LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111023\
Data File : VX038742.D
Acq On : 10 Nov 2023 20:24
Operator : JC/MD
Sample : 05316-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-1978

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\82X110723W.M
Title : SW846 8260

Signal : TIC: VX038742.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.148	6	10	21	rBV2	99948	111488	7.38%	0.744%
2	1.246	22	26	28	rBV	17467	23235	1.54%	0.155%
3	1.374	41	47	51	rBV2	18275	23424	1.55%	0.156%
4	1.453	54	60	66	rBV	26991	29299	1.94%	0.196%
5	2.154	167	175	182	rVB3	9394	16295	1.08%	0.109%
6	2.374	205	211	226	rBV	260737	430637	28.52%	2.874%
7	2.526	228	236	243	rBV	10477	20990	1.39%	0.140%
8	2.953	298	306	316	rBV	23492	54703	3.62%	0.365%
9	3.239	347	353	361	rBV2	7277	18224	1.21%	0.122%
10	4.233	506	516	531	rBV	69652	190867	12.64%	1.274%
11	4.556	563	569	584	rBV	30815	87288	5.78%	0.583%
12	5.385	693	705	722	rBV	160506	470493	31.15%	3.140%
13	5.550	722	732	752	rVB	247282	712270	47.16%	4.754%
14	5.952	788	798	806	rBV	148455	397791	26.34%	2.655%
15	6.038	806	812	834	rVB	71517	201783	13.36%	1.347%
16	6.336	852	861	881	rVB5	10378	34823	2.31%	0.232%
17	6.763	921	931	950	rBV	383462	937319	62.07%	6.256%
18	7.129	985	991	1000	rVB5	8612	20998	1.39%	0.140%
19	7.293	1012	1018	1026	rVB2	11278	22468	1.49%	0.150%
20	7.671	1073	1080	1091	rVB6	4981	16802	1.11%	0.112%
21	8.220	1165	1170	1179	rBV	12346	21537	1.43%	0.144%
22	8.415	1193	1202	1209	rBV5	18921	48526	3.21%	0.324%
23	8.647	1234	1240	1247	rBV	820148	1290737	85.47%	8.615%
24	8.720	1247	1252	1264	rVB	224636	361376	23.93%	2.412%
25	9.445	1364	1371	1375	rBV	79388	122537	8.11%	0.818%
26	9.488	1375	1378	1381	rVV	31876	47552	3.15%	0.317%
27	9.531	1381	1385	1395	rVV	117989	180126	11.93%	1.202%
28	9.616	1395	1399	1410	rVB	12046	21959	1.45%	0.147%
29	10.055	1461	1471	1484	rBV	917590	1319204	87.35%	8.805%
30	10.195	1489	1494	1502	rVV	52550	77605	5.14%	0.518%
31	10.299	1502	1511	1521	rVV	208774	318608	21.10%	2.126%
32	10.409	1522	1529	1531	rVV4	18101	30691	2.03%	0.205%
33	10.445	1531	1535	1541	rVB	93529	128458	8.51%	0.857%
34	10.653	1563	1569	1578	rBV2	735803	1086922	71.97%	7.254%
35	10.756	1582	1586	1596	rVB4	15475	39361	2.61%	0.263%
36	10.860	1598	1603	1607	rBV4	10287	15904	1.05%	0.106%

LSC Area Percent Report

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Acq On : 10 Nov 2023 20:24
Operator : JC/MD
Sample : 05316-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : NWB-1978

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\82X110723W.M
Title : SW846 8260

