LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102122\
Data File : VX032285.D
Acq On : 21 Oct 2022 13:52
Operator : JC/MD
Sample : N5185-19 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PZ-3R

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\82X101922W.M
Title : SW846 8260

Signal : TIC: VX032285.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	26	29	36	rBV	21810	21412	1.21%	0.132%
2	1.368	43	46	52	rBV	167106	165875	9.41%	1.021%
3	1.746	103	108	120	rVB	686780	932231	52.89%	5.737%
4	1.953	137	142	153	rVB	186966	265071	15.04%	1.631%
5	2.069	156	161	167	rBV	24648	33478	1.90%	0.206%
6	2.166	172	177	181	rVV	13433	21283	1.21%	0.131%
7	2.215	181	185	194	rVB	42438	63272	3.59%	0.389%
8	2.337	199	205	212	rBV2	14190	28666	1.63%	0.176%
9	2.782	258	278	281	rBV2	47634	124433	7.06%	0.766%
10	2.825	281	285	289	rVV	102077	206753	11.73%	1.272%
11	2.867	289	292	308	rVB2	50126	120443	6.83%	0.741%
12	3.099	319	330	342	rBV	74662	169413	9.61%	1.043%
13	3.319	359	366	376	rVB	8104	18068	1.03%	0.111%
14	3.447	376	387	395	rBV	27958	61995	3.52%	0.381%
15	3.733	427	434	443	rVB3	19736	48192	2.73%	0.297%
16	3.837	443	451	458	rBV3	12414	32105	1.82%	0.198%
17	4.099	485	494	503	rVB2	13556	33690	1.91%	0.207%
18	4.215	503	513	518	rVV3	10874	30564	1.73%	0.188%
19	4.306	518	528	540	rVV	121276	344022	19.52%	2.117%
20	5.196	666	674	687	rVB3	8725	27351	1.55%	0.168%
21	5.385	694	705	713	rBV	82685	242437	13.76%	1.492%
22	5.477	713	720	722	rVV2	18847	38277	2.17%	0.236%
23	5.550	725	732	741	rVB	138141	376508	21.36%	2.317%
24	5.830	762	778	789	rBV2	22284	66877	3.79%	0.412%
25	5.958	789	799	806	rVV	92094	242587	13.76%	1.493%
26	6.038	806	812	823	rVV	65346	174710	9.91%	1.075%
27	6.166	823	833	839	rVV6	14537	53623	3.04%	0.330%
28	6.251	839	847	857	rVV2	40385	128604	7.30%	0.791%
29	6.361	857	865	874	rVB3	11265	32935	1.87%	0.203%
30	6.611	896	906	915	rBV3	8309	20503	1.16%	0.126%
31	6.763	921	931	940	rBV	221602	537694	30.51%	3.309%
32	6.842	940	944	956	rVB7	11431	32940	1.87%	0.203%
33	7.379	1020	1032	1043	rBV5	33885	94656	5.37%	0.582%
34	7.659	1073	1078	1085	rVB	9802	18641	1.06%	0.115%
35	7.982	1123	1131	1140	rVB	17589	36467	2.07%	0.224%
36	8.104	1143	1151	1155	rBV2	24733	52492	2.98%	0.323%

LSC Area Percent Report

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Operator : JC/MD
Sample : N5185-19 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PZ-3R

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\82X101922W.M
Title : SW846 8260

37	8.434	1201	1205	1212	rBV2	10161	18556	1.05%	0.114%
38	8.507	1212	1217	1227	rVB2	19019	34998	1.99%	0.215%
39	8.647	1234	1240	1248	rVB	442158	704240	39.96%	4.334%
40	8.720	1248	1252	1257	rVB	18360	27248	1.55%	0.168%
41	8.848	1264	1273	1278	rVB4	8755	18723	1.06%	0.115%
42	10.055	1465	1471	1478	rVB	454376	598550	33.96%	3.683%
43	10.195	1489	1494	1501	rVB	1156630	1445277	82.00%	8.894%
44	10.305	1506	1512	1518	rVB	549583	745160	42.28%	4.586%
45	10.640	1562	1567	1574	rBV	64209	86148	4.89%	0.530%
46	10.964	1614	1620	1626	rBV	106058	131528	7.46%	0.809%
47	11.079	1634	1639	1650	rVB	383687	486888	27.62%	2.996%
48	11.305	1667	1676	1683	rBV	291298	345396	19.60%	2.125%
49	11.403	1683	1692	1696	rBV	331879	439763	24.95%	2.706%
50	11.451	1696	1700	1708	rVB	95926	116965	6.64%	0.720%
51	11.616	1721	1727	1735	rVB	195304	255638	14.50%	1.573%
52	11.750	1744	1749	1756	rVB	1434999	1762501	100.00%	10.846%
53	11.866	1762	1768	1770	rBV	14127	18647	1.06%	0.115%
54	11.890	1770	1772	1779	rVB	19834	21718	1.23%	0.134%
55	12.024	1789	1794	1799	rBV	489112	606847	34.43%	3.734%
56	12.085	1799	1804	1810	rBV	476752	593071	33.65%	3.650%
57	12.244	1824	1830	1837	rBV2	452229	570458	32.37%	3.510%
58	12.311	1837	1841	1851	rVV3	94473	160181	9.09%	0.986%
59	12.408	1851	1857	1862	rVV2	21470	27399	1.55%	0.169%
60	12.463	1862	1866	1872	rVB	65395	78370	4.45%	0.482%
61	12.530	1872	1877	1879	rBV	113000	136147	7.72%	0.838%
62	12.555	1879	1881	1886	rVV	88425	95158	5.40%	0.586%
63	12.616	1886	1891	1894	rVV	215085	266691	15.13%	1.641%
64	12.646	1894	1896	1900	rVV	29548	30561	1.73%	0.188%
65	12.701	1900	1905	1916	rVV2	88447	136879	7.77%	0.842%
66	12.847	1924	1929	1934	rVB	51637	64172	3.64%	0.395%
67	12.921	1934	1941	1944	rBV	114928	134264	7.62%	0.826%
68	12.963	1944	1948	1954	rVB	139608	162958	9.25%	1.003%
69	13.170	1978	1982	1986	rVB	97804	113176	6.42%	0.696%
70	13.256	1992	1996	1998	rBV2	12114	17629	1.00%	0.108%
71	13.292	1998	2002	2007	rVB2	199230	261672	14.85%	1.610%
72	13.420	2019	2023	2031	rVB	26078	35452	2.01%	0.218%
73	13.579	2046	2049	2056	rVV3	21800	41492	2.35%	0.255%
74	13.670	2060	2064	2069	rVB3	13856	24710	1.40%	0.152%
75	13.774	2076	2081	2092	rBV	257165	327410	18.58%	2.015%
76	14.213	2149	2153	2160	rBV3	11686	19869	1.13%	0.122%

