LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081423\
Data File : VX036974.D
Acq On : 14 Aug 2023 19:00
Operator : JC/MD
Sample : 03932-03 10X
Misc : 7.14g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB-01-Z30-32

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: VX036974.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.385	694	705	717	rBV2	81694	238851	1.42%	0.515%
2	5.550	721	732	749	rVB	130718	375933	2.24%	0.810%
3	5.958	789	799	805	rBV	86058	224297	1.33%	0.484%
4	6.038	805	812	826	rVB	121245	324288	1.93%	0.699%
5	6.763	921	931	948	rBV	219254	520735	3.10%	1.123%
6	8.647	1235	1240	1249	rVB	458022	718782	4.27%	1.550%
7	10.055	1466	1471	1477	rVB	504777	655252	3.90%	1.413%
8	10.195	1487	1494	1500	rBV	801662	1024501	6.09%	2.209%
9	11.079	1634	1639	1650	rVB	458239	641019	3.81%	1.382%
10	11.396	1685	1691	1695	rBV	154620	227961	1.36%	0.491%
11	11.610	1722	1726	1734	rVB	167257	228038	1.36%	0.492%
12	11.750	1745	1749	1757	rVB	433832	548017	3.26%	1.181%
13	12.018	1788	1793	1800	rBV	545065	762342	4.53%	1.644%
14	12.085	1800	1804	1809	rBV	199295	279188	1.66%	0.602%
15	12.244	1824	1830	1837	rBV	2913706	3574623	21.26%	7.707%
16	12.317	1837	1842	1848	rVV2	186325	261681	1.56%	0.564%
17	12.555	1873	1881	1885	rBV	140635	246162	1.46%	0.531%
18	12.610	1886	1890	1894	rVB	201305	254960	1.52%	0.550%
19	12.701	1899	1905	1910	rBV	144622	265951	1.58%	0.573%
20	12.963	1944	1948	1954	rVB	153587	246509	1.47%	0.531%
21	13.170	1974	1982	1986	rBV	424984	551926	3.28%	1.190%
22	13.286	1992	2001	2006	rBV2	377243	637946	3.79%	1.375%
23	13.341	2006	2010	2014	rVB	361625	418611	2.49%	0.903%
24	13.420	2019	2023	2029	rVB	869751	1183606	7.04%	2.552%
25	13.780	2076	2082	2088	rVB	12911218	16813932	100.00%	36.250%
26	13.865	2093	2096	2100	rVV	336580	433421	2.58%	0.934%
27	13.920	2100	2105	2111	rVB3	130913	226372	1.35%	0.488%
28	14.219	2150	2154	2158	rBV2	183733	254626	1.51%	0.549%
29	14.317	2166	2170	2176	rVB	160413	231737	1.38%	0.500%
30	14.634	2212	2222	2233	rVB	4175409	5760455	34.26%	12.419%
31	14.780	2240	2246	2254	rVB	3044200	3830446	22.78%	8.258%
32	15.207	2308	2316	2320	rBV	288558	420387	2.50%	0.906%
33	15.371	2337	2343	2347	rBV	654030	902363	5.37%	1.945%
34	15.475	2354	2360	2365	rBV	502179	782727	4.66%	1.688%
35	15.609	2377	2382	2386	rBV	522055	837267	4.98%	1.805%
36	15.646	2386	2388	2395	rVB	311007	437163	2.60%	0.942%

LSC Area Percent Report

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Instrument :
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ClientSampleId :
NEVINS-SB-01-Z30-32

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

37	15.835	2410	2419	2431	rVB2	130104	393493	2.34%	0.848%
38	16.322	2491	2499	2511	rVB2	329318	647880	3.85%	1.397%

