LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081622\
Data File : VN073943.D
Acq On : 16 Aug 2022 12:55
Operator : JC\MD
Sample : N4198-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GFD-TOTES

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_N\methods\82N081522W.M
Title : SW846 8260

Signal : TIC: VN073943.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.216	385	396	419	rBV	1478551	4324629	55.69%	8.267%
2	4.504	433	445	464	rBV	445369	1375833	17.72%	2.630%
3	7.263	901	914	926	rBV2	63381	180112	2.32%	0.344%
4	7.951	1020	1031	1036	rBV	401428	943034	12.14%	1.803%
5	8.016	1036	1042	1060	rVB	721575	1686537	21.72%	3.224%
6	8.369	1093	1102	1113	rBV	357239	823891	10.61%	1.575%
7	8.904	1184	1193	1212	rBV	949885	1958862	25.23%	3.745%
8	9.345	1261	1268	1274	rBV2	59459	116533	1.50%	0.223%
9	10.269	1418	1425	1434	rBV	79910	151756	1.95%	0.290%
10	10.380	1434	1444	1449	rBV	1330424	2434849	31.36%	4.654%
11	10.445	1449	1455	1470	rVB	4238353	7765279	100.00%	14.844%
12	11.027	1543	1554	1566	rBV	974791	1639904	21.12%	3.135%
13	11.175	1574	1579	1585	rVB	59150	94563	1.22%	0.181%
14	11.686	1655	1666	1676	rBV	1412753	2470181	31.81%	4.722%
15	11.786	1676	1683	1690	rVV	64835	128498	1.65%	0.246%
16	11.892	1692	1701	1712	rVB	228802	467403	6.02%	0.893%
17	12.222	1744	1757	1764	rBV2	277979	557278	7.18%	1.065%
18	12.292	1764	1769	1777	rVB	308067	485671	6.25%	0.928%
19	12.374	1777	1783	1790	rBV2	43533	98089	1.26%	0.188%
20	12.669	1827	1833	1844	rVB	1234069	2096033	26.99%	4.007%
21	12.786	1846	1853	1859	rVV	251072	420224	5.41%	0.803%
22	12.863	1861	1866	1870	rVV	46373	83212	1.07%	0.159%
23	12.921	1870	1876	1880	rVV	257058	447098	5.76%	0.855%
24	12.957	1880	1882	1885	rVV	127285	173268	2.23%	0.331%
25	13.004	1885	1890	1901	rVB2	287662	720599	9.28%	1.378%
26	13.157	1910	1916	1923	rBV	238276	407944	5.25%	0.780%
27	13.304	1932	1941	1947	rBV	476646	809052	10.42%	1.547%
28	13.498	1969	1974	1979	rBV3	79072	139629	1.80%	0.267%
29	13.616	1987	1994	2004	rVV2	1673055	3412123	43.94%	6.523%
30	13.710	2004	2010	2017	rVV	868207	1372670	17.68%	2.624%
31	13.780	2017	2022	2023	rVV4	89047	139622	1.80%	0.267%
32	13.810	2023	2027	2031	rVV2	414573	735022	9.47%	1.405%
33	13.845	2031	2033	2043	rVB3	205110	393868	5.07%	0.753%
34	13.933	2043	2048	2053	rBV3	171684	284007	3.66%	0.543%
35	14.004	2054	2060	2066	rBV2	120195	206363	2.66%	0.394%
36	14.068	2067	2071	2074	rBV	122736	209572	2.70%	0.401%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081622\
Data File : VN073943.D
Acq On : 16 Aug 2022 12:55
Operator : JC\MD
Sample : N4198-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GFD-TOTES

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_N\methods\82N081522W.M
Title : SW846 8260

37	14.098	2074	2076	2081	rVB	138225	175492	2.26%	0.335%
38	14.157	2081	2086	2091	rVB	197650	292533	3.77%	0.559%
39	14.216	2091	2096	2099	rBV2	67593	107842	1.39%	0.206%
40	14.268	2099	2105	2116	rBV2	269366	586272	7.55%	1.121%
41	14.398	2122	2127	2131	rBV2	97038	150789	1.94%	0.288%
42	14.468	2131	2139	2144	rVV6	227869	527871	6.80%	1.009%
43	14.516	2144	2147	2151	rVV	202070	280641	3.61%	0.536%
44	14.568	2151	2156	2158	rVV2	185865	280499	3.61%	0.536%
45	14.604	2158	2162	2169	rVB3	365678	593893	7.65%	1.135%
46	14.698	2174	2178	2182	rVB2	70021	102103	1.31%	0.195%
47	14.745	2182	2186	2190	rBV	257480	436347	5.62%	0.834%
48	14.786	2190	2193	2199	rVB2	173572	274049	3.53%	0.524%
49	14.868	2199	2207	2212	rBV2	648844	1426711	18.37%	2.727%
50	14.915	2212	2215	2224	rVB6	98016	195519	2.52%	0.374%
51	15.021	2226	2233	2239	rBV	570995	969048	12.48%	1.852%
52	15.133	2247	2252	2255	rBV4	149414	251068	3.23%	0.480%
53	15.245	2265	2271	2275	rBV2	211477	449437	5.79%	0.859%
54	15.321	2281	2284	2291	rVB6	62938	113324	1.46%	0.217%
55	15.439	2292	2304	2309	rBV2	439904	1198507	15.43%	2.291%
56	15.492	2309	2313	2317	rBV	96107	136513	1.76%	0.261%
57	15.545	2318	2322	2324	rBV5	77554	111552	1.44%	0.213%
58	15.627	2333	2336	2346	rVB4	145766	293771	3.78%	0.562%
59	15.733	2346	2354	2359	rBV3	230212	488583	6.29%	0.934%
60	15.792	2360	2364	2373	rVV7	67805	177314	2.28%	0.339%
61	15.939	2377	2389	2400	rVB	399920	1054160	13.58%	2.015%
62	16.115	2411	2419	2425	rBV4	109952	292994	3.77%	0.560%
63	16.262	2436	2444	2452	rBV	286648	637769	8.21%	1.219%
64	16.462	2472	2478	2484	rVB2	156251	308842	3.98%	0.590%
65	16.527	2484	2489	2496	rBV	134128	279689	3.60%	0.535%
66	16.739	2517	2525	2531	rBV5	129905	365632	4.71%	0.699%