LSC Area Percent Report

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ALS Vial : 7 Sample Multiplier: 1

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ClientSampleId :
PZ-3R

Integration Parameters: RTEINT.P
Integrator: RTE
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Sampling : 1 Min Area: 3 % of largest Peak
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Title : SW846 8260

77	14.640	2213	2223	2231	rBV	93180	118060	6.70%	0.727%
78	14.780	2241	2246	2254	rVB	58233	71502	4.06%	0.440%

Sum of corrected areas: 16250340

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Acq On : 21 Oct 2022 13:52
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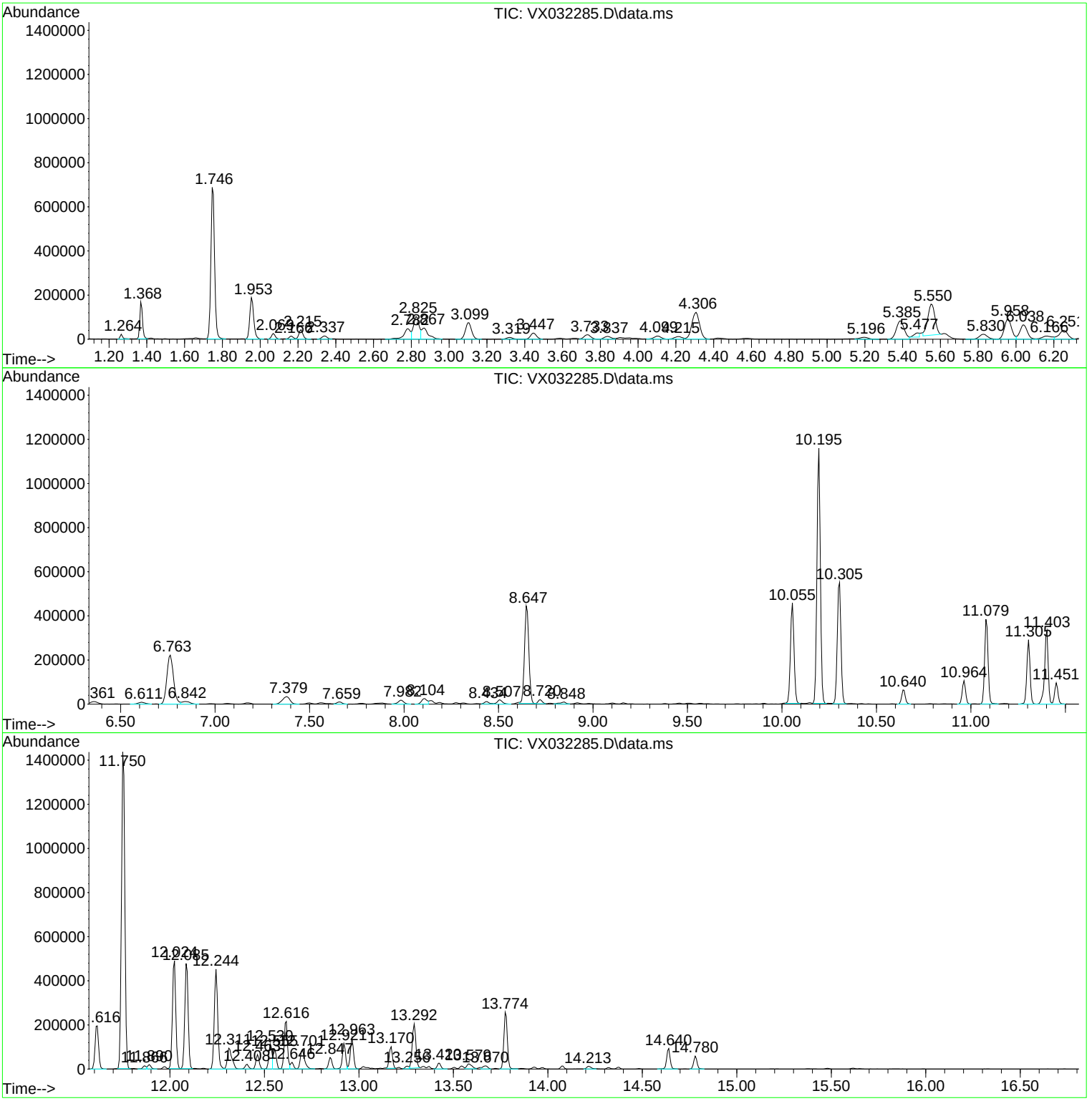
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PZ-3R

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102122\
Data File : VX032285.D
Acq On : 21 Oct 2022 13:52
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Instrument :
MSVOA_X
ClientSampleId :
PZ-3R

