LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071521\
Data File : VX023306.D
Acq On : 15 Jul 2021 17:59
Operator : JC/MD
Sample : M3058-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 210714106-02-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\82X070221W.M
Title : SW846 8260

Signal : TIC: VX023306.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	26	28	42	rVB	120390	236054	2.94%	0.527%
2	2.386	204	213	223	rBV2	53528	106024	1.32%	0.236%
3	2.971	298	309	328	rBV	3297964	7243658	90.36%	16.157%
4	4.599	560	576	589	rBV	2514376	8016065	100.00%	17.880%
5	5.013	632	644	660	rBV	623832	1889920	23.58%	4.215%
6	5.397	695	707	720	rVV2	133297	382646	4.77%	0.853%
7	5.562	722	734	747	rVB	232326	658250	8.21%	1.468%
8	5.964	790	800	808	rBV	147279	381352	4.76%	0.851%
9	6.086	808	820	830	rBV4	49313	197617	2.47%	0.441%
10	6.245	838	846	855	rVB	79480	222883	2.78%	0.497%
11	6.769	922	932	946	rVB	353449	833129	10.39%	1.858%
12	8.580	1221	1229	1234	rBV2	69452	129244	1.61%	0.288%
13	8.653	1234	1241	1247	rBV	732520	1124579	14.03%	2.508%
14	8.720	1247	1252	1261	rVB	63539	104918	1.31%	0.234%
15	8.805	1261	1266	1271	rBV	67078	105062	1.31%	0.234%
16	10.055	1460	1471	1483	rBV	715210	1066899	13.31%	2.380%
17	10.201	1490	1495	1500	rBV2	45741	99937	1.25%	0.223%
18	10.305	1508	1512	1518	rVB	136783	198996	2.48%	0.444%
19	10.384	1518	1525	1535	rVB3	37985	93415	1.17%	0.208%
20	10.647	1563	1568	1578	rBV	83653	140698	1.76%	0.314%
21	10.951	1613	1618	1627	rBV4	58165	121853	1.52%	0.272%
22	11.085	1634	1640	1646	rBV	595156	793307	9.90%	1.769%
23	11.482	1699	1705	1707	rVV3	82536	151170	1.89%	0.337%
24	11.506	1707	1709	1715	rVB	106108	120744	1.51%	0.269%
25	11.756	1746	1750	1752	rVV2	69046	86029	1.07%	0.192%
26	11.890	1760	1772	1776	rBV4	118127	216535	2.70%	0.483%
27	12.024	1788	1794	1801	rBV2	753885	1144756	14.28%	2.553%
28	12.244	1824	1830	1836	rBV3	74980	135052	1.68%	0.301%
29	12.427	1854	1860	1864	rBV	212600	257716	3.21%	0.575%
30	12.524	1872	1876	1878	rBV2	90912	119802	1.49%	0.267%
31	12.579	1883	1885	1890	rVB2	100495	116022	1.45%	0.259%
32	12.671	1896	1900	1906	rVB4	49214	91932	1.15%	0.205%
33	12.768	1909	1916	1920	rVV2	527292	731654	9.13%	1.632%
34	12.908	1928	1939	1943	rBV	1904500	2437038	30.40%	5.436%
35	12.969	1943	1949	1958	rVB2	212184	446003	5.56%	0.995%
36	13.164	1977	1981	1985	rBV3	61934	102960	1.28%	0.230%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071521\
Data File : VX023306.D
Acq On : 15 Jul 2021 17:59
Operator : JC/MD
Sample : M3058-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 210714106-02-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\82X070221W.M
Title : SW846 8260

37	13.213	1985	1989	1991	rVV3	52818	82439	1.03%	0.184%
38	13.268	1995	1998	2007	rVB3	188288	312258	3.90%	0.696%
39	13.384	2008	2017	2020	rBV3	69086	135327	1.69%	0.302%
40	13.475	2027	2032	2035	rVV2	403798	588215	7.34%	1.312%
41	13.512	2035	2038	2046	rVB	1555081	1878402	23.43%	4.190%
42	13.591	2046	2051	2060	rBV	602177	830944	10.37%	1.853%
43	13.689	2060	2067	2071	rBV6	42351	85932	1.07%	0.192%
44	13.774	2077	2081	2088	rVB2	498034	660329	8.24%	1.473%
45	13.847	2088	2093	2096	rBV3	65034	113795	1.42%	0.254%
46	13.933	2101	2107	2109	rVV4	138760	277796	3.47%	0.620%
47	13.957	2109	2111	2120	rVB	221138	291983	3.64%	0.651%
48	14.042	2121	2125	2128	rVB	152526	162506	2.03%	0.362%
49	14.097	2128	2134	2138	rBV	301626	414296	5.17%	0.924%
50	14.317	2167	2170	2175	rBV4	67239	87506	1.09%	0.195%
51	14.414	2182	2186	2194	rBV3	69713	159050	1.98%	0.355%
52	14.640	2215	2223	2231	rVB	511809	764469	9.54%	1.705%
53	14.719	2231	2236	2240	rBV	902590	1124578	14.03%	2.508%
54	14.762	2240	2243	2244	rVV	341394	393183	4.90%	0.877%
55	14.780	2244	2246	2252	rVB	392420	483486	6.03%	1.078%
56	15.213	2309	2317	2321	rBV2	217155	324382	4.05%	0.724%
57	15.353	2333	2340	2348	rBV3	293246	606962	7.57%	1.354%
58	15.487	2355	2362	2375	rBV2	1199331	2063495	25.74%	4.603%
59	15.615	2378	2383	2387	rVV	186919	316141	3.94%	0.705%
60	15.652	2387	2389	2394	rVB	94238	125162	1.56%	0.279%
61	15.841	2412	2420	2426	rBV2	51631	153172	1.91%	0.342%
62	16.097	2456	2462	2469	rBV2	89843	183750	2.29%	0.410%
63	16.188	2469	2477	2481	rBV4	94104	204678	2.55%	0.457%
64	16.328	2494	2500	2506	rBV	630431	1131835	14.12%	2.525%
65	16.536	2528	2534	2541	rBV3	32526	86910	1.08%	0.194%
66	16.688	2550	2559	2568	rVB	207584	486600	6.07%	1.085%