Sum of corrected areas: 52311972

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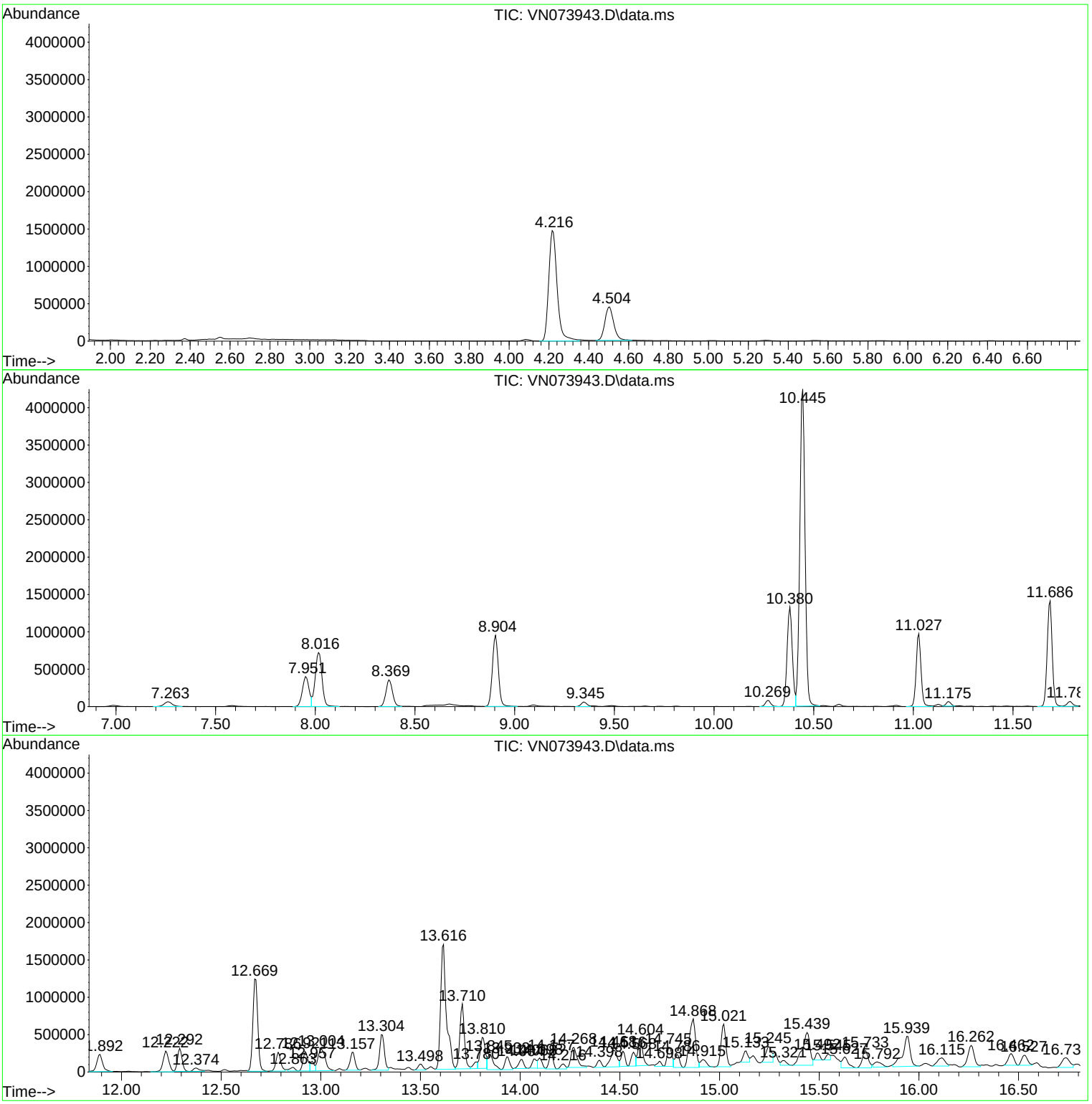
Sample : N4198-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GFD-TOTES

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081522W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081622\
Data File : VN073943.D
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Operator : JC\MD
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Quant Title : SW846 8260

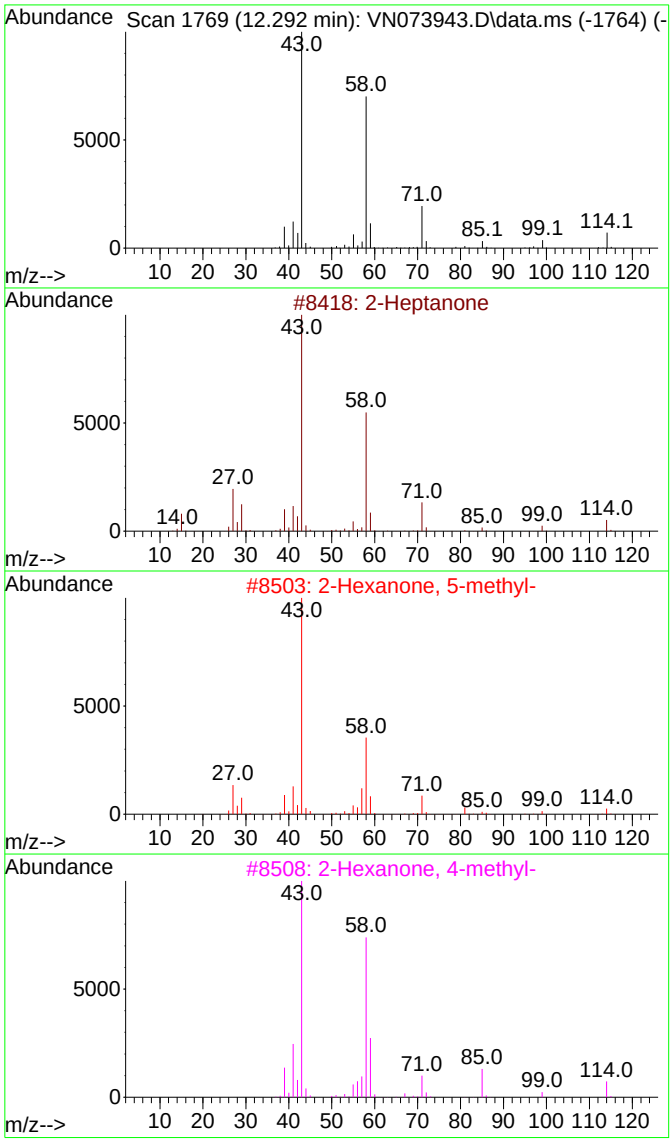
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