Sum of corrected areas: 46383448

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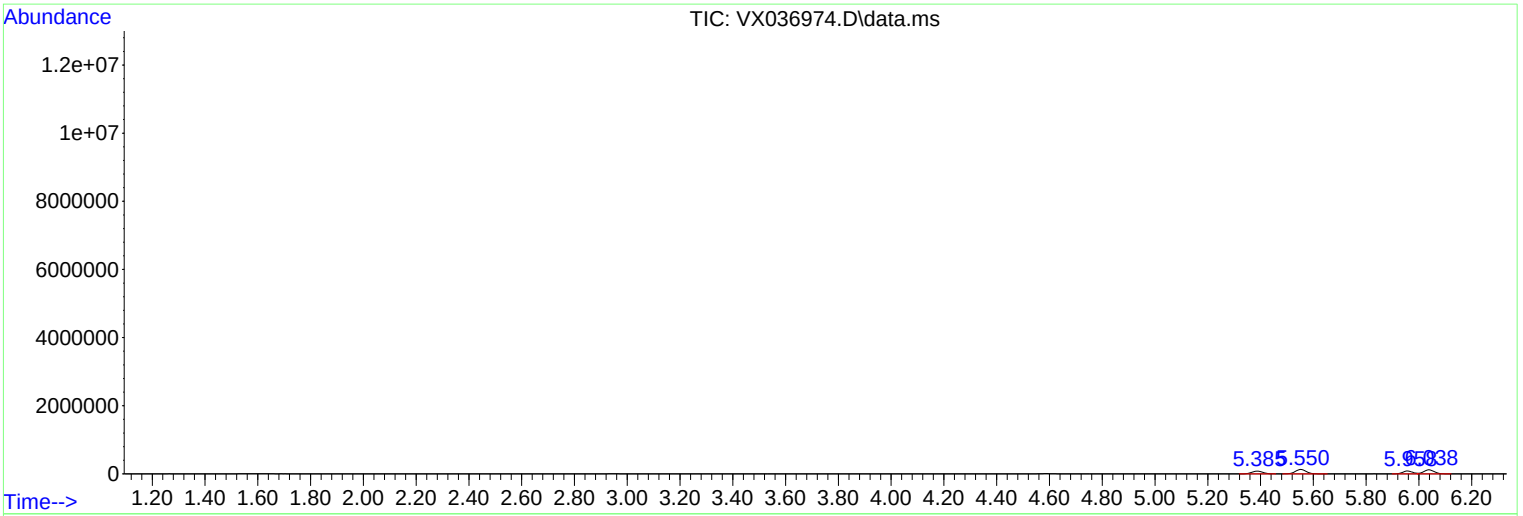
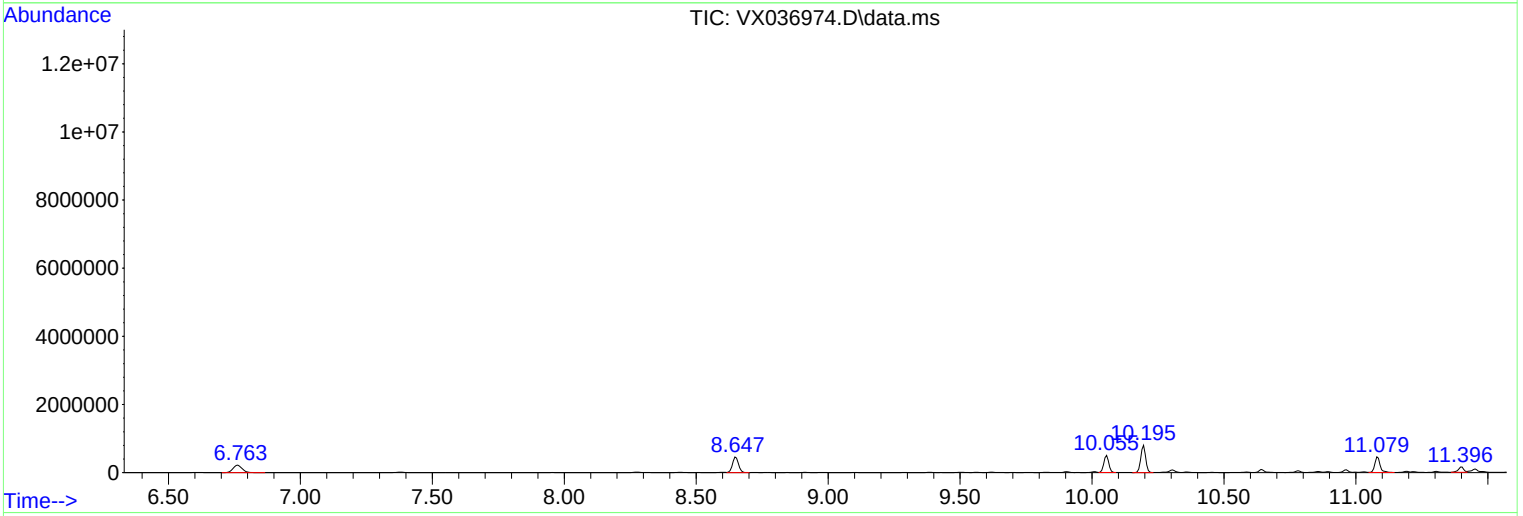
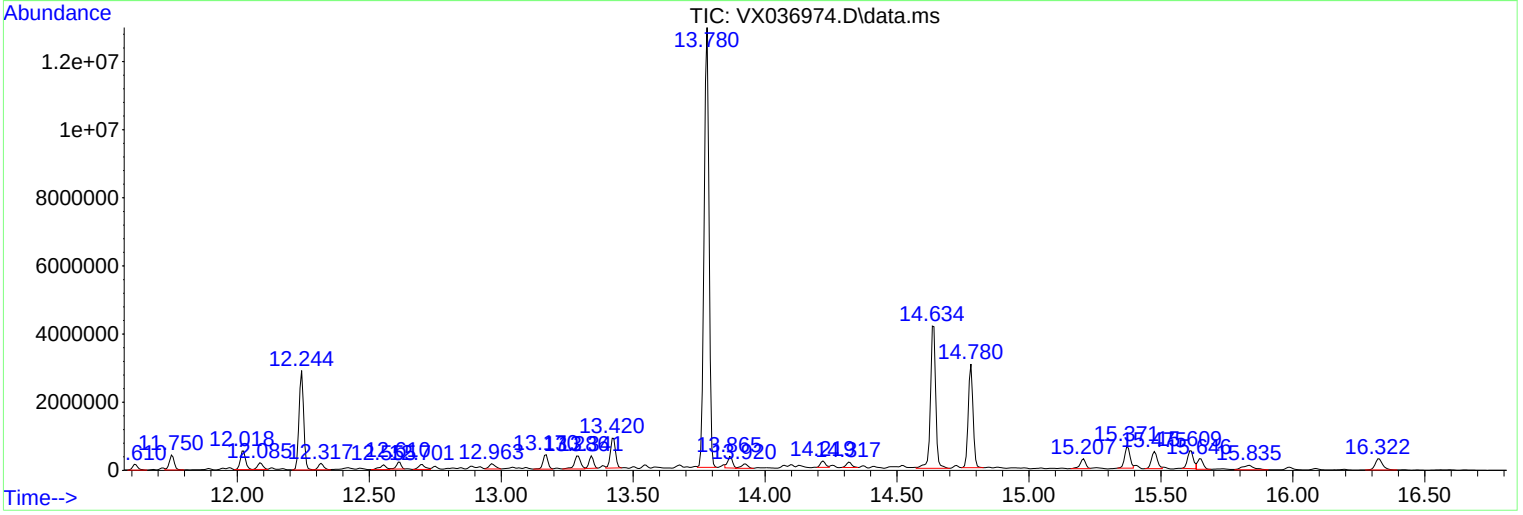
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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