37	11.079	1634	1639	1646	rBV	855877	1094010	72.44%	7.302%
38	11.311	1668	1677	1681	rBV	15273	22355	1.48%	0.149%
39	11.378	1685	1688	1695	rVV	30311	59956	3.97%	0.400%
40	11.451	1695	1700	1712	rVB	31593	56461	3.74%	0.377%
41	11.573	1714	1720	1723	rBV	17220	26215	1.74%	0.175%
42	11.634	1723	1730	1738	rVB2	64117	107138	7.09%	0.715%
43	11.750	1744	1749	1754	rBV	154359	206670	13.68%	1.379%
44	11.811	1754	1759	1762	rVV	156587	210823	13.96%	1.407%
45	11.847	1762	1765	1770	rVB2	49286	64738	4.29%	0.432%
46	12.018	1788	1793	1801	rBV	1147244	1510198	100.00%	10.080%
47	12.085	1801	1804	1808	rBV	60669	71785	4.75%	0.479%
48	12.134	1808	1812	1818	rVB	47651	63779	4.22%	0.426%
49	12.219	1821	1826	1828	rBV	66235	90455	5.99%	0.604%
50	12.414	1852	1858	1864	rBV	456621	580702	38.45%	3.876%
51	12.799	1915	1921	1926	rBV	84737	120235	7.96%	0.802%
52	12.963	1944	1948	1953	rVB2	24346	35181	2.33%	0.235%
53	13.170	1977	1982	1986	rVB	13885	18017	1.19%	0.120%
54	13.292	1997	2002	2006	rBV2	26052	36501	2.42%	0.244%
55	13.341	2006	2010	2018	rVB3	37750	50528	3.35%	0.337%
56	13.426	2018	2024	2029	rVB	49000	68270	4.52%	0.456%
57	13.500	2032	2036	2040	rBV2	11364	15758	1.04%	0.105%
58	13.542	2040	2043	2046	rBV2	12277	16166	1.07%	0.108%
59	13.713	2067	2071	2075	rBV2	26934	36178	2.40%	0.241%
60	13.774	2076	2081	2087	rVV	545579	681045	45.10%	4.545%
61	13.835	2087	2091	2093	rVV2	15171	25045	1.66%	0.167%
62	13.865	2093	2096	2103	rVB2	21735	36460	2.41%	0.243%
63	14.225	2150	2155	2159	rBV4	18137	34220	2.27%	0.228%
64	14.317	2166	2170	2176	rVB2	11369	16453	1.09%	0.110%
65	14.371	2176	2179	2183	rBV	12520	15280	1.01%	0.102%
66	14.481	2192	2197	2200	rBV3	12096	19305	1.28%	0.129%
67	14.634	2214	2222	2233	rVB	139236	208417	13.80%	1.391%
68	14.780	2241	2246	2254	rBV	129620	171019	11.32%	1.141%
69	15.207	2308	2316	2321	rVB2	18187	32095	2.13%	0.214%
70	15.377	2337	2344	2347	rBV	12241	21051	1.39%	0.141%
71	15.475	2354	2360	2368	rBV	30879	52715	3.49%	0.352%
72	15.615	2377	2383	2386	rBV	39775	64267	4.26%	0.429%
73	15.652	2386	2389	2394	rVB	27814	39833	2.64%	0.266%
74	15.828	2411	2418	2426	rVB2	13113	33819	2.24%	0.226%
75	15.975	2436	2442	2451	rBV4	7623	19508	1.29%	0.130%
76	16.085	2456	2460	2469	rVB2	10908	17913	1.19%	0.120%

LSC Area Percent Report

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Data File : VX038742.D
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Sample : 05316-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
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ClientSampleId :
NWB-1978

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X110723W.M
Title : SW846 8260

