LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120822\
Data File : VX033334.D
Acq On : 08 Dec 2022 19:22
Operator : JC/MD
Sample : N5906-14
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-42

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\82X120722W.M
Title : SW846 8260

Signal : TIC: VX033334.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	41	rBV	843412	992739	2.94%	0.413%
2	1.374	41	47	53	rVV	1996141	2345047	6.94%	0.975%
3	1.752	103	109	124	rBV	5892217	7950381	23.54%	3.307%
4	1.959	138	143	156	rVB2	1668507	2679836	7.93%	1.115%
5	2.069	156	161	168	rVV	583649	784115	2.32%	0.326%
6	2.166	172	177	181	rVV	231873	343619	1.02%	0.143%
7	2.215	181	185	196	rVV	859823	1265899	3.75%	0.527%
8	2.343	198	206	226	rVB	181495	373025	1.10%	0.155%
9	2.782	258	278	281	rBV3	452550	1567557	4.64%	0.652%
10	2.831	281	286	289	rVV	967551	2024686	5.99%	0.842%
11	2.867	289	292	306	rVB2	738480	1854923	5.49%	0.772%
12	3.105	322	331	346	rVB2	835363	1904054	5.64%	0.792%
13	3.325	355	367	378	rBV3	179842	450525	1.33%	0.187%
14	3.446	378	387	399	rVB	302249	658351	1.95%	0.274%
15	3.666	416	423	428	rBV	191558	448674	1.33%	0.187%
16	3.733	428	434	443	rVB	412554	971158	2.88%	0.404%
17	3.837	443	451	457	rBV	277960	700940	2.08%	0.292%
18	4.105	485	495	505	rVB	316811	818561	2.42%	0.340%
19	4.306	518	528	540	rVB	1352928	3808441	11.27%	1.584%
20	5.196	664	674	689	rVB	208403	668519	1.98%	0.278%
21	5.477	710	720	728	rBV2	425328	1413652	4.18%	0.588%
22	5.830	765	778	791	rBV4	154506	490177	1.45%	0.204%
23	6.044	803	813	823	rBV	1427727	3735060	11.06%	1.554%
24	6.165	823	833	835	rBV3	145162	362760	1.07%	0.151%
25	6.257	842	848	857	rVB2	302122	887214	2.63%	0.369%
26	6.361	857	865	875	rVB2	155023	447974	1.33%	0.186%
27	6.763	924	931	937	rBV	252572	640565	1.90%	0.266%
28	6.848	937	945	953	rVB4	230497	756943	2.24%	0.315%
29	7.178	990	999	1009	rBV3	159629	385063	1.14%	0.160%
30	7.379	1019	1032	1045	rBV4	648233	1739396	5.15%	0.723%
31	8.141	1153	1157	1163	rVB	394332	674948	2.00%	0.281%
32	8.507	1210	1217	1226	rVB	411133	718951	2.13%	0.299%
33	8.720	1246	1252	1258	rBV	2396135	3616744	10.71%	1.504%
34	8.842	1265	1272	1279	rBV	209162	371372	1.10%	0.154%
35	10.055	1461	1471	1476	rBV	513405	815157	2.41%	0.339%
36	10.201	1489	1495	1500	rVB	11602657	16157917	47.83%	6.721%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120822\
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Acq On : 08 Dec 2022 19:22
Operator : JC/MD
Sample : N5906-14
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-42

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\82X120722W.M
Title : SW846 8260

37	10.311	1506	1513	1518	rVB	22253989	33779147	100.00%	14.050%
38	10.646	1562	1568	1573	rBV	12861878	16896643	50.02%	7.028%
39	10.963	1613	1620	1628	rVB	1055860	1320489	3.91%	0.549%
40	11.079	1635	1639	1644	rVB	334274	426718	1.26%	0.177%
41	11.305	1667	1676	1683	rVB	3016418	3733936	11.05%	1.553%
42	11.384	1683	1689	1696	rBV	11423492	21014861	62.21%	8.741%
43	11.457	1696	1701	1706	rVB	6725172	8262011	24.46%	3.437%
44	11.616	1721	1727	1736	rBV	6266639	7638527	22.61%	3.177%
45	11.762	1744	1751	1755	rBV	19256562	26172682	77.48%	10.886%
46	11.969	1779	1785	1789	rBV	371000	478412	1.42%	0.199%
47	12.024	1789	1794	1799	rVB2	576968	832356	2.46%	0.346%
48	12.091	1799	1805	1810	rBV	6432145	7913142	23.43%	3.291%
49	12.244	1825	1830	1833	rBV	5055748	6496333	19.23%	2.702%
50	12.317	1838	1842	1850	rVB2	2425489	3428920	10.15%	1.426%
51	12.408	1852	1857	1862	rBV2	430780	577276	1.71%	0.240%
52	12.463	1862	1866	1872	rVB	615518	707295	2.09%	0.294%
53	12.530	1872	1877	1879	rBV	1497288	1843442	5.46%	0.767%
54	12.555	1879	1881	1886	rVB	1332364	1465337	4.34%	0.609%
55	12.616	1886	1891	1894	rBV	2386728	2814849	8.33%	1.171%
56	12.646	1894	1896	1900	rVB	497032	512127	1.52%	0.213%
57	12.701	1900	1905	1913	rBV2	1469188	2056540	6.09%	0.855%
58	12.847	1924	1929	1934	rBV	664613	804521	2.38%	0.335%
59	12.920	1934	1941	1945	rVV	1341385	1706459	5.05%	0.710%
60	12.963	1945	1948	1954	rVB	2026529	2290612	6.78%	0.953%
61	13.170	1978	1982	1986	rVB	1540323	1807401	5.35%	0.752%
62	13.292	1997	2002	2007	rVB2	2952505	3721414	11.02%	1.548%
63	13.420	2019	2023	2029	rVB	531172	707579	2.09%	0.294%
64	13.542	2040	2043	2046	rVV	289963	393648	1.17%	0.164%
65	13.585	2046	2050	2056	rVV3	304561	584436	1.73%	0.243%
66	13.664	2060	2063	2069	rVB2	285212	426772	1.26%	0.178%
67	13.780	2076	2082	2091	rVB	6355286	8324354	24.64%	3.462%
68	13.865	2091	2096	2101	rVB	254821	362092	1.07%	0.151%
69	14.219	2149	2154	2159	rBV2	204575	381048	1.13%	0.158%
70	14.640	2218	2223	2233	rVB	2349927	3066407	9.08%	1.275%
71	14.780	2241	2246	2255	rBV	1320343	1645998	4.87%	0.685%