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

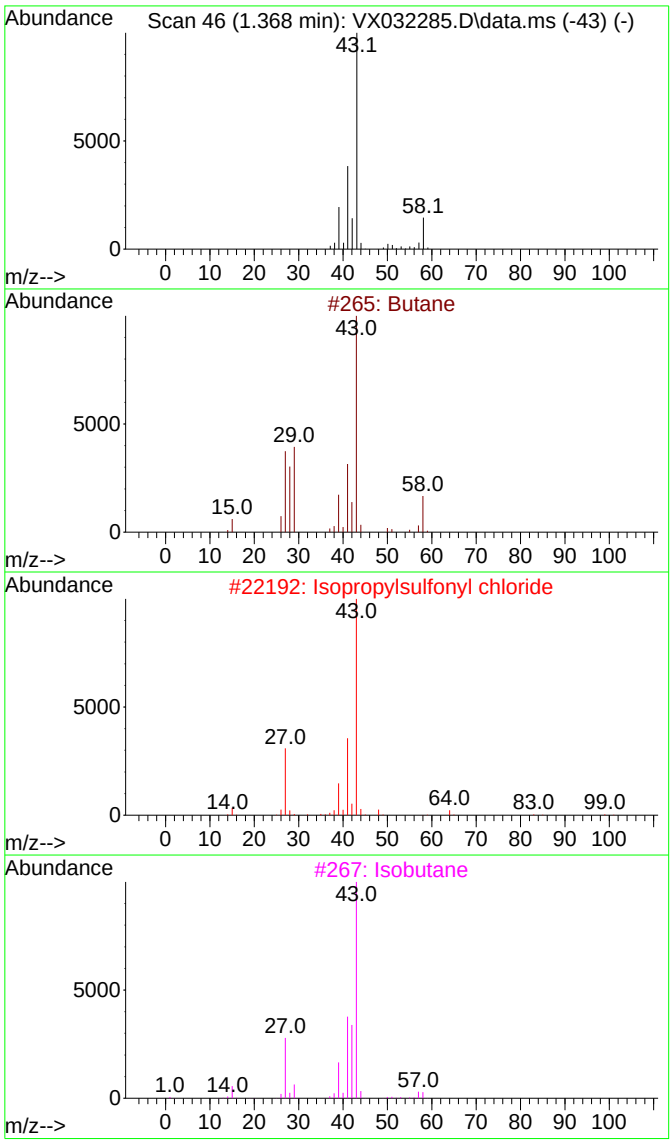
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

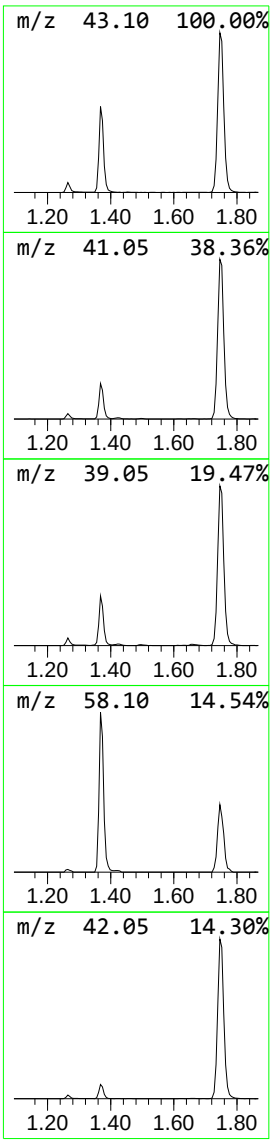
****

Peak Number 1 Butane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.368	22.03 ug/l	165875	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	80
2	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
3	Isobutane	58	C4H10	000075-28-5	9
4	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
5	Acetone	58	C3H6O	000067-64-1	5





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102122\
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Operator : JC/MD
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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PZ-3R

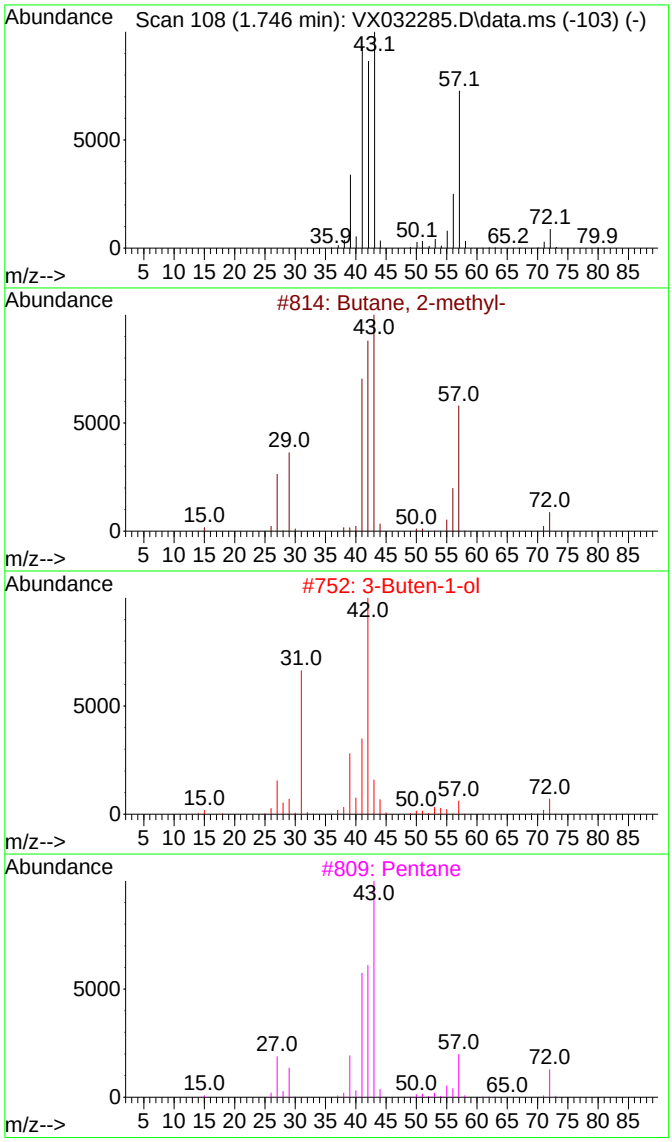
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

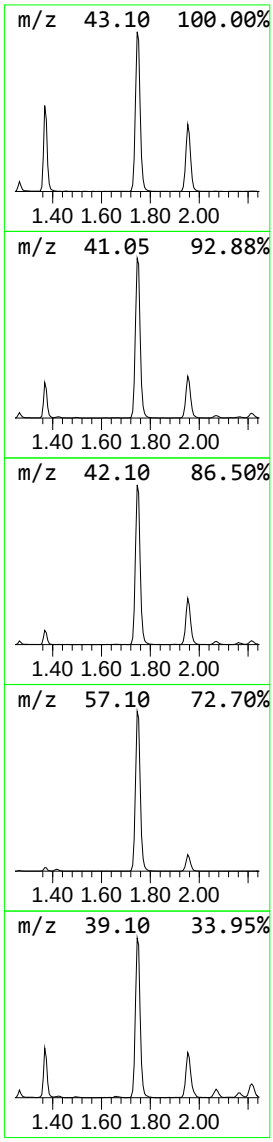
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.746	123.80 ug/l	932231	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	90
2	3-Buten-1-ol	72	C4H8O	000627-27-0	47
3	Pentane	72	C5H12	000109-66-0	36
4	1-Butene	56	C4H8	000106-98-9	10
5	Methane, isocyanato-	57	C2H3NO	000624-83-9	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102122\
Data File : VX032285.D
Acq On : 21 Oct 2022 13:52
Operator : JC/MD
Sample : N5185-19 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PZ-3R

