LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102423\
Data File : VX038462.D
Acq On : 24 Oct 2023 17:50
Operator : JC/MD
Sample : 04938-18 10X
Misc : 5.51g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
0-3(5-10)

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\82X100523W.M
Title : SW846 8260

Signal : TIC: VX038462.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.593	68	83	87	rBV6	17820	68977	2.36%	0.489%
2	5.385	689	705	720	rBV2	111801	329627	11.26%	2.338%
3	5.550	720	732	747	rVV	176209	505297	17.26%	3.583%
4	5.958	786	799	817	rBV	109835	303673	10.38%	2.154%
5	6.763	920	931	949	rBV	276564	676967	23.13%	4.801%
6	8.647	1234	1240	1248	rBV	602472	941369	32.16%	6.676%
7	8.720	1248	1252	1264	rVB	17082	31796	1.09%	0.225%
8	10.055	1465	1471	1482	rBV	657394	894490	30.56%	6.343%
9	10.195	1489	1494	1505	rBV	85780	116313	3.97%	0.825%
10	10.299	1505	1511	1519	rBV	316135	431276	14.73%	3.058%
11	10.640	1562	1567	1579	rVB	132682	182935	6.25%	1.297%
12	11.079	1634	1639	1653	rVB	581152	743617	25.41%	5.273%
13	11.305	1672	1676	1683	rVB	32381	40915	1.40%	0.290%
14	11.378	1683	1688	1691	rBV	102845	161504	5.52%	1.145%
15	11.451	1695	1700	1708	rVB	94708	141261	4.83%	1.002%
16	11.610	1722	1726	1736	rBV2	44997	82308	2.81%	0.584%
17	11.750	1740	1749	1755	rBV	310946	391268	13.37%	2.775%
18	11.811	1755	1759	1762	rBV	28540	35755	1.22%	0.254%
19	12.018	1788	1793	1800	rBV	817981	1048118	35.81%	7.433%
20	12.085	1800	1804	1808	rVV	117024	145770	4.98%	1.034%
21	12.128	1808	1811	1817	rVB	86164	107886	3.69%	0.765%
22	12.244	1822	1830	1838	rBV3	120167	231098	7.90%	1.639%
23	12.317	1838	1842	1848	rBV3	41982	68249	2.33%	0.484%
24	12.414	1848	1858	1864	rVV	553005	740437	25.30%	5.251%
25	12.530	1873	1877	1879	rBV	21570	30191	1.03%	0.214%
26	12.609	1884	1890	1894	rVV3	40641	57544	1.97%	0.408%
27	12.963	1944	1948	1954	rBV	65067	89084	3.04%	0.632%
28	13.067	1960	1965	1968	rBV2	30978	44697	1.53%	0.317%
29	13.237	1990	1993	1996	rBV2	29306	31188	1.07%	0.221%
30	13.286	1996	2001	2006	rVV2	71348	103453	3.53%	0.734%
31	13.341	2006	2010	2015	rVV	223349	257406	8.79%	1.825%
32	13.426	2018	2024	2033	rVV	243332	330398	11.29%	2.343%
33	13.499	2033	2036	2040	rVB2	30124	37499	1.28%	0.266%
34	13.585	2046	2050	2060	rVB7	19027	38526	1.32%	0.273%
35	13.774	2076	2081	2089	rVB	2432895	2926885	100.00%	20.756%
36	13.865	2091	2096	2104	rVB	69814	95176	3.25%	0.675%

LSC Area Percent Report

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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
0-3(5-10)

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\82X100523W.M
Title : SW846 8260

37	14.219	2150	2154	2157	rBV2	24123	32516	1.11%	0.231%
38	14.316	2164	2170	2177	rBV2	26126	52091	1.78%	0.369%
39	14.438	2181	2190	2200	rBV	137259	192593	6.58%	1.366%
40	14.633	2218	2222	2232	rVB	562095	720815	24.63%	5.112%
41	14.725	2233	2237	2241	rBV2	18002	30979	1.06%	0.220%
42	14.780	2241	2246	2253	rVB	363085	462518	15.80%	3.280%
43	15.206	2308	2316	2319	rBV	28983	54144	1.85%	0.384%
44	15.475	2355	2360	2364	rBV	27338	45220	1.54%	0.321%
45	15.615	2378	2383	2386	rBV	30828	47521	1.62%	0.337%