Sum of corrected areas: 240418727

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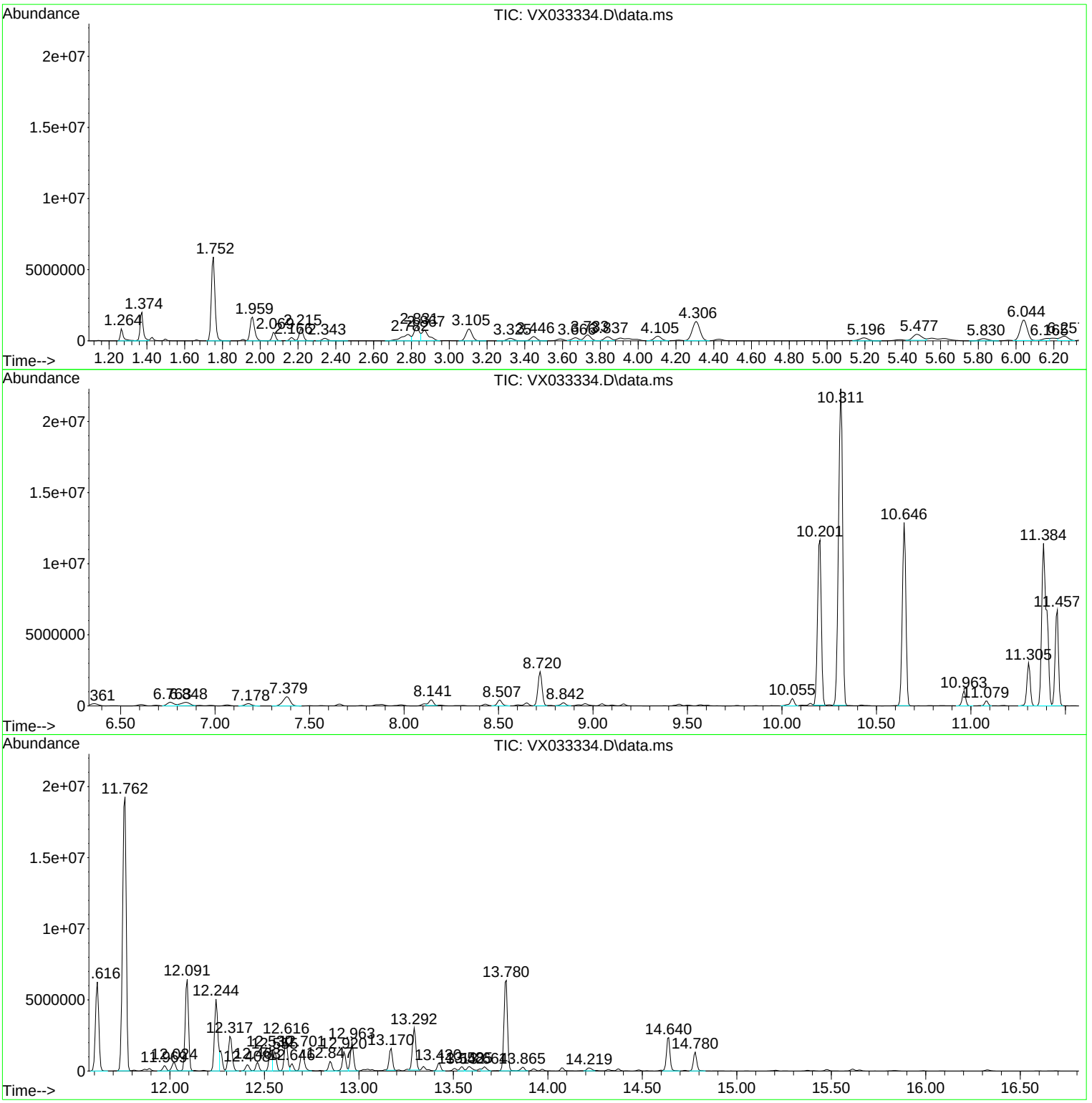
Acq On : 08 Dec 2022 19:22
Operator : JC/MD
Sample : N5906-14
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-42