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

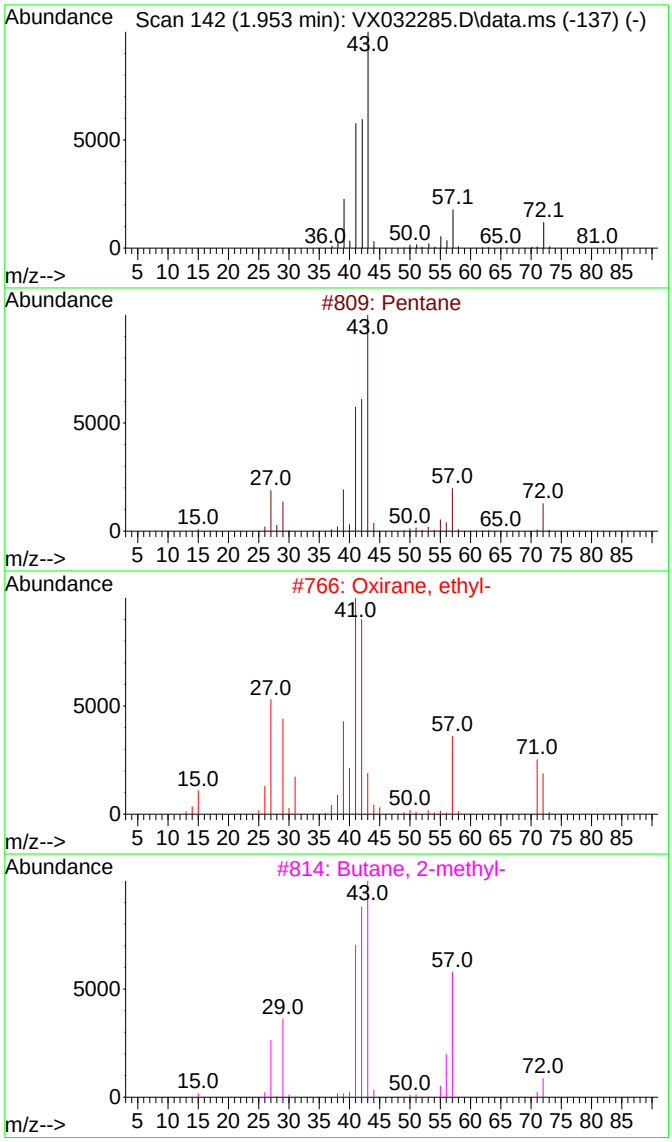
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

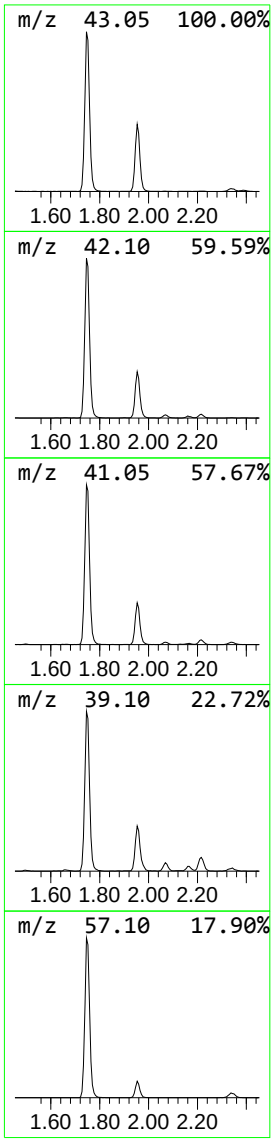
****

Peak Number 3 Pentane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.953	35.20 ug/l	265071	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	91
2	Oxirane, ethyl-	72	C4H8O	000106-88-7	50
3	Butane, 2-methyl-	72	C5H12	000078-78-4	50
4	1-Propene, 2-methoxy-	72	C4H8O	000116-11-0	9
5	Cyclobutylamine	71	C4H9N	002516-34-9	9





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Instrument :
MSVOA_X
ClientSampleId :
PZ-3R

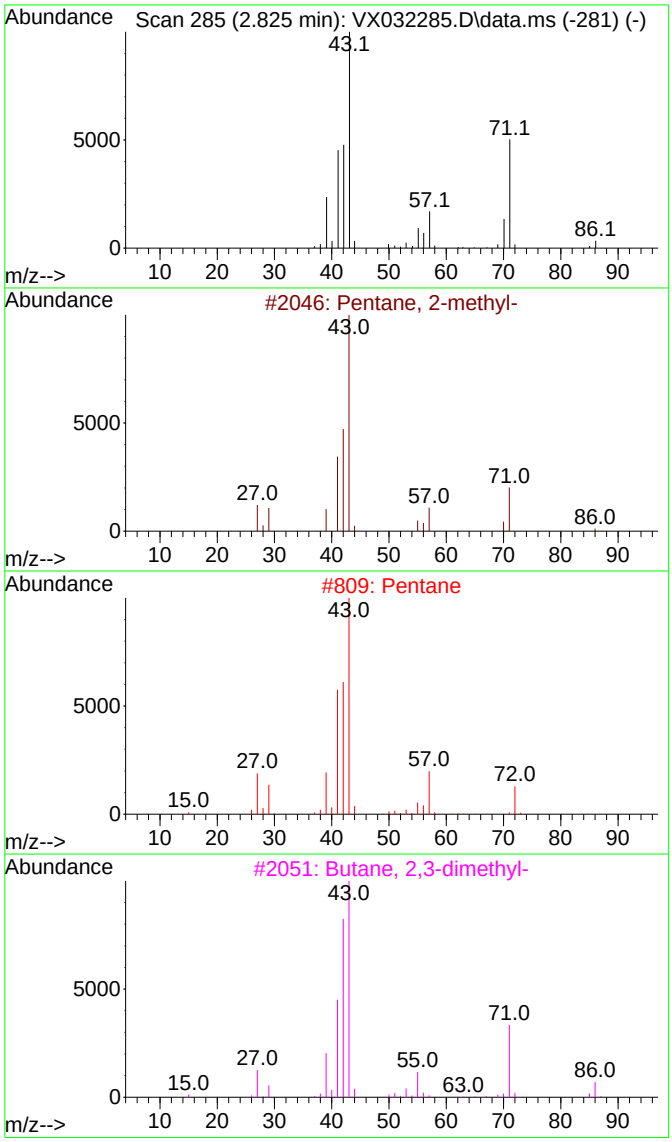
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

