LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081423\
Data File : VX036975.D
Acq On : 14 Aug 2023 19:24
Operator : JC/MD
Sample : 03983-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
713-F

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\82X072123W.M
Title : SW846 8260

Signal : TIC: VX036975.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	18	rBV	30417	33592	1.94%	0.188%
2	1.356	41	44	50	rBV	20258	22183	1.28%	0.124%
3	1.453	56	60	71	rVB	131062	155592	9.00%	0.873%
4	2.380	205	212	230	rBV	140692	236219	13.66%	1.326%
5	2.538	230	238	244	rBV	40549	73790	4.27%	0.414%
6	2.965	298	308	326	rBV	151583	333757	19.30%	1.873%
7	3.697	416	428	446	rBV	322927	873291	50.49%	4.900%
8	4.227	500	515	528	rBV4	66214	275951	15.95%	1.548%
9	4.556	559	569	588	rBV	237277	669273	38.69%	3.756%
10	5.001	629	642	662	rBV	204065	657268	38.00%	3.688%
11	5.391	694	706	720	rBV	81118	234848	13.58%	1.318%
12	5.556	720	733	747	rVB	125720	357533	20.67%	2.006%
13	5.958	787	799	804	rBV	85163	216500	12.52%	1.215%
14	6.038	804	812	834	rVB	491428	1345979	77.82%	7.553%
15	6.336	853	861	879	rVB3	13997	45017	2.60%	0.253%
16	6.763	921	931	945	rBV	209671	495370	28.64%	2.780%
17	7.464	1039	1046	1051	rBV2	9243	19934	1.15%	0.112%
18	7.525	1051	1056	1062	rVB	17330	32052	1.85%	0.180%
19	7.641	1070	1075	1080	rBV	14269	27225	1.57%	0.153%
20	8.574	1222	1228	1234	rBV	25003	41877	2.42%	0.235%
21	8.647	1234	1240	1246	rVV	428540	673363	38.93%	3.778%
22	8.720	1246	1252	1263	rVB	1129798	1729699	100.00%	9.706%
23	9.446	1365	1371	1374	rBV3	12969	25072	1.45%	0.141%
24	9.488	1374	1378	1382	rVV	31453	48310	2.79%	0.271%
25	9.531	1382	1385	1395	rVV	39717	65356	3.78%	0.367%
26	9.878	1433	1442	1447	rBV2	12012	17899	1.03%	0.100%
27	10.055	1462	1471	1484	rBV	455513	687314	39.74%	3.857%
28	10.195	1489	1494	1500	rVV	283875	378512	21.88%	2.124%
29	10.299	1500	1511	1519	rVV	762381	1062042	61.40%	5.960%
30	10.409	1522	1529	1531	rVV3	11675	24353	1.41%	0.137%
31	10.445	1531	1535	1541	rVB2	33956	52749	3.05%	0.296%
32	10.506	1541	1545	1551	rBV	29399	36288	2.10%	0.204%
33	10.640	1562	1567	1579	rVB2	459513	700727	40.51%	3.932%
34	10.769	1581	1588	1595	rBV2	18316	41291	2.39%	0.232%
35	10.964	1614	1620	1625	rVB	12795	17928	1.04%	0.101%
36	11.079	1634	1639	1645	rBV	383980	495242	28.63%	2.779%

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713-F

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
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Title : SW846 8260

37	11.134	1645	1648	1652	rVV2	16970	29767	1.72%	0.167%
38	11.305	1672	1676	1681	rVB	16106	22004	1.27%	0.123%
39	11.378	1681	1688	1694	rVV	77375	130522	7.55%	0.732%
40	11.451	1694	1700	1714	rVB	50161	84829	4.90%	0.476%
41	11.573	1714	1720	1722	rBV	13385	19709	1.14%	0.111%
42	11.610	1722	1726	1735	rVB	45539	79920	4.62%	0.448%
43	11.750	1744	1749	1754	rBV	172305	212402	12.28%	1.192%
44	11.805	1754	1758	1761	rBV	34023	48791	2.82%	0.274%
45	11.866	1766	1768	1779	rVB	36884	55590	3.21%	0.312%
46	11.957	1779	1783	1788	rVB2	13223	20220	1.17%	0.113%
47	12.018	1788	1793	1797	rBV	456844	598990	34.63%	3.361%
48	12.061	1797	1800	1802	rVV	58506	79592	4.60%	0.447%
49	12.085	1802	1804	1808	rVB	82217	88626	5.12%	0.497%
50	12.128	1808	1811	1820	rVB	30533	41527	2.40%	0.233%
51	12.213	1820	1825	1838	rBV	634177	919581	53.16%	5.160%
52	12.415	1852	1858	1863	rBV	400164	534262	30.89%	2.998%
53	12.488	1867	1870	1875	rVV	34457	44699	2.58%	0.251%
54	12.799	1917	1921	1926	rBV	22447	29324	1.70%	0.165%
55	12.847	1926	1929	1932	rVV	32458	38270	2.21%	0.215%
56	12.878	1932	1934	1939	rVB2	26082	29637	1.71%	0.166%
57	12.963	1944	1948	1951	rBV2	14411	19052	1.10%	0.107%
58	13.286	1992	2001	2006	rBV2	18930	30430	1.76%	0.171%
59	13.341	2006	2010	2017	rVB3	17069	25927	1.50%	0.145%
60	13.420	2018	2023	2029	rVB	31489	42698	2.47%	0.240%
61	13.774	2073	2081	2088	rVV	986952	1217865	70.41%	6.834%
62	13.847	2088	2093	2094	rVV3	20653	31319	1.81%	0.176%
63	13.866	2094	2096	2100	rVV	28923	36770	2.13%	0.206%
64	13.914	2100	2104	2110	rVB3	19085	29241	1.69%	0.164%
65	14.634	2214	2222	2232	rVB	186965	252330	14.59%	1.416%
66	14.780	2240	2246	2251	rBV	120601	158019	9.14%	0.887%
67	15.207	2307	2316	2320	rBV	30391	43742	2.53%	0.245%
68	15.371	2338	2343	2347	rBV	42796	63029	3.64%	0.354%
69	15.475	2354	2360	2372	rBV	48940	82097	4.75%	0.461%
70	15.609	2377	2382	2386	rVV	61126	98242	5.68%	0.551%
71	15.646	2386	2388	2394	rVB	34089	47485	2.75%	0.266%
72	15.835	2410	2419	2424	rBV2	19093	50166	2.90%	0.282%
73	15.975	2435	2442	2455	rBV3	48443	115856	6.70%	0.650%
74	16.085	2455	2460	2467	rVB3	15261	27080	1.57%	0.152%
75	16.322	2492	2499	2512	rBV2	61283	137906	7.97%	0.774%