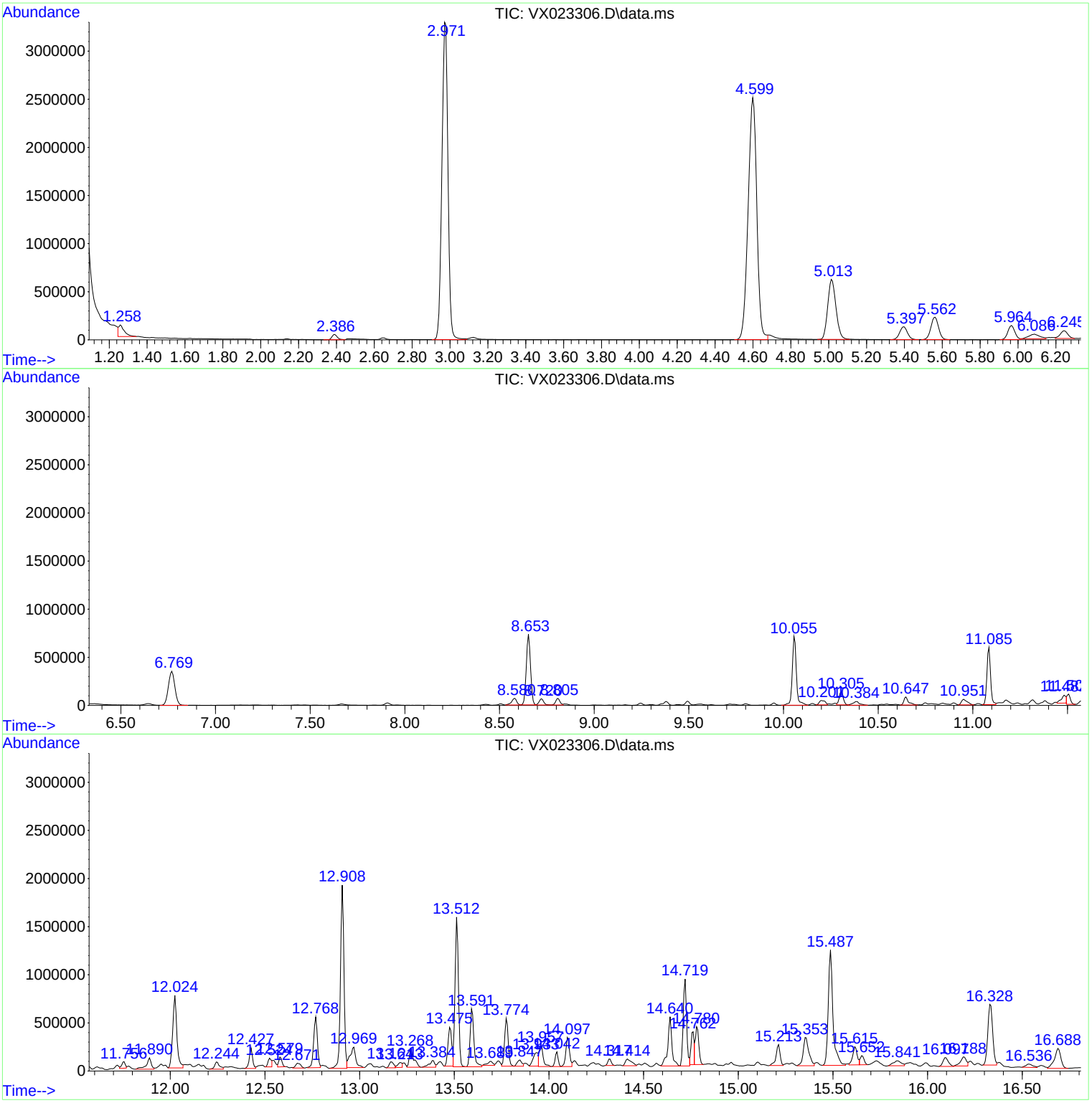
Sum of corrected areas: 44833500

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071521\
Data File : VX023306.D
Acq On : 15 Jul 2021 17:59
Operator : JC/MD
Sample : M3058-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
210714106-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X070221W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071521\
Data File : VX023306.D
Acq On : 15 Jul 2021 17:59
Operator : JC/MD
Sample : M3058-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
210714106-02-VOA