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120822\
Data File : VX033334.D
Acq On : 08 Dec 2022 19:22
Operator : JC/MD
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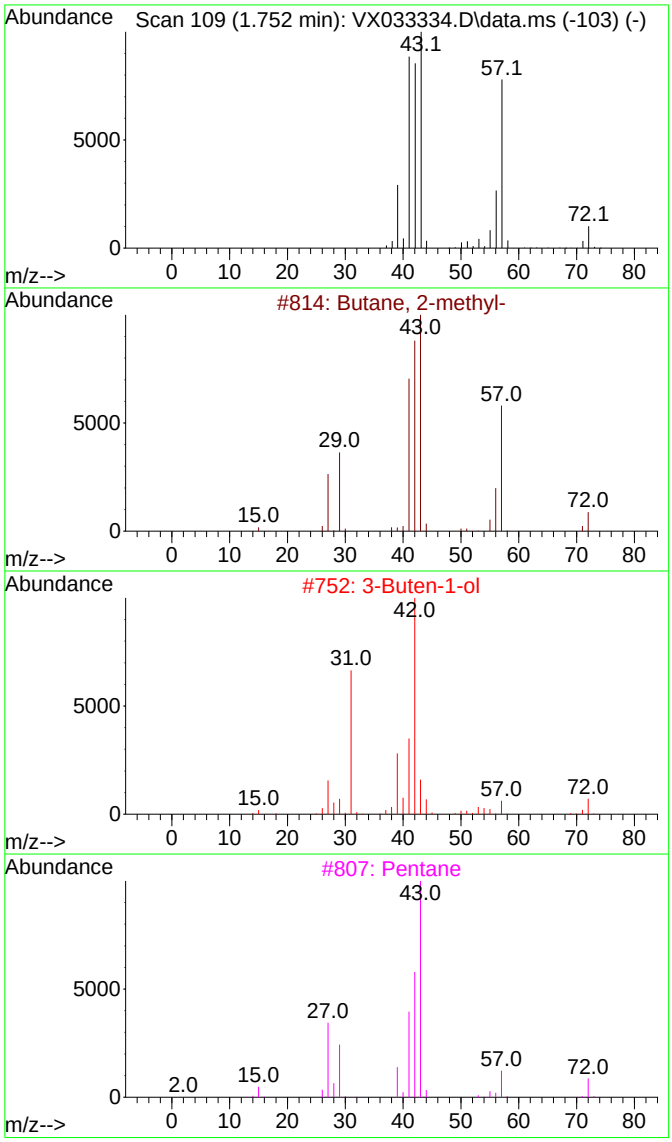
Quant Title : SW846 8260

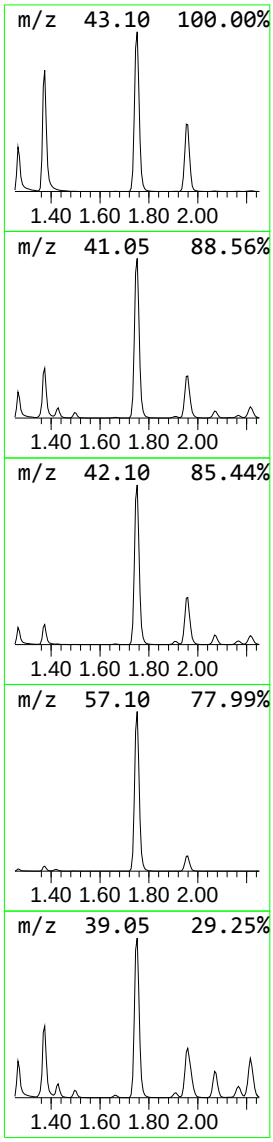
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	281.20 ug/l	7950380	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	87
2	3-Buten-1-ol	72	C4H8O	000627-27-0	43
3	Pentane	72	C5H12	000109-66-0	42
4	1-Butene	56	C4H8	000106-98-9	10
5	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	10





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120822\
Data File : VX033334.D
Acq On : 08 Dec 2022 19:22
Operator : JC/MD
Sample : N5906-14
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-42

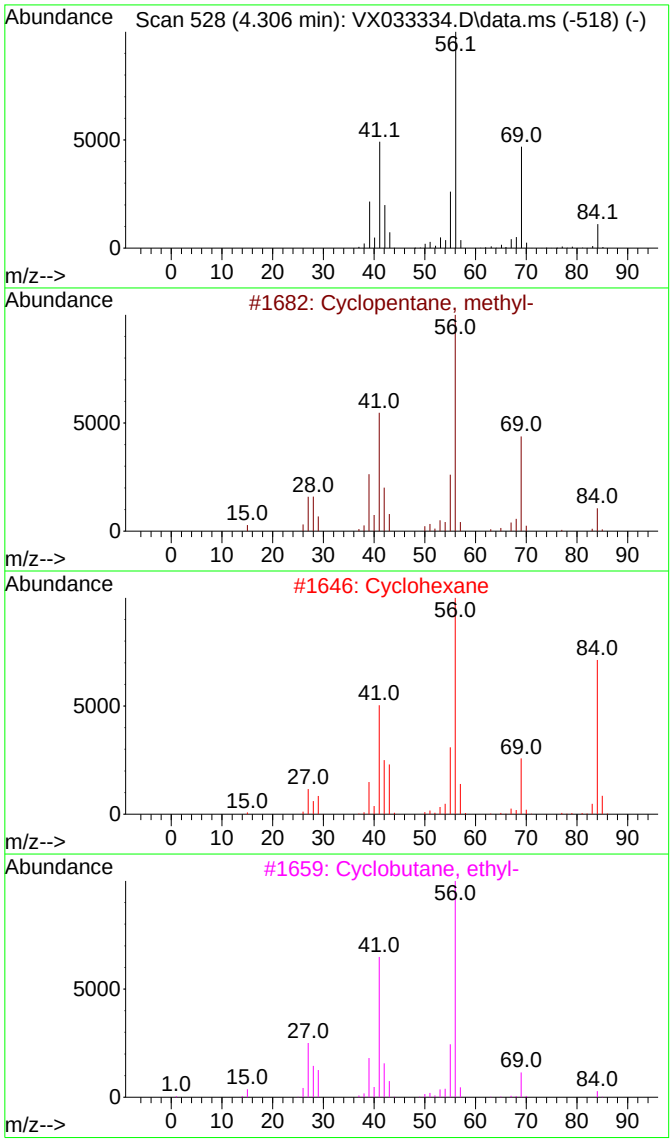
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