Sum of corrected areas: 14101350

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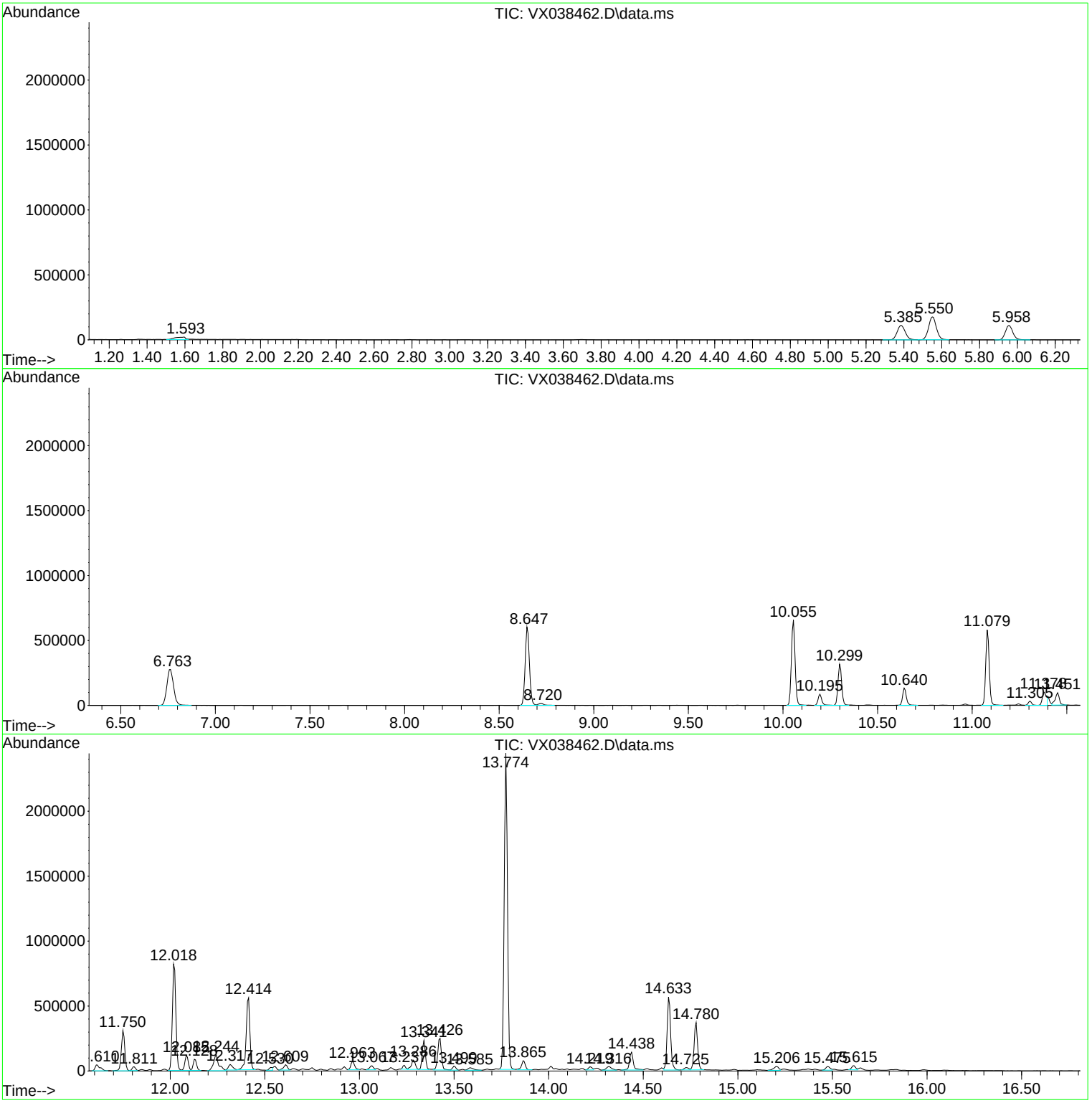
Instrument :
MSVOA_X
ClientSampleId :
0-3(5-10)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102423\
Data File : VX038462.D
Acq On : 24 Oct 2023 17:50
Operator : JC/MD
Sample : 04938-18 10X
Misc : 5.51g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
0-3(5-10)

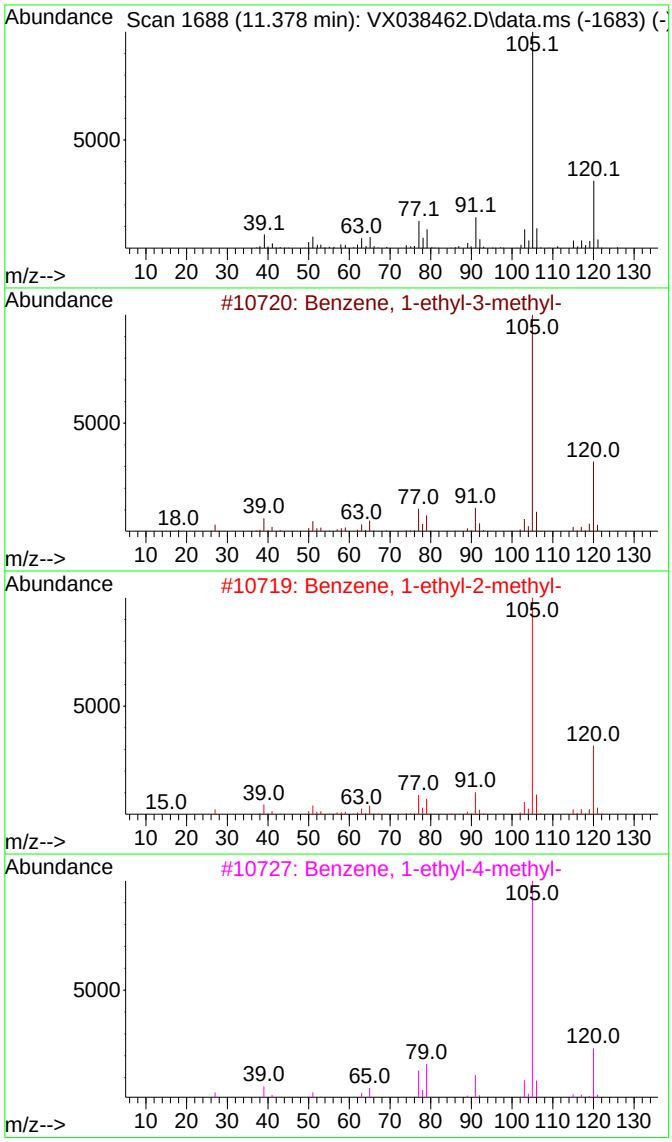
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

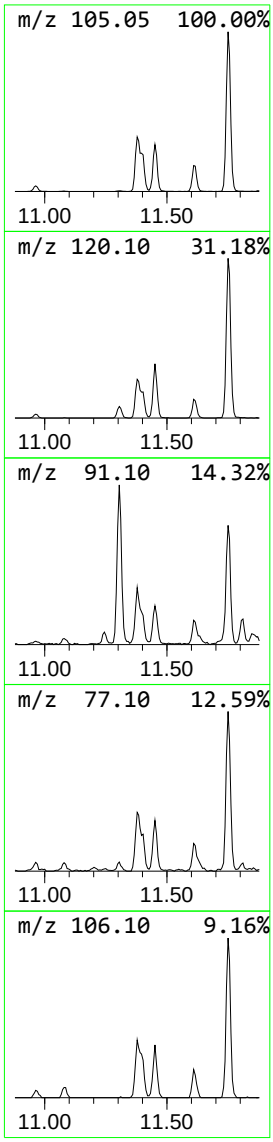
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Benzene, 1-ethyl-3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	7.70 ug/l	161504	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	91





