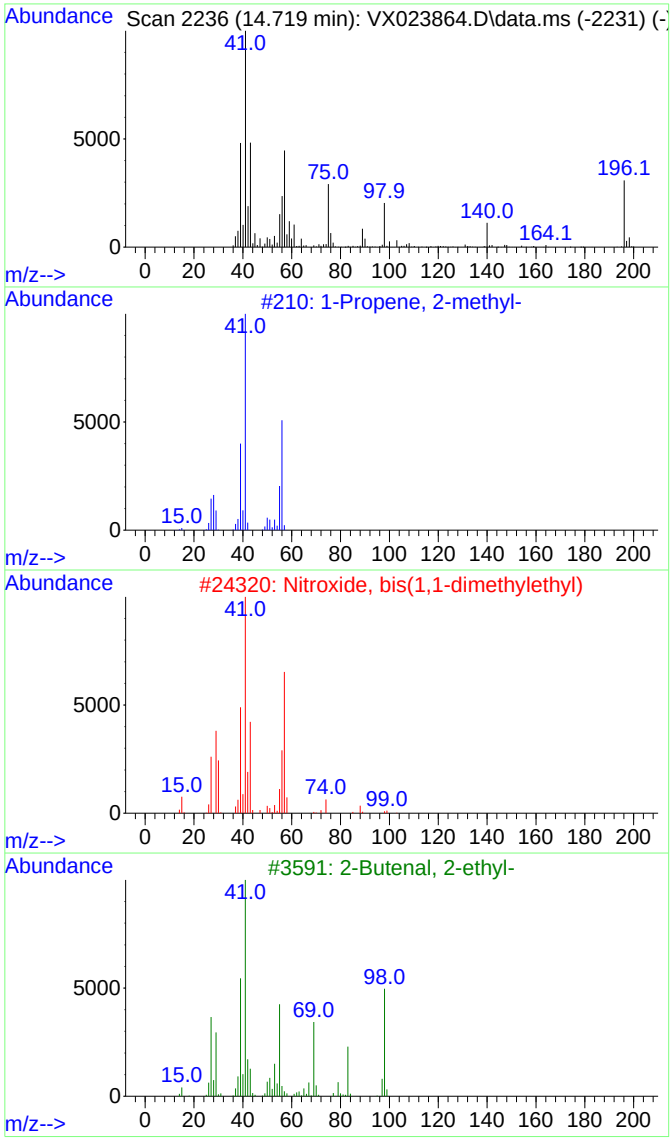
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

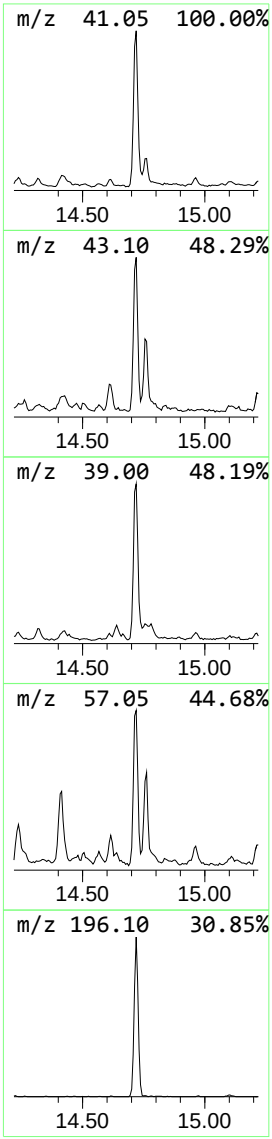
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 unknown39.47 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.719	39.47 ug/l	555332	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 2-methyl-	56	C4H8	000115-11-7	30
2	Nitroxide, bis(1,1-dimethylethyl)	144	C8H18NO	002406-25-9	16
3	2-Butenal, 2-ethyl-	98	C6H10O	019780-25-7	12
4	2(5H)-Furanone, 3-methyl-	98	C5H6O2	022122-36-7	12
5	Hydrazinecarboxylic acid, 2-cycl...	214	C11H22N2O2	060295-21-8	10