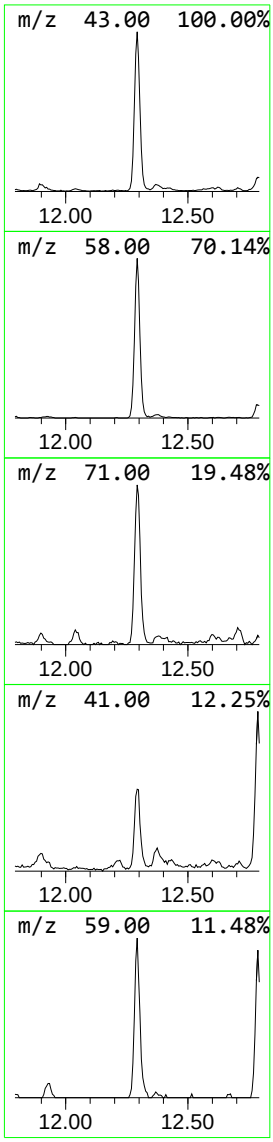
****

Peak Number 1 2-Heptanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.292	9.83 ug/l	485671	Chlorobenzene-d5	11.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone	114	C7H14O	000110-43-0	91
2	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	83
3	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	53
4	2-Pentanone, 4,4-dimethyl-	114	C7H14O	000590-50-1	49
5	N-Cyclohexyl-N'-[2-(dimethylamin...	213	C11H23N3O	097943-37-8	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081622\
Data File : VN073943.D
Acq On : 16 Aug 2022 12:55
Operator : JC\MD
Sample : N4198-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GFD-TOTES

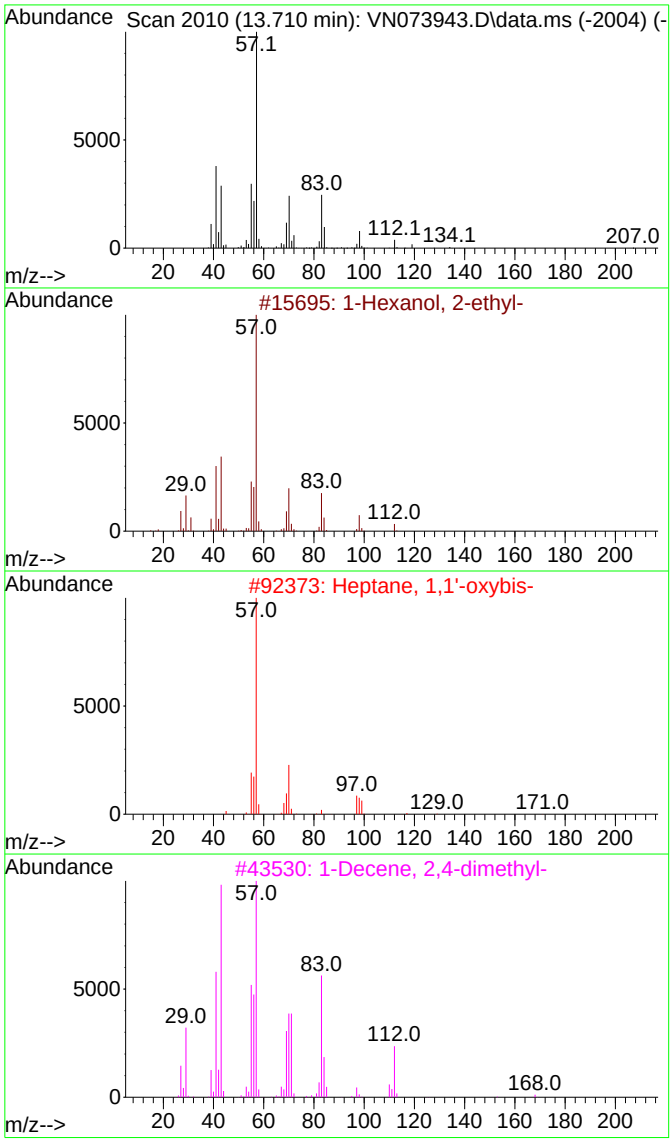
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081522W.M
Quant Title : SW846 8260

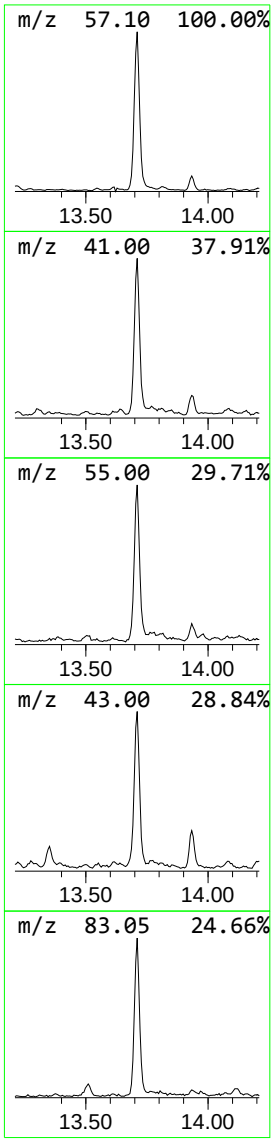
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.710	20.11 ug/l	1372670	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
3	1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	50
4	2-Ethyl-1-hexanol, pentafluoropr...	276	C11H17F5O2	959012-82-9	47
5	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081622\
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Acq On : 16 Aug 2022 12:55
Operator : JC\MD
Sample : N4198-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GFD-TOTES