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ClientSampleId :
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Quant Title : SW846 8260

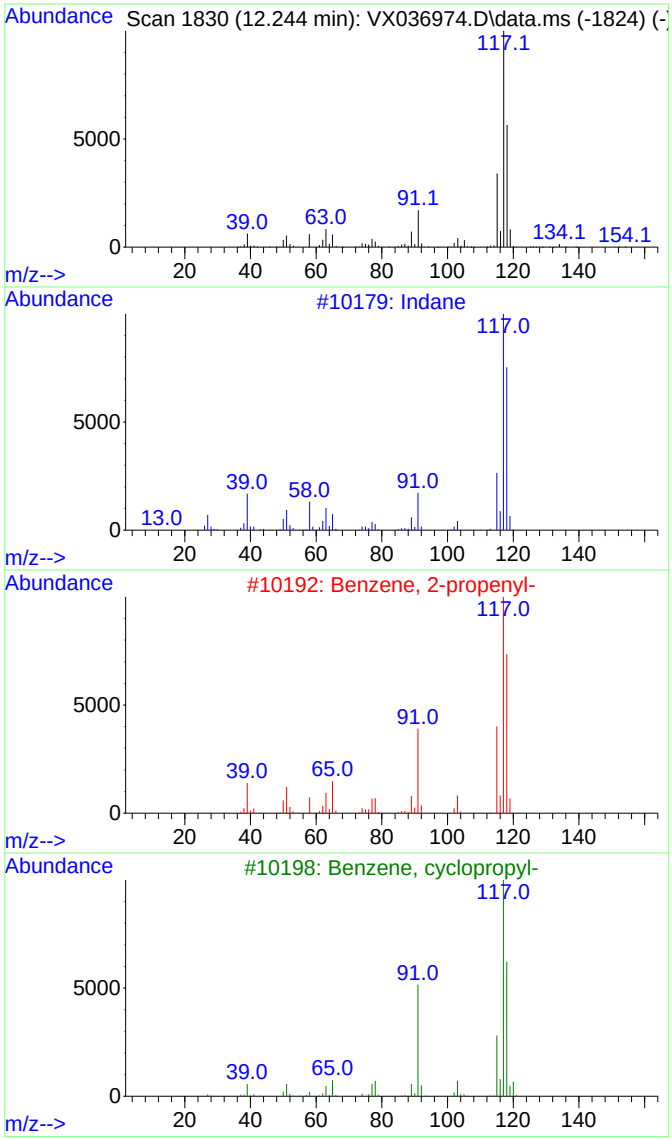
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

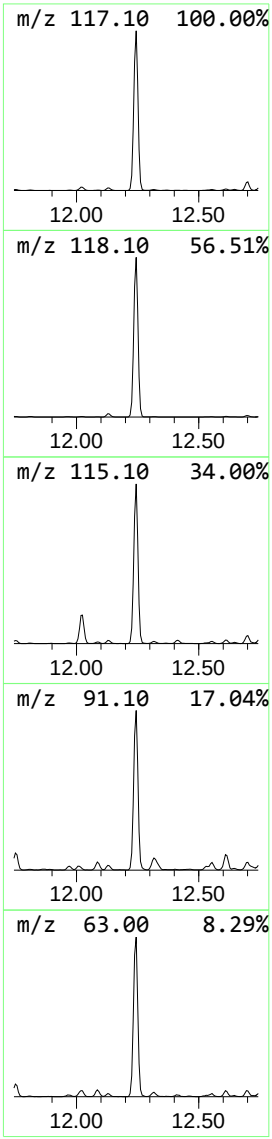
****

Peak Number 1 Indane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	234.45 ug/l	3574620	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	91
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	83
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	80
4	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	72
5	Deltacyclene	118	C9H10	007785-10-6	53





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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB-01-Z30-32