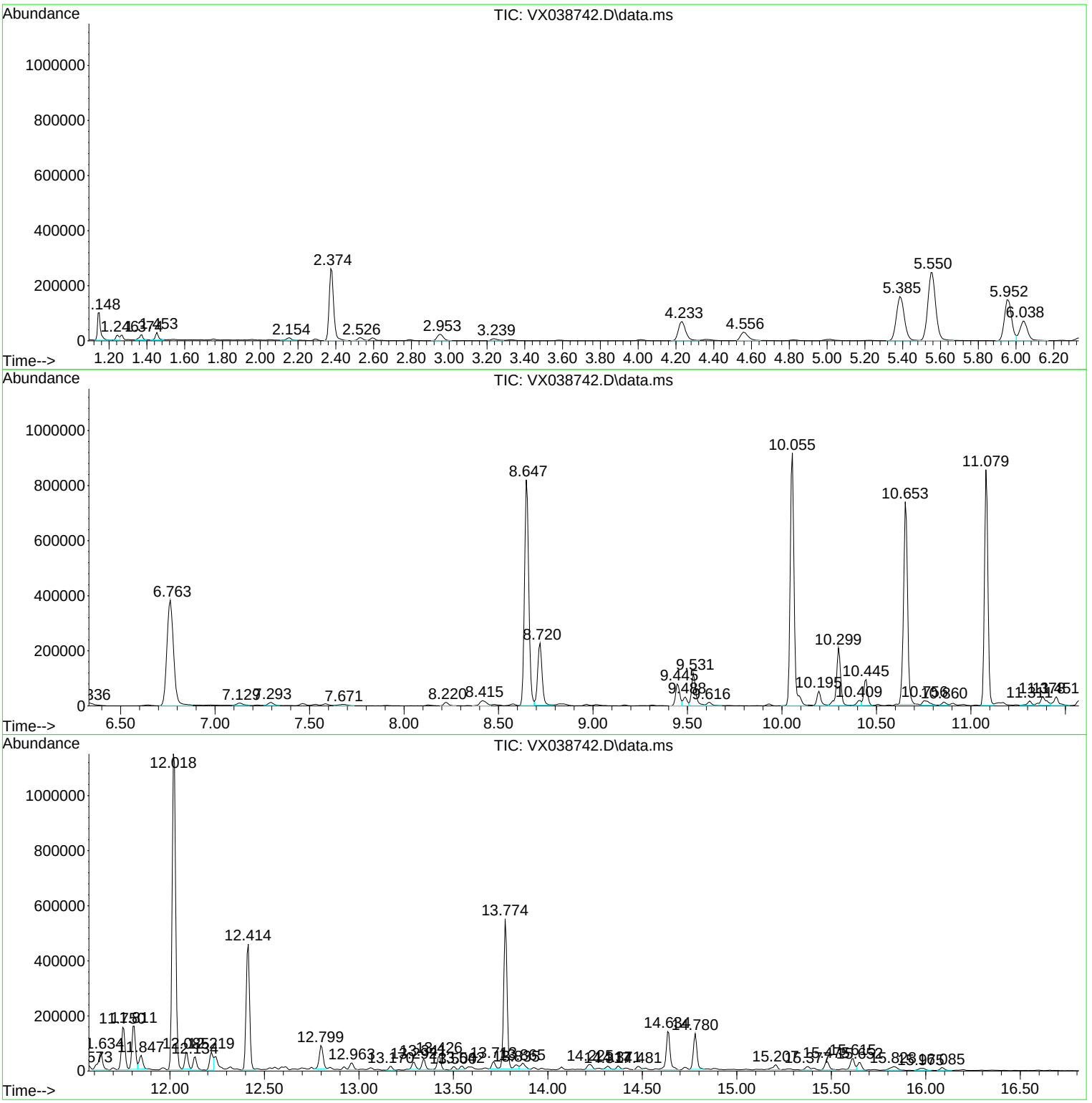
Sum of corrected areas: 14982864

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111023\
Data File : VX038742.D
Acq On : 10 Nov 2023 20:24
Operator : JC/MD
Sample : 05316-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-1978

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X110723W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111023\
Data File : VX038742.D
Acq On : 10 Nov 2023 20:24
Operator : JC/MD
Sample : 05316-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-1978

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X110723W.M
Quant Title : SW846 8260

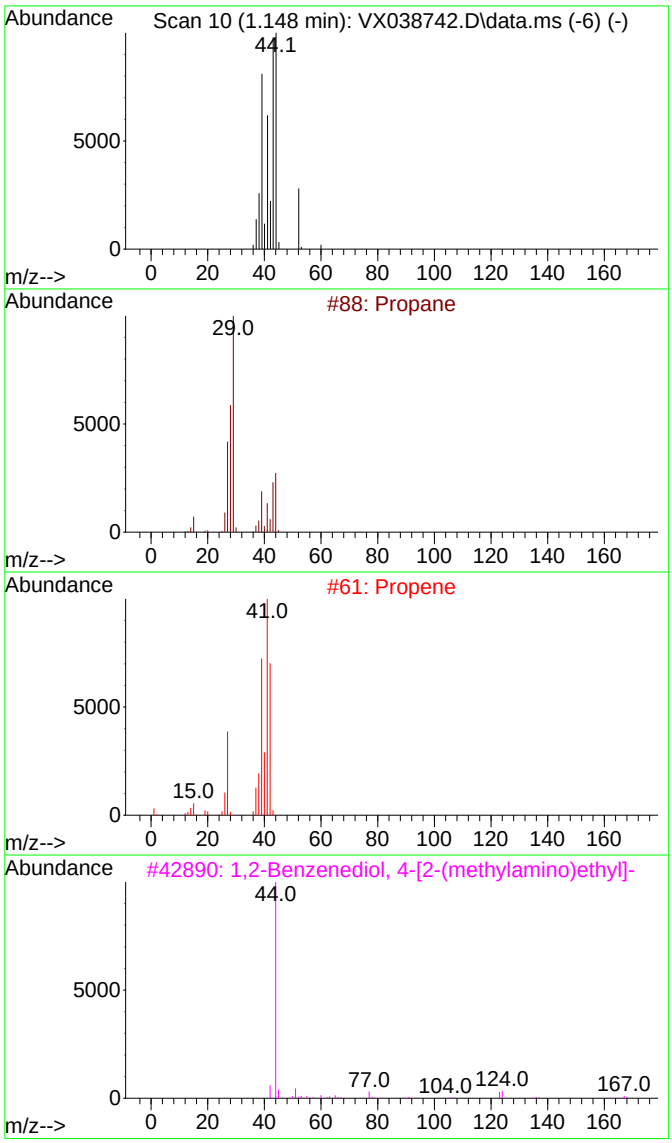
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

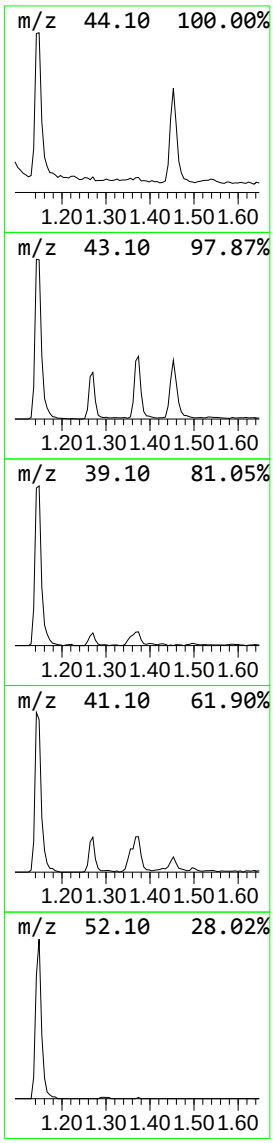
****

Peak Number 1 Propane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.148	7.83 ug/l	111488	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane	44	C3H8	000074-98-6	80
2	Propene	42	C3H6	000115-07-1	9
3	1,2-Benzenediol, 4-[2-(methylami...	167	C9H13NO2	000501-15-5	2
4	Cyclopropene	40	C3H4	002781-85-3	2
5	Methylenecyclopropane	54	C4H6	006142-73-0	2