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Integration Parameters: RTEINT.P
Integrator: RTE
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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Title : SW846 8260

Sum of corrected areas: 17820912

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081423\
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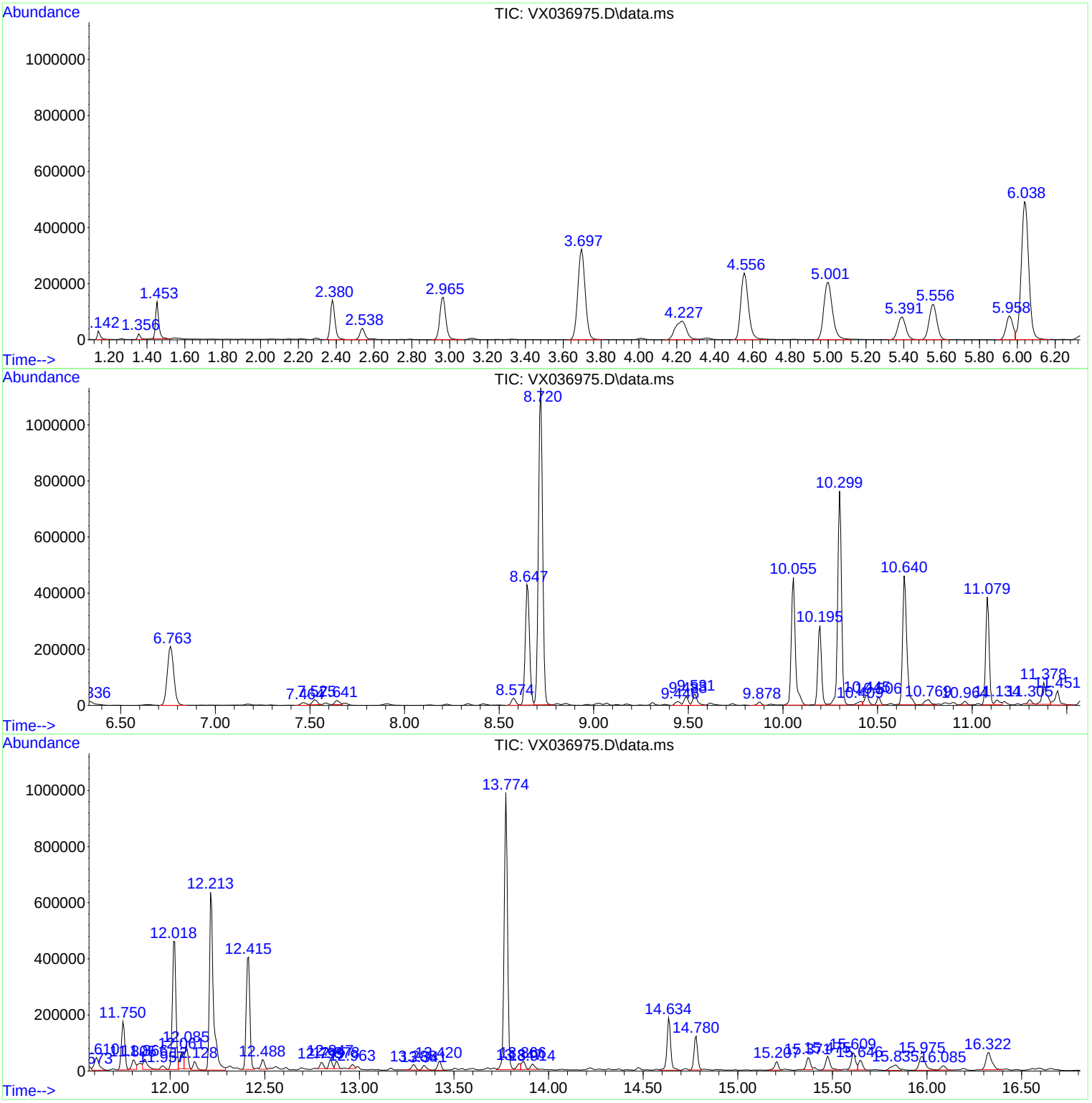
MSVOA_X
ClientSampleId :
713-F