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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
0-3(5-10)

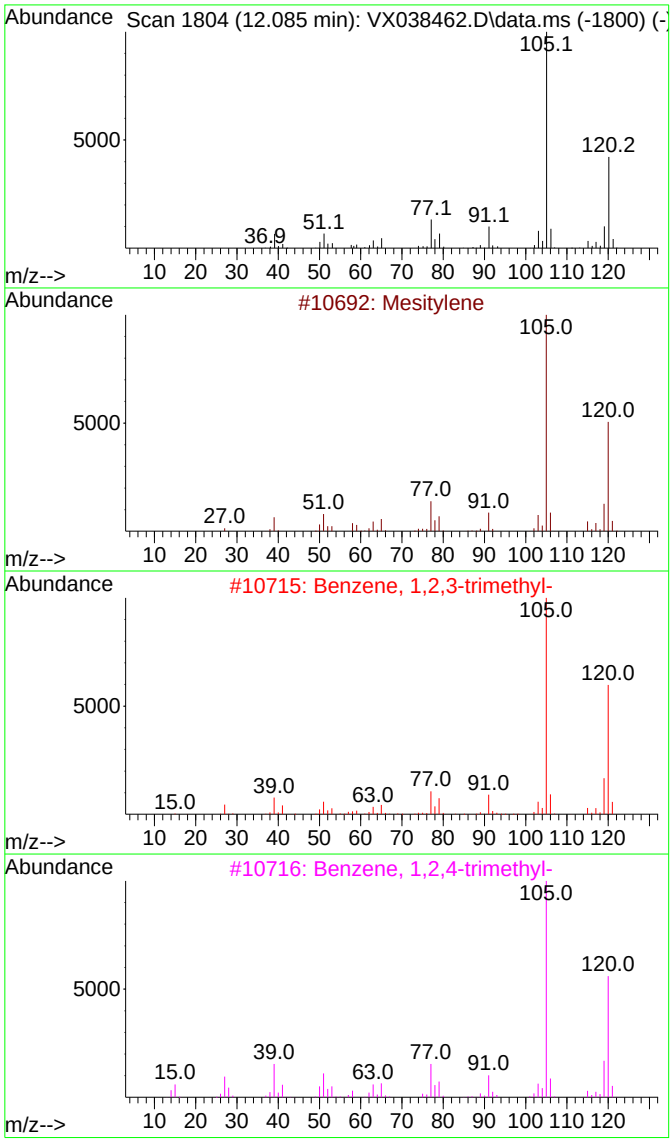
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

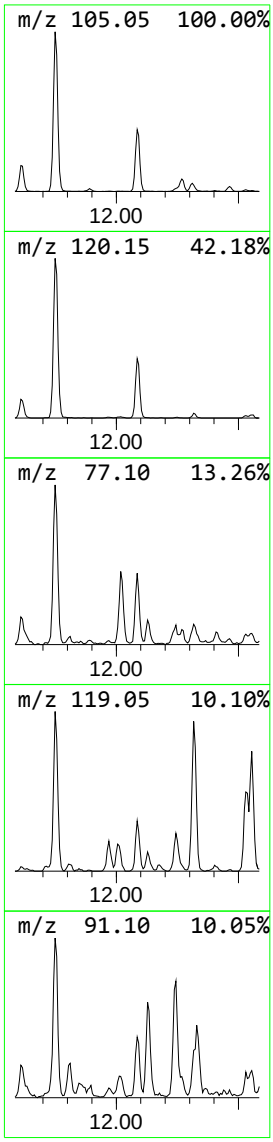
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzene, 1,2,3-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	6.95 ug/l	145770	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	93
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90





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Data File : VX038462.D
Acq On : 24 Oct 2023 17:50
Operator : JC/MD
Sample : 04938-18 10X
Misc : 5.51g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
0-3(5-10)

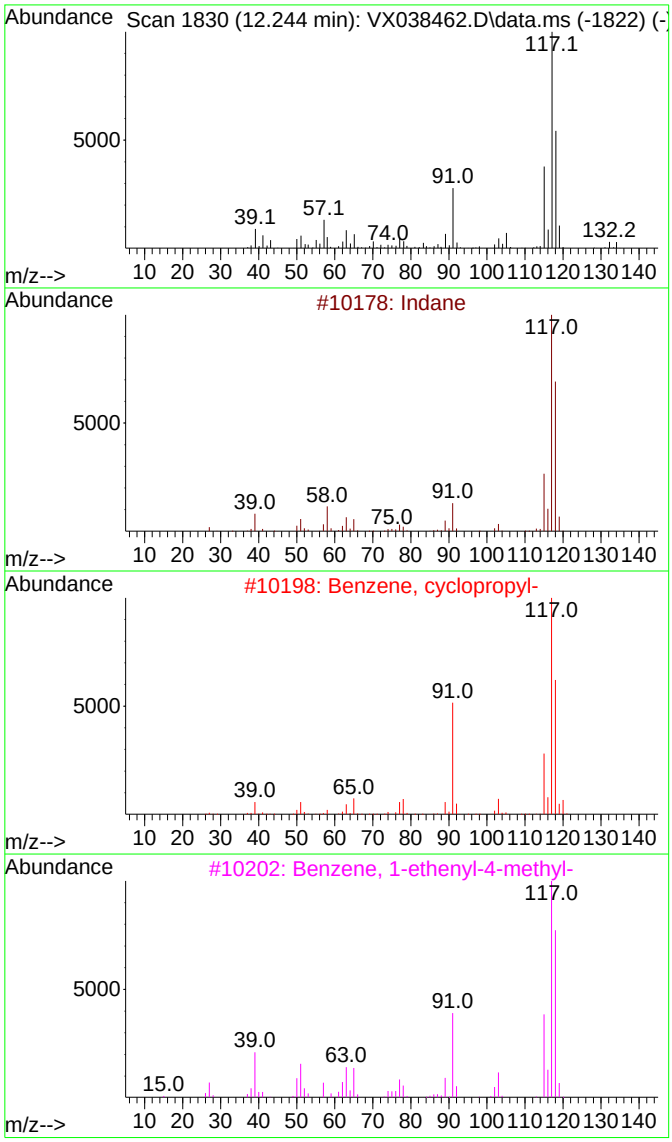
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