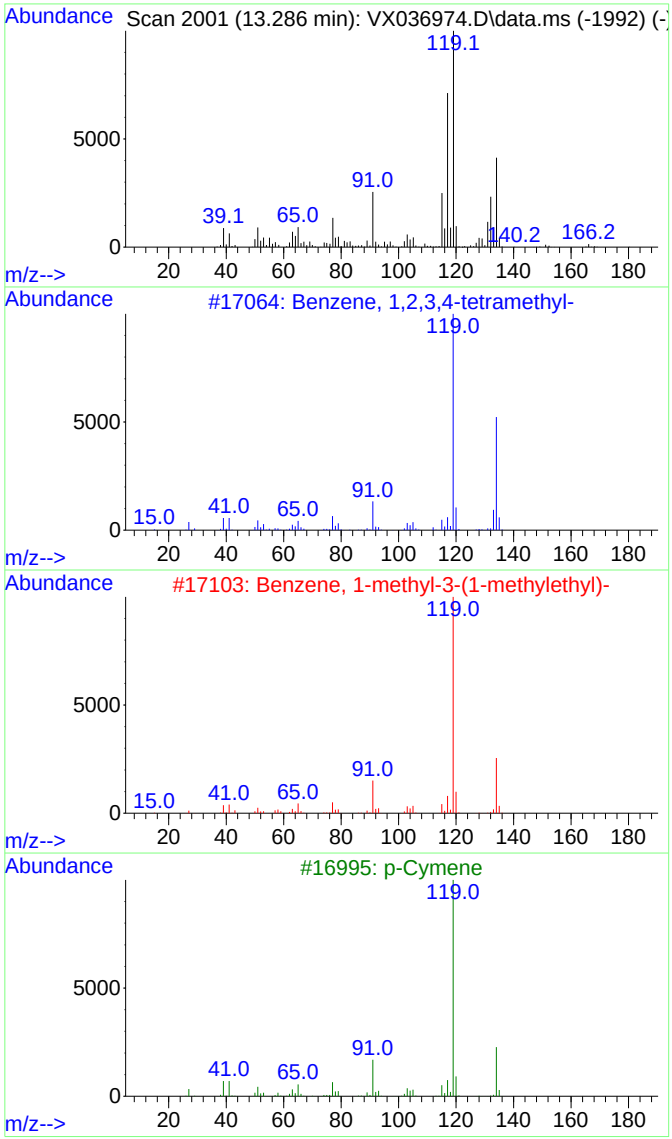
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

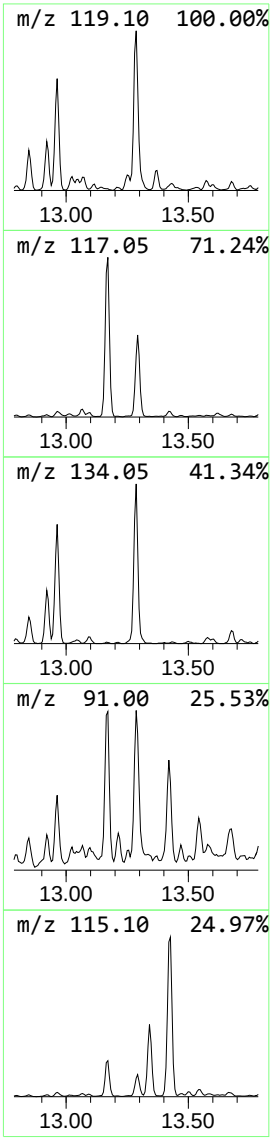
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.286	41.84 ug/l	637946	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	64
2	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	60
3	p-Cymene	134	C10H14	000099-87-6	60
4	o-Cymene	134	C10H14	000527-84-4	60
5	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	60





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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB-01-Z30-32

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

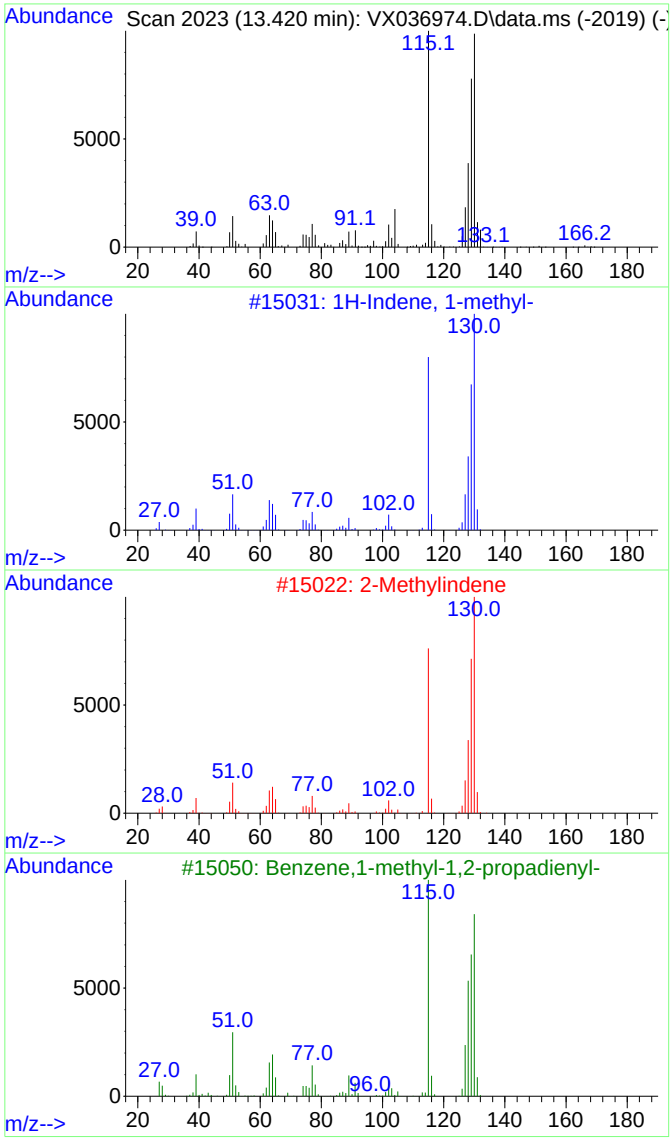
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