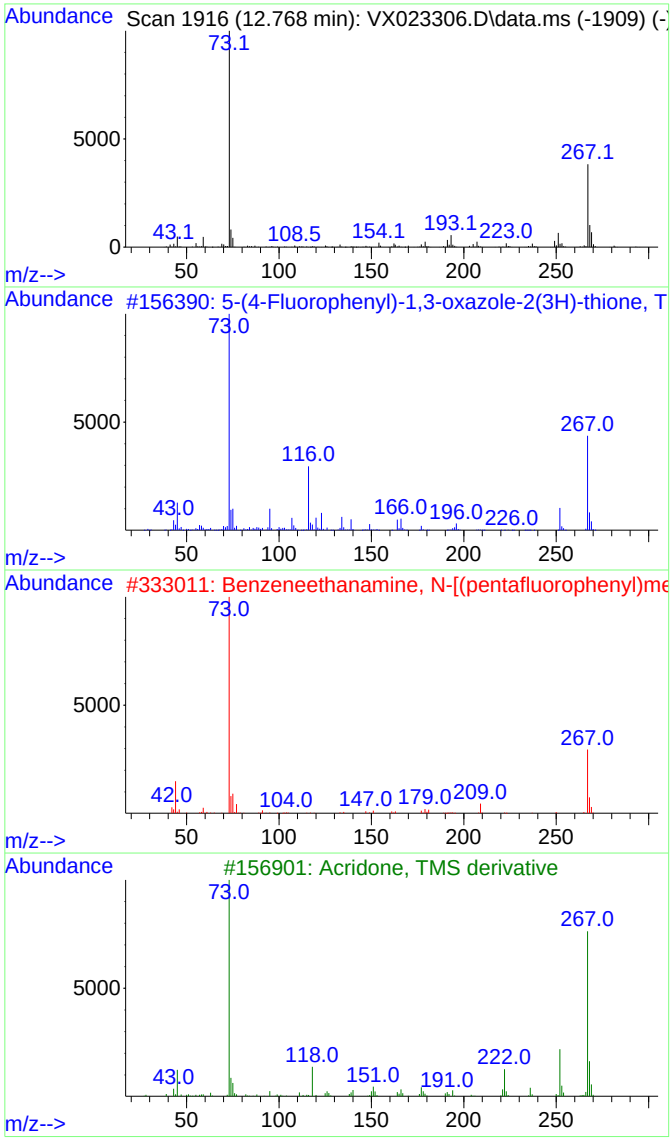
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X070221W.M
Quant Title : SW846 8260

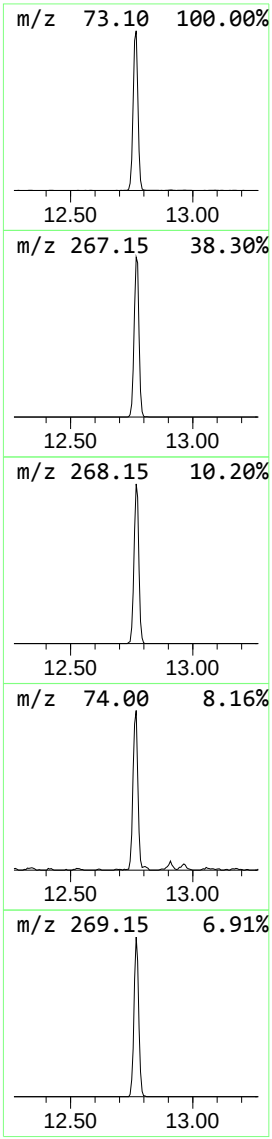
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 5-(4-Fluorophenyl)-1,3-oxaz... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.768	31.96 ug/l	731654	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-(4-Fluorophenyl)-1,3-oxazole-2...	267	C12H14FNOSSi	1000497-07-6	59
2	Benzeneethanamine, N-[(pentafluo...	475	C21H26F5NO2Si2	055429-85-1	59
3	Acridone, TMS derivative	267	C16H17NOSi	1000478-16-0	59
4	11H-Dibenzo[b,e][1,4]diazepin-11...	267	C16H17N3O	013450-73-2	55
5	Salicylic acid, 2TMS derivative	282	C13H22O3Si2	003789-85-3	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071521\
Data File : VX023306.D
Acq On : 15 Jul 2021 17:59
Operator : JC/MD
Sample : M3058-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
210714106-02-VOA

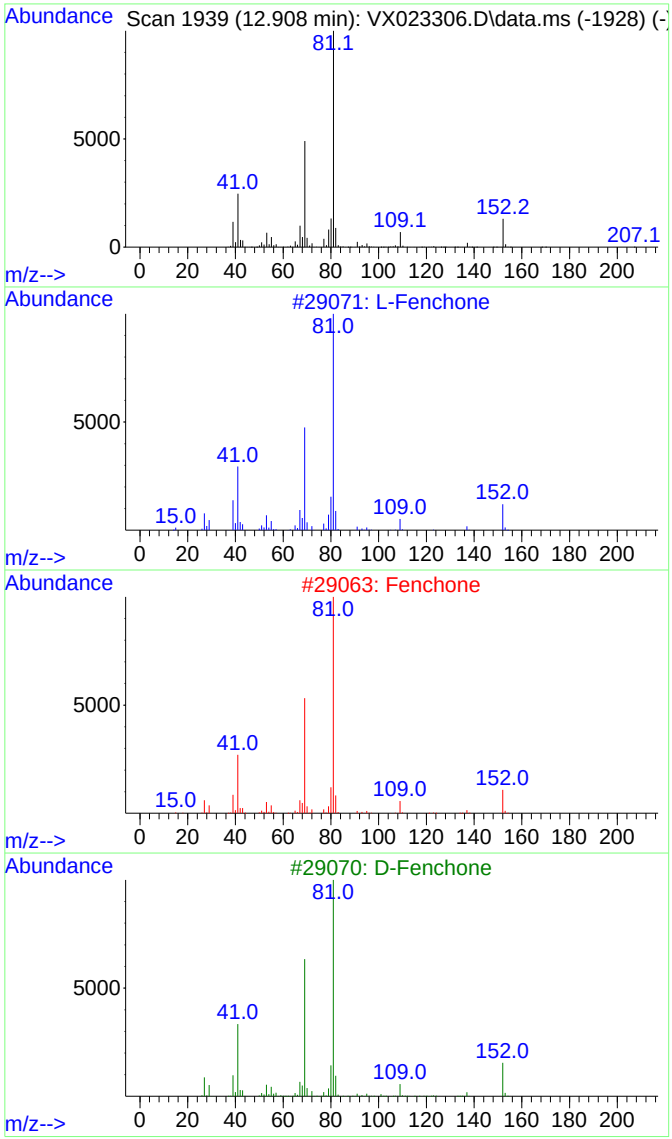
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X070221W.M
Quant Title : SW846 8260