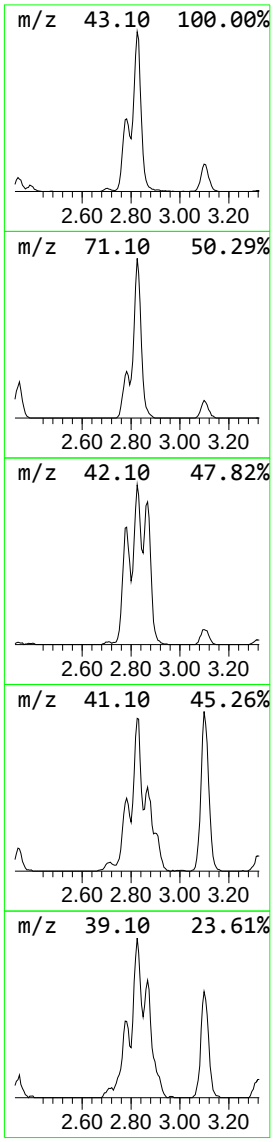
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Pentane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.825	27.46 ug/l	206753	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	78
2	Pentane	72	C5H12	000109-66-0	49
3	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	38
4	Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	33
5	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	28





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102122\
Data File : VX032285.D
Acq On : 21 Oct 2022 13:52
Operator : JC/MD
Sample : N5185-19 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PZ-3R

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

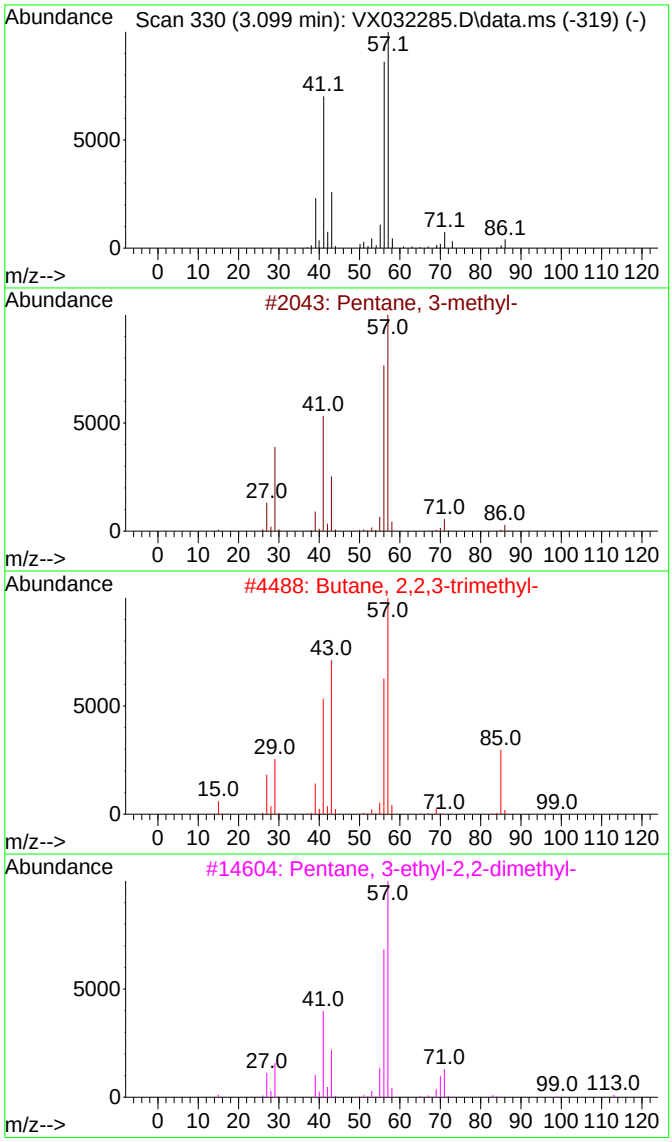
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

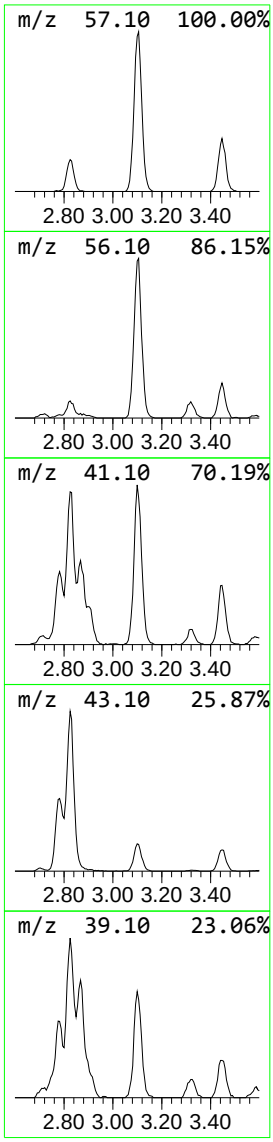
****

Peak Number 5 Pentane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.099	22.50 ug/l	169413	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	78
3	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	43
4	Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	43
5	Butyl isocyanatoacetate	157	C7H11NO3	017046-22-9	40





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Data File : VX032285.D
Acq On : 21 Oct 2022 13:52
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PZ-3R