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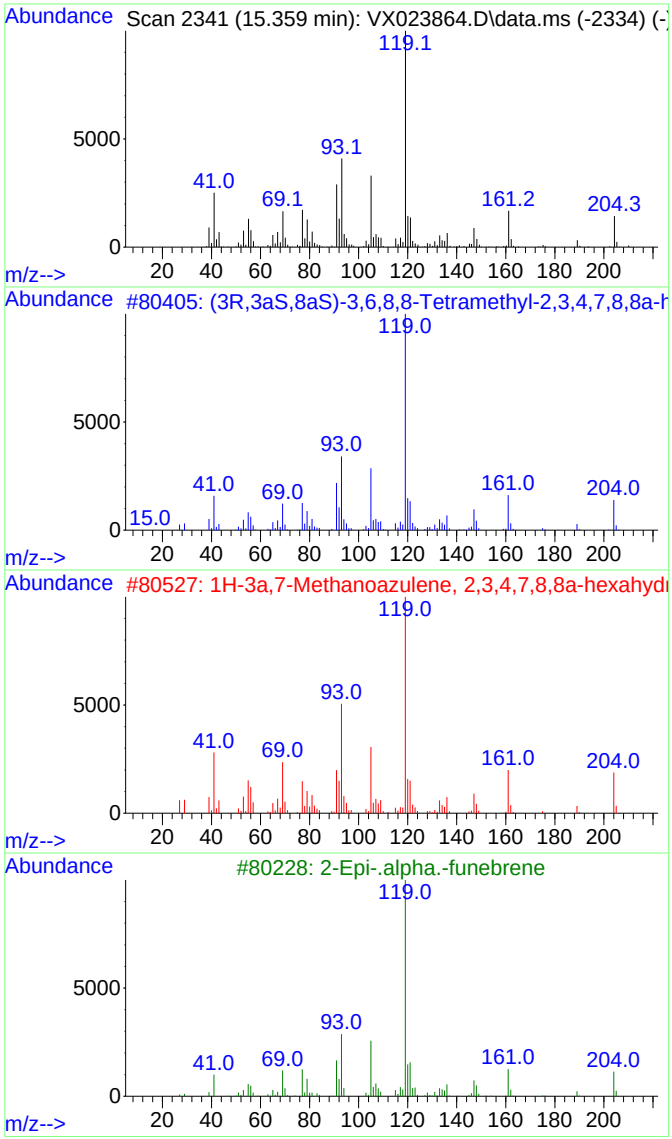
Quant Title : SW846 8260

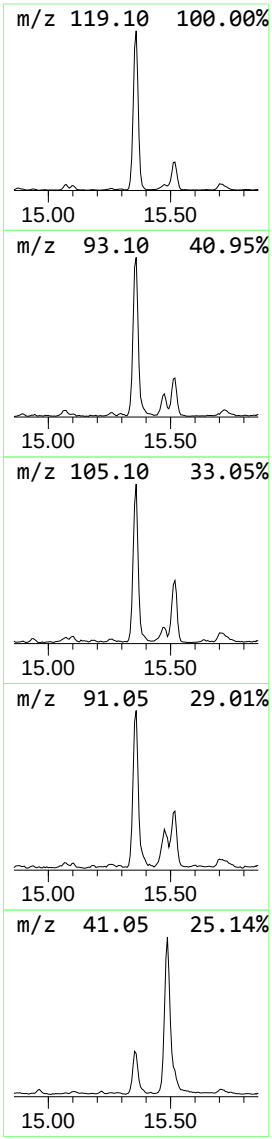
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (3R,3aS,8aS)-3,6,8,8-Tetram... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.359	95.19 ug/l	1339220	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(3R,3aS,8aS)-3,6,8,8-Tetramethyl...	204	C15H24	022567-43-7	99
2	1H-3a,7-Methanoazulene, 2,3,4,7,...	204	C15H24	000469-61-4	98
3	2-Epi-.alpha.-funebrene	204	C15H24	065354-33-8	93
4	(R)-1-Methyl-4-(6-methylhept-5-e...	204	C15H24	028976-67-2	87
5	(1S,5S)-2-Methyl-5-((R)-6-methyl...	204	C15H24	159407-35-9	83





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ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
210818092-02-VOA

