LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080222\
Data File : VX030350.D
Acq On : 02 Aug 2022 14:20
Operator : JC/MD
Sample : N3861-14 4X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
2-INCH

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\82X072522W.M
Title : SW846 8260

Signal : TIC: VX030350.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.746	103	108	118	rVB	74165	99150	1.43%	0.268%
2	2.215	179	185	194	rVB	63495	101660	1.46%	0.275%
3	2.867	287	292	300	rVB	73212	140196	2.02%	0.379%
4	2.947	300	305	318	rVB	32769	81051	1.17%	0.219%
5	3.105	322	331	341	rBV3	30766	75983	1.09%	0.206%
6	3.733	421	434	444	rBV4	38625	109934	1.58%	0.297%
7	4.306	516	528	541	rBV	292138	834662	12.01%	2.258%
8	5.196	665	674	688	rVB2	28346	86699	1.25%	0.235%
9	5.391	694	706	713	rBV	145861	431162	6.20%	1.167%
10	5.477	713	720	727	rVV2	195875	592394	8.52%	1.603%
11	5.562	727	734	746	rVB	153912	441478	6.35%	1.194%
12	5.964	789	800	807	rBV	170941	453081	6.52%	1.226%
13	6.044	807	813	824	rVV2	65078	175068	2.52%	0.474%
14	6.208	825	840	856	rVB7	65164	293661	4.22%	0.795%
15	6.763	921	931	940	rBV	255670	638300	9.18%	1.727%
16	7.385	1020	1033	1045	rBV2	145209	368569	5.30%	0.997%
17	7.885	1112	1115	1124	rVB3	42207	78938	1.14%	0.214%
18	8.147	1146	1158	1164	rBV	119559	232484	3.34%	0.629%
19	8.507	1210	1217	1227	rVB2	124748	208494	3.00%	0.564%
20	8.653	1234	1241	1248	rBV	820601	1286940	18.51%	3.482%
21	8.842	1265	1272	1281	rVB	44371	80731	1.16%	0.218%
22	8.958	1281	1291	1300	rBV	171532	297131	4.27%	0.804%
23	9.049	1300	1306	1312	rBV	154623	238470	3.43%	0.645%
24	10.055	1461	1471	1476	rBV	606768	835044	12.01%	2.259%
25	10.195	1490	1494	1499	rBV	323030	410542	5.91%	1.111%
26	10.305	1506	1512	1517	rVB	92832	136360	1.96%	0.369%
27	10.964	1613	1620	1626	rVB	811638	1004543	14.45%	2.718%
28	11.085	1635	1640	1646	rVB	633151	823461	11.85%	2.228%
29	11.305	1666	1676	1687	rBV	2019209	2385067	34.31%	6.453%
30	11.402	1687	1692	1696	rVV	74880	97129	1.40%	0.263%
31	11.451	1696	1700	1707	rVB	47164	69944	1.01%	0.189%
32	11.616	1721	1727	1735	rBV	254671	320261	4.61%	0.866%
33	11.866	1762	1768	1770	rBV	60356	75481	1.09%	0.204%
34	11.890	1770	1772	1779	rVB	79289	92773	1.33%	0.251%
35	12.024	1788	1794	1800	rVB	856471	1032882	14.86%	2.795%
36	12.091	1800	1805	1809	rBV	118887	147366	2.12%	0.399%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080222\
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Acq On : 02 Aug 2022 14:20
Operator : JC/MD
Sample : N3861-14 4X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
2-INCH

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\82X072522W.M
Title : SW846 8260

37	12.244	1825	1830	1837	rBV	5632769	6951966	100.00%	18.809%
38	12.317	1837	1842	1851	rVB2	176355	335409	4.82%	0.907%
39	12.408	1852	1857	1863	rBV	121484	153539	2.21%	0.415%
40	12.616	1885	1891	1894	rBV	1499606	1829051	26.31%	4.949%
41	12.646	1894	1896	1900	rVV	379911	415038	5.97%	1.123%
42	12.701	1900	1905	1912	rVB	1351644	1784103	25.66%	4.827%
43	12.841	1921	1928	1934	rBV3	42709	77488	1.11%	0.210%
44	12.921	1934	1941	1946	rVB	932581	1192053	17.15%	3.225%
45	13.030	1954	1959	1964	rBV2	52169	83505	1.20%	0.226%
46	13.170	1978	1982	1992	rVB	1203953	1450025	20.86%	3.923%
47	13.292	1992	2002	2008	rBV2	2454135	3297851	47.44%	8.923%
48	13.427	2019	2024	2030	rVB	120966	148011	2.13%	0.400%
49	13.506	2032	2037	2040	rBV2	64945	92107	1.32%	0.249%
50	13.542	2040	2043	2047	rVV	205890	302316	4.35%	0.818%
51	13.585	2047	2050	2054	rVV3	201439	281935	4.06%	0.763%
52	13.640	2054	2059	2060	rVV2	110633	142920	2.06%	0.387%
53	13.664	2060	2063	2074	rVV2	215699	338787	4.87%	0.917%
54	13.780	2074	2082	2090	rVB	258452	373755	5.38%	1.011%
55	13.926	2099	2106	2110	rBV2	83420	123954	1.78%	0.335%
56	13.969	2110	2113	2118	rVB	76034	95433	1.37%	0.258%
57	14.079	2125	2131	2137	rBV	125089	180696	2.60%	0.489%
58	14.213	2149	2153	2164	rVB	107590	183465	2.64%	0.496%
59	14.371	2175	2179	2185	rVB	85789	110049	1.58%	0.298%
60	14.640	2218	2223	2233	rVB	976471	1280960	18.43%	3.466%
61	14.780	2241	2246	2256	rVB	757517	959084	13.80%	2.595%