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081423\
Data File : VX036975.D
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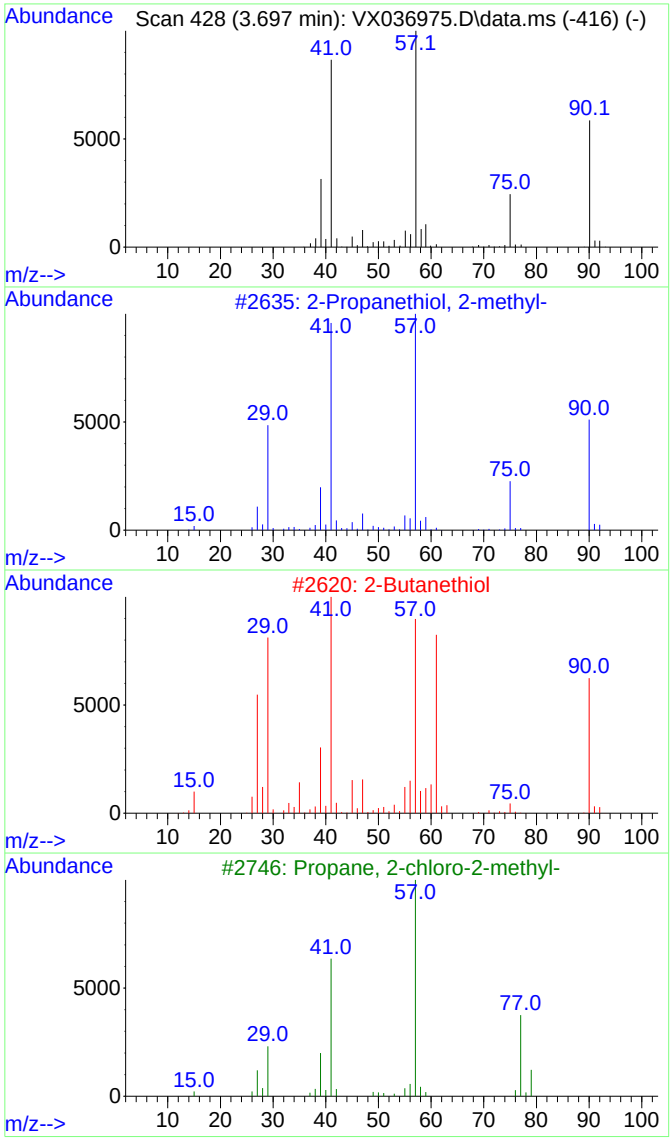
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

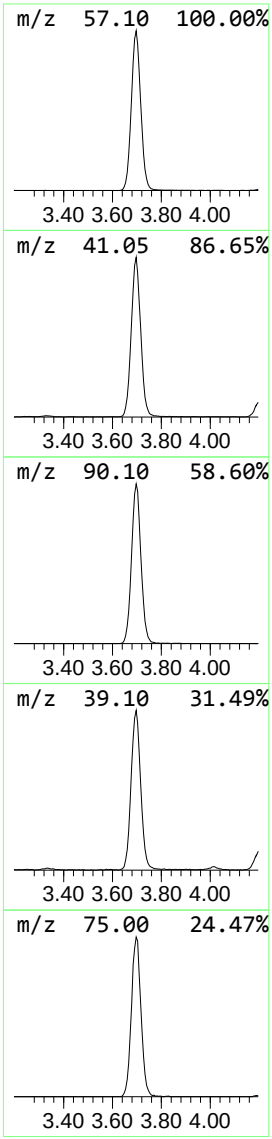
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Propanethiol, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.697	122.13 ug/l	873291	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	91
2	2-Butanethiol	90	C4H10S	000513-53-1	42
3	Propane, 2-chloro-2-methyl-	92	C4H9Cl	000507-20-0	22
4	Ethynyl tert-butyl sulfoxide	130	C6H10OS	041463-34-7	16
5	Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	14





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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

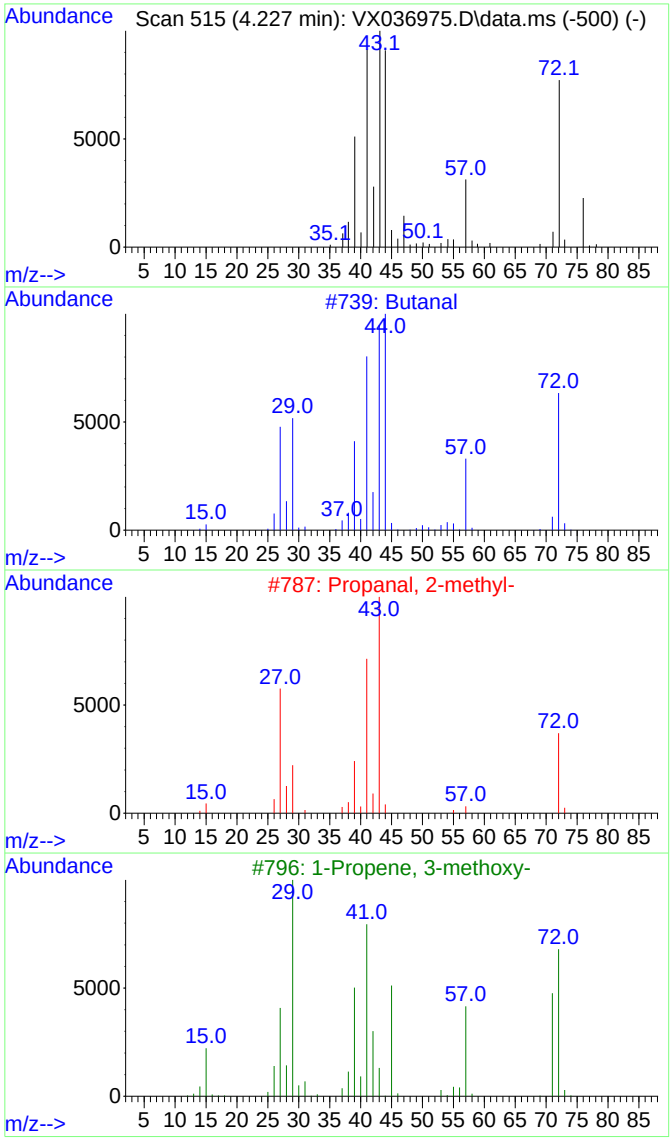
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