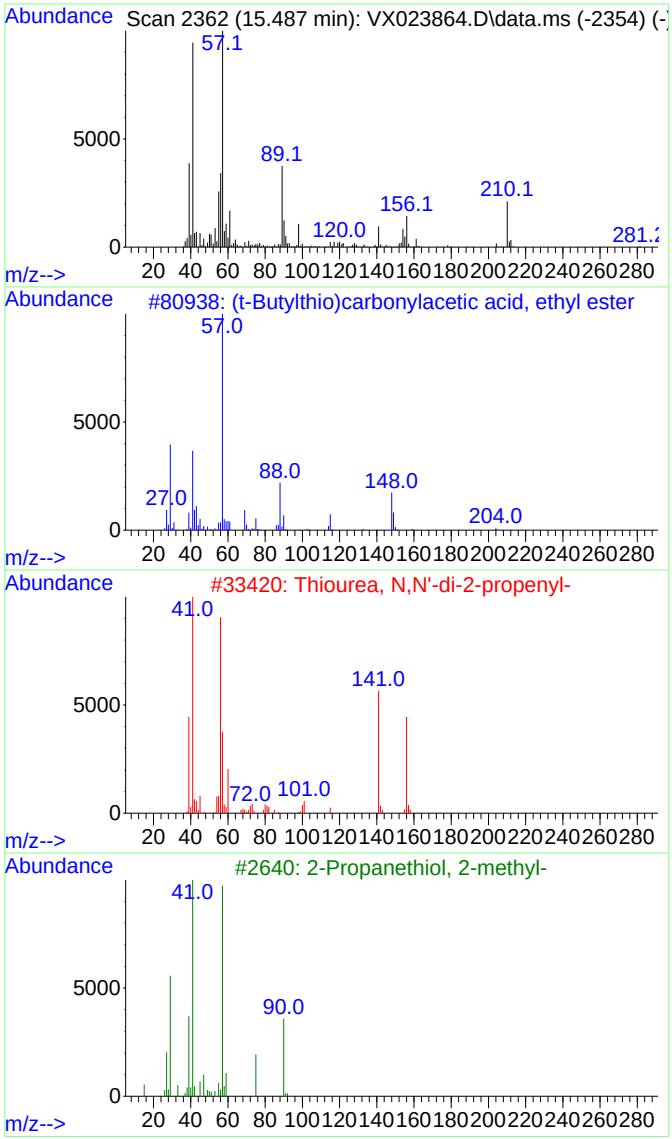
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

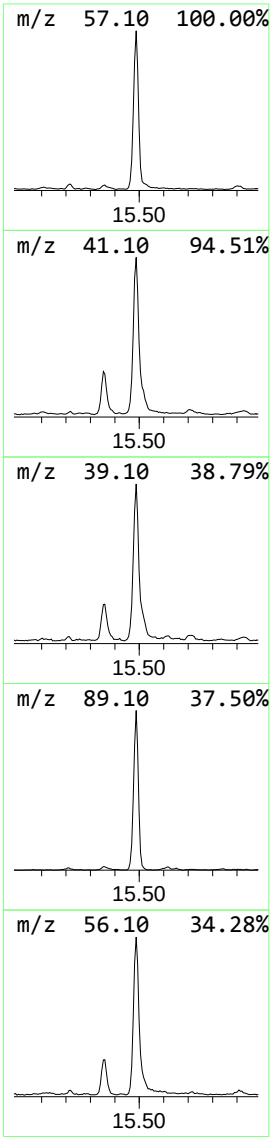
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 unknown15.487 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.487	111.53 ug/l	1569000	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(t-Butylthio)carbonylacetic acid...	204	C9H16O3S	1000192-52-7	14
2	Thiourea, N,N'-di-2-propenyl-	156	C7H12N2S	006601-20-3	11
3	2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	10
4	1-[(chloromethyl)sulfonyl]butane	170	C5H11ClO2S	1000404-59-5	10
5	N-(tert-Butoxycarbonyl)sulfamide	196	C5H12N2O4S	148017-28-1	10





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Operator : JC/MD
Sample : M3479-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
210818092-02-VOA