Sum of corrected areas: 36960589

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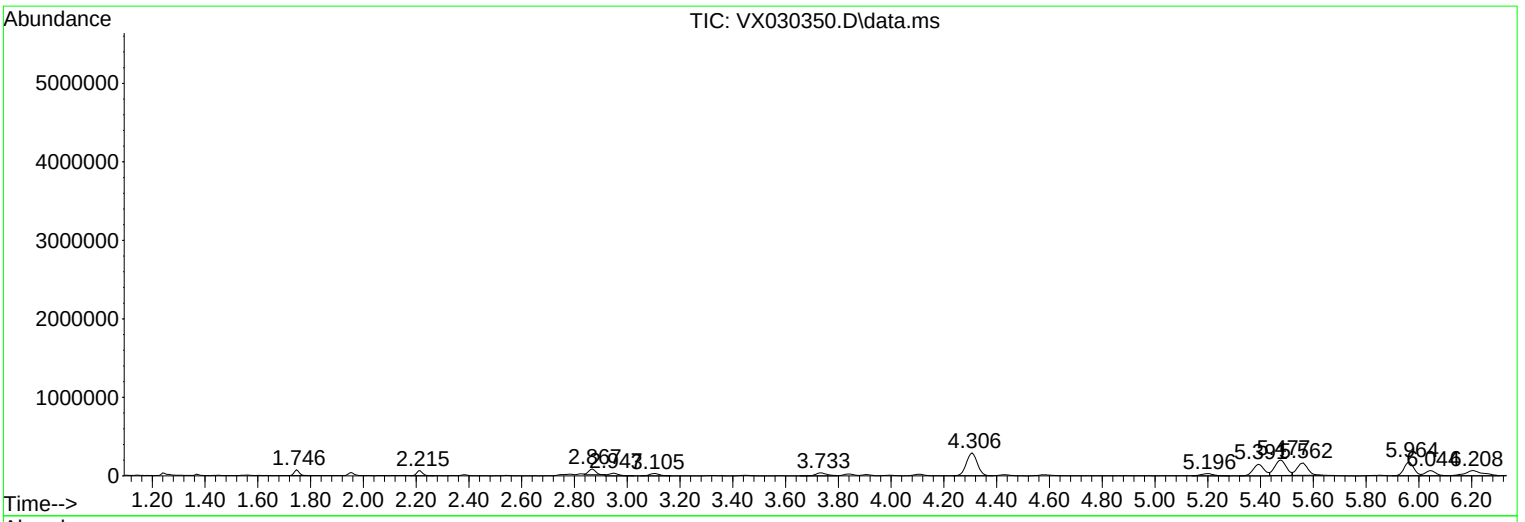
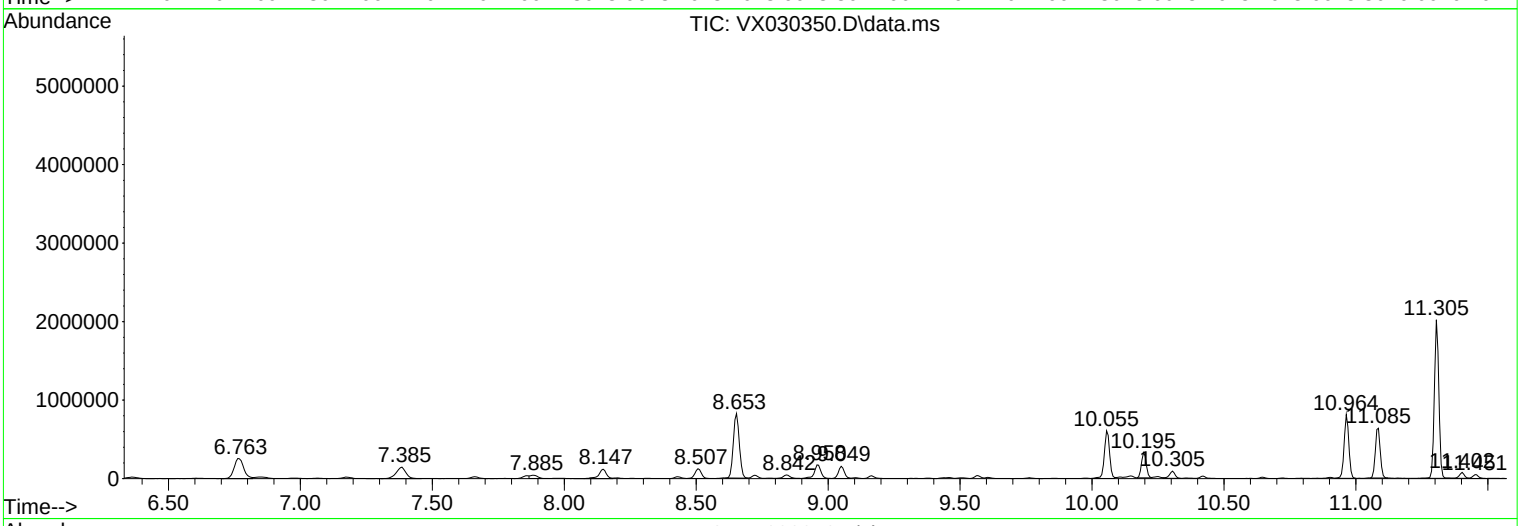
ALS Vial : 12 Sample Multiplier: 1