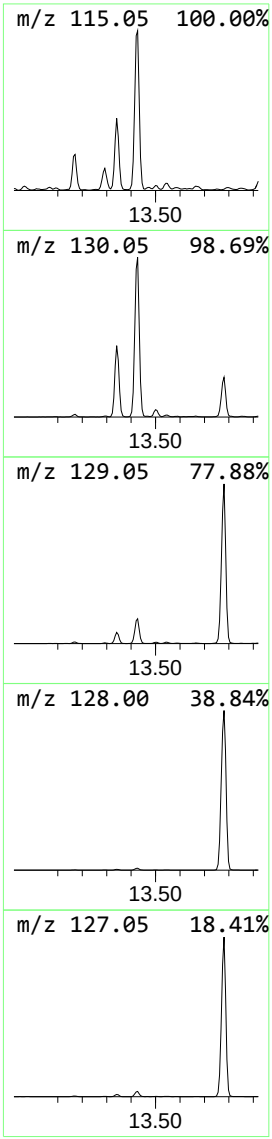
****

Peak Number 3 1H-Indene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.420	77.63 ug/l	1183610	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	96
2	2-Methylindene	130	C10H10	002177-47-1	96
3	Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	96
4	Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	96
5	1H-Indene, 3-methyl-	130	C10H10	000767-60-2	95





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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB-01-Z30-32

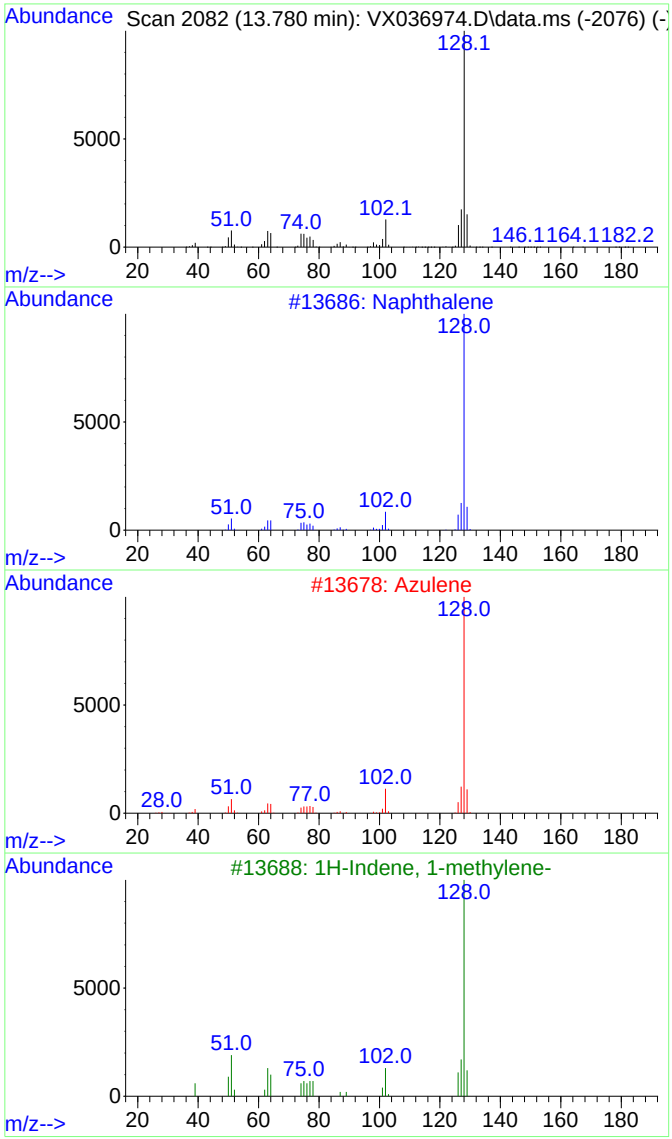
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

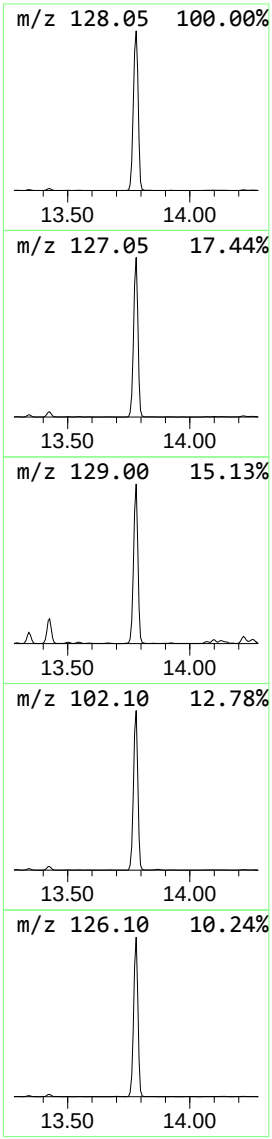
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1H-Indene, 1-methylene- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.780	1102.78 ug/l	16813900	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	94
3	1H-Indene, 1-methylene-	128	C10H8	002471-84-3	78
4	4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	72
5	1,3-Dicyanobenzene	128	C8H4N2	000626-17-5	53