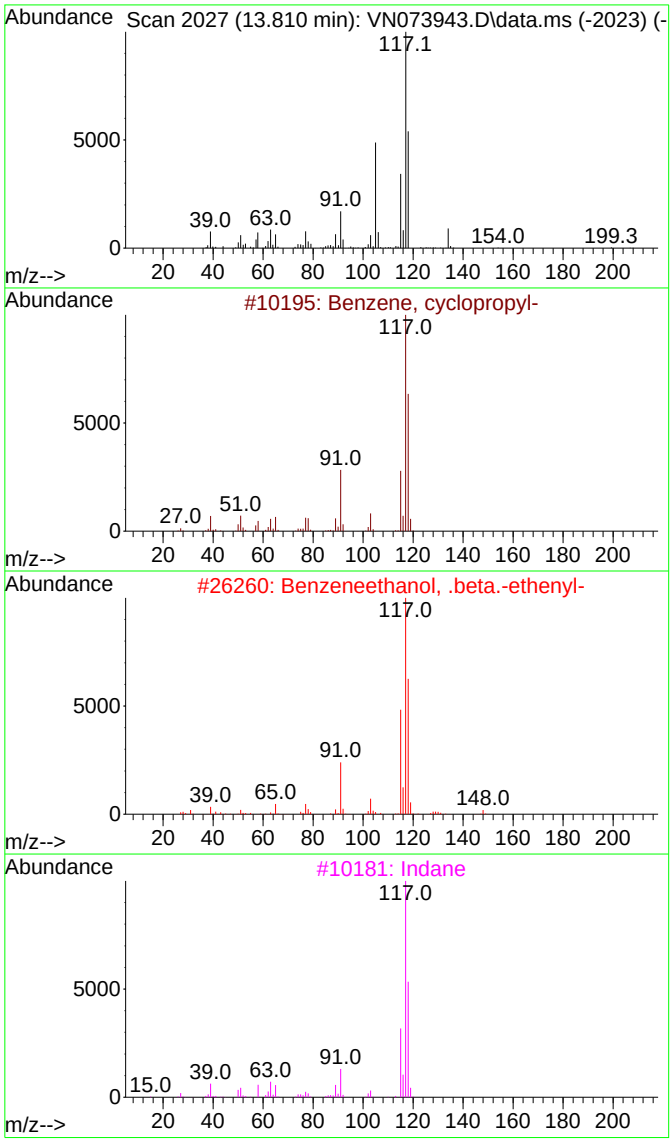
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081522W.M
Quant Title : SW846 8260

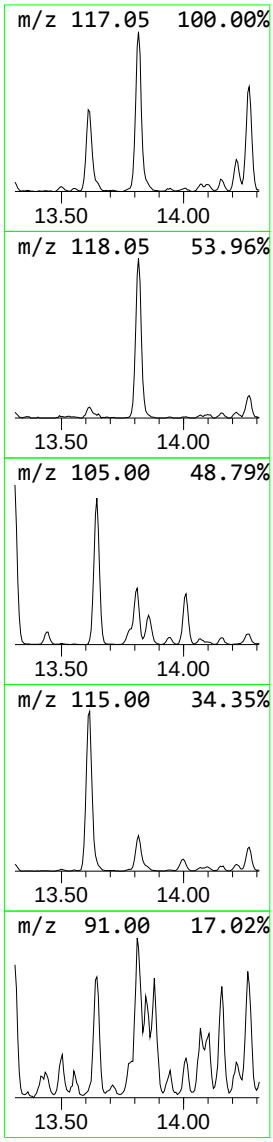
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzene, cyclopropyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.810	10.77 ug/l	735022	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
2	Benzeneethanol, .beta.-ethenyl-	148	C10H12O	006052-63-7	72
3	Indane	118	C9H10	000496-11-7	70
4	Benzene, 2-propenyl-	118	C9H10	000300-57-2	68
5	Deltacyclene	118	C9H10	007785-10-6	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081622\
Data File : VN073943.D
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Operator : JC\MD
Sample : N4198-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GFD-TOTES

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081522W.M
Quant Title : SW846 8260

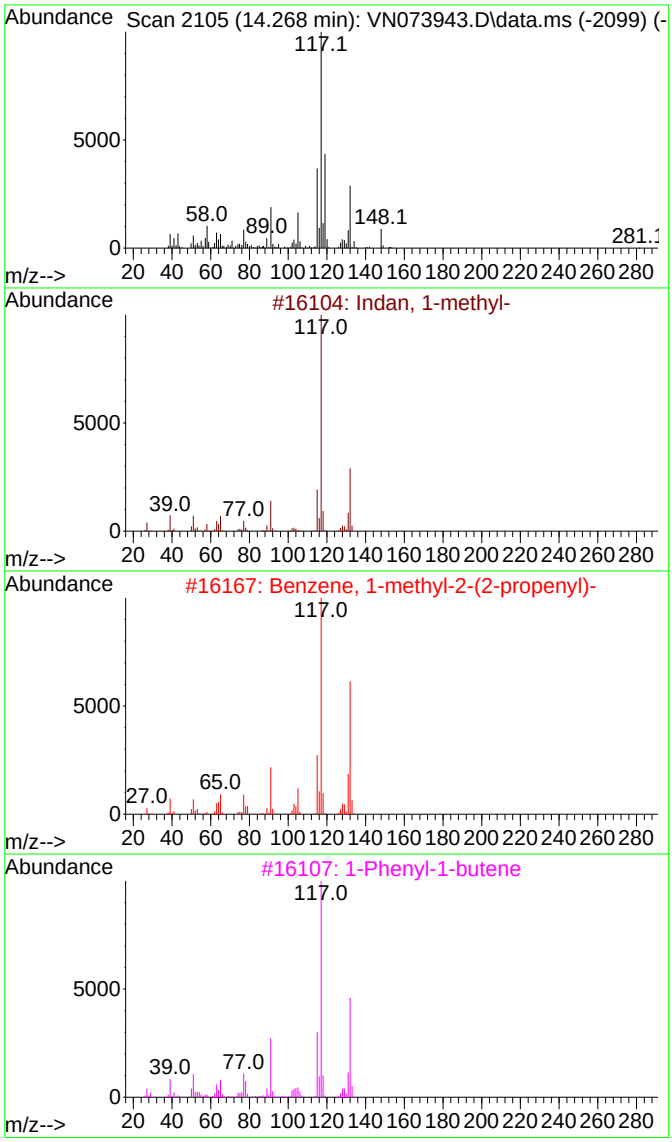
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