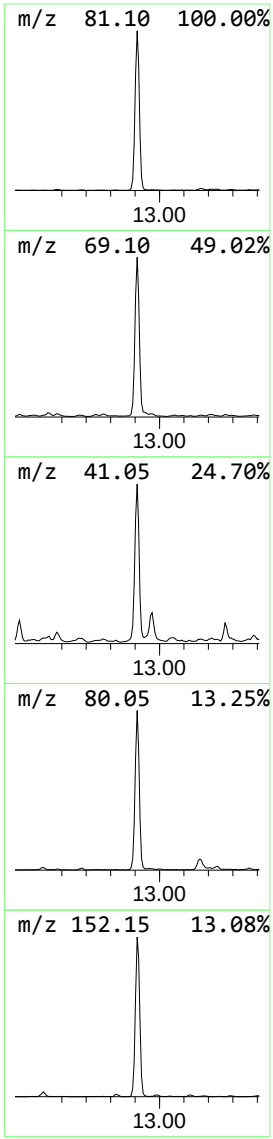
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 L-Fenchone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.908	106.44 ug/l	2437040	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	L-Fenchone	152	C10H16O	007787-20-4	95
2	Fenchone	152	C10H16O	001195-79-5	95
3	D-Fenchone	152	C10H16O	004695-62-9	94
4	Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	45
5	Ethanone, 1-(2-methyl-2-cyclopen...	124	C8H12O	001767-84-6	45





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071521\
Data File : VX023306.D
Acq On : 15 Jul 2021 17:59
Operator : JC/MD
Sample : M3058-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
210714106-02-VOA

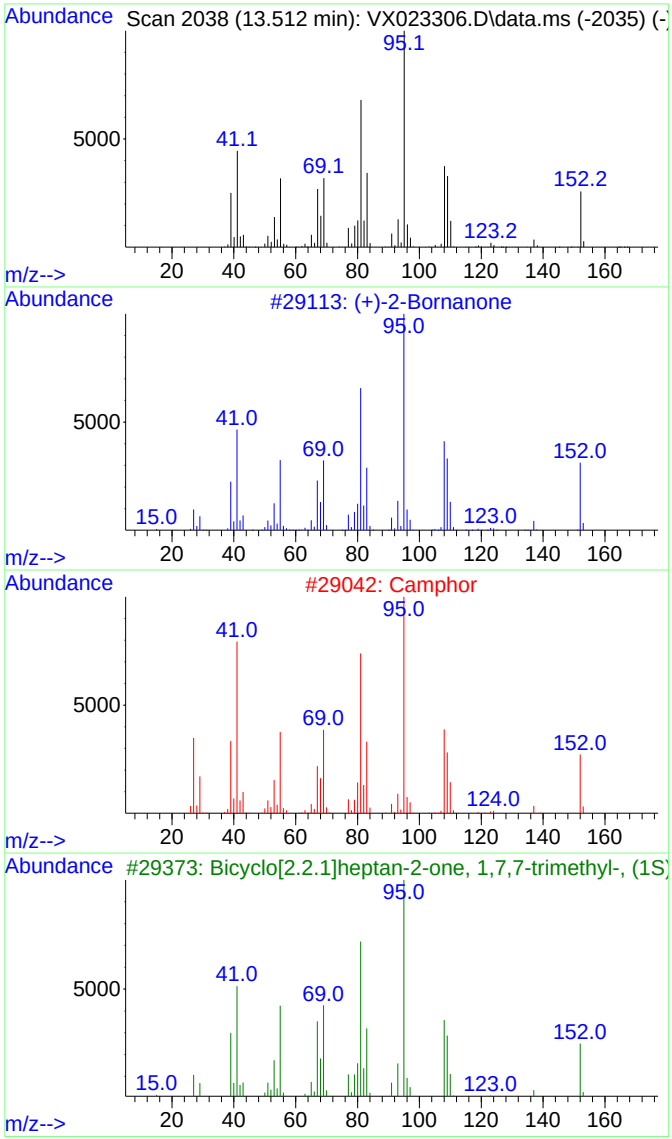
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X070221W.M
Quant Title : SW846 8260

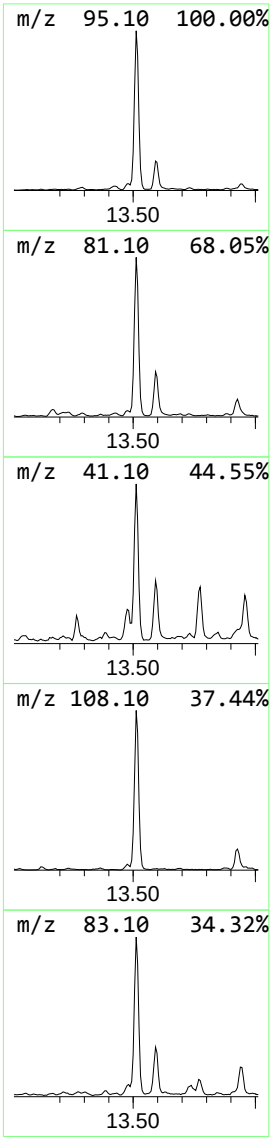
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (+)-2-Bornanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.512	82.04 ug/l	1878400	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-2-Bornanone	152	C10H16O	000464-49-3	98
2	Camphor	152	C10H16O	000076-22-2	98
3	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	97
4	5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	58
5	2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	49