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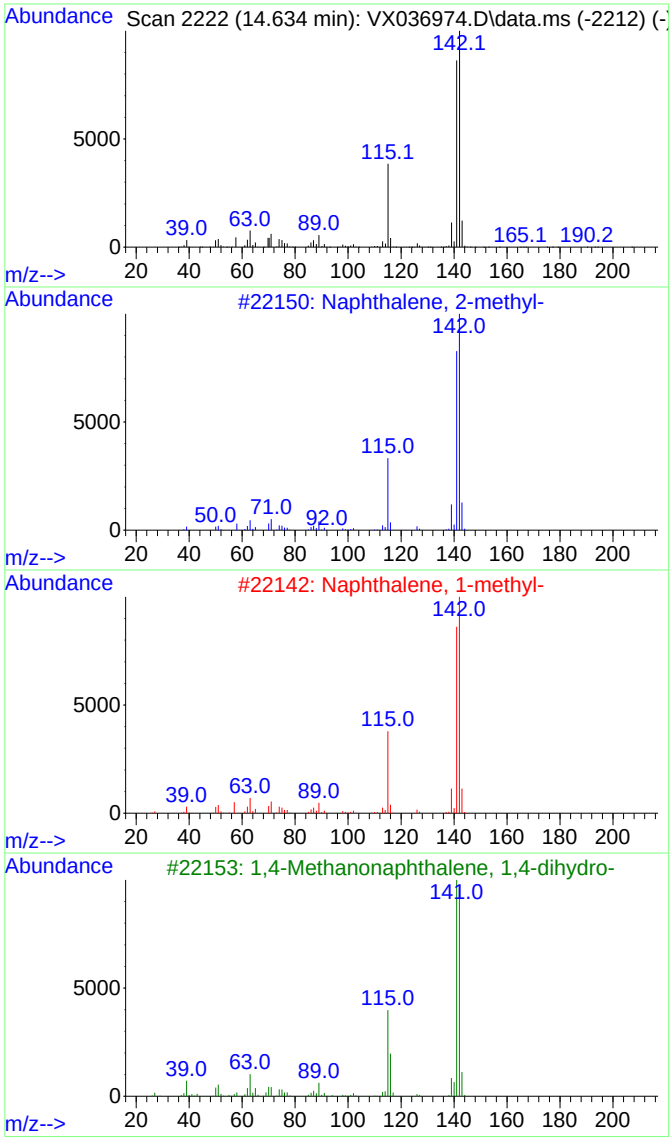
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

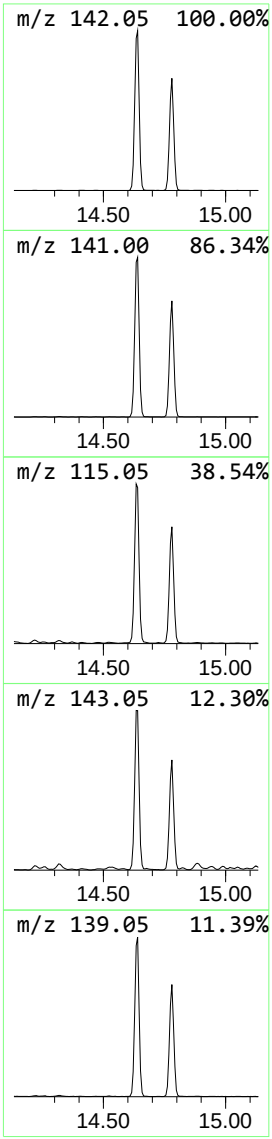
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1,4-Methanonaphthalene, 1,4... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.634	377.81 ug/l	5760460	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	72