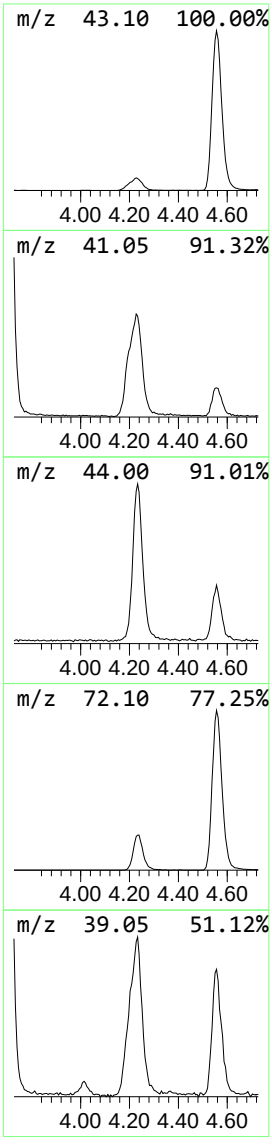
****

Peak Number 3 Butanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.227	38.59 ug/l	275951	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	81
2	Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
3	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	38
4	2-Propanone, hydrazone	72	C3H8N2	005281-20-9	32
5	DL-Cystine	240	C6H12N2O4S2	000923-32-0	32





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081423\
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ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
713-F

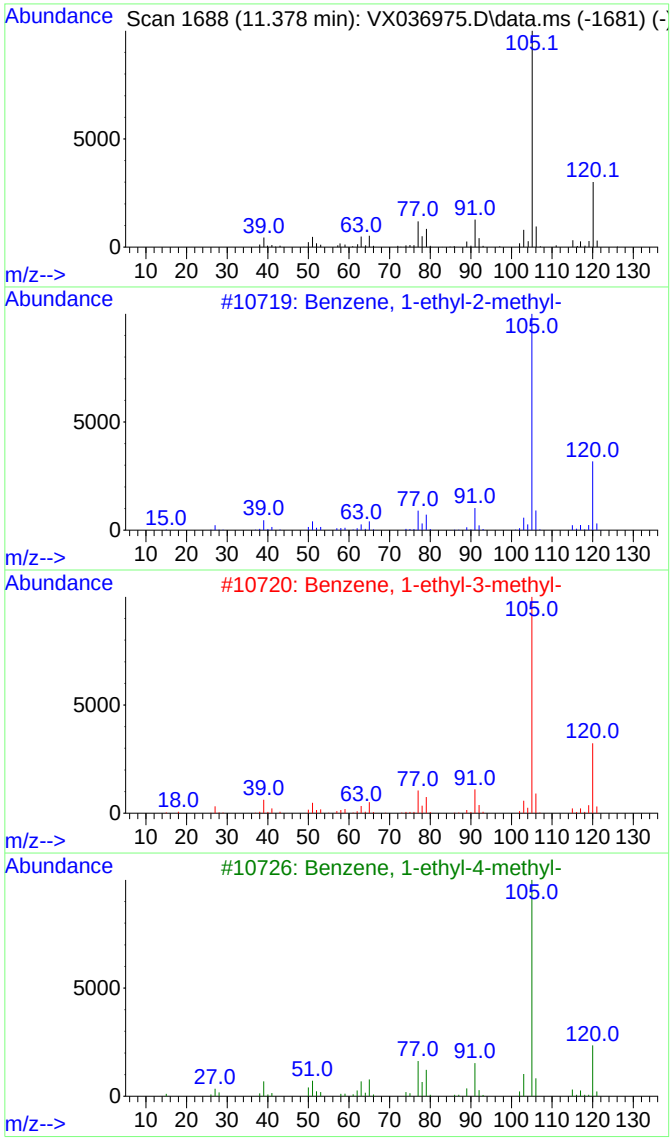
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

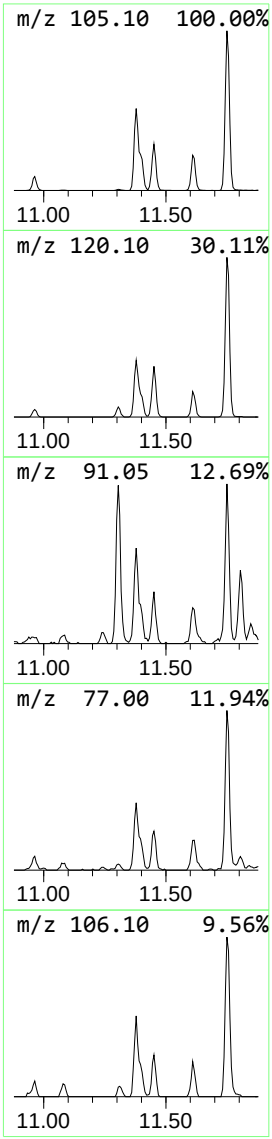
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 1-ethyl-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	10.90 ug/l	130522	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081423\
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Instrument :
MSVOA_X
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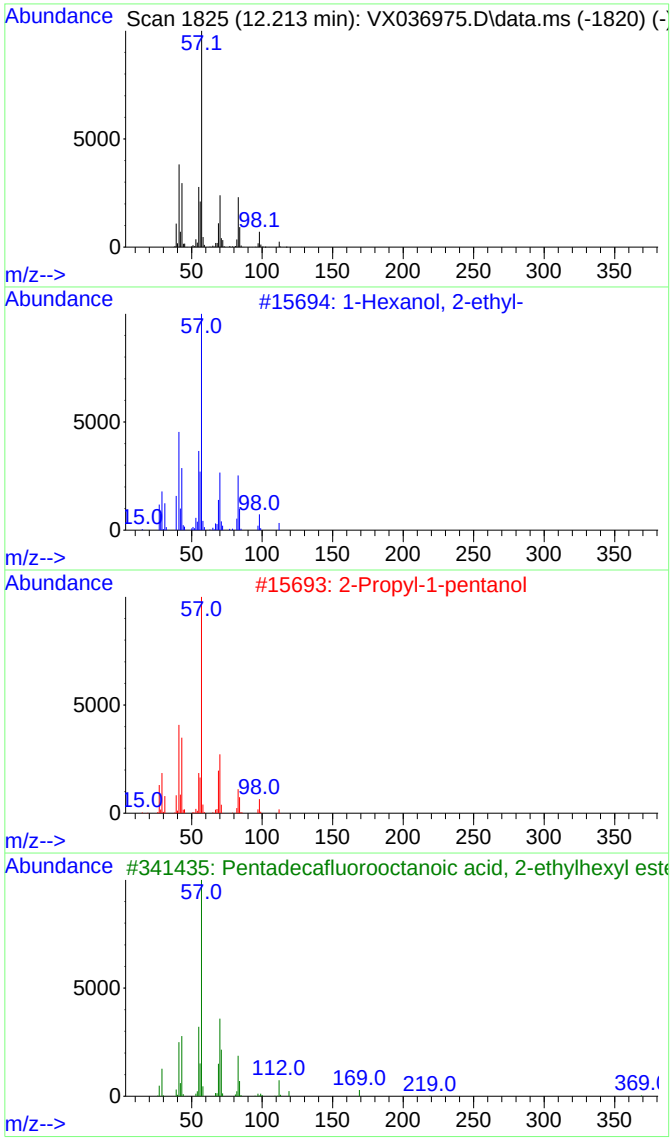
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