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071521\
Data File : VX023306.D
Acq On : 15 Jul 2021 17:59
Operator : JC/MD
Sample : M3058-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
210714106-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X070221W.M
Quant Title : SW846 8260

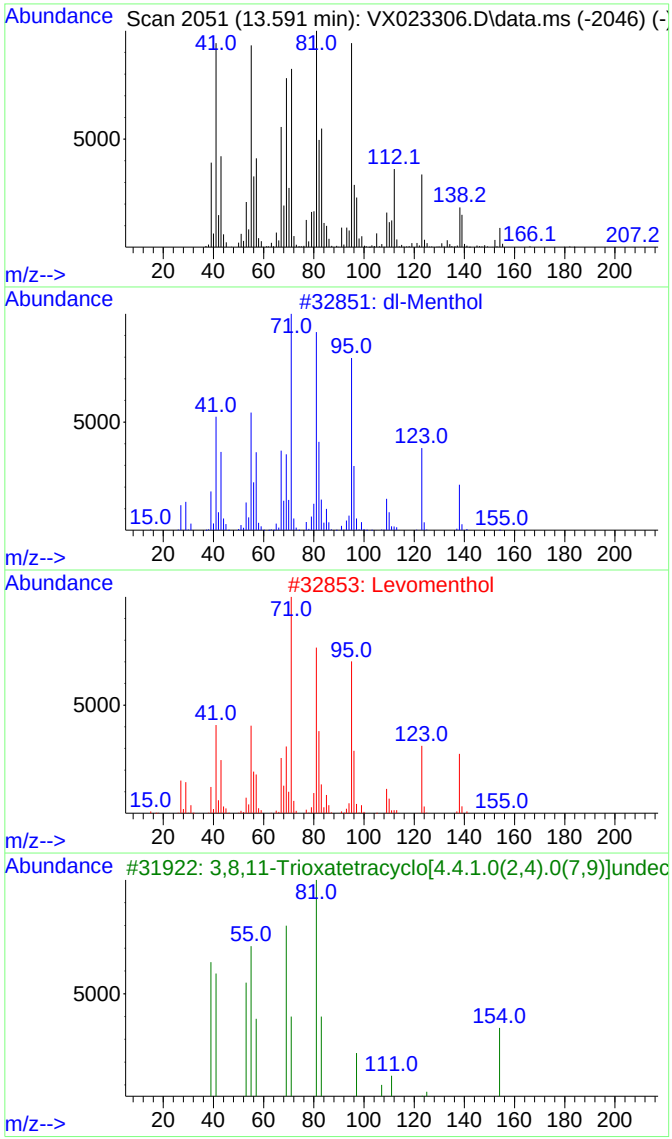
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

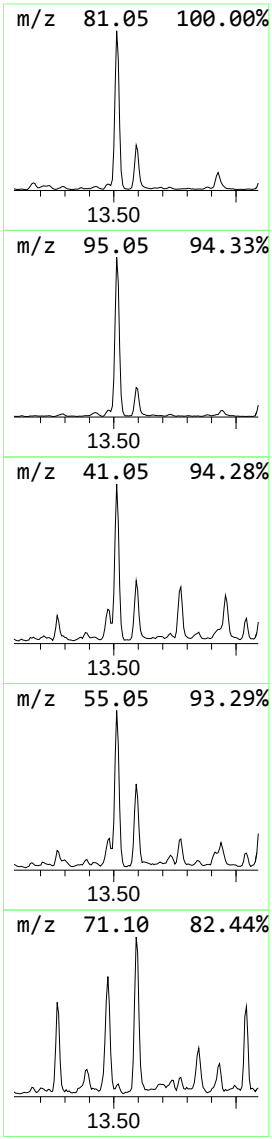
****

Peak Number 5 dl-Menthol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.591	36.29 ug/l	830944	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	dl-Menthol	156	C10H20O	000089-78-1	58
2	Levomenthol	156	C10H20O	002216-51-5	52
3	3,8,11-Trioxatetracyclo[4.4.1.0(...	154	C8H10O3	050267-13-5	46
4	Oxirane, tetradecyl-	240	C16H32O	007320-37-8	41
5	9-Methylbicyclo[3.3.1]nonane	138	C10H18	025107-01-1	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071521\
Data File : VX023306.D
Acq On : 15 Jul 2021 17:59
Operator : JC/MD
Sample : M3058-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
210714106-02-VOA