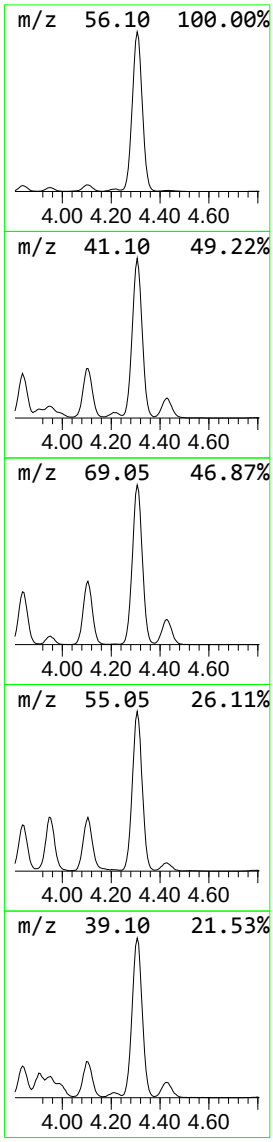
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Cyclopentane, methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	134.70 ug/l	3808440	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	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
5	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120822\
Data File : VX033334.D
Acq On : 08 Dec 2022 19:22
Operator : JC/MD
Sample : N5906-14
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-42

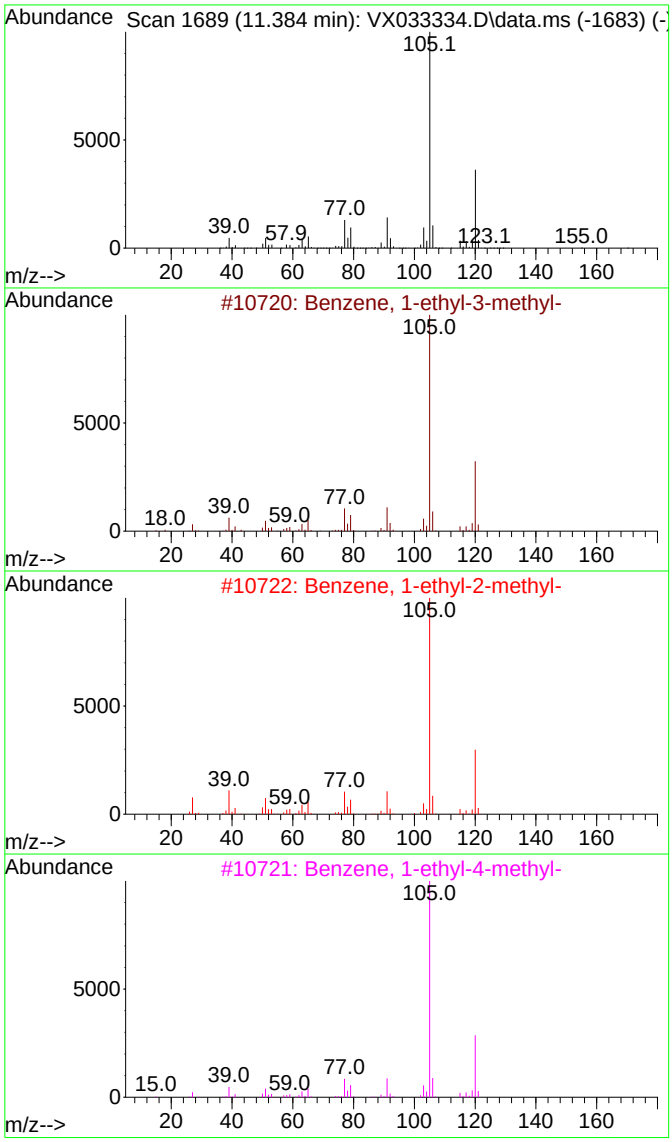
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

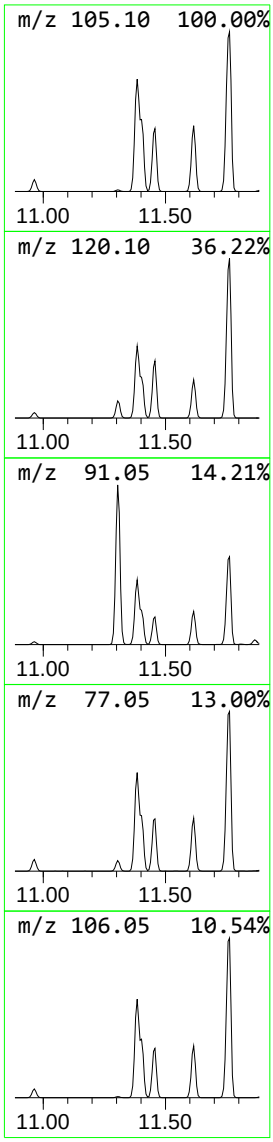
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzene, 1-ethyl-3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.384	1262.37 ug/l	21014900	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	97
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	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	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120822\
Data File : VX033334.D
Acq On : 08 Dec 2022 19:22
Operator : JC/MD
Sample : N5906-14
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-42