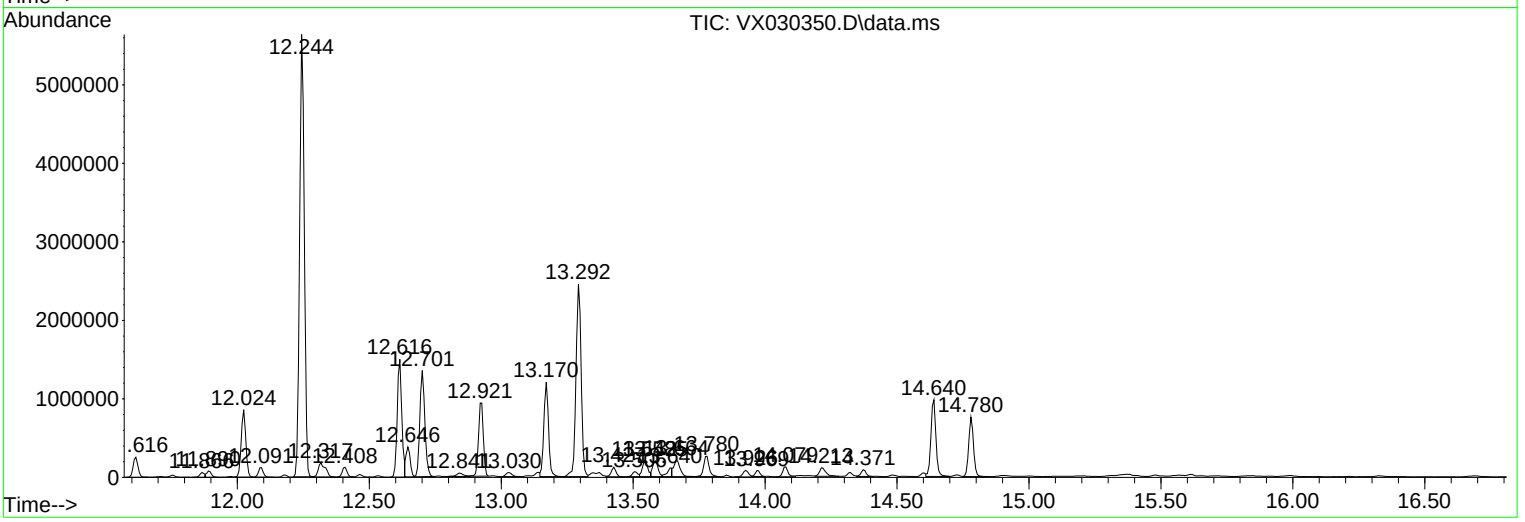
Instrument :
MSVOA_X
ClientSampleId :
2-INCH

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

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







Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080222\
Data File : VX030350.D
Acq On : 02 Aug 2022 14:20
Operator : JC/MD
Sample : N3861-14 4X
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
2-INCH

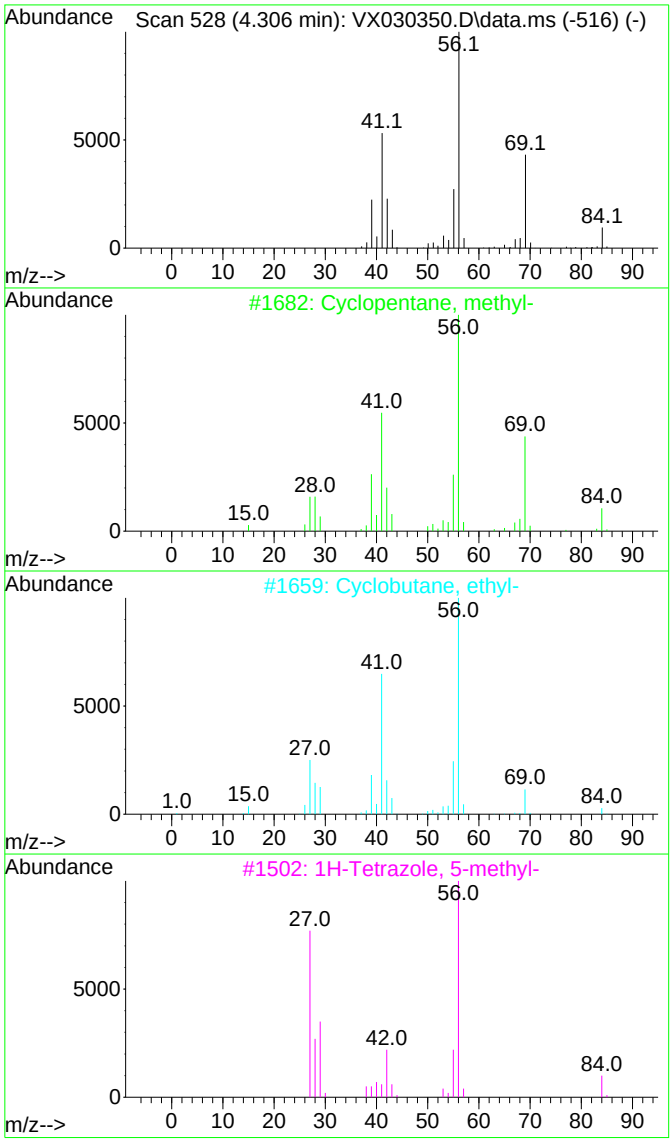
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

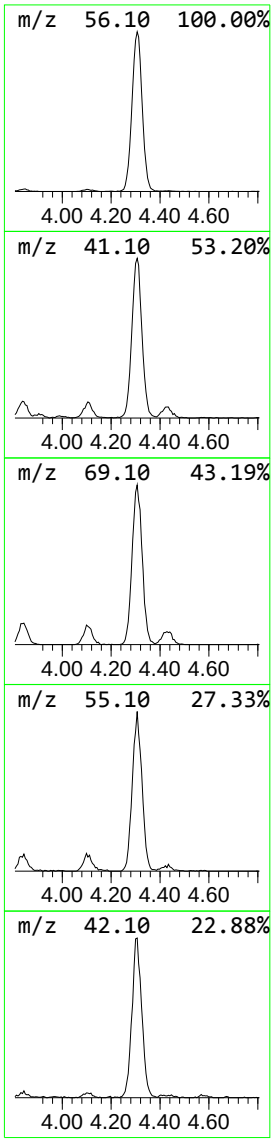
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	94.53 ug/l	834662	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	Cyclobutane, ethyl-	84	C6H12	004806-61-5	80
3	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
4	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	59
5	2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080222\
Data File : VX030350.D
Acq On : 02 Aug 2022 14:20
Operator : JC/MD
Sample : N3861-14 4X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
2-INCH