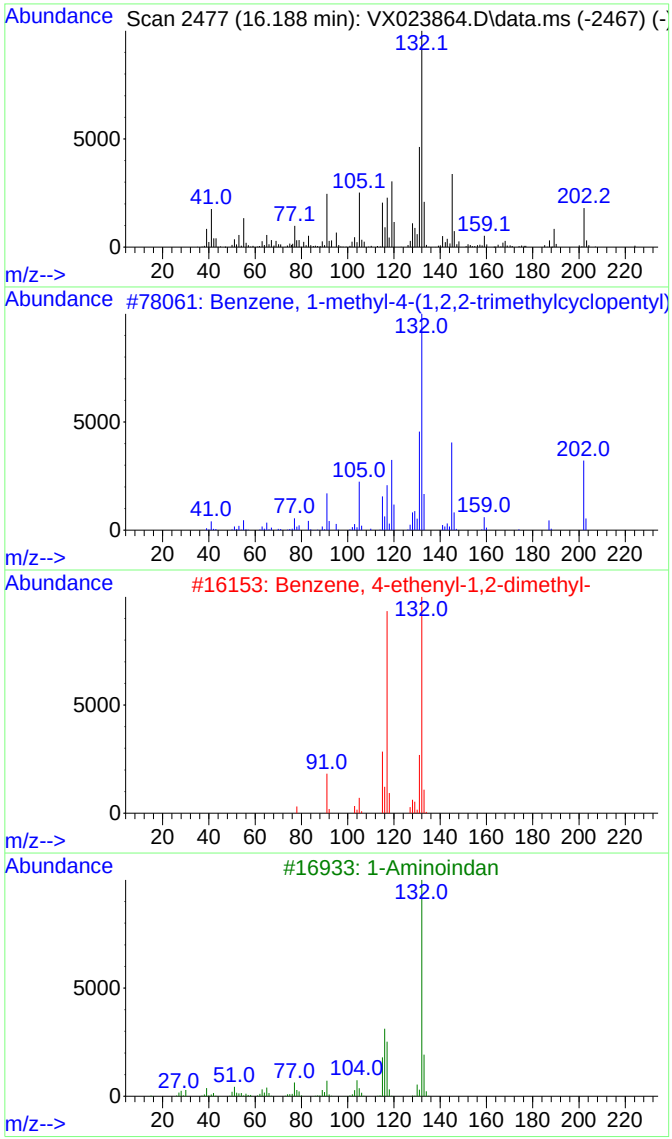
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

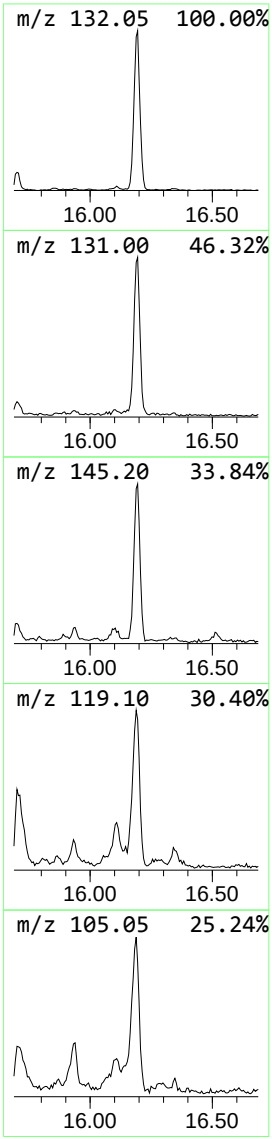
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1-methyl-4-(1,2,2-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.188	33.35 ug/l	469228	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-4-(1,2,2-trime...	202	C15H22	016982-00-6	98
2	Benzene, 4-ethenyl-1,2-dimethyl-	132	C10H12	027831-13-6	46
3	1-Aminoindan	133	C9H11N	034698-41-4	43
4	1H-Indol-4-amine	132	C8H8N2	005192-23-4	43
5	Methyl-3-phenylaziridine, 2-	133	C9H11N	007763-71-5	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082021\
Data File : VX023864.D
Acq On : 20 Aug 2021 01:39
Operator : JC/MD
Sample : M3479-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
210818092-02-VOA