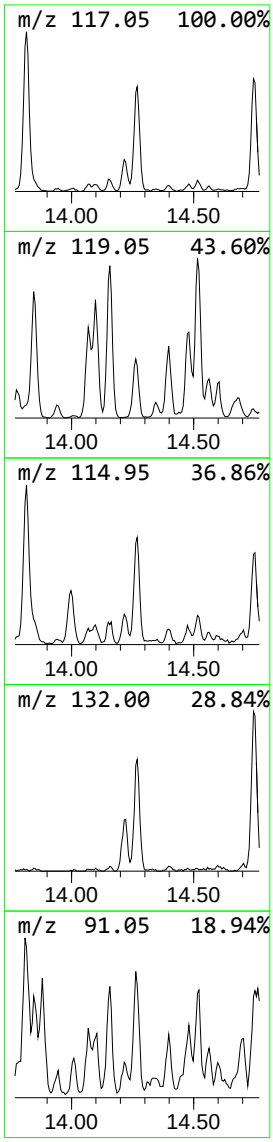
****

Peak Number 4 Indan, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.269	8.59 ug/l	586272	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indan, 1-methyl-	132	C10H12	000767-58-8	70
2	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	68
3	1-Phenyl-1-butene	132	C10H12	000824-90-8	68
4	(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	68
5	Benzene, 2-butenyl-	132	C10H12	001560-06-1	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081622\
Data File : VN073943.D
Acq On : 16 Aug 2022 12:55
Operator : JC\MD
Sample : N4198-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GFD-TOTES

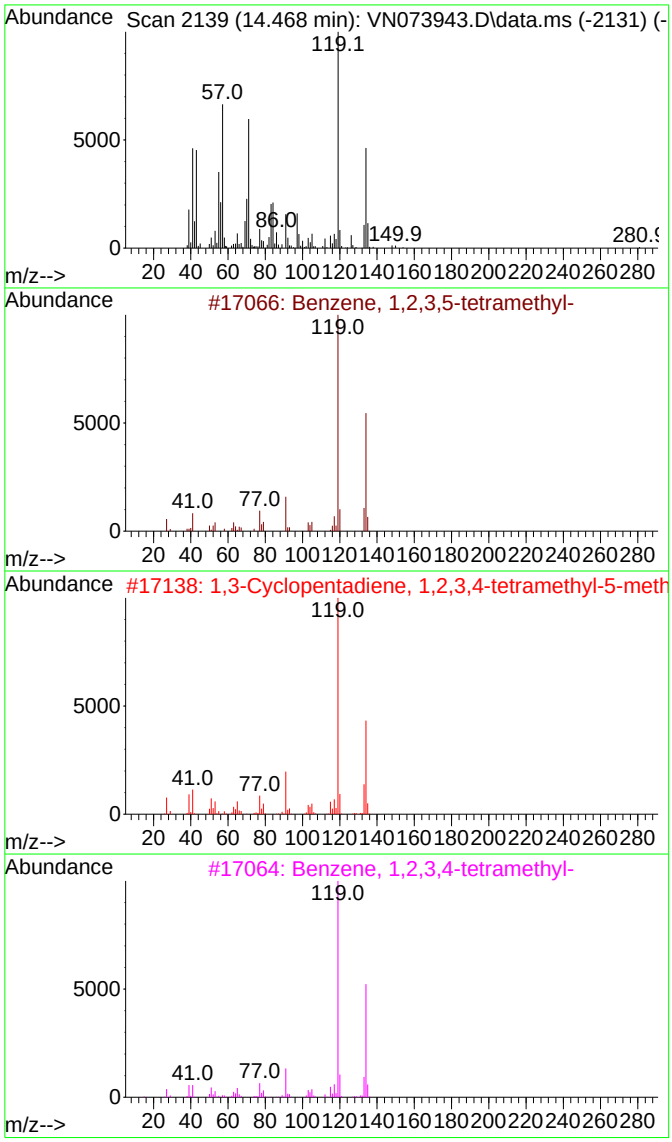
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081522W.M
Quant Title : SW846 8260

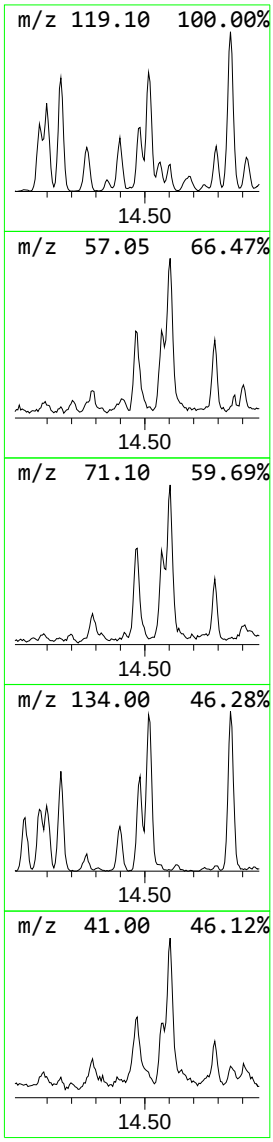
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.468	7.74 ug/l	527871	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	86
2	1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	86
3	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	50
4	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	50
5	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	46





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081622\
Data File : VN073943.D
Acq On : 16 Aug 2022 12:55
Operator : JC\MD
Sample : N4198-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GFD-TOTES

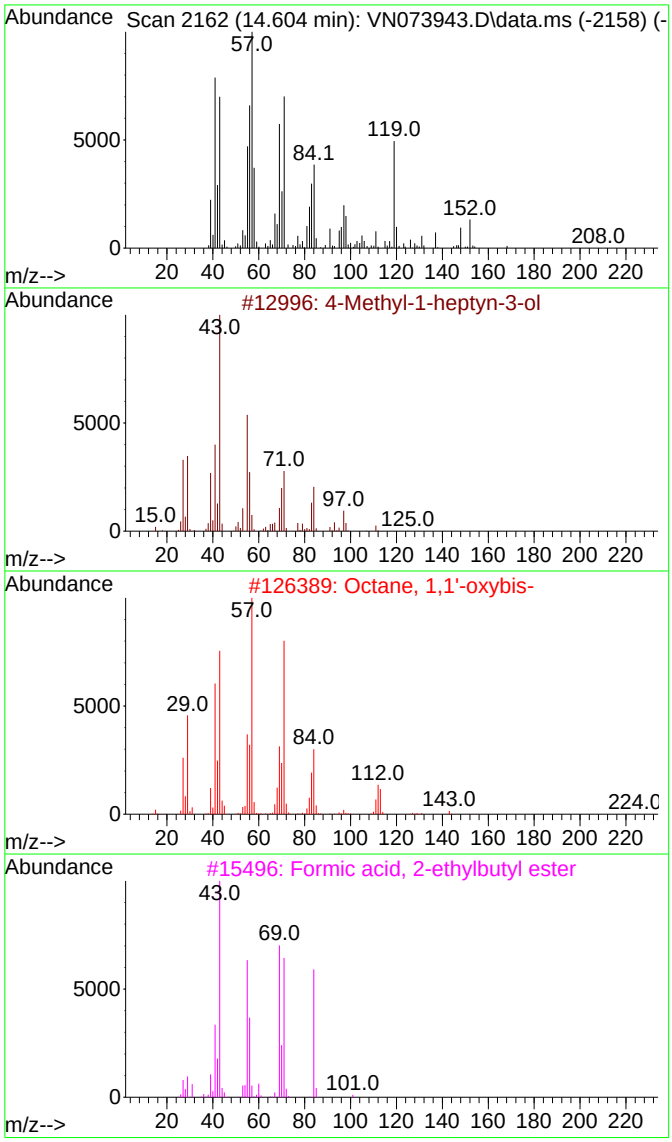
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081522W.M
Quant Title : SW846 8260