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

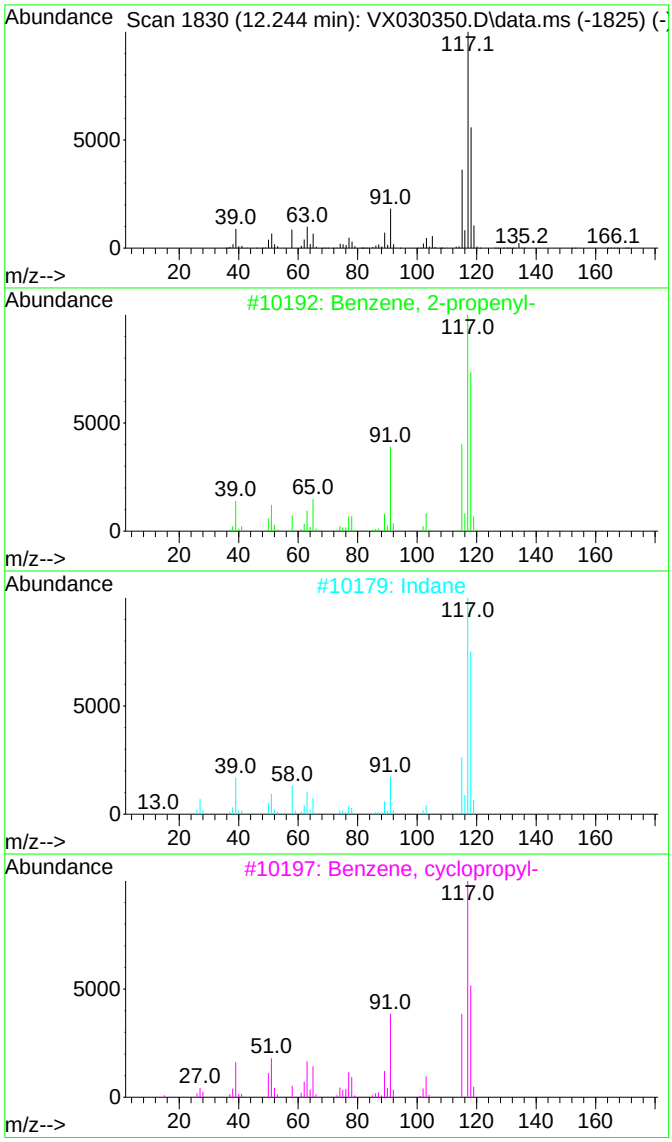
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

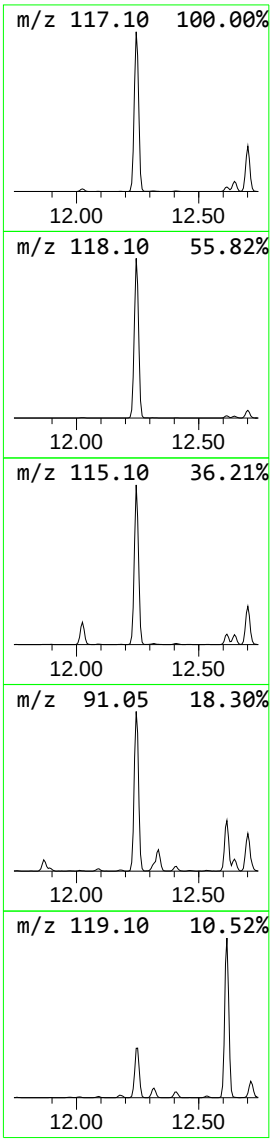
****

Peak Number 3 Benzene, 2-propenyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	336.53 ug/l	6951970	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-propenyl-	118	C9H10	000300-57-2	87
2	Indane	118	C9H10	000496-11-7	87
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
4	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	76
5	Deltacyclene	118	C9H10	007785-10-6	58





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080222\
Data File : VX030350.D
Acq On : 02 Aug 2022 14:20
Operator : JC/MD
Sample : N3861-14 4X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
2-INCH

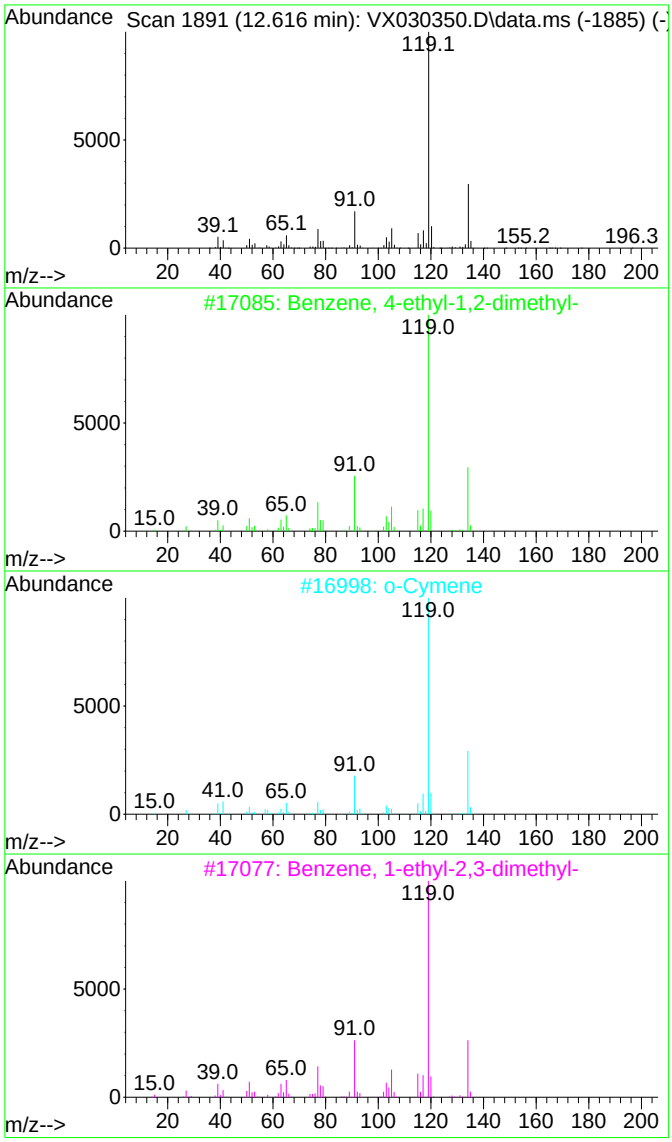
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

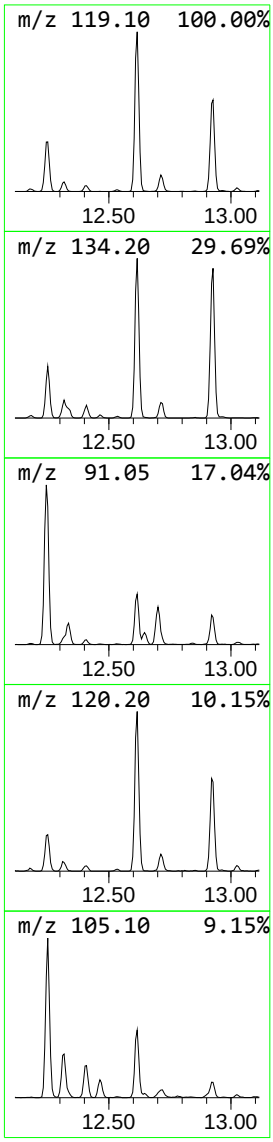
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	88.54 ug/l	1829050	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
2	o-Cymene	134	C10H14	000527-84-4	95
3	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
4	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94
5	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	94