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111023\
Data File : VX038742.D
Acq On : 10 Nov 2023 20:24
Operator : JC/MD
Sample : 05316-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-1978

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X110723W.M
Quant Title : SW846 8260

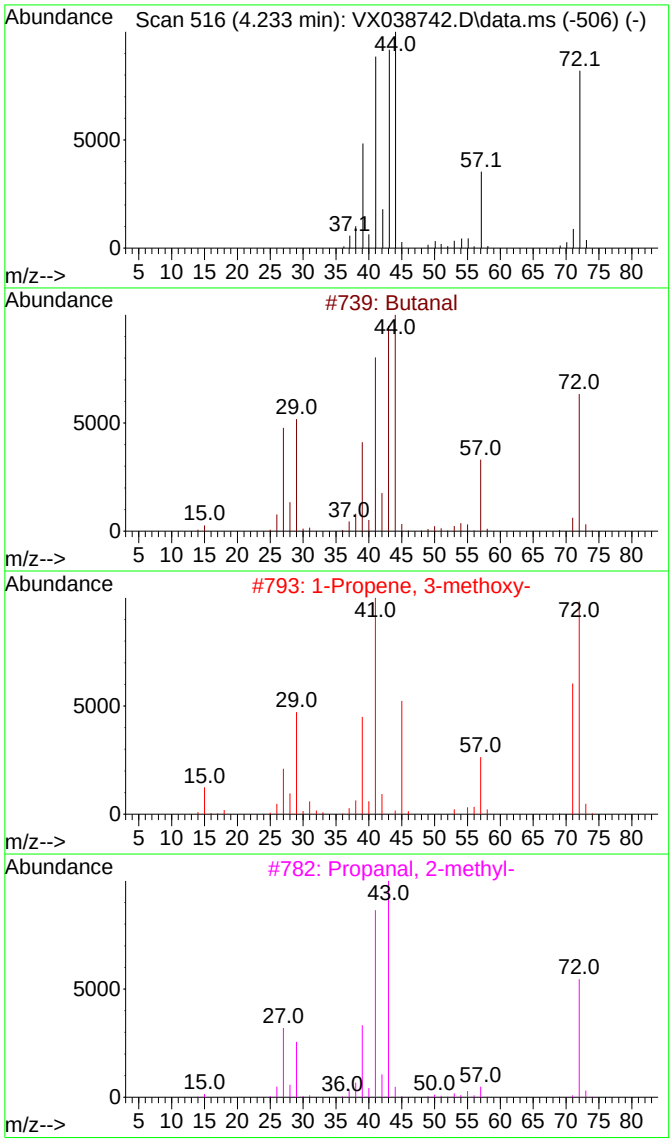
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

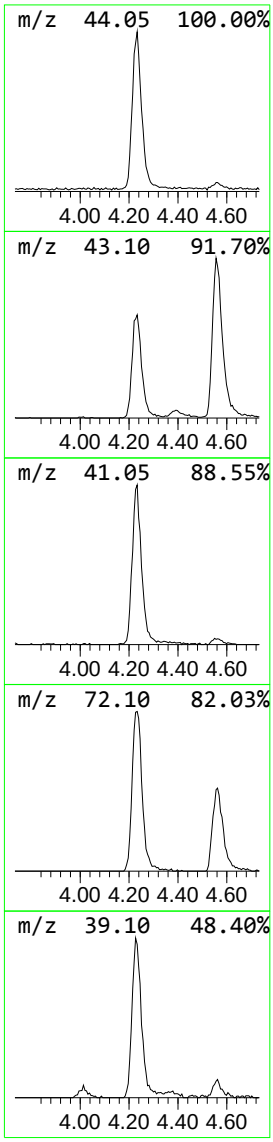
****

Peak Number 2 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.233	13.40 ug/l	190867	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	47
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	46
4	2-Propanone, hydrazone	72	C3H8N2	005281-20-9	43
5	Ethene, ethoxy-	72	C4H8O	000109-92-2	42





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111023\
Data File : VX038742.D
Acq On : 10 Nov 2023 20:24
Operator : JC/MD
Sample : 05316-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-1978