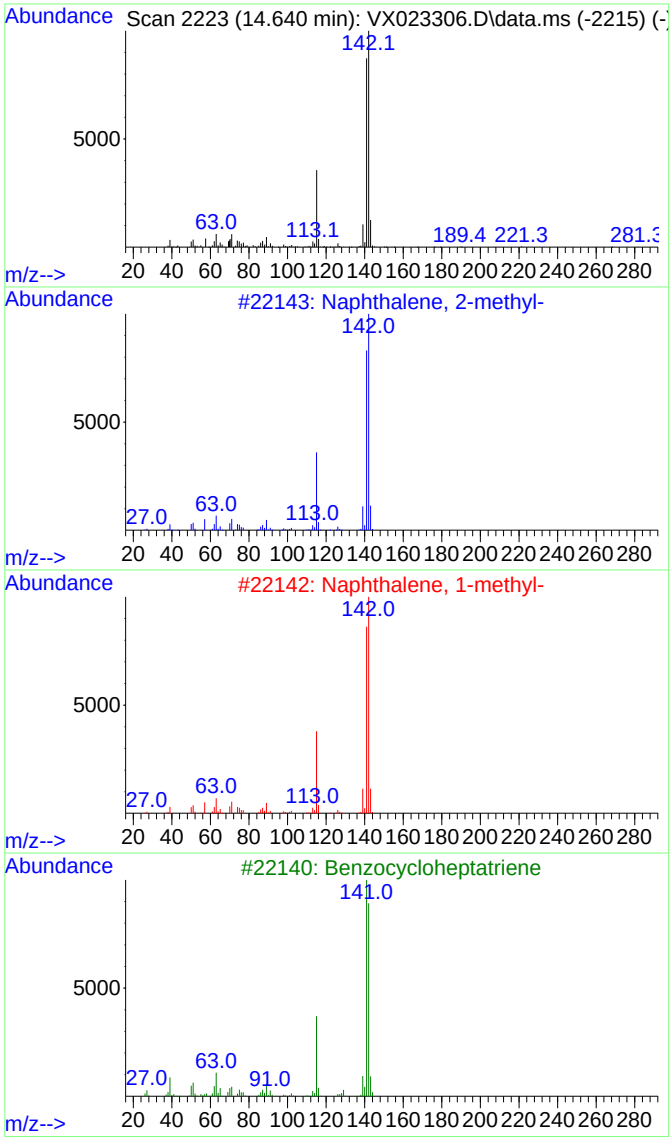
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X070221W.M
Quant Title : SW846 8260

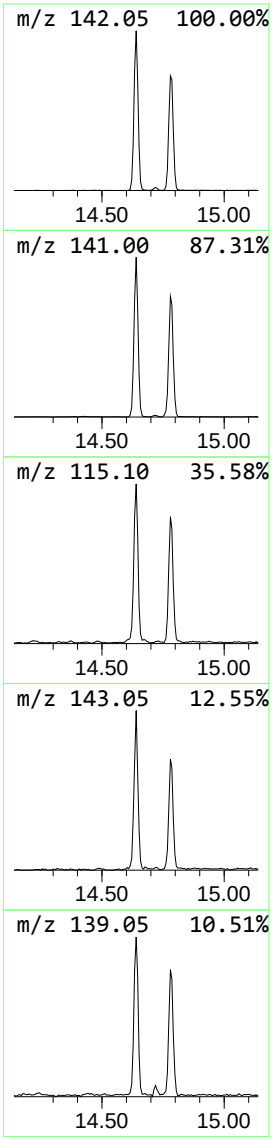
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Naphthalene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	33.39 ug/l	764469	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3	Benzocycloheptatriene	142	C11H10	000264-09-5	91
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071521\
Data File : VX023306.D
Acq On : 15 Jul 2021 17:59
Operator : JC/MD
Sample : M3058-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
210714106-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X070221W.M
Quant Title : SW846 8260

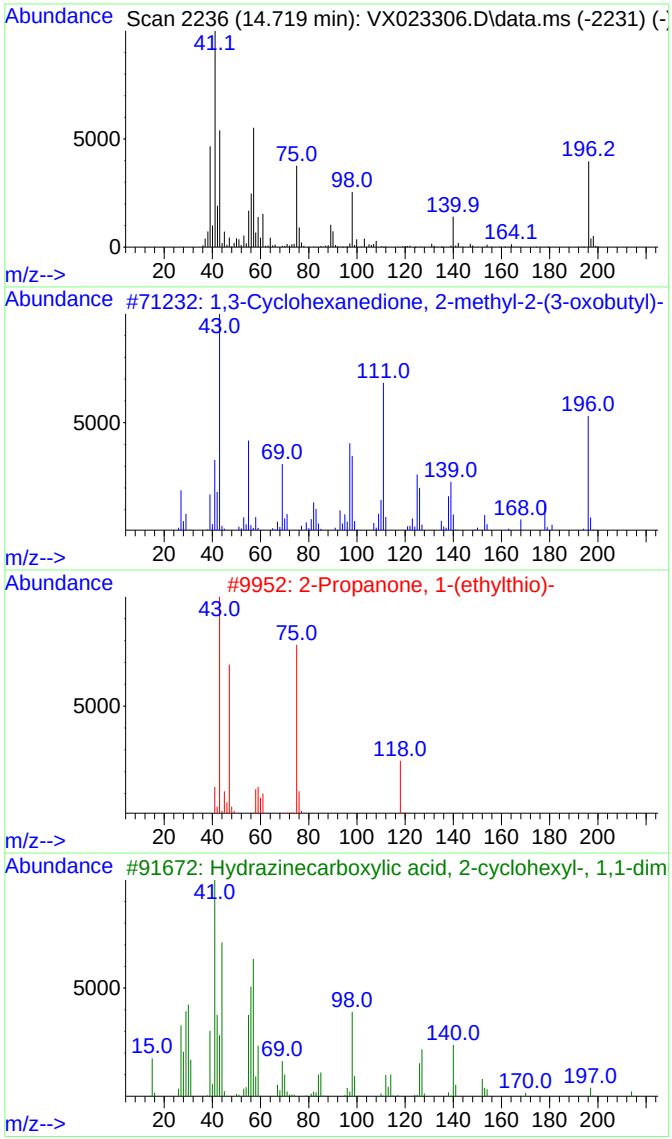
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