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080222\
Data File : VX030350.D
Acq On : 02 Aug 2022 14:20
Operator : JC/MD
Sample : N3861-14 4X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
2-INCH

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

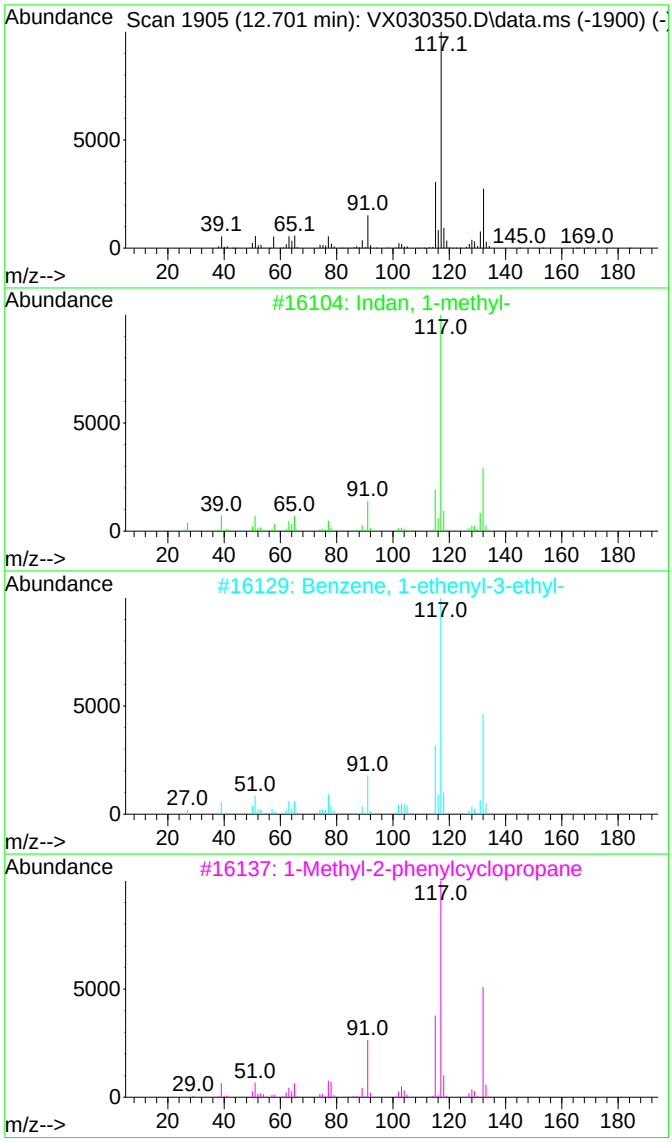
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

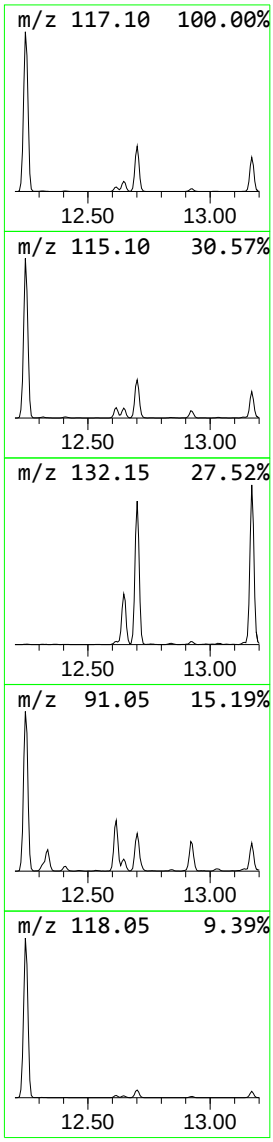
****

Peak Number 5 Indan, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	86.37 ug/l	1784100	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indan, 1-methyl-	132	C10H12	000767-58-8	90
2	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90
3	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	87
4	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	86
5	Benzene, 2-butenyl-	132	C10H12	001560-06-1	83





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080222\
Data File : VX030350.D
Acq On : 02 Aug 2022 14:20
Operator : JC/MD
Sample : N3861-14 4X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
2-INCH

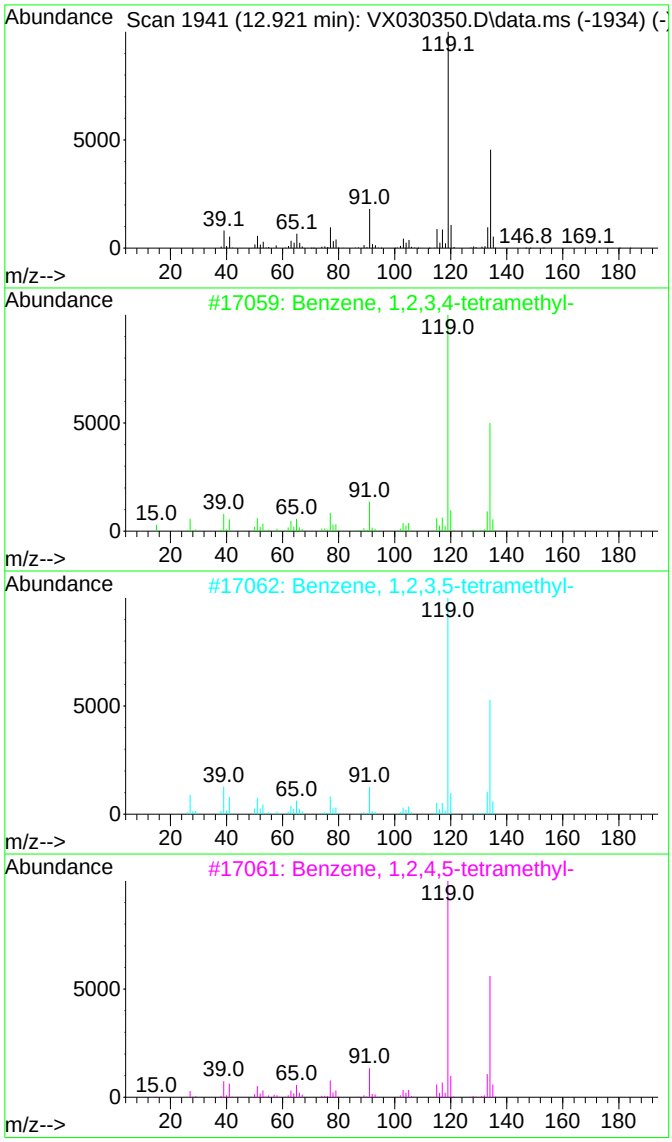
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