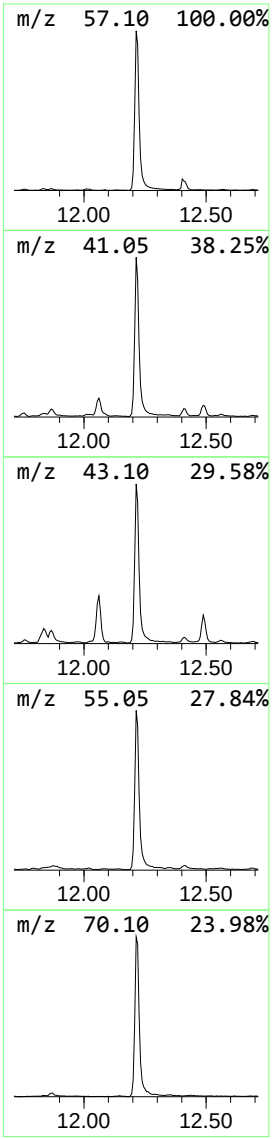
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.213	76.76 ug/l	919581	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	64
3	Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	53
4	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50
5	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	50





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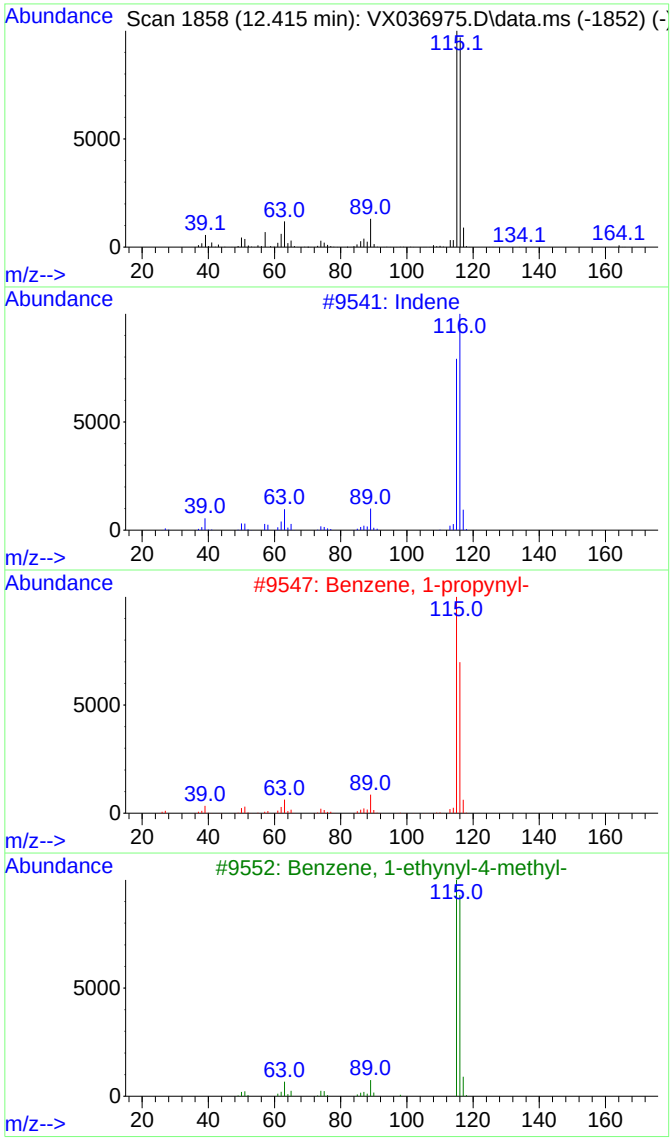
Quant Title : SW846 8260

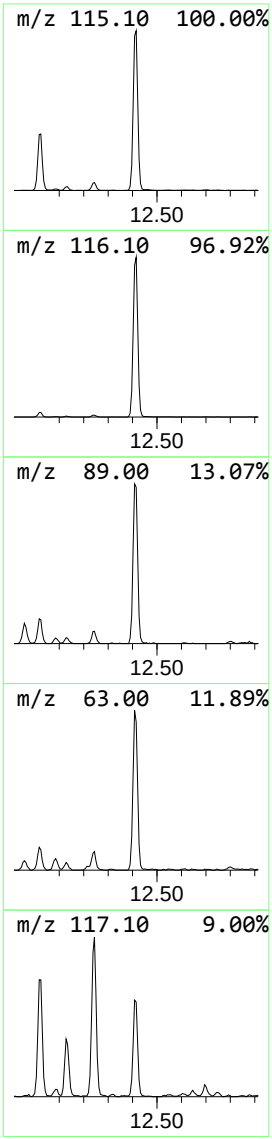
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Indene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.415	44.60 ug/l	534262	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	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	91
4	3-Methylphenylacetylene	116	C9H8	000766-82-5	91
5	2-Methylphenylacetylene	116	C9H8	000766-47-2	91