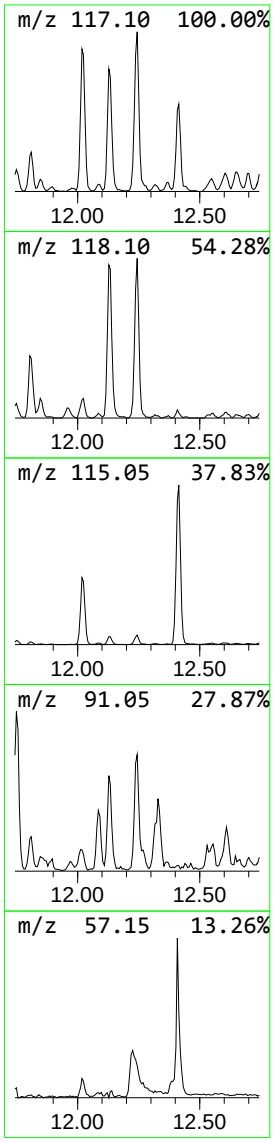
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Indane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	11.02 ug/l	231098	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	81
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	59
3	Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	59
4	Deltacyclene	118	C9H10	007785-10-6	58
5	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	55





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102423\
Data File : VX038462.D
Acq On : 24 Oct 2023 17:50
Operator : JC/MD
Sample : 04938-18 10X
Misc : 5.51g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
0-3(5-10)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

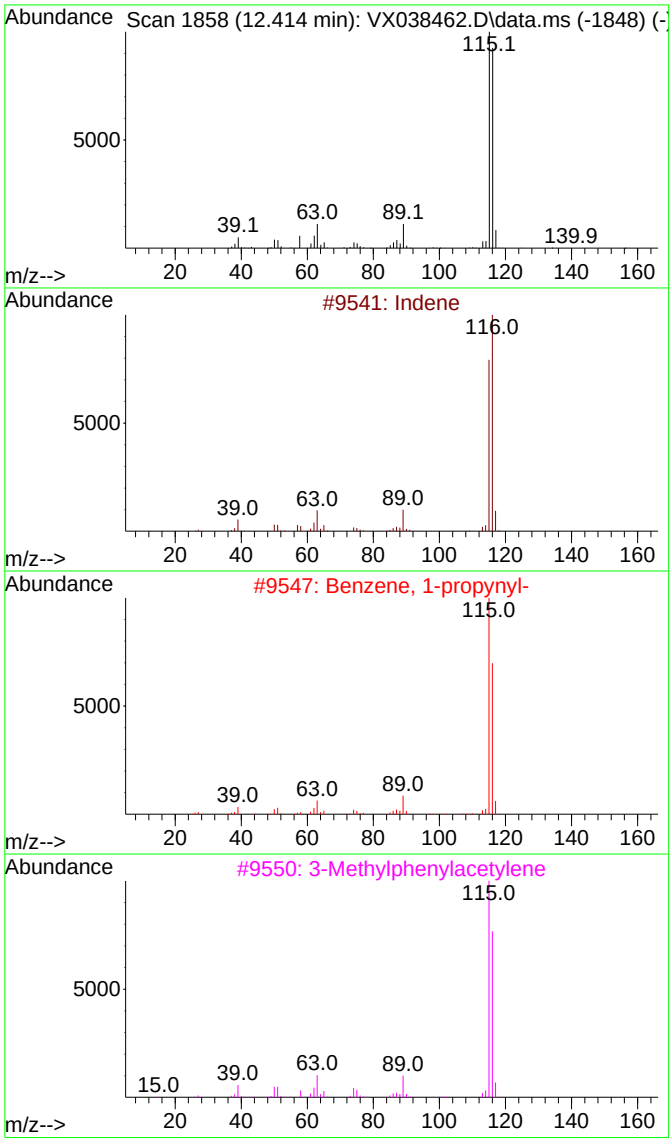
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

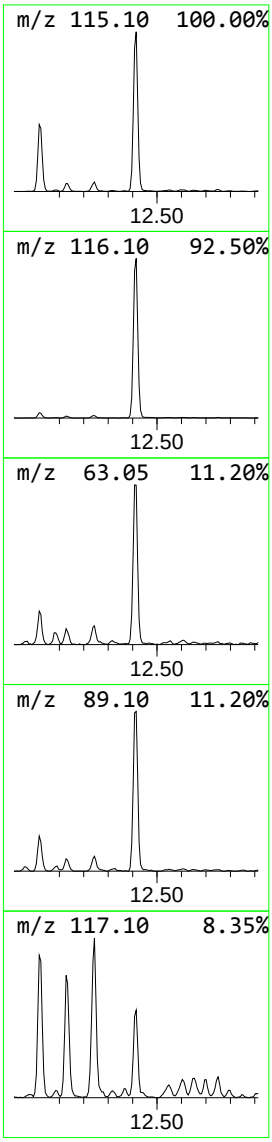
****

Peak Number 4 Indene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.414	35.32 ug/l	740437	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	1-Propyne, 3-phenyl-	116	C9H8	010147-11-2	90