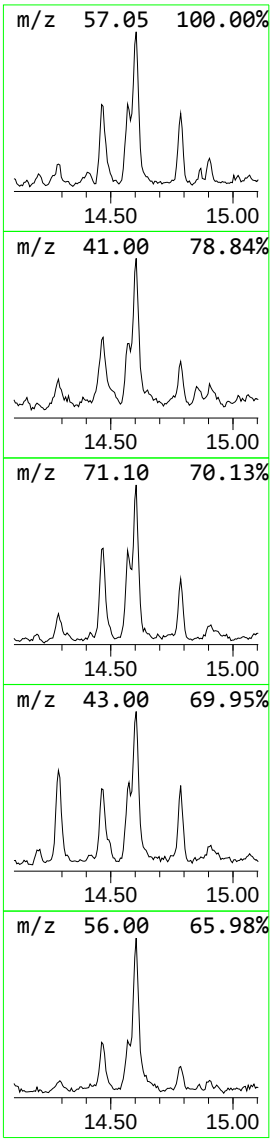
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 unknown14.604 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.604	8.70 ug/l	593893	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methyl-1-heptyn-3-ol	126	C8H14O	1000342-45-3	35
2	Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	35
3	Formic acid, 2-ethylbutyl ester	130	C7H14O2	1000367-92-2	27
4	1-Pentene, 3-methyl-	84	C6H12	000760-20-3	25
5	Cyclohexane	84	C6H12	000110-82-7	22





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081622\
Data File : VN073943.D
Acq On : 16 Aug 2022 12:55
Operator : JC\MD
Sample : N4198-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GFD-TOTES

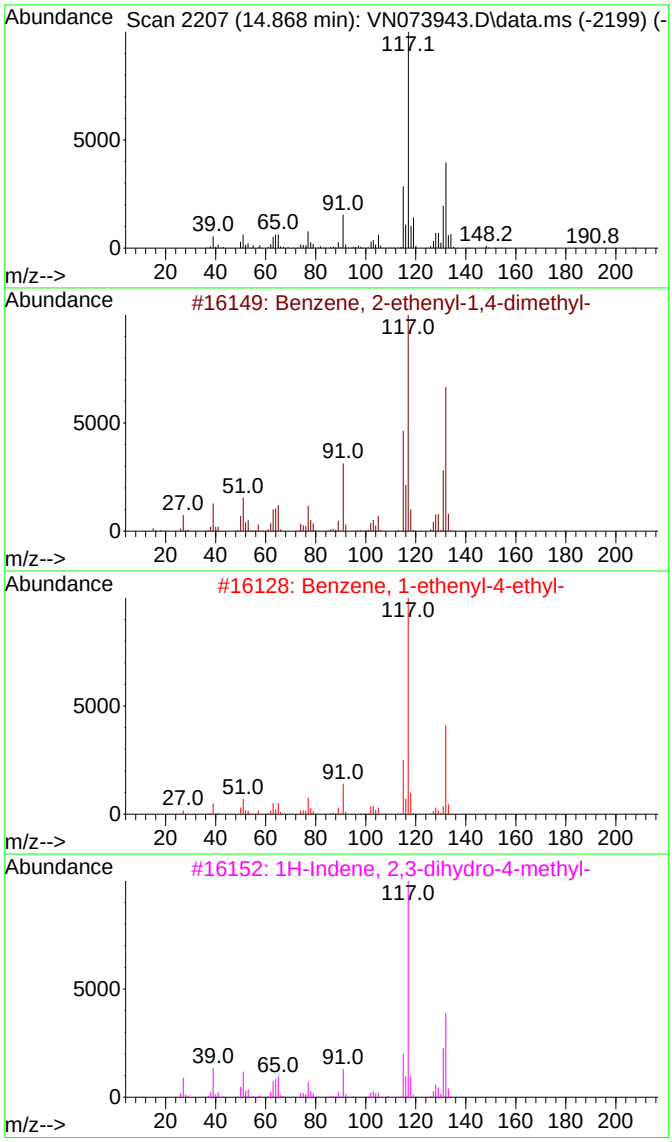
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081522W.M
Quant Title : SW846 8260

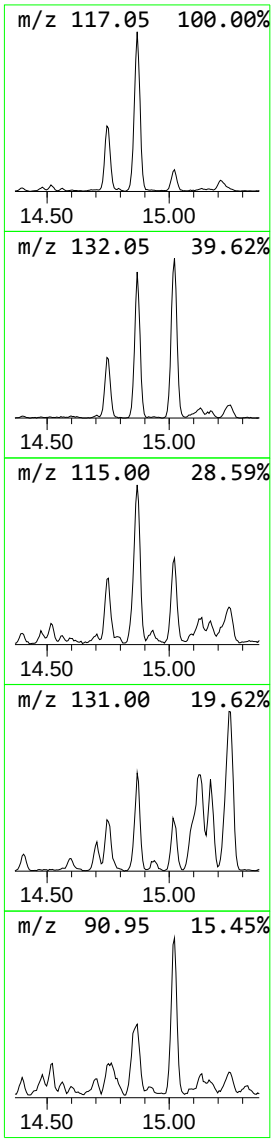
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.868	20.91 ug/l	1426710	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
3	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	90
4	3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
5	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87





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Data File : VN073943.D
Acq On : 16 Aug 2022 12:55
Operator : JC\MD
Sample : N4198-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GFD-TOTES