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

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

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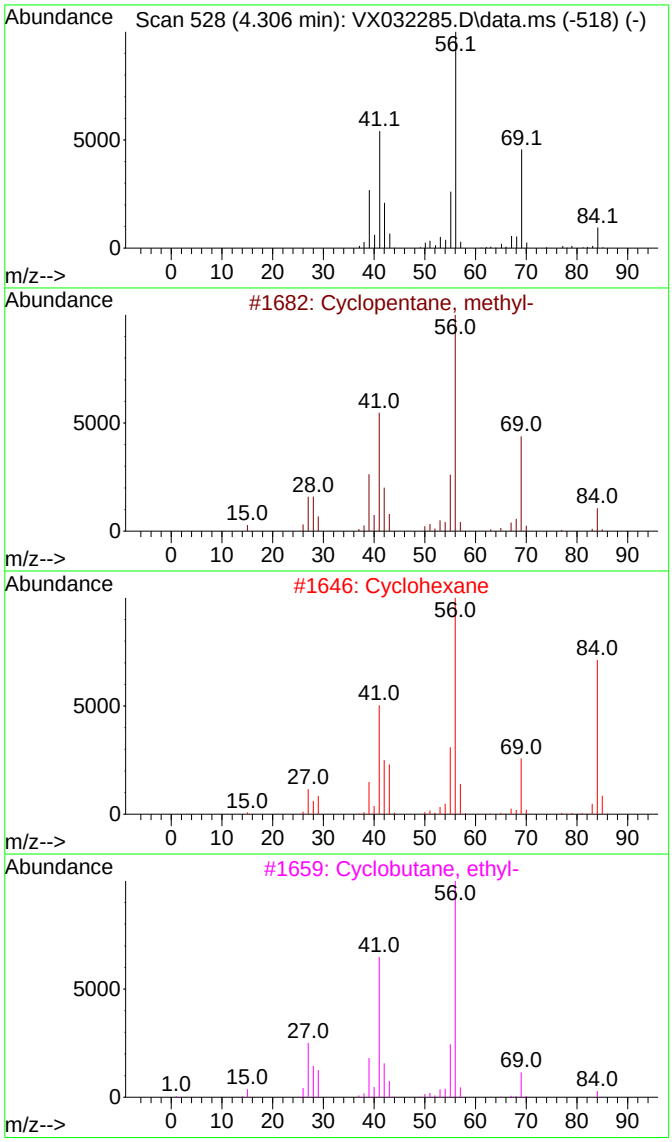
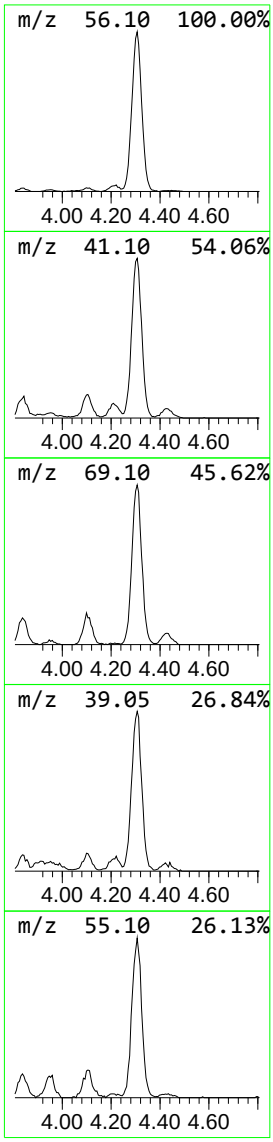
Peak Number 6 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	45.69 ug/l	344022	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	Cyclohexane	84	C6H12	000110-82-7	78
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
4	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	53
5	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102122\
Data File : VX032285.D
Acq On : 21 Oct 2022 13:52
Operator : JC/MD
Sample : N5185-19 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PZ-3R

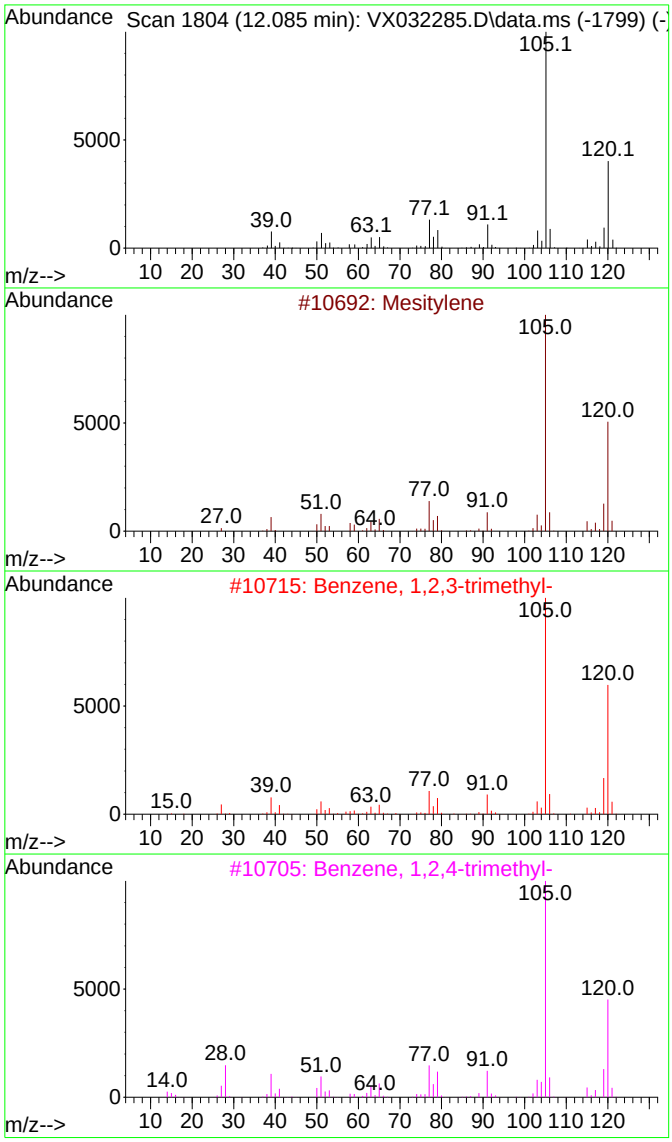
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

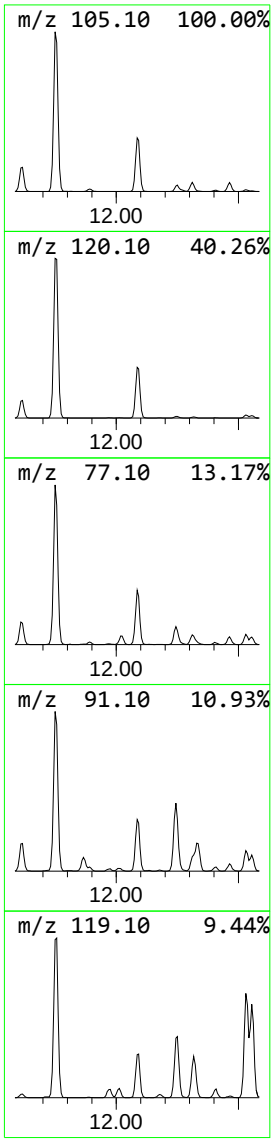
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1,2,3-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	48.87 ug/l	593071	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Mesitylene	120	C9H12	000108-67-8	97
2	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102122\
Data File : VX032285.D
Acq On : 21 Oct 2022 13:52
Operator : JC/MD
Sample : N5185-19 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PZ-3R