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Operator : JC/MD
Sample : 04938-18 10X
Misc : 5.51g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
0-3(5-10)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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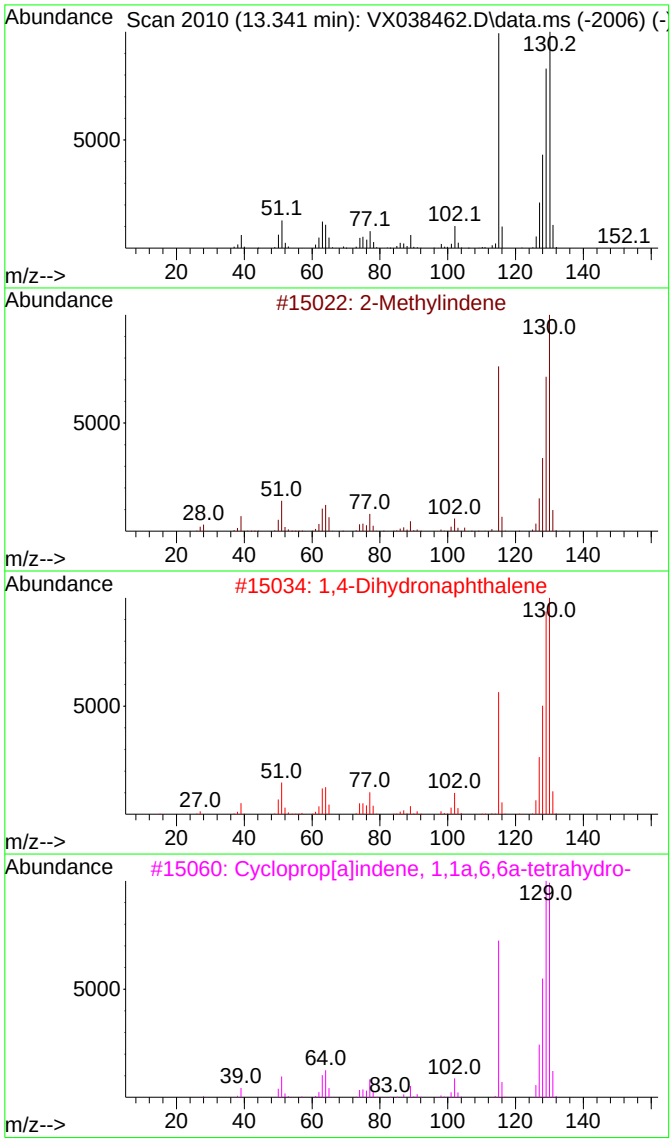
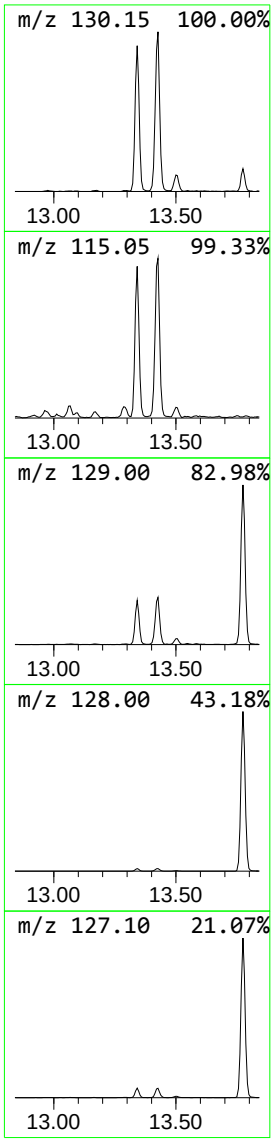
****

Peak Number 5 2-Methylindene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	12.28 ug/l	257406	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methylindene	130	C10H10	002177-47-1	96
2	1,4-Dihydronaphthalene	130	C10H10	000612-17-9	95
3	Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	95
4	Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	94
5	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	94





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Instrument :
MSVOA_X
ClientSampleId :
0-3(5-10)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

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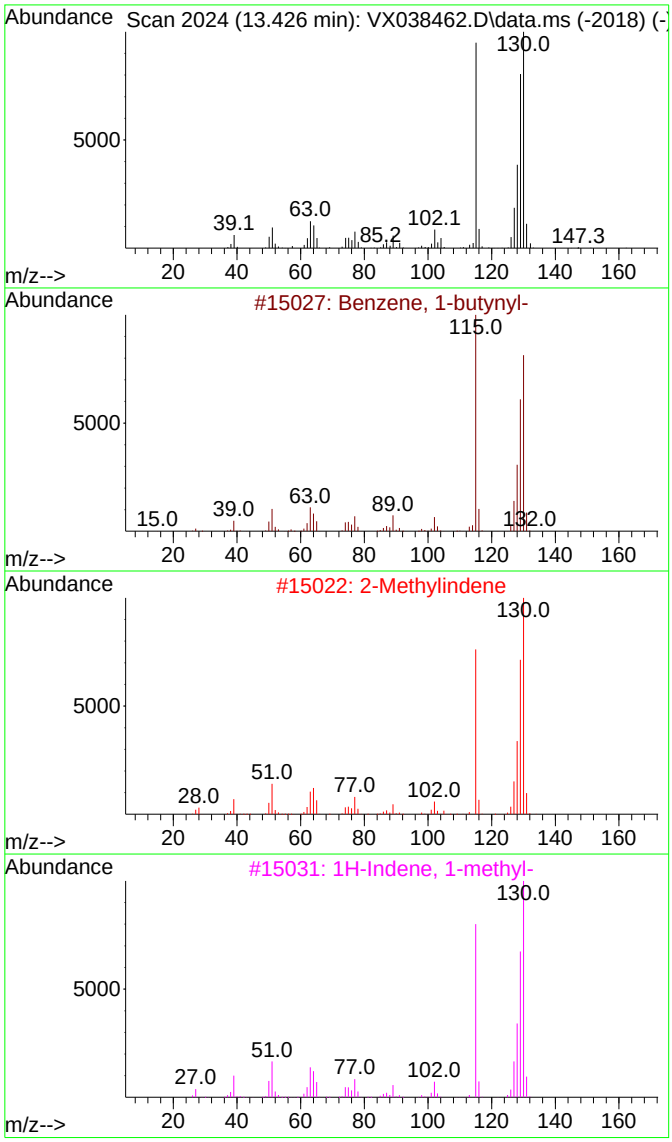
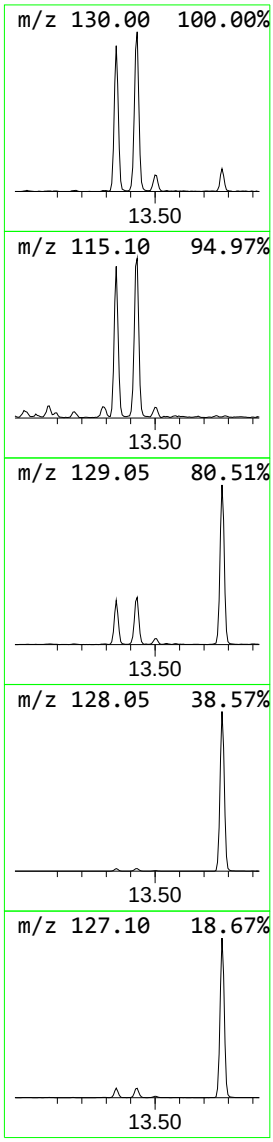
Peak Number 6 Benzene, 1-butynyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.426	15.76 ug/l	330398	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-butynyl-	130	C10H10	000622-76-4	95
2	2-Methylindene	130	C10H10	002177-47-1	95
3	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	94
4	Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	93
5	1H-Indene, 3-methyl-	130	C10H10	000767-60-2	93