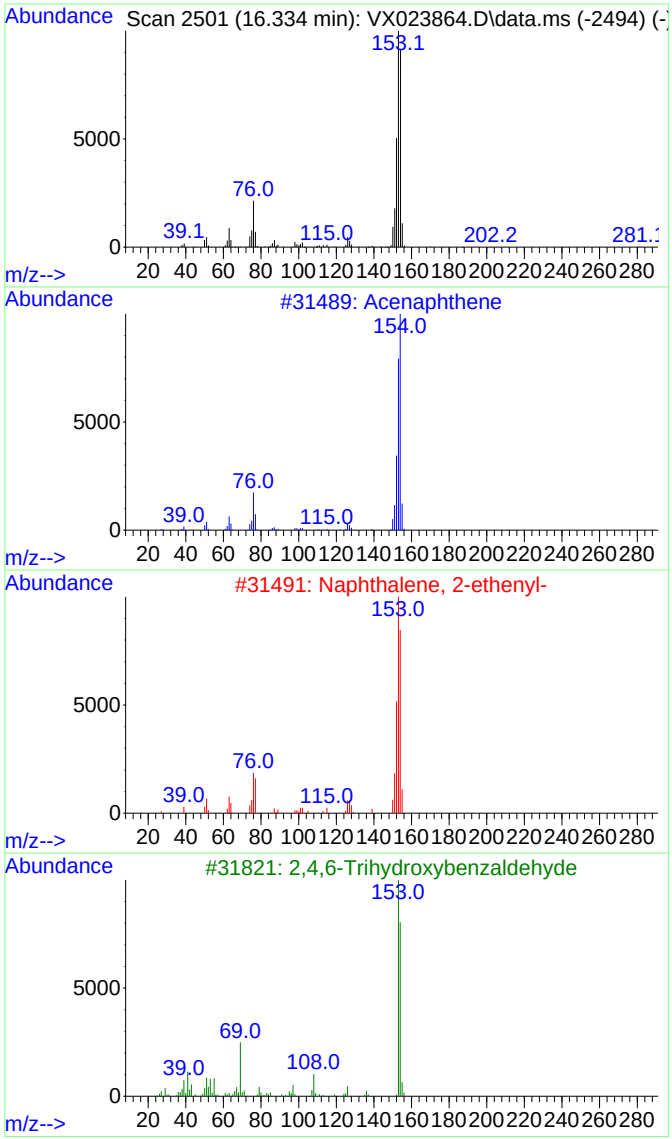
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

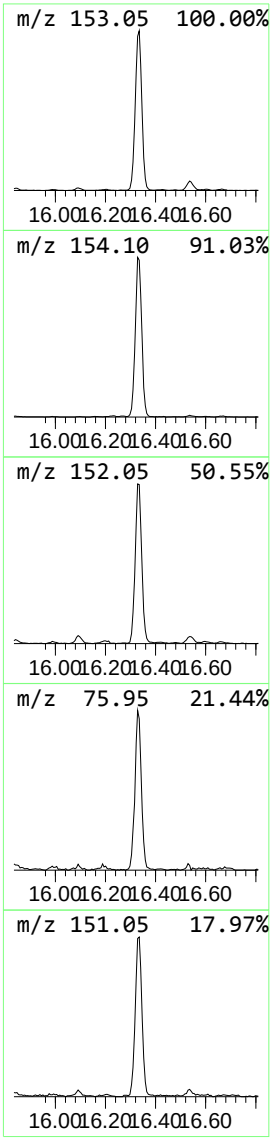
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Acenaphthene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.334	50.53 ug/l	710844	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acenaphthene	154	C12H10	000083-32-9	93
2	Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	68
3	2,4,6-Trihydroxybenzaldehyde	154	C7H6O4	000487-70-7	50
4	3-Fluoro-para-anisaldehyde	154	C8H7FO2	000351-54-2	50
5	1,4-Ethenonaphthalene, 1,4-dihydro-	154	C12H10	007322-47-6	42





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082021\
Data File : VX023864.D
Acq On : 20 Aug 2021 01:39
Operator : JC/MD
Sample : M3479-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 210818092-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Dimethyl ether	1.258	55.0	ug/l	475309	1	5.562	432255	50.0
Benzeneethanami...	12.768	44.1	ug/l	620932	4	12.024	703411	50.0
Fenchone	12.908	101.9	ug/l	1433160	4	12.024	703411	50.0
Cyclohexene,1-(...	13.591	37.1	ug/l	522163	4	12.024	703411	50.0
unknown39.47	14.719	39.5	ug/l	555332	4	12.024	703411	50.0
(3R,3aS,8aS)-3,...	15.359	95.2	ug/l	1339220	4	12.024	703411	50.0
unknown15.487	15.487	111.5	ug/l	1569000	4	12.024	703411	50.0
Benzene, 1-meth...	16.188	33.4	ug/l	469228	4	12.024	703411	50.0
Acenaphthene	16.334	50.5	ug/l	710844	4	12.024	703411	50.0