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Instrument :
MSVOA_X
ClientSampleId :
713-F

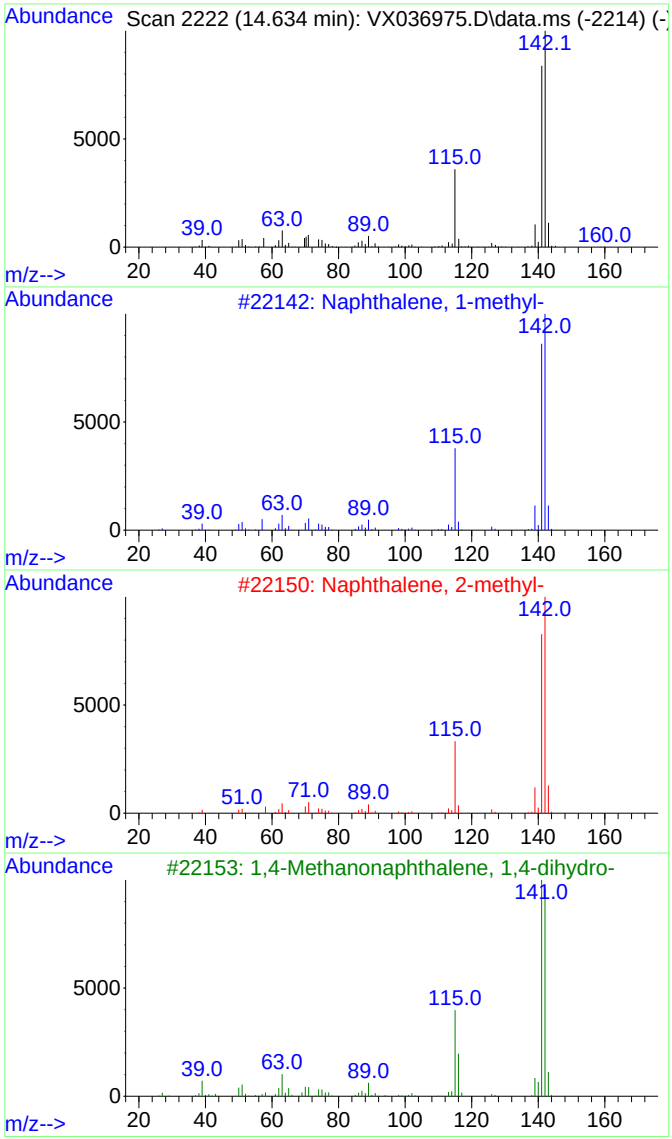
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

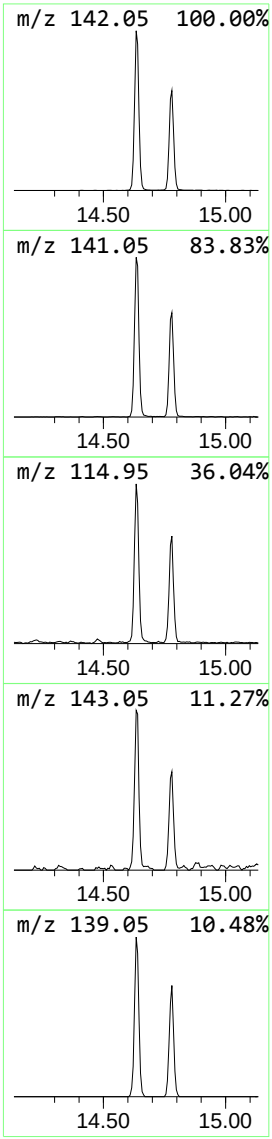
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Naphthalene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.634	21.06 ug/l	252330	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	93
4	Benzocycloheptatriene	142	C11H10	000264-09-5	90
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081423\
Data File : VX036975.D
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Sample : 03983-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
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ClientSampleId :
713-F

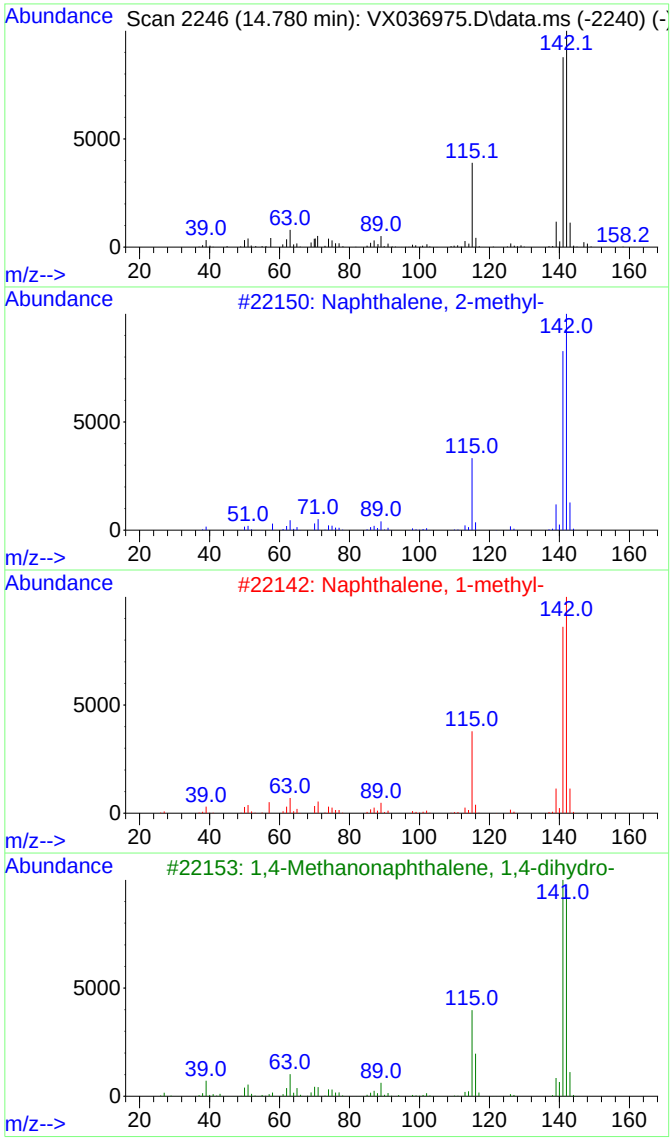
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