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Instrument :
MSVOA_X
ClientSampleId :
0-3(5-10)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

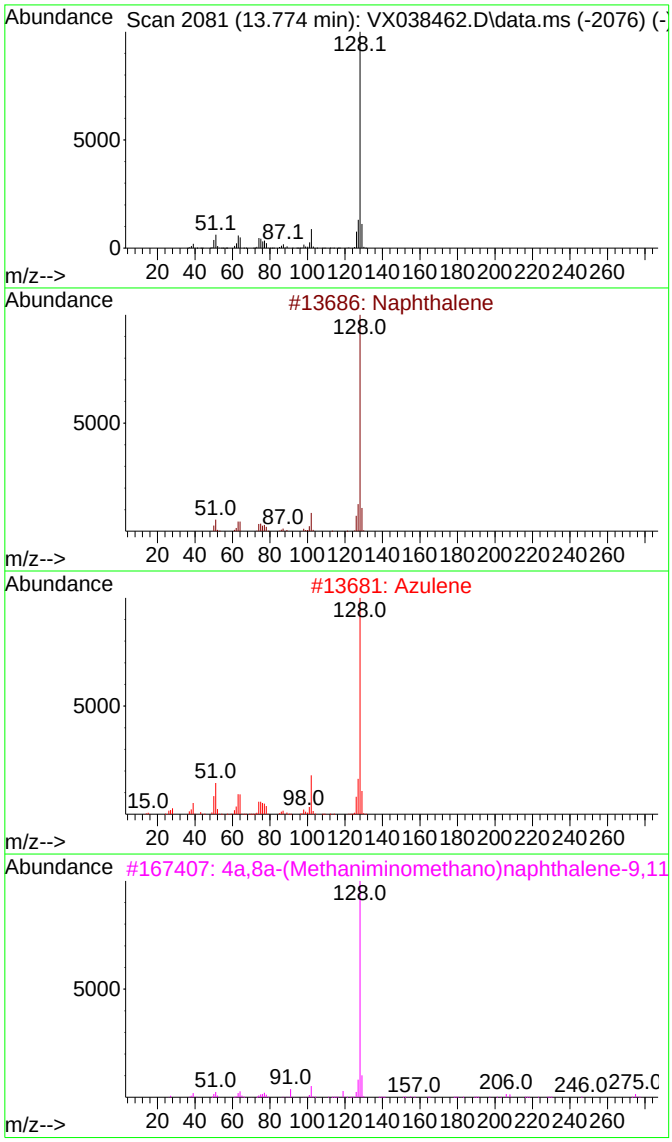
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

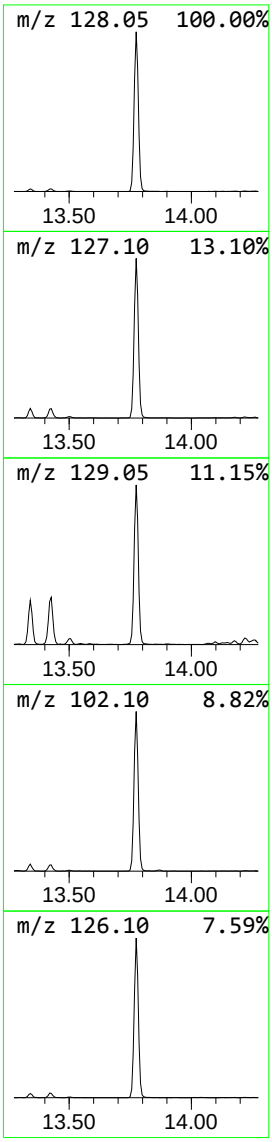
****

Peak Number 7 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	139.63 ug/l	2926890	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene	128	C10H8	000091-20-3	95
2	Azulene	128	C10H8	000275-51-4	91
3	4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	78
4	4-Phenylbut-3-ene-1-yne	128	C10H8	1000222-12-0	64
5	1,3-Dicyanobenzene	128	C8H4N2	000626-17-5	59





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Data File : VX038462.D
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
0-3(5-10)