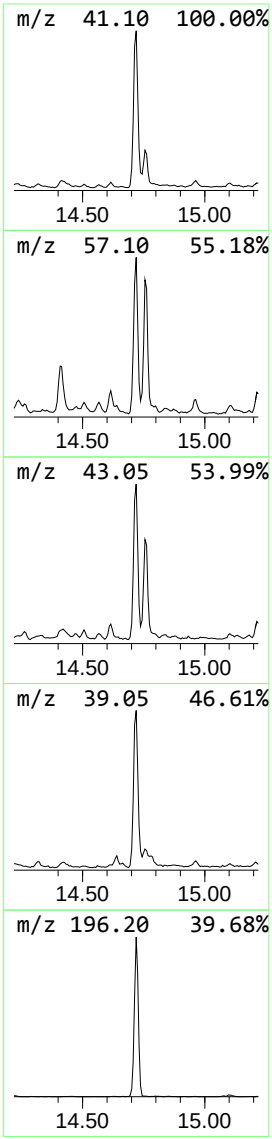
****

Peak Number 7 unknown14.719 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.719	49.12 ug/l	1124580	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclohexanedione, 2-methyl-2...	196	C11H16O3	005073-65-4	16
2	2-Propanone, 1-(ethylthio)-	118	C5H10OS	020996-62-7	14
3	Hydrazinecarboxylic acid, 2-cycl...	214	C11H22N2O2	060295-21-8	10
4	3-Methyl-3-hexene	98	C7H14	003404-65-7	9
5	1-Butanamine, 3-methyl-N-(3-meth...	155	C10H21N	035448-31-8	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071521\
Data File : VX023306.D
Acq On : 15 Jul 2021 17:59
Operator : JC/MD
Sample : M3058-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
210714106-02-VOA

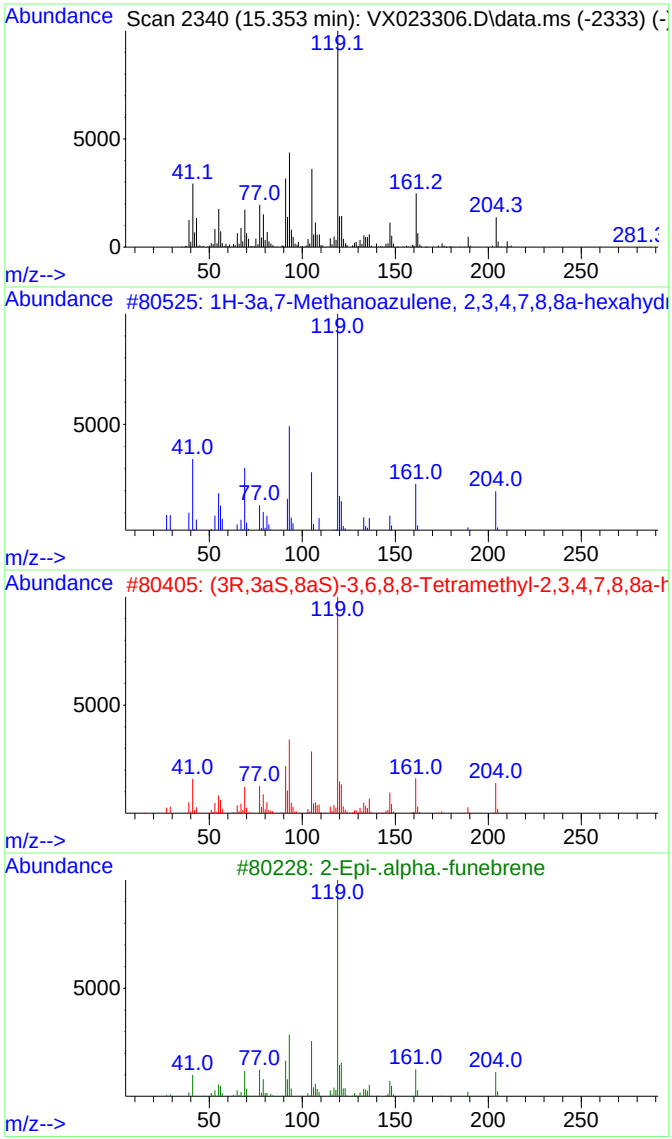
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X070221W.M
Quant Title : SW846 8260

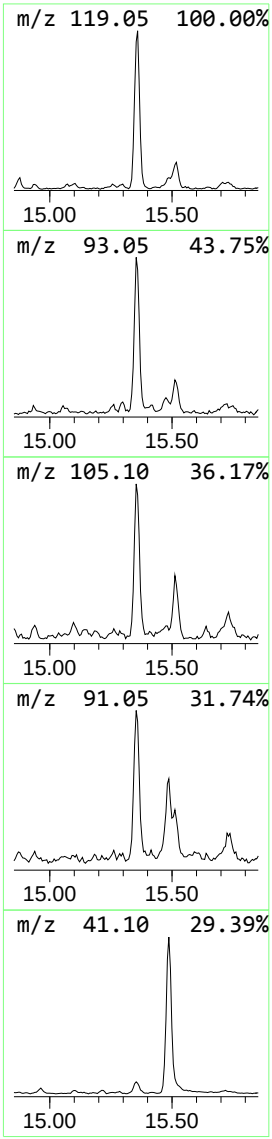
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1H-3a,7-Methanoazulene, 2,3... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.353	26.51 ug/l	606962	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-3a,7-Methanoazulene, 2,3,4,7,...	204	C15H24	000469-61-4	98
2	(3R,3aS,8aS)-3,6,8,8-Tetramethyl...	204	C15H24	022567-43-7	97
3	2-Epi-.alpha.-funebrene	204	C15H24	065354-33-8	90
4	Cubenene	204	C15H24	029837-12-5	90
5	3,5,5,9-Tetramethyl-4a,5,6,7,8,9...	204	C15H24	1000412-94-8	86