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TIC Library : C:\Database\NIST20.L
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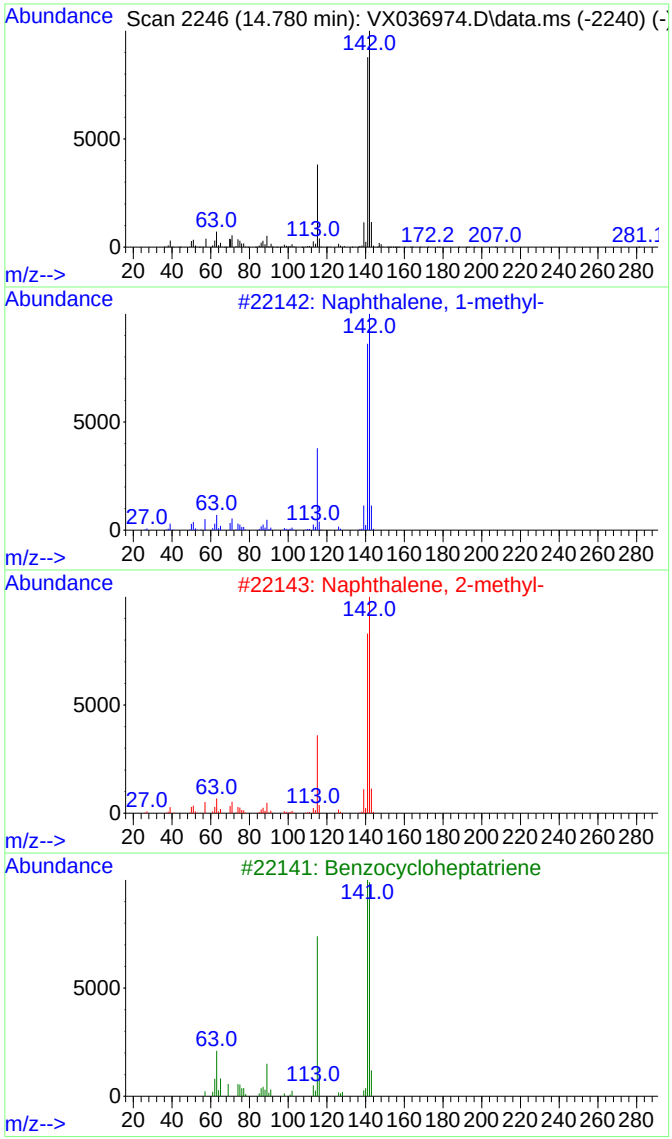
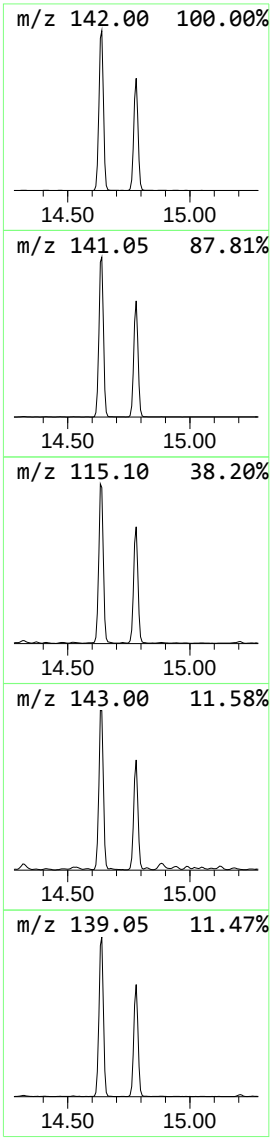
****
Peak Number 6 Benzocycloheptatriene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	251.23 ug/l	3830450	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	64





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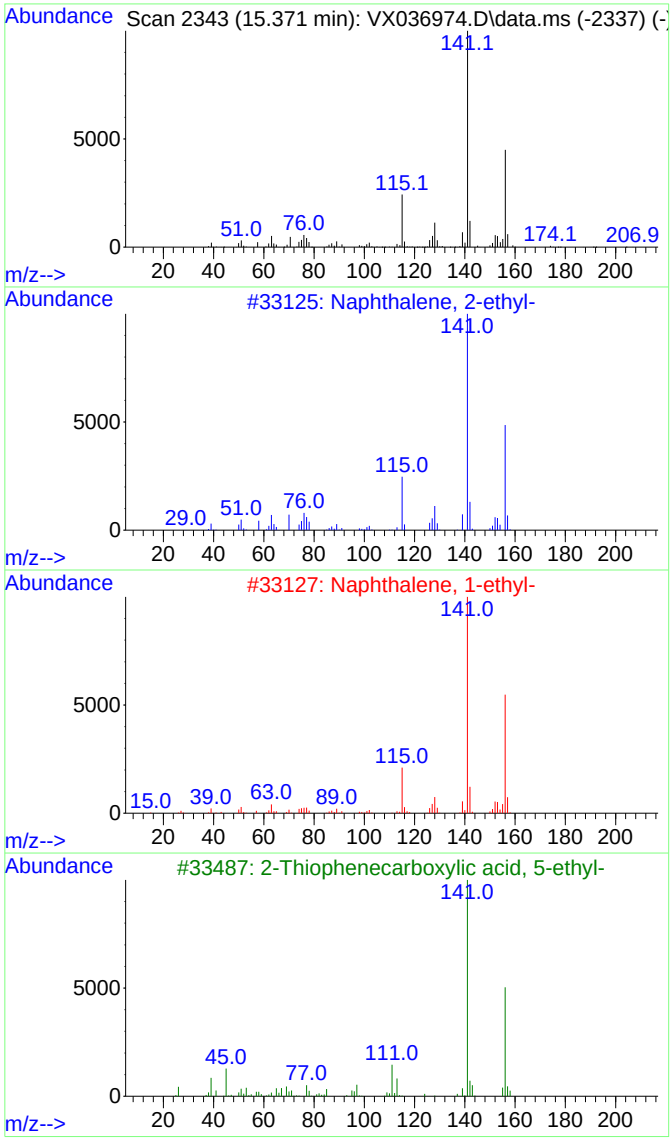
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