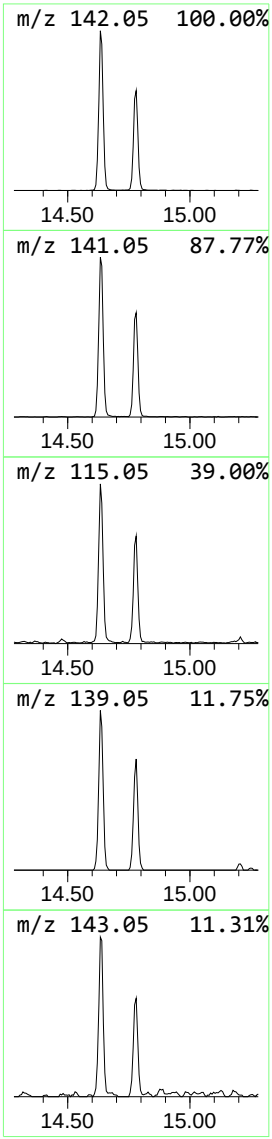
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Naphthalene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	13.19 ug/l	158019	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	94
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081423\
Data File : VX036975.D
Acq On : 14 Aug 2023 19:24
Operator : JC/MD
Sample : 03983-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
713-F

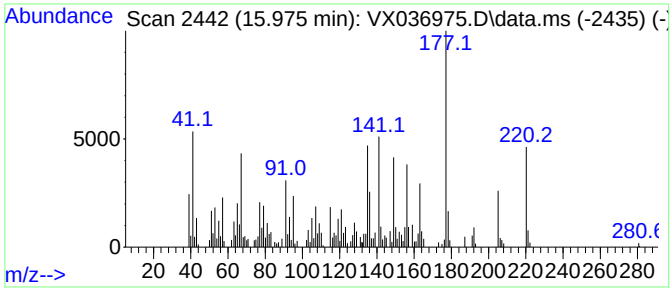
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

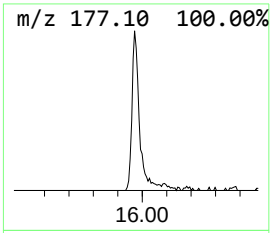
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

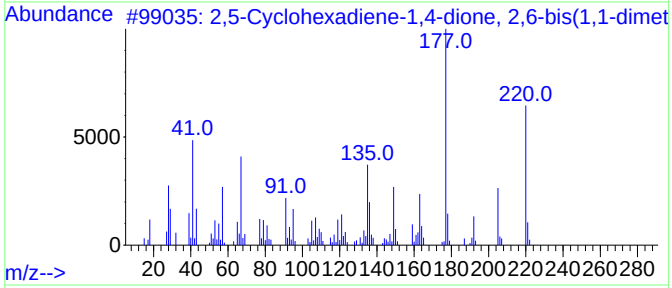
****
Peak Number 9 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 10

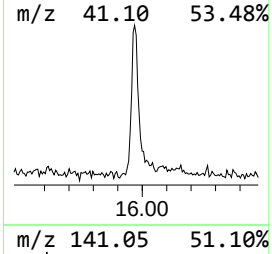
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.975	9.67 ug/l	115856	1,4-Dichlorobenzene-d4	12.024

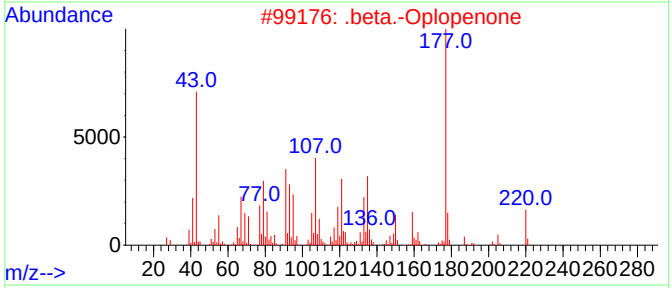
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	94
2	.beta.-Oplopenone	220	C15H24O	028305-60-4	42
3	2H-1-benzopyran-6-ol, 3,4-dihydr...	220	C14H20O2	1000396-25-4	42
4	N-[4-(Ethyl-methyl-amino)-phenyl...	192	C11H16N2O	099981-45-0	38
5	Octamethyl-1,4-cyclohexadiene	192	C14H24	172684-93-4	35