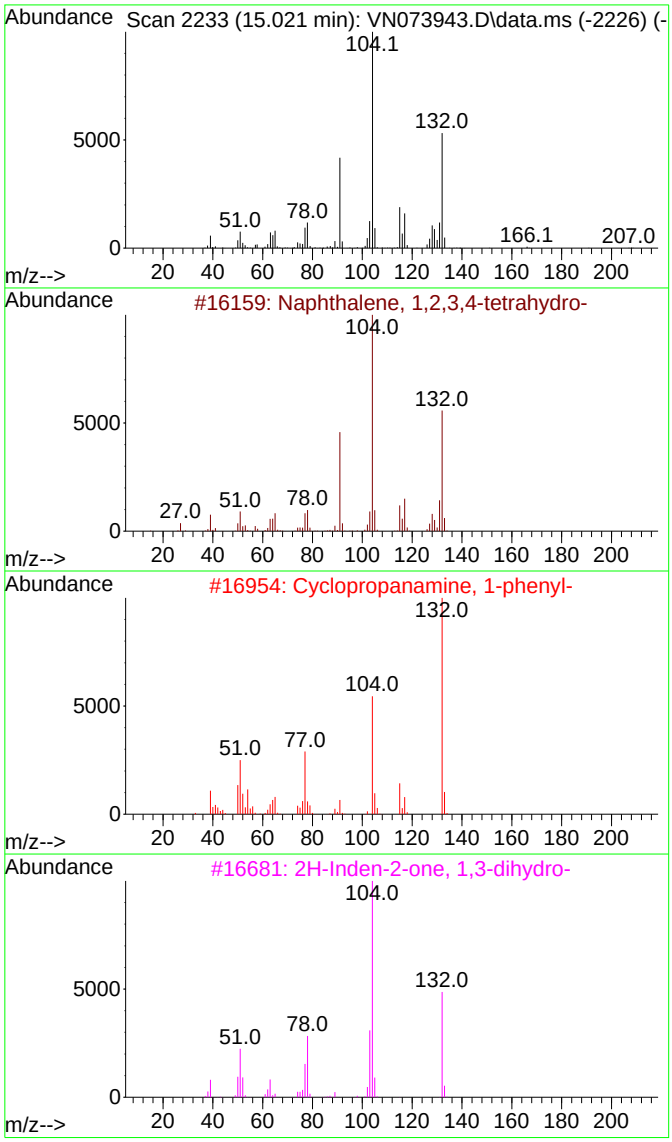
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081522W.M
Quant Title : SW846 8260

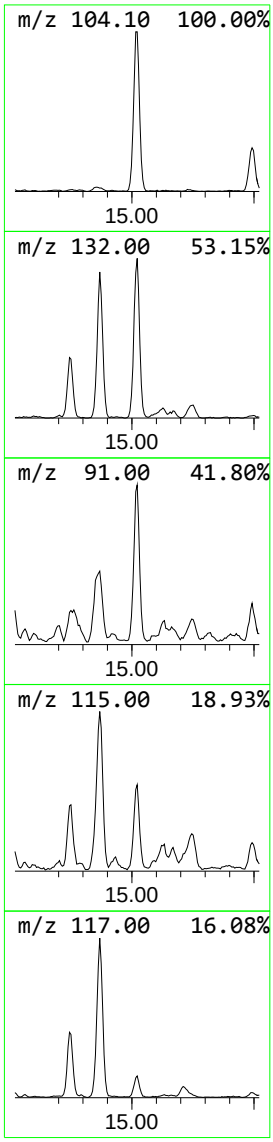
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.021	14.20 ug/l	969048	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	96
2	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	59
3	2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	53
4	Indan, epoxide	132	C9H8O	000768-22-9	50
5	2-Methylbenzyl cyanide	131	C9H9N	022364-68-7	49





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081622\
Data File : VN073943.D
Acq On : 16 Aug 2022 12:55
Operator : JC\MD
Sample : N4198-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GFD-TOTES

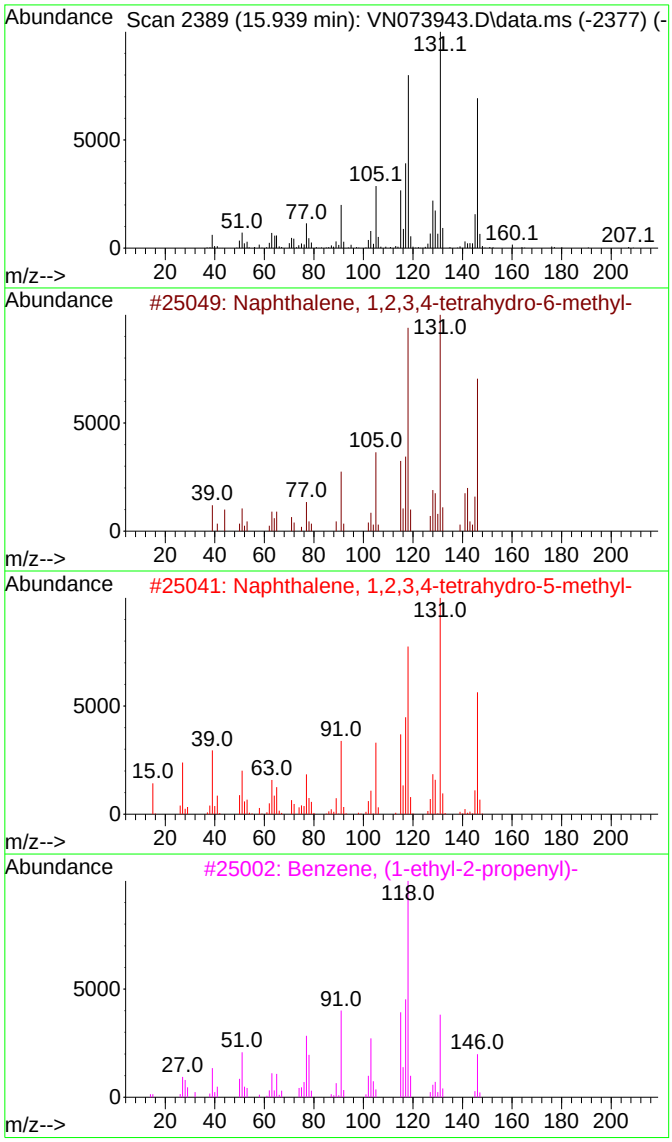
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081522W.M
Quant Title : SW846 8260