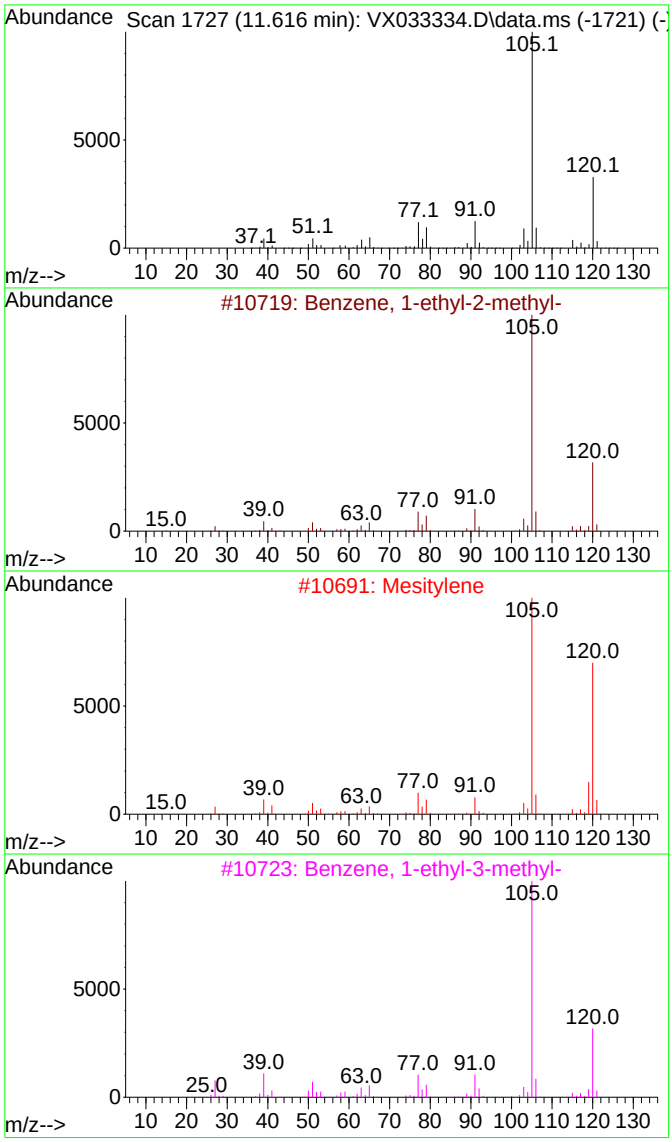
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

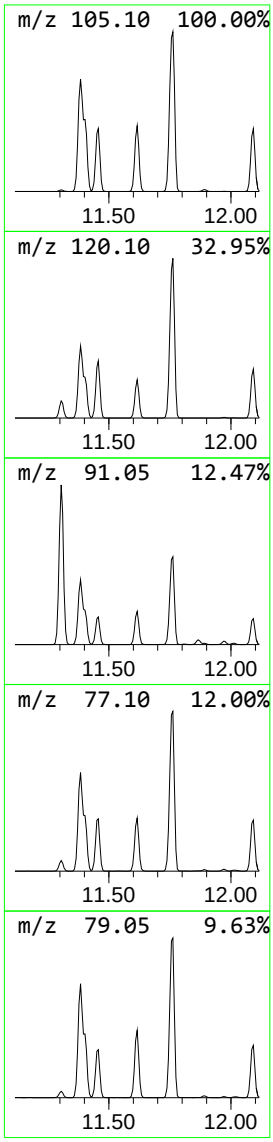
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 1-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	458.85 ug/l	7638530	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	94
2	Mesitylene	120	C9H12	000108-67-8	91
3	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120822\
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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-42

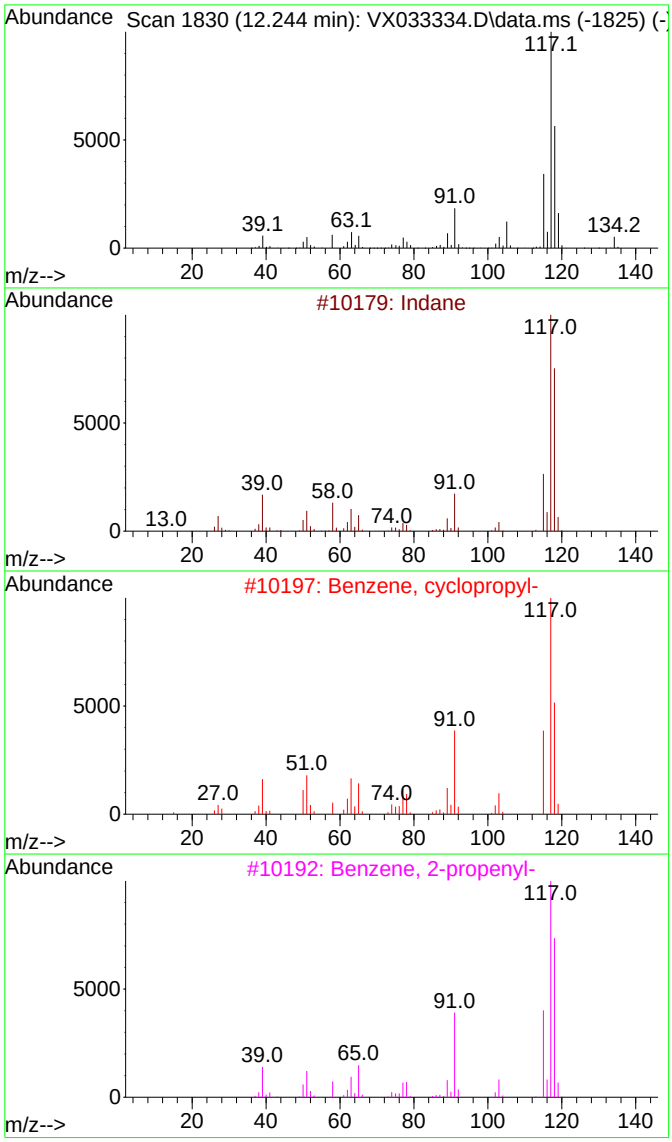
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