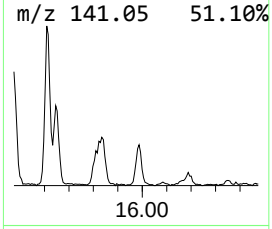


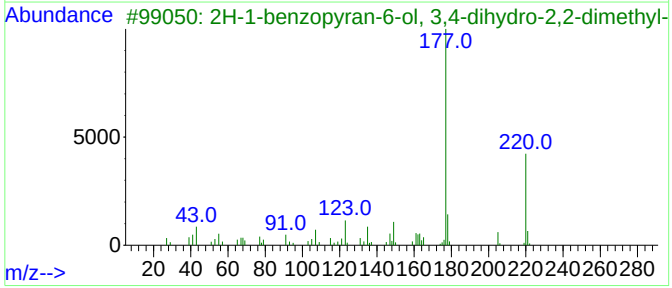


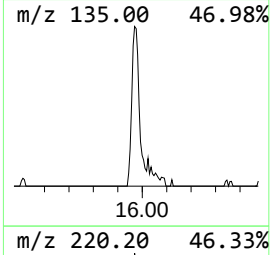


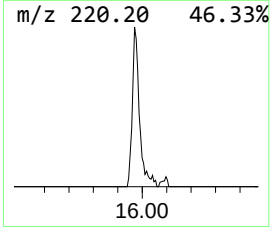












Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081423\
Data File : VX036975.D
Acq On : 14 Aug 2023 19:24
Operator : JC/MD
Sample : 03983-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
713-F

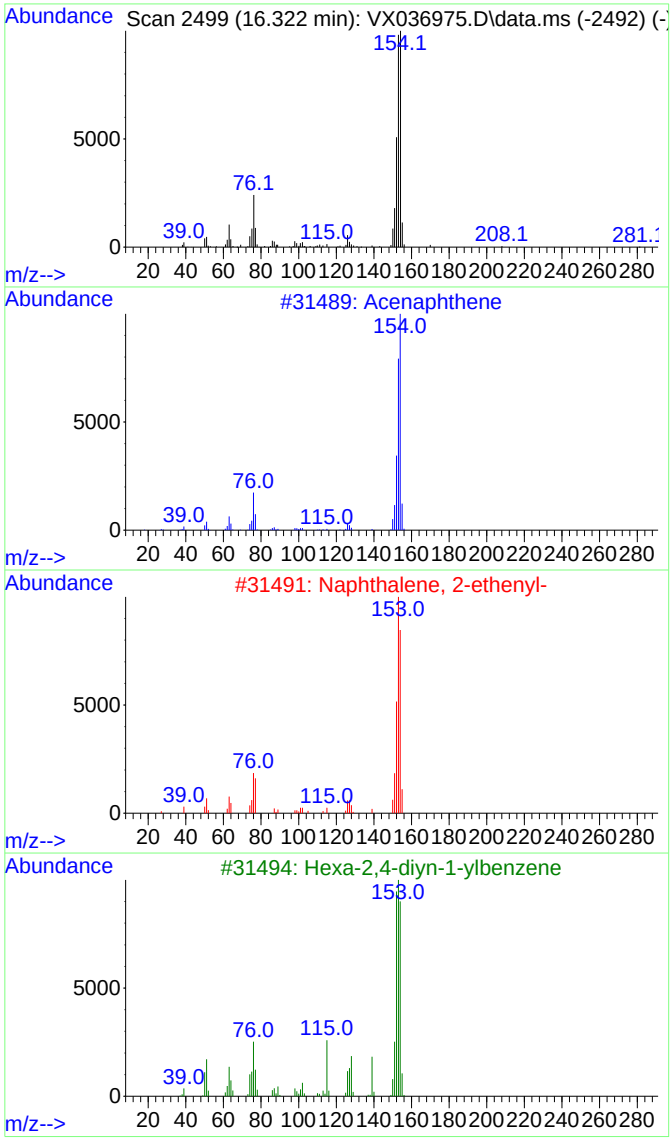
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

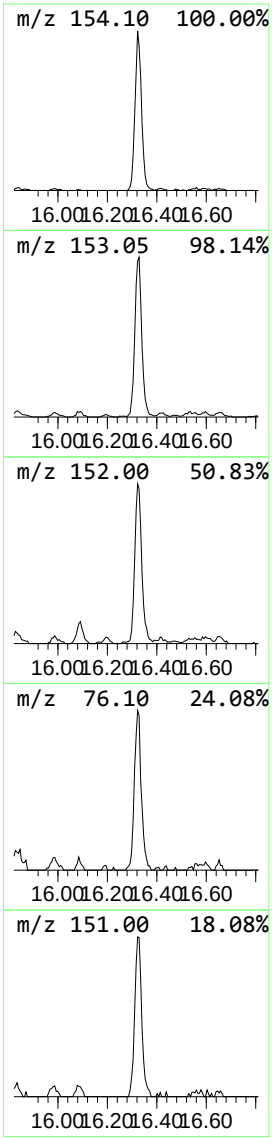
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Acenaphthene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.322	11.51 ug/l	137906	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acenaphthene	154	C12H10	000083-32-9	94
2	Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	68
3	Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	59
4	Biphenyl	154	C12H10	000092-52-4	52
5	1,4-Ethenonaphthalene, 1,4-dihydro-	154	C12H10	007322-47-6	45





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081423\
Data File : VX036975.D
Acq On : 14 Aug 2023 19:24
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Sample : 03983-05
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ALS Vial : 23 Sample Multiplier: 1

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MSVOA_X
ClientSampleId :
713-F

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.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-Propanethiol,...	3.697	122.1	ug/l	873291	1	5.556	357533	50.0
Butanal	4.227	38.6	ug/l	275951	1	5.556	357533	50.0
Benzene, 1-ethy...	11.378	10.9	ug/l	130522	4	12.024	598990	50.0
1-Hexanol, 2-et...	12.213	76.8	ug/l	919581	4	12.024	598990	50.0
Indene	12.415	44.6	ug/l	534262	4	12.024	598990	50.0
Naphthalene, 1-...	14.634	21.1	ug/l	252330	4	12.024	598990	50.0
Naphthalene, 2-...	14.780	13.2	ug/l	158019	4	12.024	598990	50.0
2,5-Cyclohexadi...	15.975	9.7	ug/l	115856	4	12.024	598990	50.0
Acenaphthene	16.322	11.5	ug/l	137906	4	12.024	598990	50.0