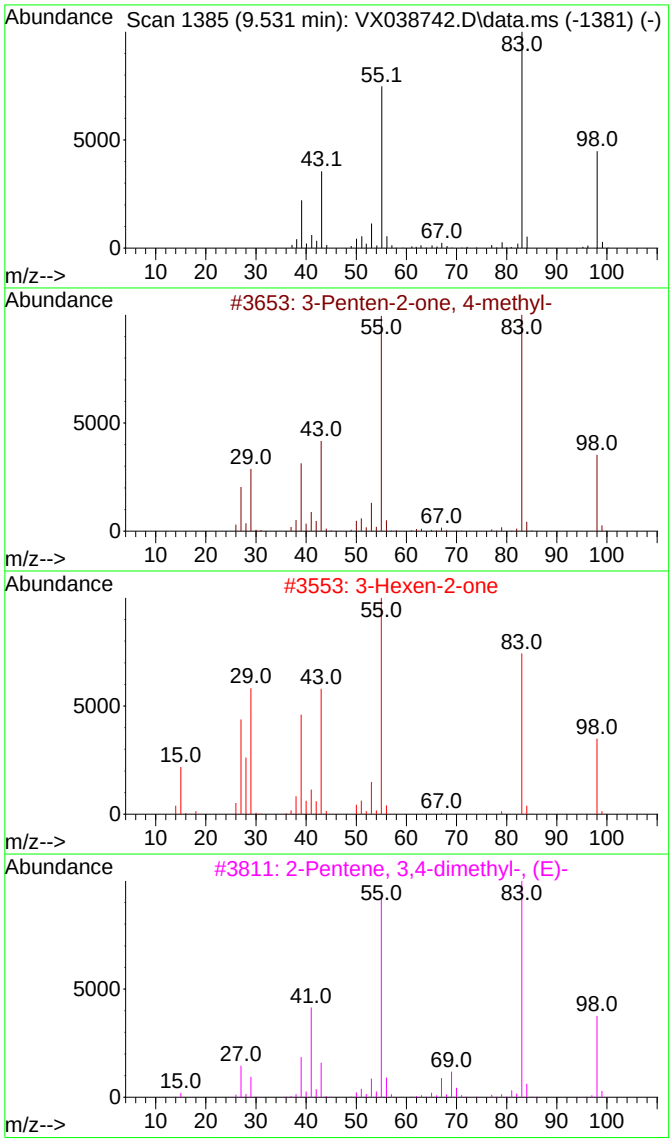
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X110723W.M
Quant Title : SW846 8260

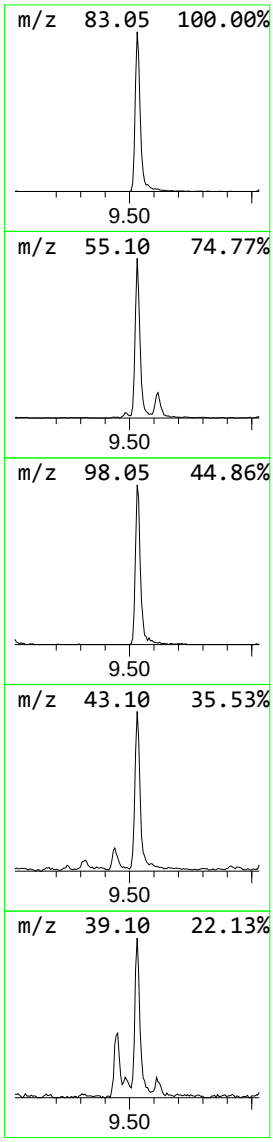
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.531	6.83 ug/l	180126	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78
4	Cyclohexane, methyl-	98	C7H14	000108-87-2	72
5	2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111023\
Data File : VX038742.D
Acq On : 10 Nov 2023 20:24
Operator : JC/MD
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ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-1978

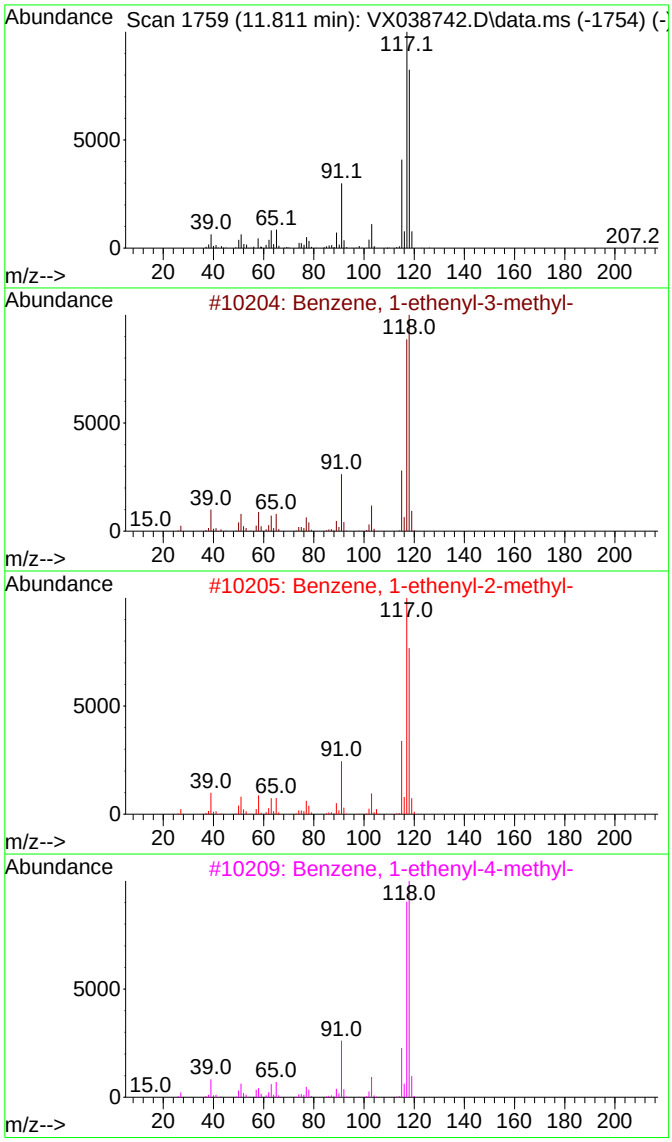
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X110723W.M
Quant Title : SW846 8260