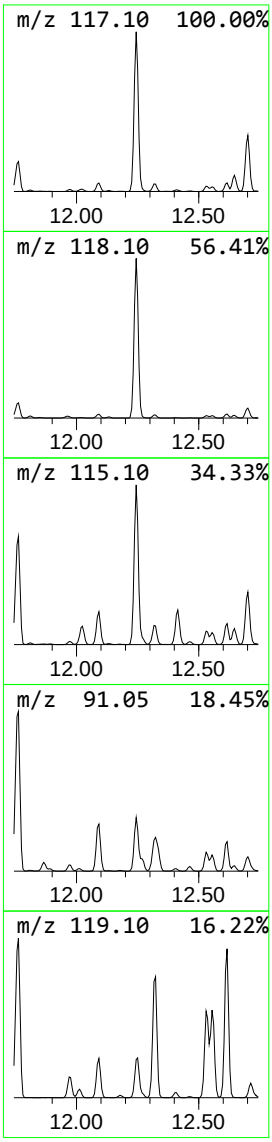
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Indane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	390.24 ug/l	6496330	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, cyclopropyl-	118	C9H10	000873-49-4	76
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
4	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	59
5	Deltacyclene	118	C9H10	007785-10-6	58





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Data File : VX033334.D
Acq On : 08 Dec 2022 19:22
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-42

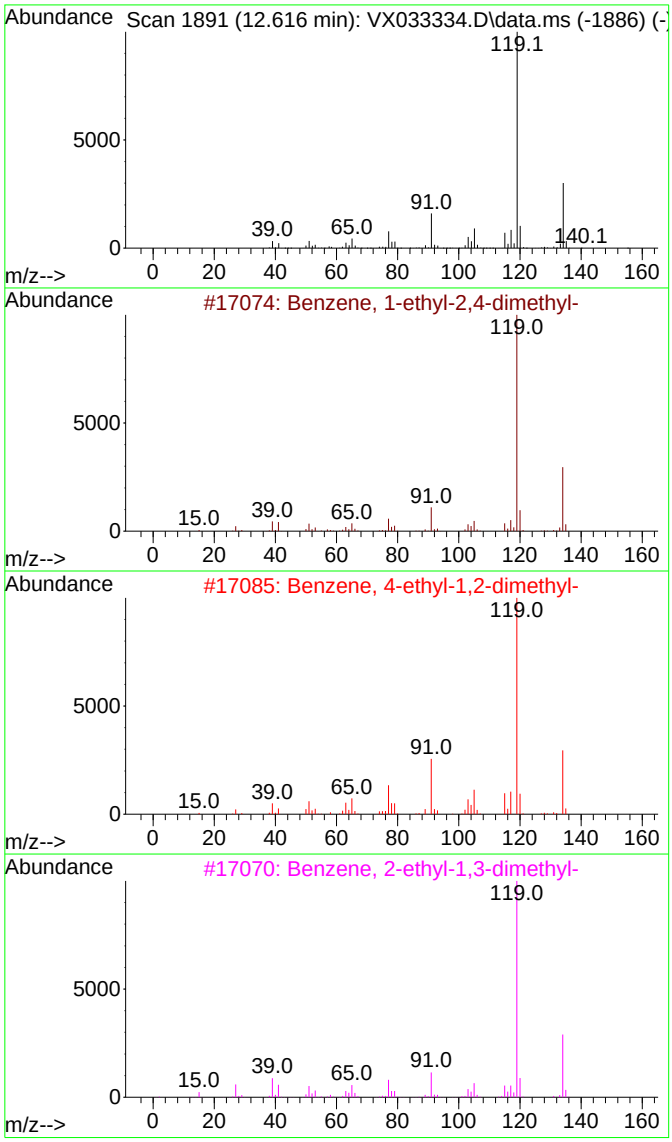
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

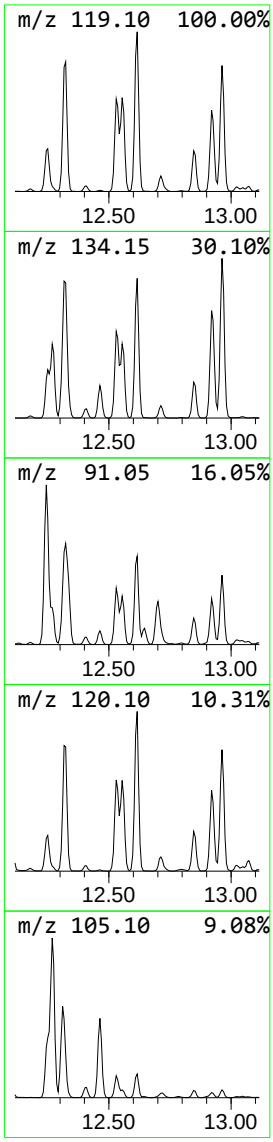
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	169.09 ug/l	2814850	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	97
2	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
3	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
4	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120822\
Data File : VX033334.D
Acq On : 08 Dec 2022 19:22
Operator : JC/MD
Sample : N5906-14
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-42