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

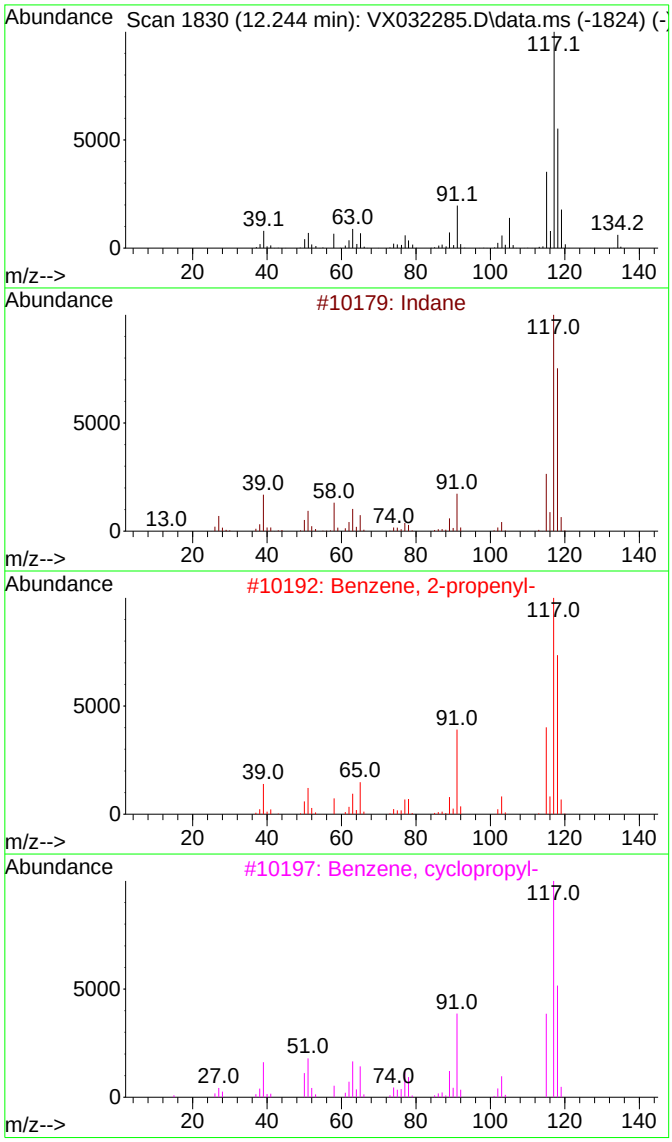
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

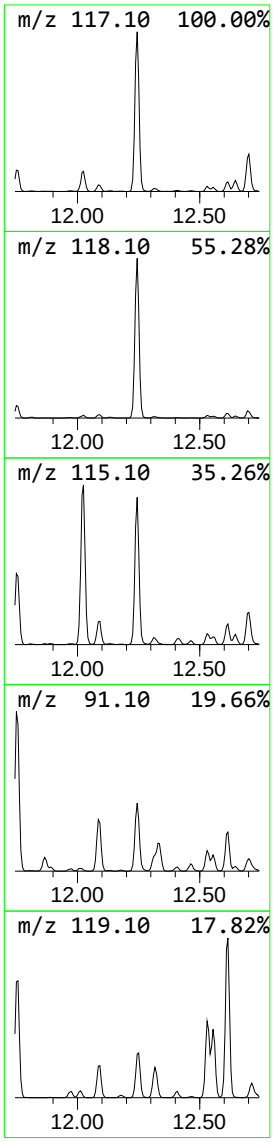
****

Peak Number 8 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	47.00 ug/l	570458	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	76
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	70
4	Deltacyclene	118	C9H10	007785-10-6	58
5	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	55





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102122\
Data File : VX032285.D
Acq On : 21 Oct 2022 13:52
Operator : JC/MD
Sample : N5185-19 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PZ-3R

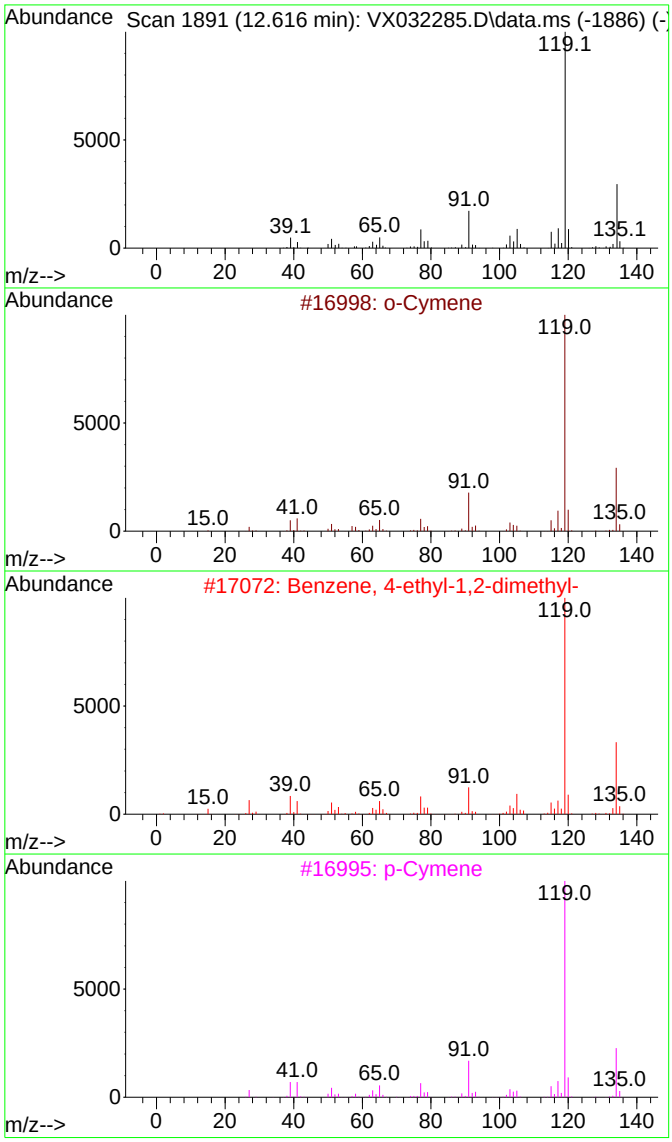
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