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071521\
Data File : VX023306.D
Acq On : 15 Jul 2021 17:59
Operator : JC/MD
Sample : M3058-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
210714106-02-VOA

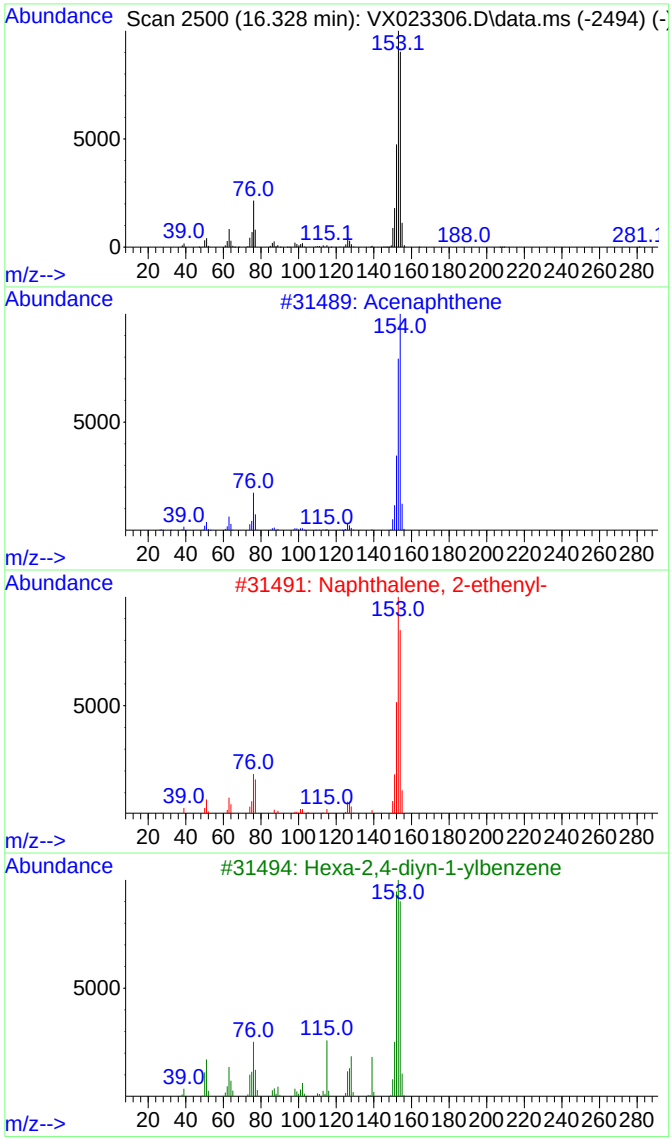
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X070221W.M
Quant Title : SW846 8260

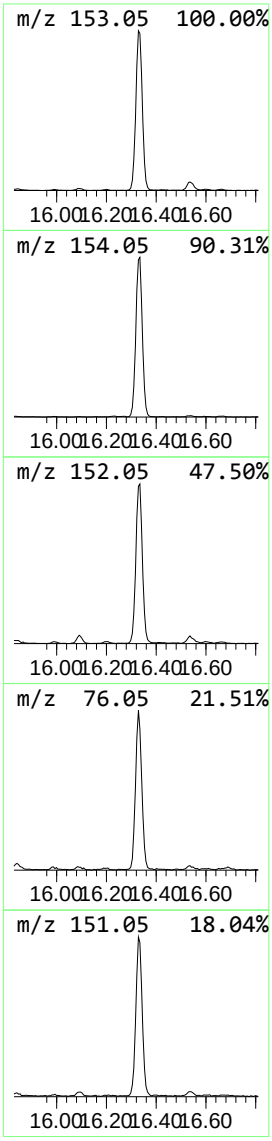
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Acenaphthene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.328	49.44 ug/l	1131840	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	64
3	Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	59
4	2,4,6-Trihydroxybenzaldehyde	154	C7H6O4	000487-70-7	50
5	3-Fluoro-para-anisaldehyde	154	C8H7FO2	000351-54-2	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071521\
Data File : VX023306.D
Acq On : 15 Jul 2021 17:59
Operator : JC/MD
Sample : M3058-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 210714106-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X070221W.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
5-(4-Fluorophen...	12.768	32.0	ug/l	731654	4	12.024	1144760	50.0
L-Fenchone	12.908	106.4	ug/l	2437040	4	12.024	1144760	50.0
(+)-2-Bornanone	13.512	82.0	ug/l	1878400	4	12.024	1144760	50.0
dl-Menthol	13.591	36.3	ug/l	830944	4	12.024	1144760	50.0
Naphthalene, 1-...	14.640	33.4	ug/l	764469	4	12.024	1144760	50.0
unknown14.719	14.719	49.1	ug/l	1124580	4	12.024	1144760	50.0
1H-3a,7-Methano...	15.353	26.5	ug/l	606962	4	12.024	1144760	50.0
Acenaphthene	16.328	49.4	ug/l	1131840	4	12.024	1144760	50.0