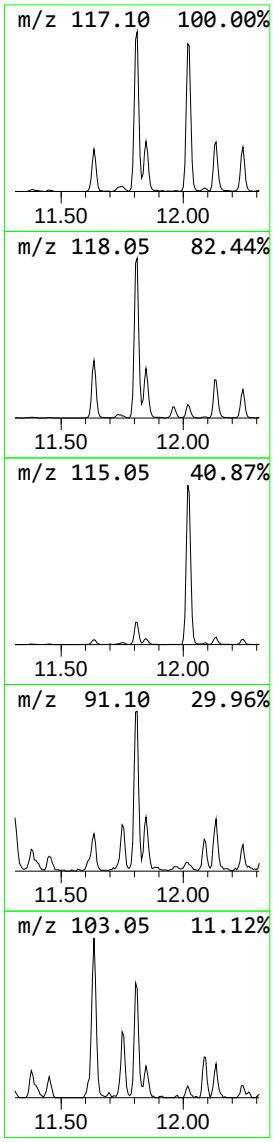
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 1-ethenyl-3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.811	6.98 ug/l	210823	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	96
2	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	94
3	Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	94
4	Benzene, 1,1'-(1-ethenyl-1,3-pro...	222	C17H18	061141-97-7	86
5	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	81





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111023\
Data File : VX038742.D
Acq On : 10 Nov 2023 20:24
Operator : JC/MD
Sample : 05316-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-1978

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X110723W.M
Quant Title : SW846 8260

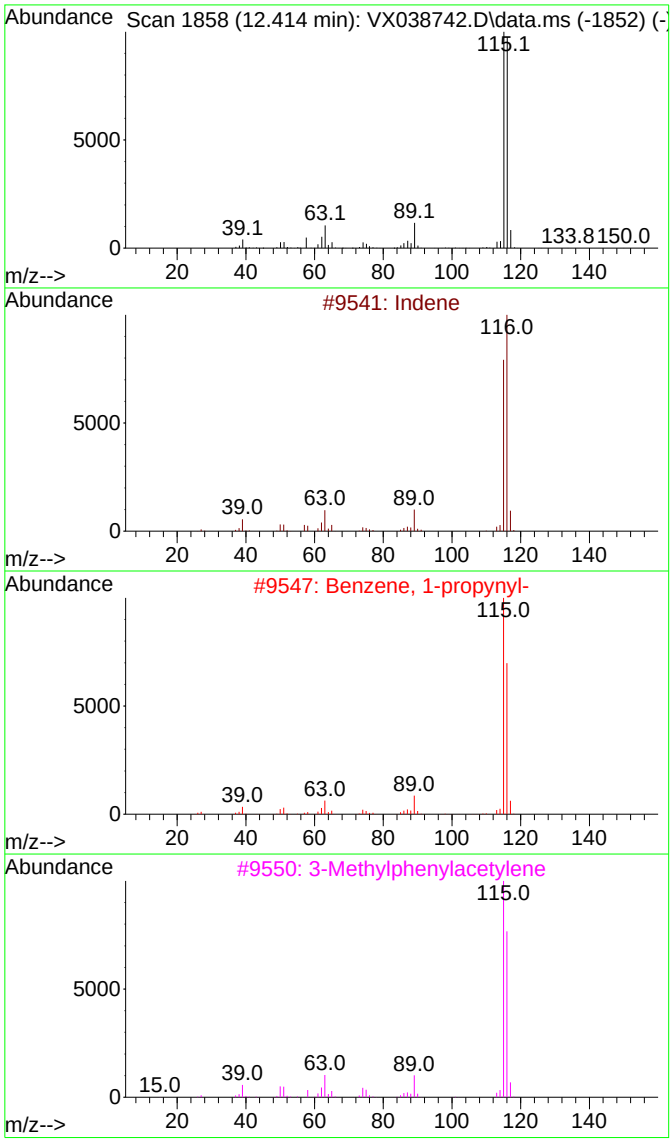
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