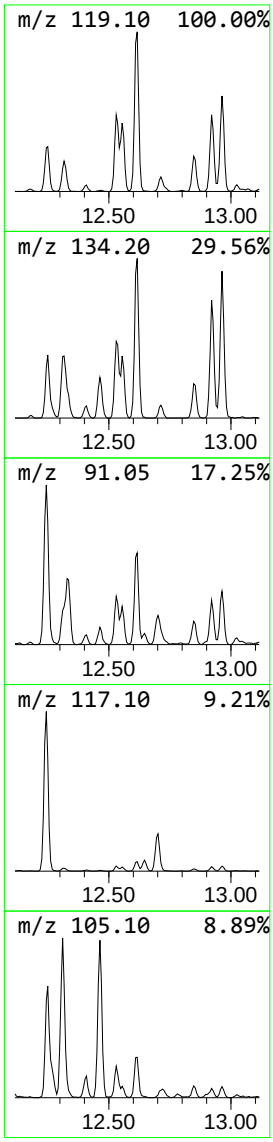
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 o-Cymene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	21.97 ug/l	266691	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Cymene	134	C10H14	000527-84-4	97
2	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
3	p-Cymene	134	C10H14	000099-87-6	95
4	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102122\
Data File : VX032285.D
Acq On : 21 Oct 2022 13:52
Operator : JC/MD
Sample : N5185-19 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PZ-3R

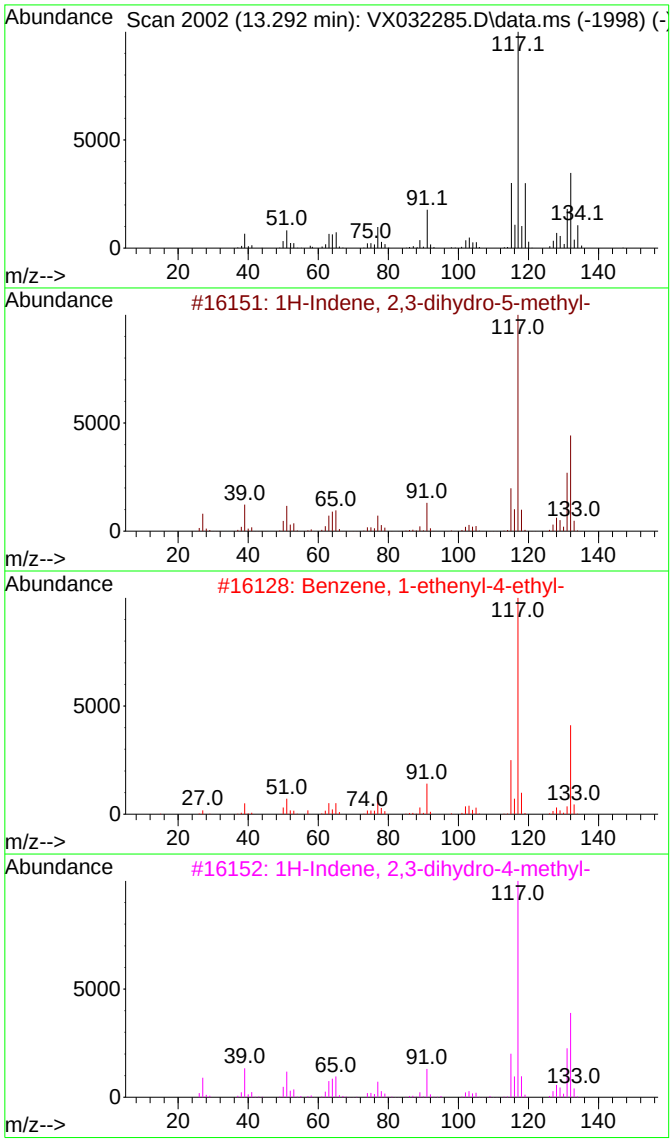
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

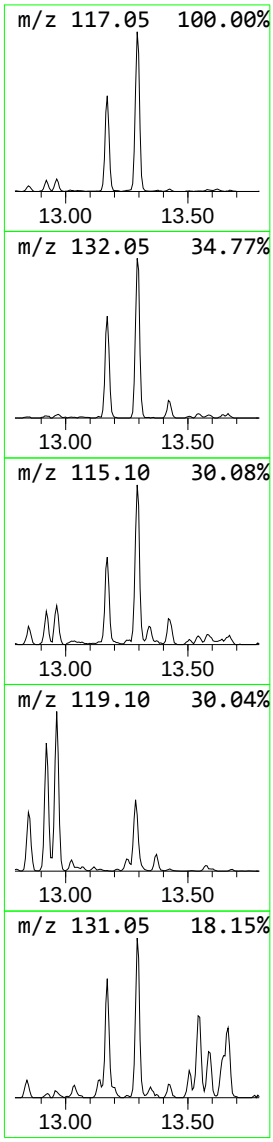
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	21.56 ug/l	261672	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	95
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	93
4	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	92
5	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102122\
Data File : VX032285.D
Acq On : 21 Oct 2022 13:52
Operator : JC/MD
Sample : N5185-19 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PZ-3R

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.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
Butane	1.368	22.0	ug/l	165875	1	5.556	376508	50.0
Butane, 2-methyl-	1.746	123.8	ug/l	932231	1	5.556	376508	50.0
Pentane	1.953	35.2	ug/l	265071	1	5.556	376508	50.0
Pentane, 2-methyl-	2.825	27.5	ug/l	206753	1	5.556	376508	50.0
Pentane, 3-methyl-	3.099	22.5	ug/l	169413	1	5.556	376508	50.0
Cyclopentane, m...	4.306	45.7	ug/l	344022	1	5.556	376508	50.0
Benzene, 1,2,3-...	12.085	48.9	ug/l	593071	4	12.024	606847	50.0
Indane	12.244	47.0	ug/l	570458	4	12.024	606847	50.0
o-Cymene	12.616	22.0	ug/l	266691	4	12.024	606847	50.0
1H-Indene, 2,3-...	13.292	21.6	ug/l	261672	4	12.024	606847	50.0