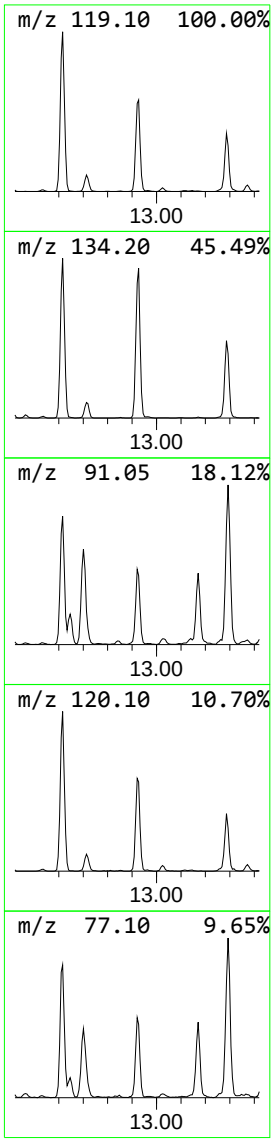
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.921	57.71 ug/l	1192050	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
2	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
3	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
4	o-Cymene	134	C10H14	000527-84-4	95
5	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94





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Data File : VX030350.D
Acq On : 02 Aug 2022 14:20
Operator : JC/MD
Sample : N3861-14 4X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
2-INCH

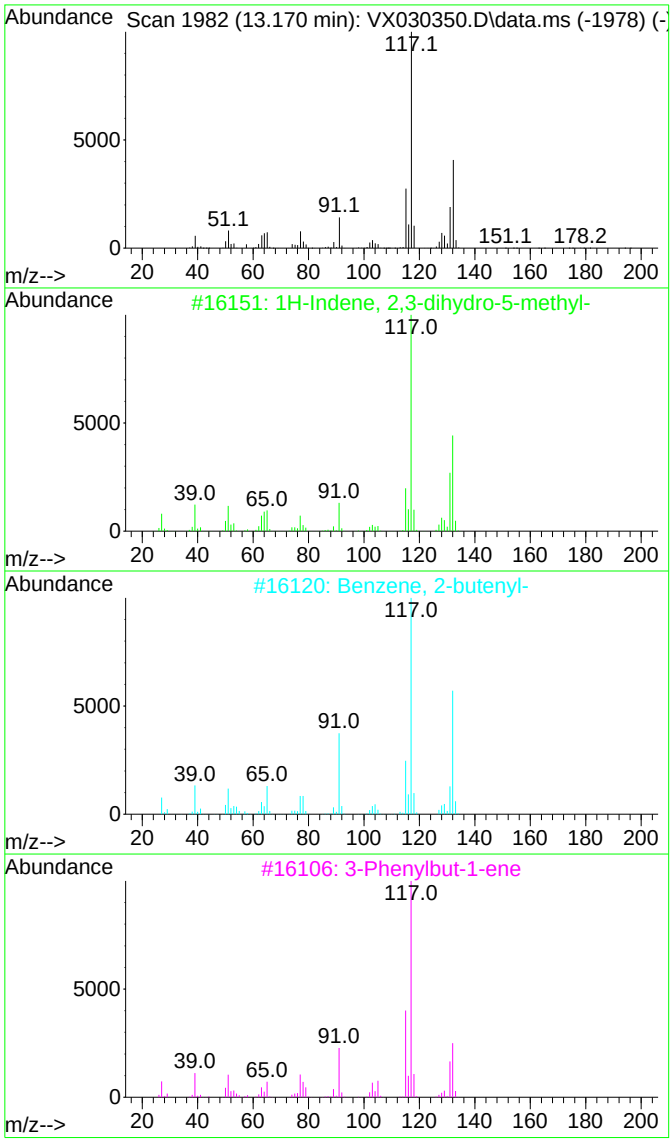
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

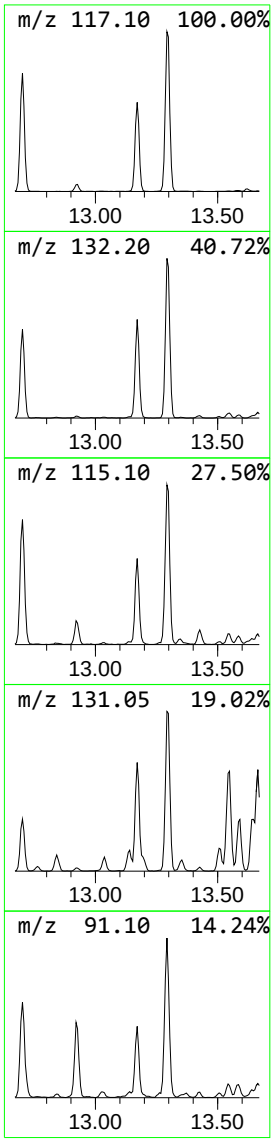
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.171	70.19 ug/l	1450030	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	94
2	Benzene, 2-butenyl-	132	C10H12	001560-06-1	91
3	3-Phenylbut-1-ene	132	C10H12	000934-10-1	91
4	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	91
5	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080222\
Data File : VX030350.D
Acq On : 02 Aug 2022 14:20
Operator : JC/MD
Sample : N3861-14 4X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
2-INCH