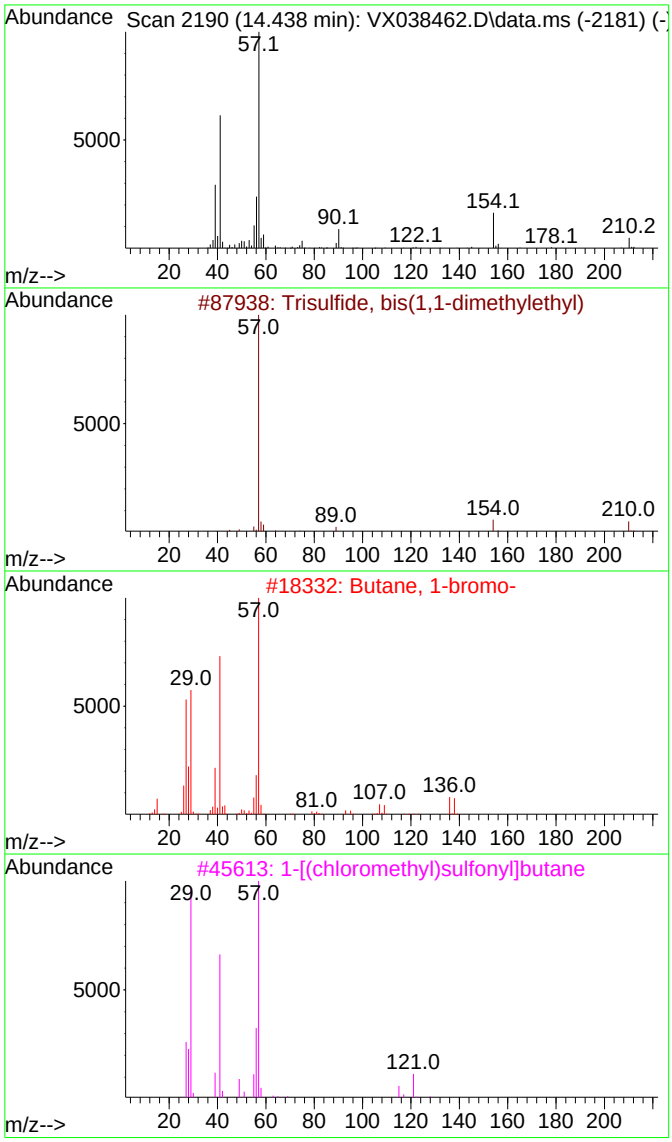
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

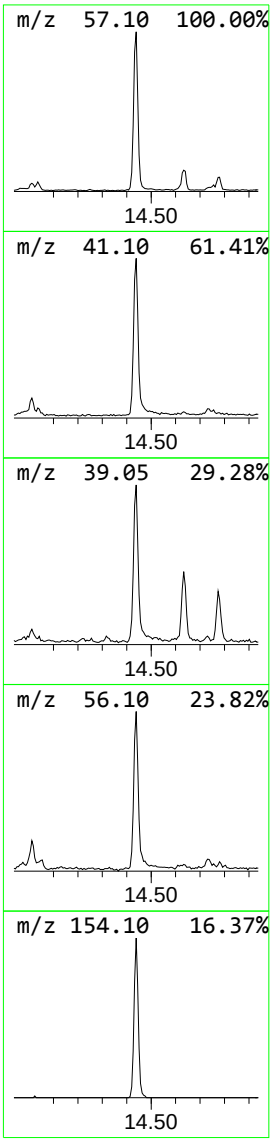
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 unknown14.438 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.438	9.19 ug/l	192593	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trisulfide, bis(1,1-dimethylethyl)	210	C8H18S3	004253-90-1	46
2	Butane, 1-bromo-	136	C4H9Br	000109-65-9	32
3	1-[(chloromethyl)sulfonyl]butane	170	C5H11ClO2S	1000404-59-5	23
4	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	23
5	Ethanedioic acid, dibutyl ester	202	C10H18O4	002050-60-4	23





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102423\
Data File : VX038462.D
Acq On : 24 Oct 2023 17:50
Operator : JC/MD
Sample : 04938-18 10X
Misc : 5.51g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
0-3(5-10)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

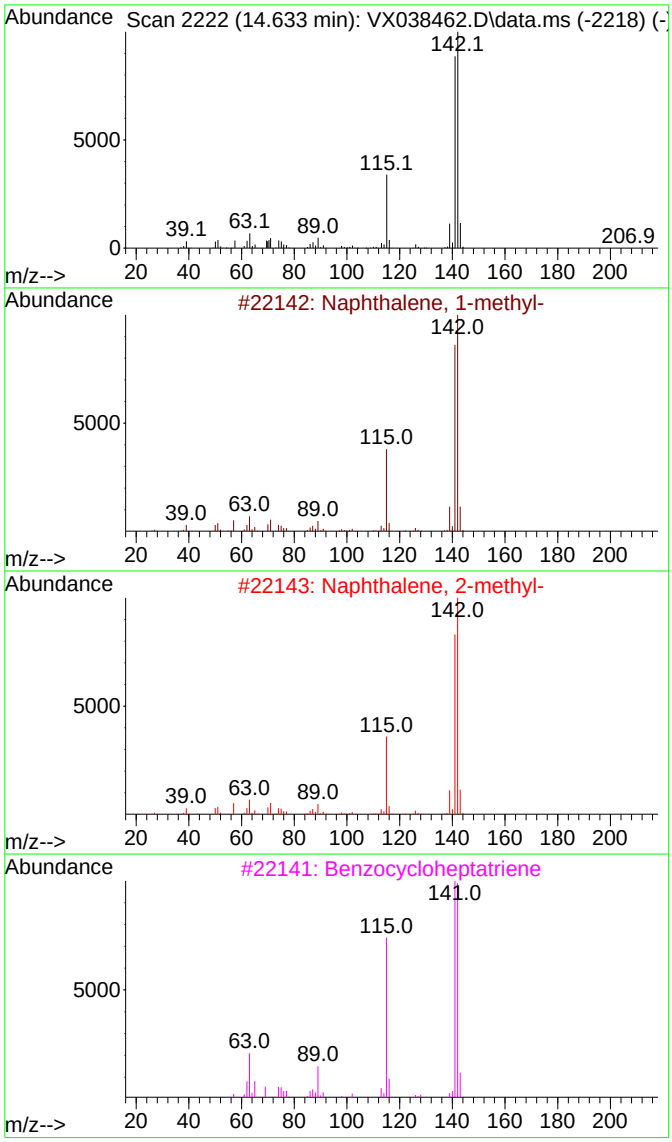
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