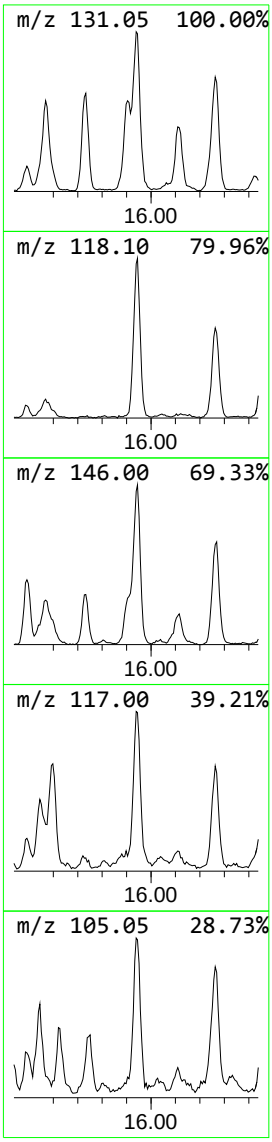
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.939	15.45 ug/l	1054160	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	95
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	87
3	Benzene, (1-ethyl-2-propenyl)-	146	C11H14	019947-22-9	80
4	Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	70
5	1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081622\
Data File : VN073943.D
Acq On : 16 Aug 2022 12:55
Operator : JC\MD
Sample : N4198-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GFD-TOTES

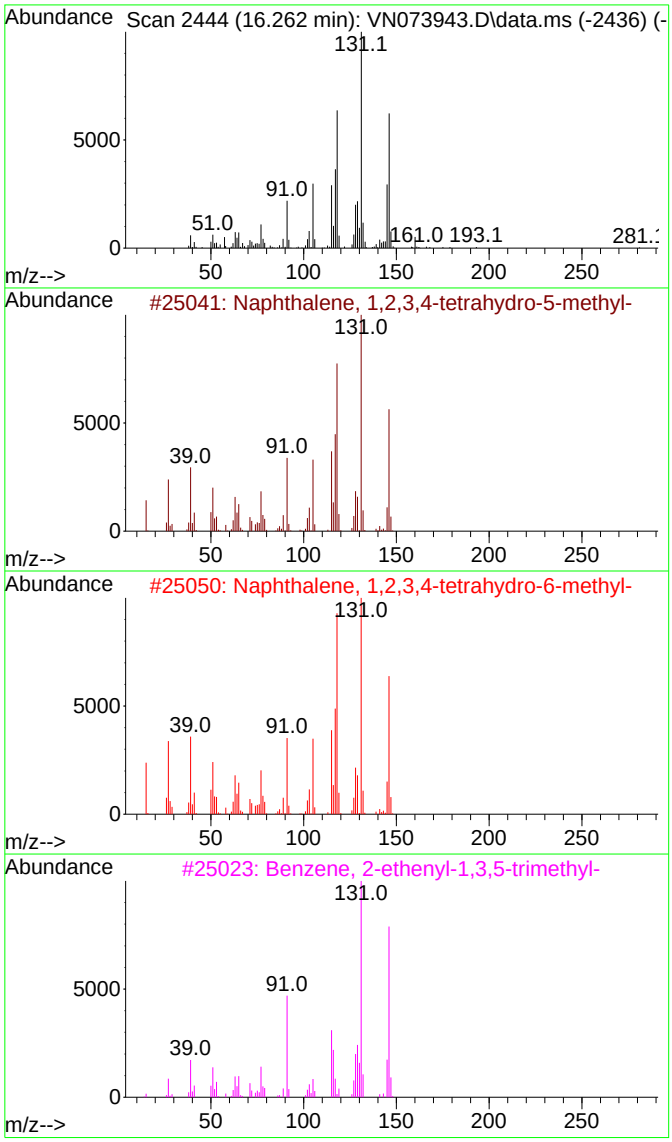
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081522W.M
Quant Title : SW846 8260

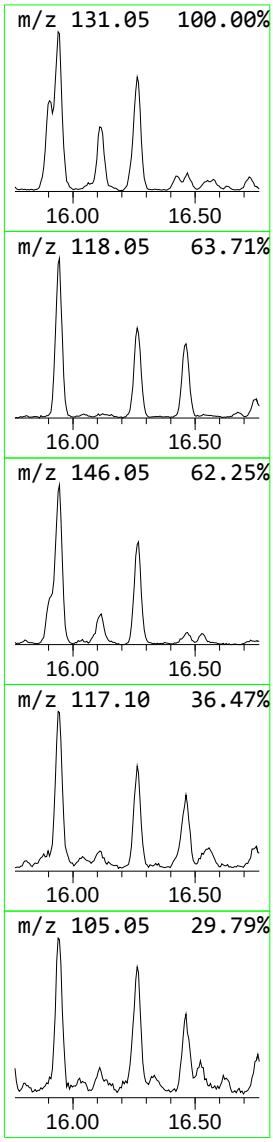
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.262	9.35 ug/l	637769	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	93
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	90
3	Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	83
4	1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	74
5	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	70





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081622\
Data File : VN073943.D
Acq On : 16 Aug 2022 12:55
Operator : JC\MD
Sample : N4198-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GFD-TOTES

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081522W.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
2-Heptanone	12.292	9.8	ug/l	485671	3	11.686	2470180	50.0
1-Hexanol, 2-et...	13.710	20.1	ug/l	1372670	4	13.616	3412120	50.0
Benzene, cyclop...	13.810	10.8	ug/l	735022	4	13.616	3412120	50.0
Indan, 1-methyl-	14.269	8.6	ug/l	586272	4	13.616	3412120	50.0
Benzene, 1,2,3,...	14.468	7.7	ug/l	527871	4	13.616	3412120	50.0
unknown14.604	14.604	8.7	ug/l	593893	4	13.616	3412120	50.0
Benzene, 2-ethe...	14.868	20.9	ug/l	1426710	4	13.616	3412120	50.0
Naphthalene, 1,...	15.021	14.2	ug/l	969048	4	13.616	3412120	50.0
Naphthalene, 1,...	15.939	15.4	ug/l	1054160	4	13.616	3412120	50.0
Naphthalene, 1,...	16.262	9.3	ug/l	637769	4	13.616	3412120	50.0