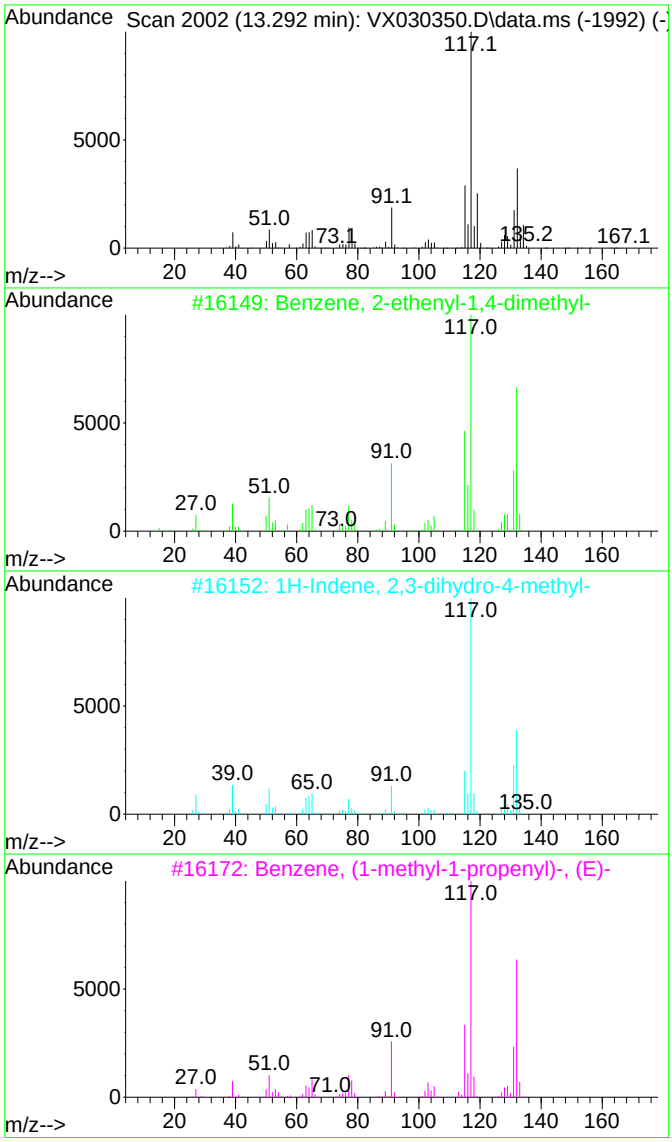
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

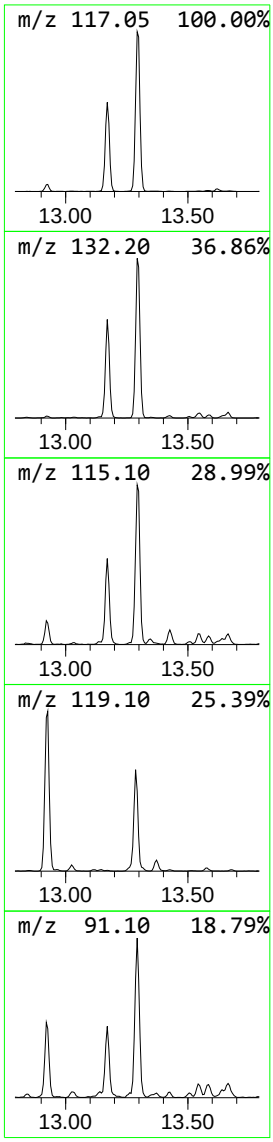
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	159.64 ug/l	3297850	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	95
2	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	93
3	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	91
4	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	89
5	1-Phenyl-1-butene	132	C10H12	000824-90-8	87





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Data File : VX030350.D
Acq On : 02 Aug 2022 14:20
Operator : JC/MD
Sample : N3861-14 4X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
2-INCH

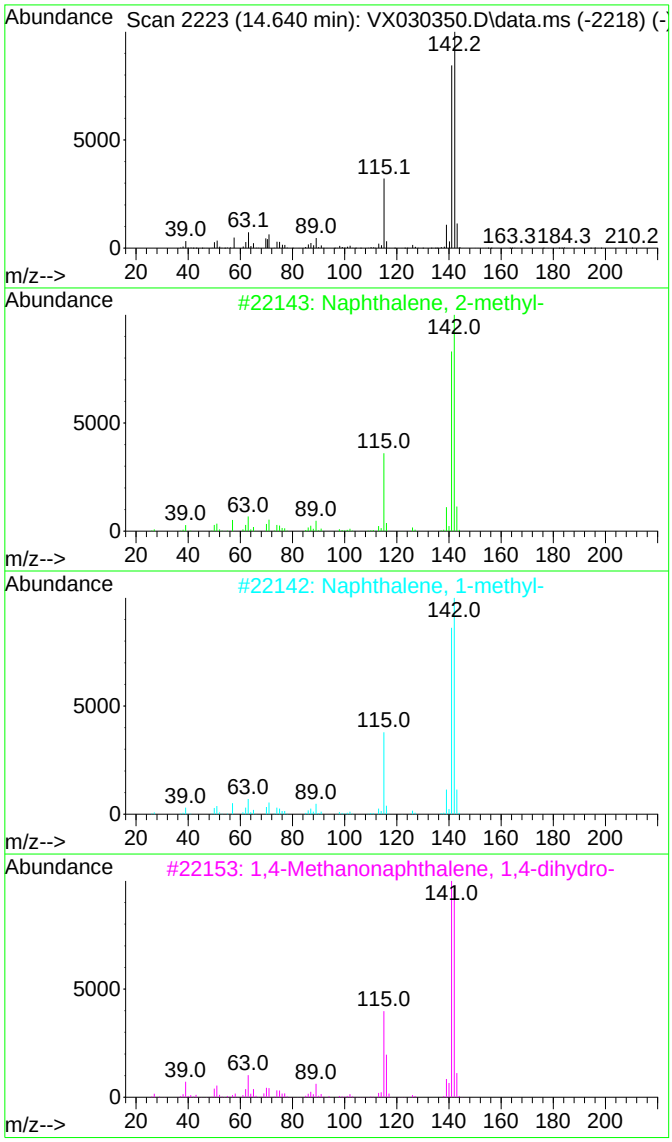
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