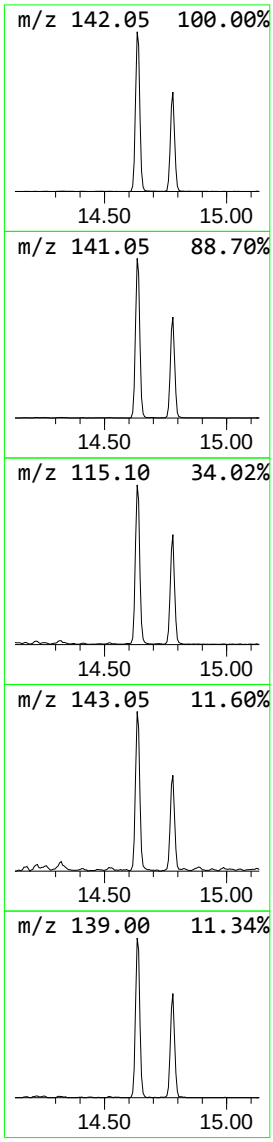
****

Peak Number 9 Benzocycloheptatriene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.633	34.39 ug/l	720815	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	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102423\
Data File : VX038462.D
Acq On : 24 Oct 2023 17:50
Operator : JC/MD
Sample : 04938-18 10X
Misc : 5.51g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
0-3(5-10)

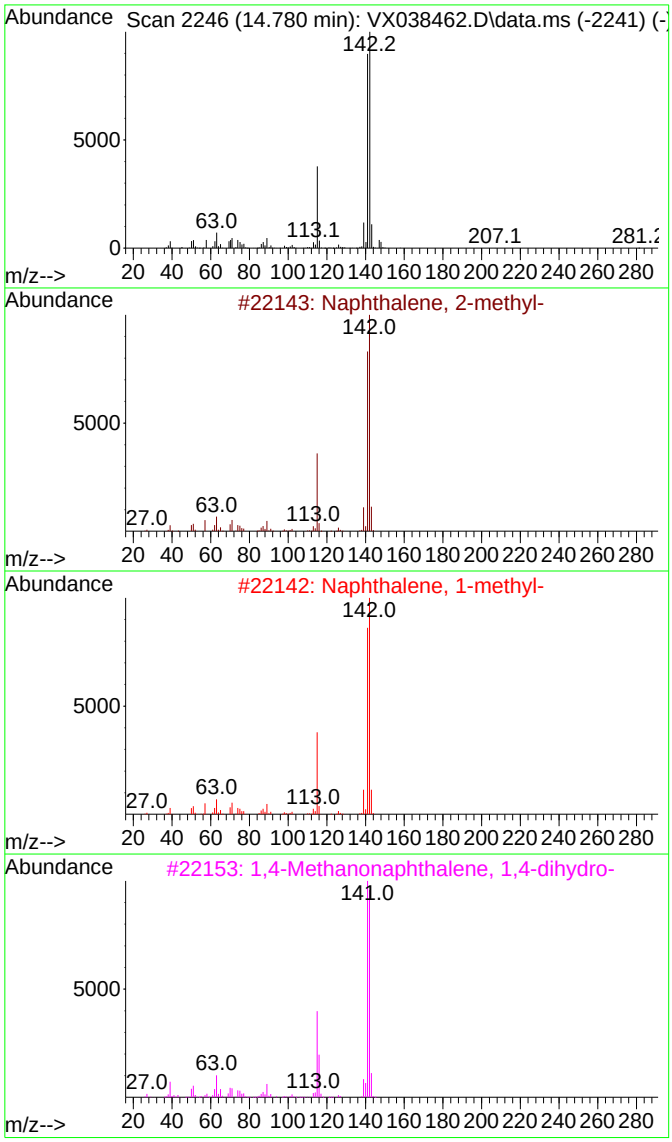
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

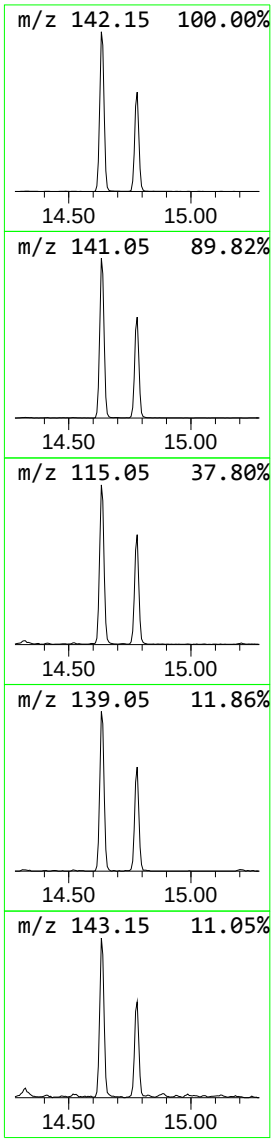
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1,4-Methanonaphthalene, 1,4... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	22.06 ug/l	462518	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	90
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102423\
Data File : VX038462.D
Acq On : 24 Oct 2023 17:50
Operator : JC/MD
Sample : 04938-18 10X
Misc : 5.51g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
0-3(5-10)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.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
Benzene, 1-ethy...	11.378	7.7	ug/l	161504	4	12.024	1048120	50.0
Benzene, 1,2,3-...	12.085	7.0	ug/l	145770	4	12.024	1048120	50.0
Indane	12.244	11.0	ug/l	231098	4	12.024	1048120	50.0
Indene	12.414	35.3	ug/l	740437	4	12.024	1048120	50.0
2-Methylindene	13.341	12.3	ug/l	257406	4	12.024	1048120	50.0
Benzene, 1-buty...	13.426	15.8	ug/l	330398	4	12.024	1048120	50.0
Azulene	13.774	139.6	ug/l	2926890	4	12.024	1048120	50.0
unknown14.438	14.438	9.2	ug/l	192593	4	12.024	1048120	50.0
Benzocyclohepta...	14.633	34.4	ug/l	720815	4	12.024	1048120	50.0
1,4-Methanonaph...	14.780	22.1	ug/l	462518	4	12.024	1048120	50.0