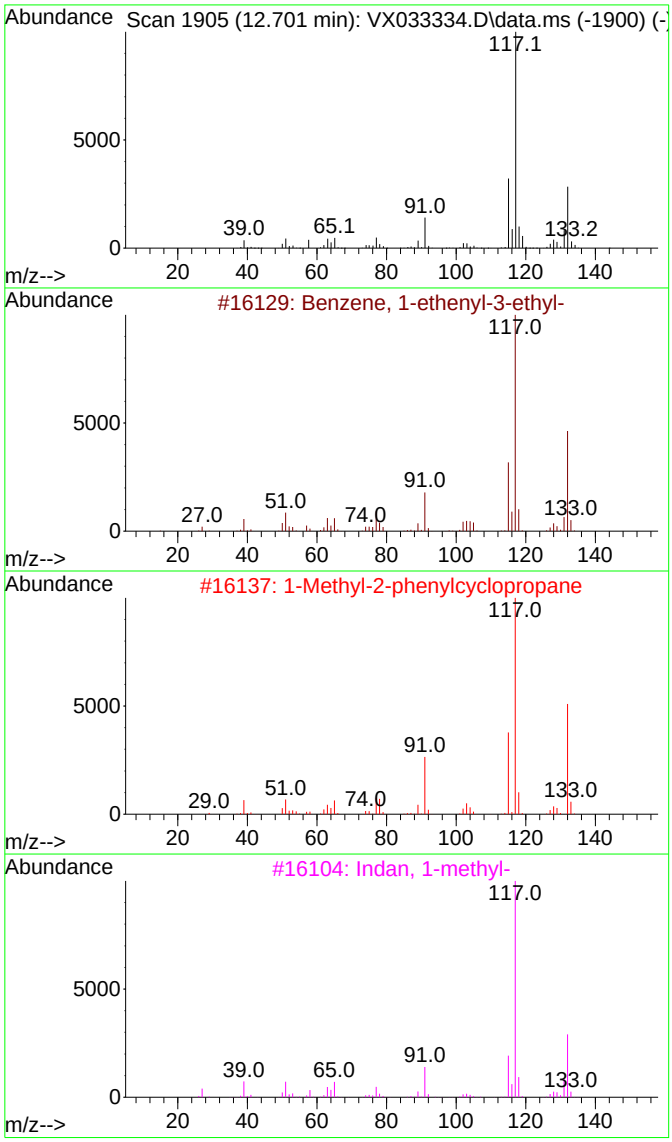
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

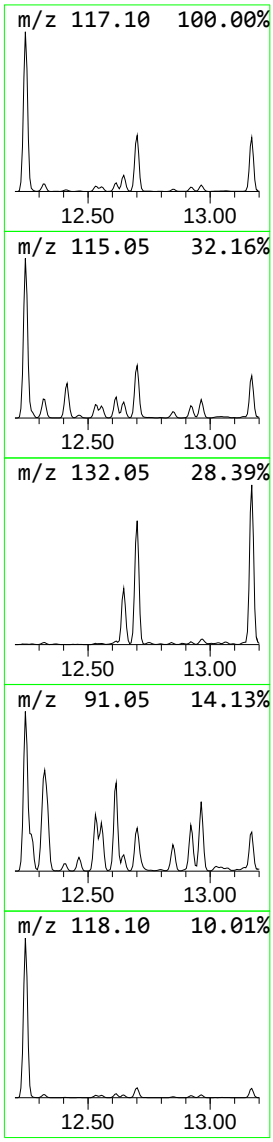
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	123.54 ug/l	2056540	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90
2	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	87
3	Indan, 1-methyl-	132	C10H12	000767-58-8	87
4	Benzene, 2-butenyl-	132	C10H12	001560-06-1	83
5	3-Phenylbut-1-ene	132	C10H12	000934-10-1	83





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Data File : VX033334.D
Acq On : 08 Dec 2022 19:22
Operator : JC/MD
Sample : N5906-14
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-42

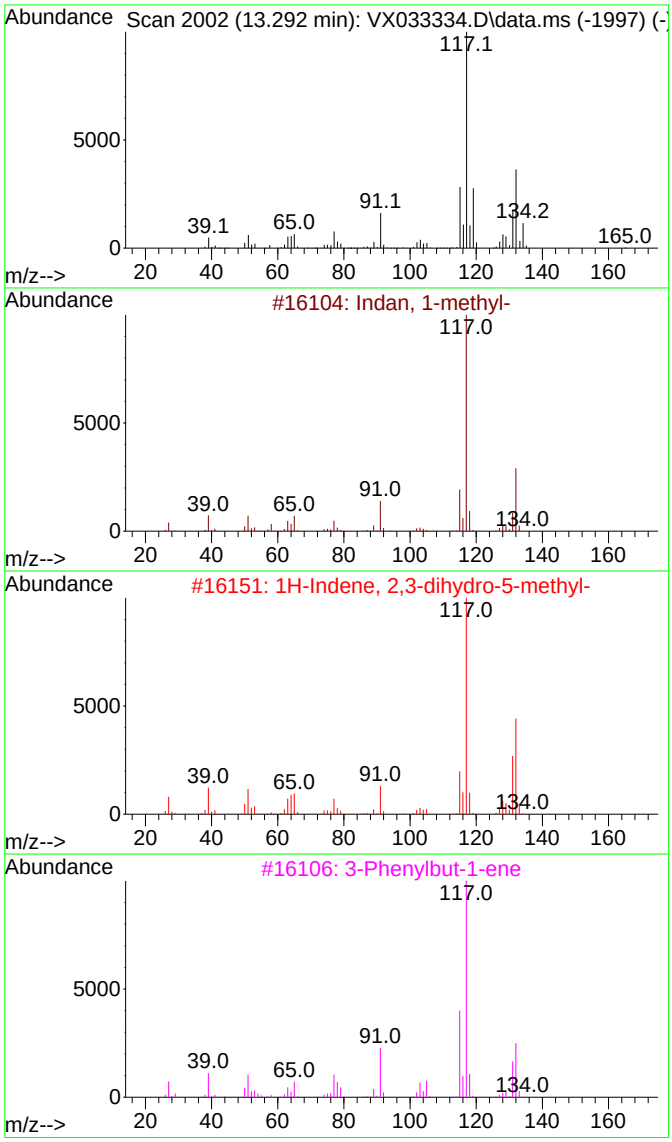
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