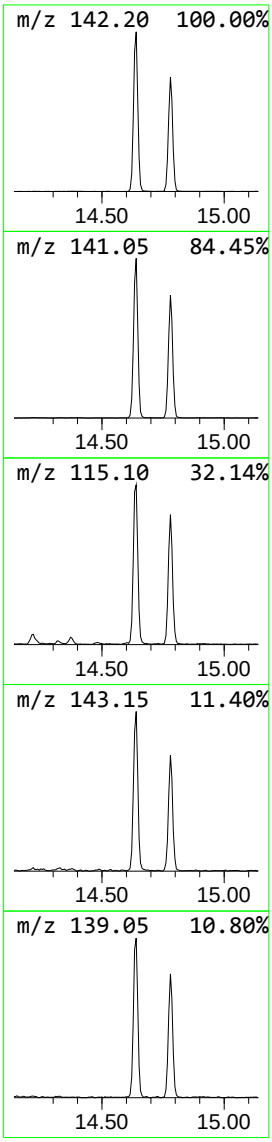
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Naphthalene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	62.01 ug/l	1280960	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	1-Naphthaleneacetamide	185	C12H11NO	000086-86-2	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080222\
Data File : VX030350.D
Acq On : 02 Aug 2022 14:20
Operator : JC/MD
Sample : N3861-14 4X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
2-INCH

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

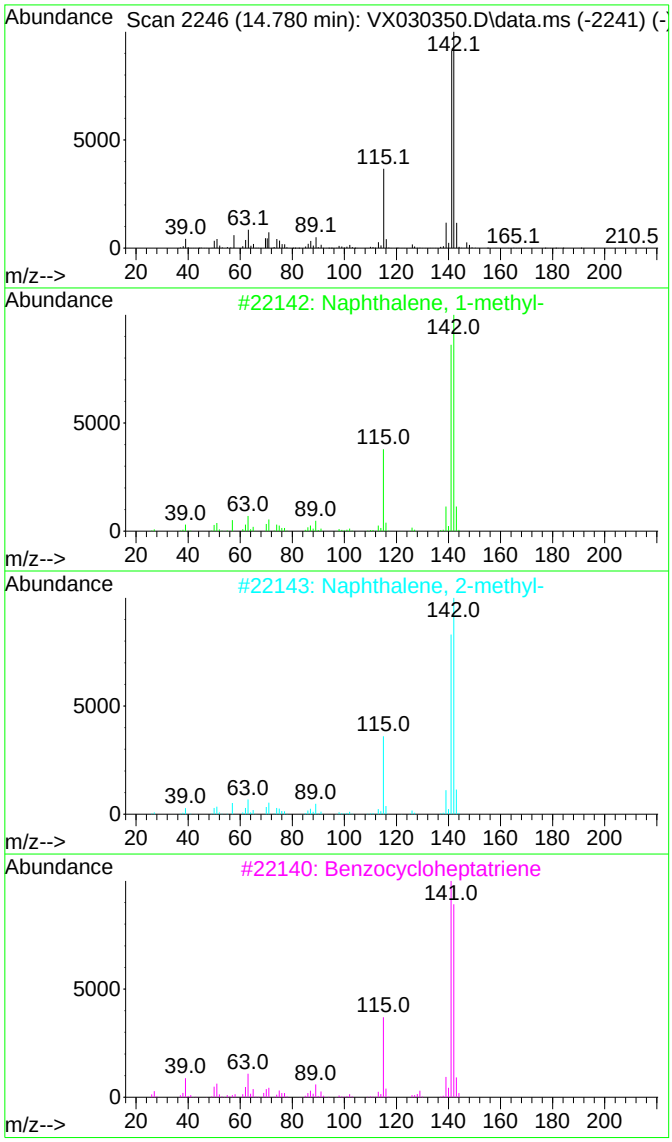
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

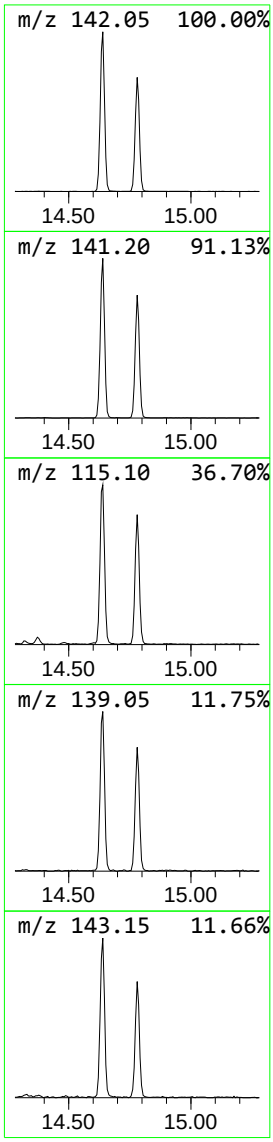
****

Peak Number 10 Benzocycloheptatriene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	46.43 ug/l	959084	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	Benzocycloheptatriene	142	C11H10	000264-09-5	91
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080222\
Data File : VX030350.D
Acq On : 02 Aug 2022 14:20
Operator : JC/MD
Sample : N3861-14 4X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
2-INCH

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.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
Cyclopentane, m...	4.306	94.5	ug/l	834662	1	5.562	441478	50.0
Benzene, 2-prop...	12.244	336.5	ug/l	6951970	4	12.024	1032880	50.0
Benzene, 4-ethy...	12.616	88.5	ug/l	1829050	4	12.024	1032880	50.0
Indan, 1-methyl-	12.701	86.4	ug/l	1784100	4	12.024	1032880	50.0
Benzene, 1,2,3,...	12.921	57.7	ug/l	1192050	4	12.024	1032880	50.0
1H-Indene, 2,3-...	13.171	70.2	ug/l	1450030	4	12.024	1032880	50.0
Benzene, 2-ethe...	13.292	159.6	ug/l	3297850	4	12.024	1032880	50.0
Naphthalene, 1-...	14.640	62.0	ug/l	1280960	4	12.024	1032880	50.0
Benzocyclohepta...	14.780	46.4	ug/l	959084	4	12.024	1032880	50.0