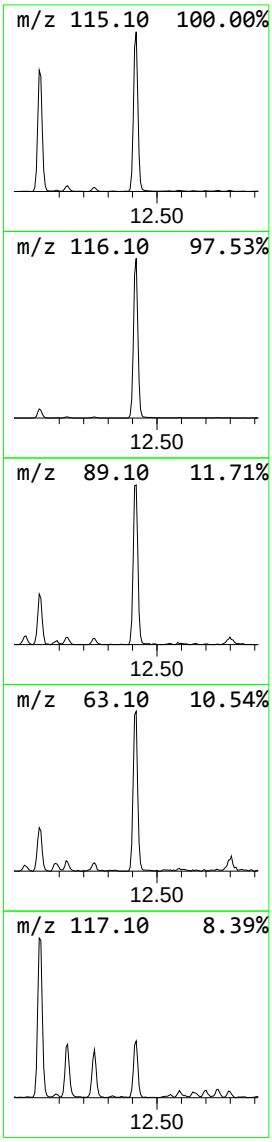
****

Peak Number 5 Indene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.415	19.23 ug/l	580702	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene	116	C9H8	000095-13-6	97
2	Benzene, 1-propynyl-	116	C9H8	000673-32-5	94
3	3-Methylphenylacetylene	116	C9H8	000766-82-5	91
4	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	91
5	2-Methylphenylacetylene	116	C9H8	000766-47-2	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111023\
Data File : VX038742.D
Acq On : 10 Nov 2023 20:24
Operator : JC/MD
Sample : 05316-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-1978

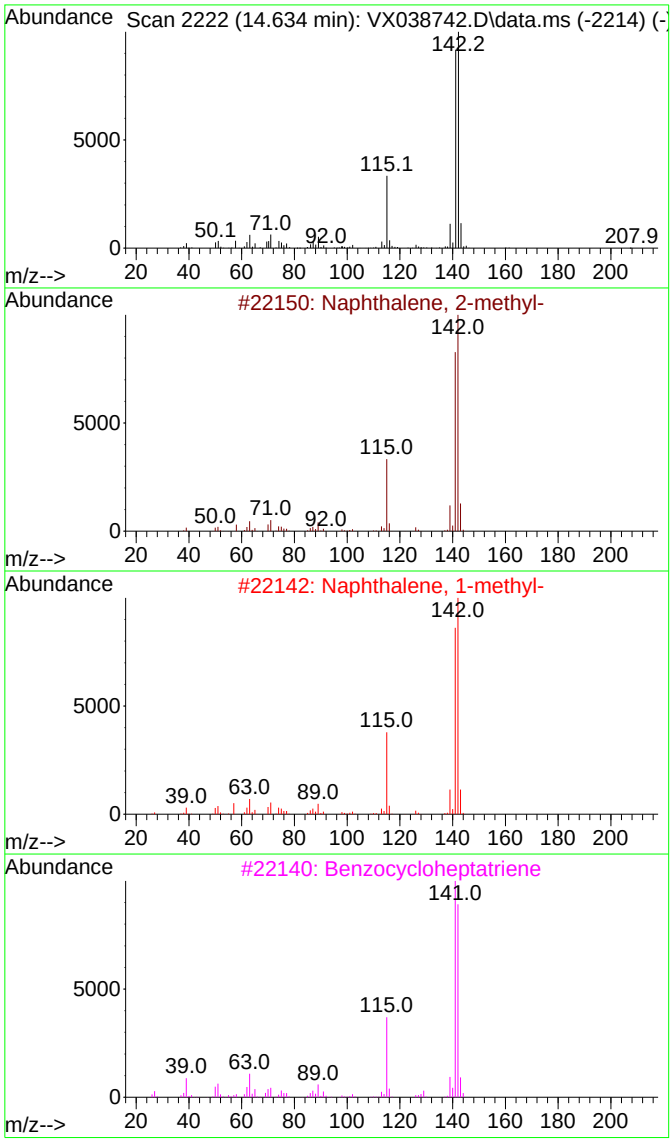
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X110723W.M
Quant Title : SW846 8260

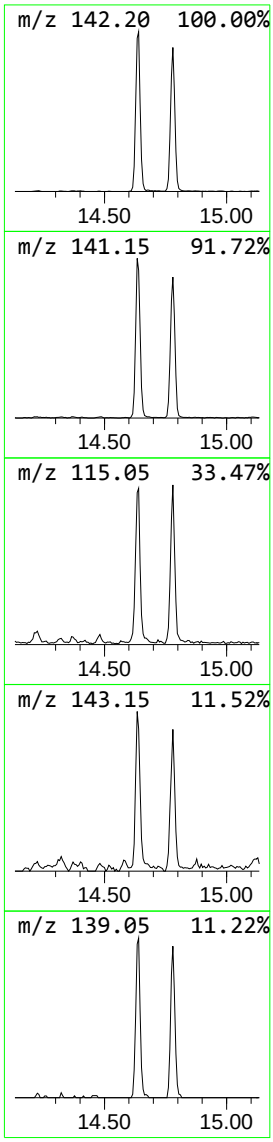
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Naphthalene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.634	6.90 ug/l	208417	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\VX111023\
Data File : VX038742.D
Acq On : 10 Nov 2023 20:24
Operator : JC/MD
Sample : 05316-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-1978