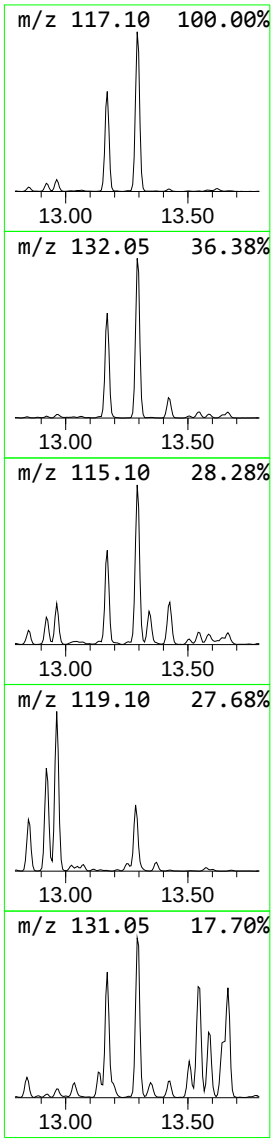
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Indan, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	223.55 ug/l	3721410	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indan, 1-methyl-	132	C10H12	000767-58-8	93
2	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	89
3	3-Phenylbut-1-ene	132	C10H12	000934-10-1	81
4	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	81
5	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	81





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120822\
Data File : VX033334.D
Acq On : 08 Dec 2022 19:22
Operator : JC/MD
Sample : N5906-14
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-42

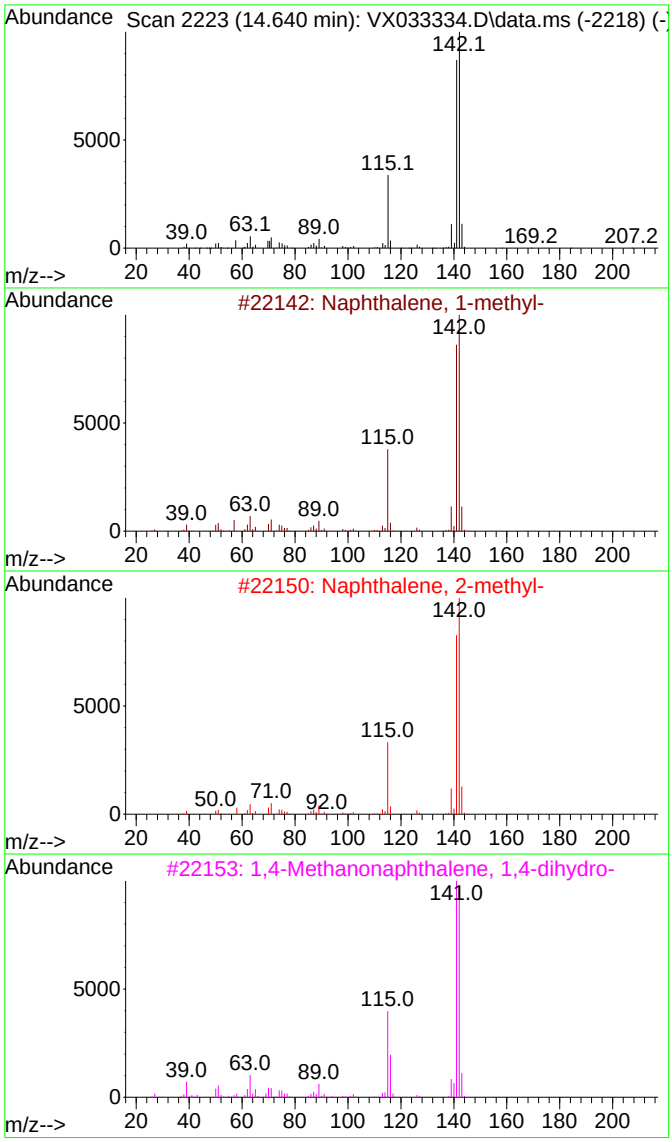
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

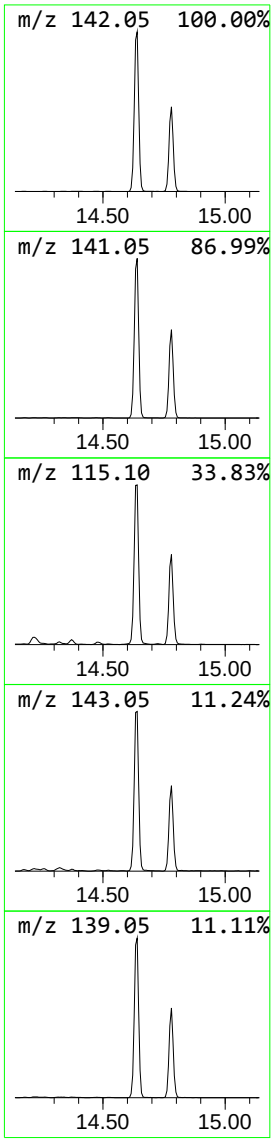
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	184.20 ug/l	3066410	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	91
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120822\
Data File : VX033334.D
Acq On : 08 Dec 2022 19:22
Operator : JC/MD
Sample : N5906-14
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-42

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.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, 2-methyl-	1.752	281.2	ug/l	7950380	1	5.556	1413650	50.0
Cyclopentane, m...	4.306	134.7	ug/l	3808440	1	5.556	1413650	50.0
Benzene, 1-ethy...	11.384	1262.4	ug/l	21014900	4	12.024	832356	50.0
Benzene, 1-ethy...	11.616	458.9	ug/l	7638530	4	12.024	832356	50.0
Indane	12.244	390.2	ug/l	6496330	4	12.024	832356	50.0
Benzene, 1-ethy...	12.616	169.1	ug/l	2814850	4	12.024	832356	50.0
Benzene, 1-ethe...	12.701	123.5	ug/l	2056540	4	12.024	832356	50.0
Indan, 1-methyl-	13.292	223.6	ug/l	3721410	4	12.024	832356	50.0
Naphthalene, 1-...	14.640	184.2	ug/l	3066410	4	12.024	832356	50.0