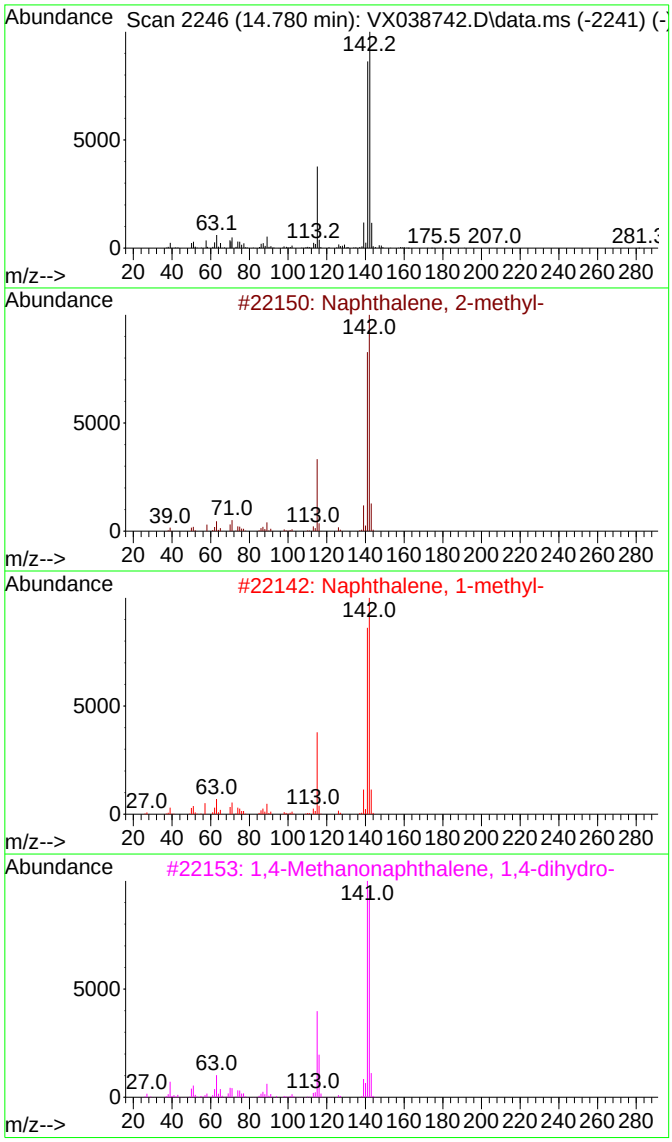
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X110723W.M
Quant Title : SW846 8260

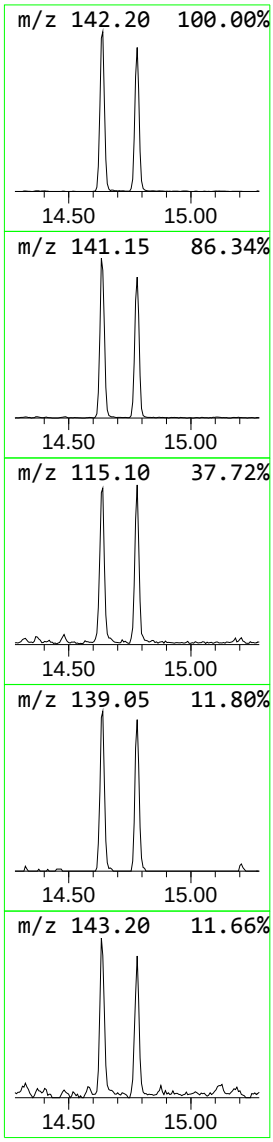
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Naphthalene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	5.66 ug/l	171019	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	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111023\
Data File : VX038742.D
Acq On : 10 Nov 2023 20:24
Operator : JC/MD
Sample : 05316-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-1978

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X110723W.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
Propane	1.148	7.8	ug/l	111488	1	5.556	712270	50.0
Butanal	4.233	13.4	ug/l	190867	1	5.556	712270	50.0
3-Penten-2-one,...	9.531	6.8	ug/l	180126	3	10.055	1319200	50.0
Benzene, 1-ethe...	11.811	7.0	ug/l	210823	4	12.024	1510200	50.0
Indene	12.415	19.2	ug/l	580702	4	12.024	1510200	50.0
Naphthalene, 2-...	14.634	6.9	ug/l	208417	4	12.024	1510200	50.0
Naphthalene, 1-...	14.780	5.7	ug/l	171019	4	12.024	1510200	50.0