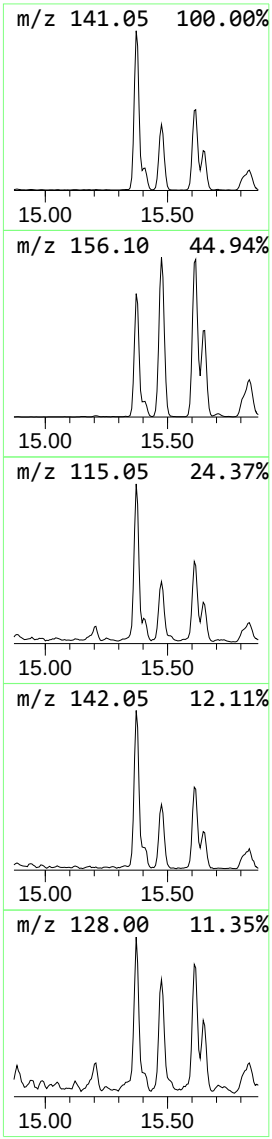
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2-Thiophenecarboxylic acid,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.371	59.18 ug/l	902363	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-ethyl-	156	C12H12	000939-27-5	96
2	Naphthalene, 1-ethyl-	156	C12H12	001127-76-0	96
3	2-Thiophenecarboxylic acid, 5-et...	156	C7H8O2S	023229-72-3	59
4	Naphthalene, 1-propyl-	170	C13H14	002765-18-6	59
5	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	58





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ClientSampleId :
NEVINS-SB-01-Z30-32

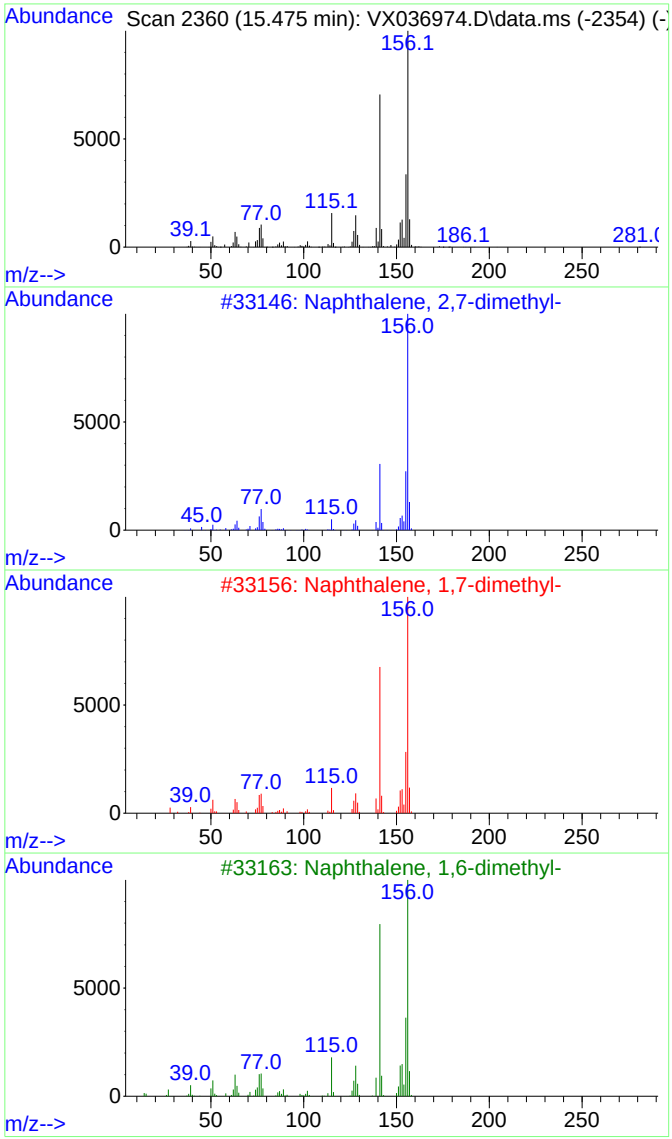
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

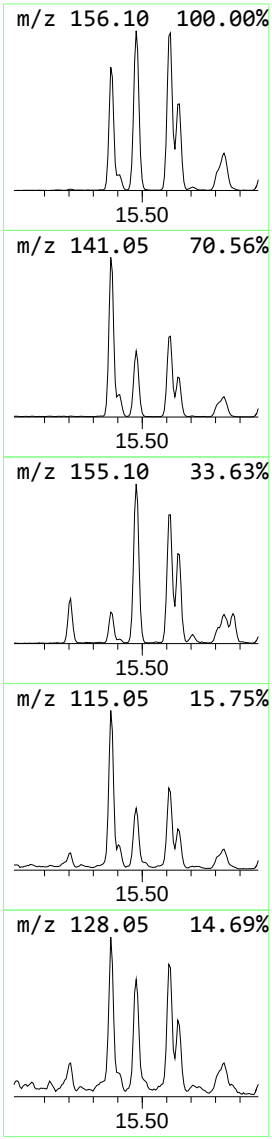
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.475	51.34 ug/l	782727	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
2	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
3	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
4	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	97
5	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081423\
Data File : VX036974.D
Acq On : 14 Aug 2023 19:00
Operator : JC/MD
Sample : 03932-03 10X
Misc : 7.14g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB-01-Z30-32

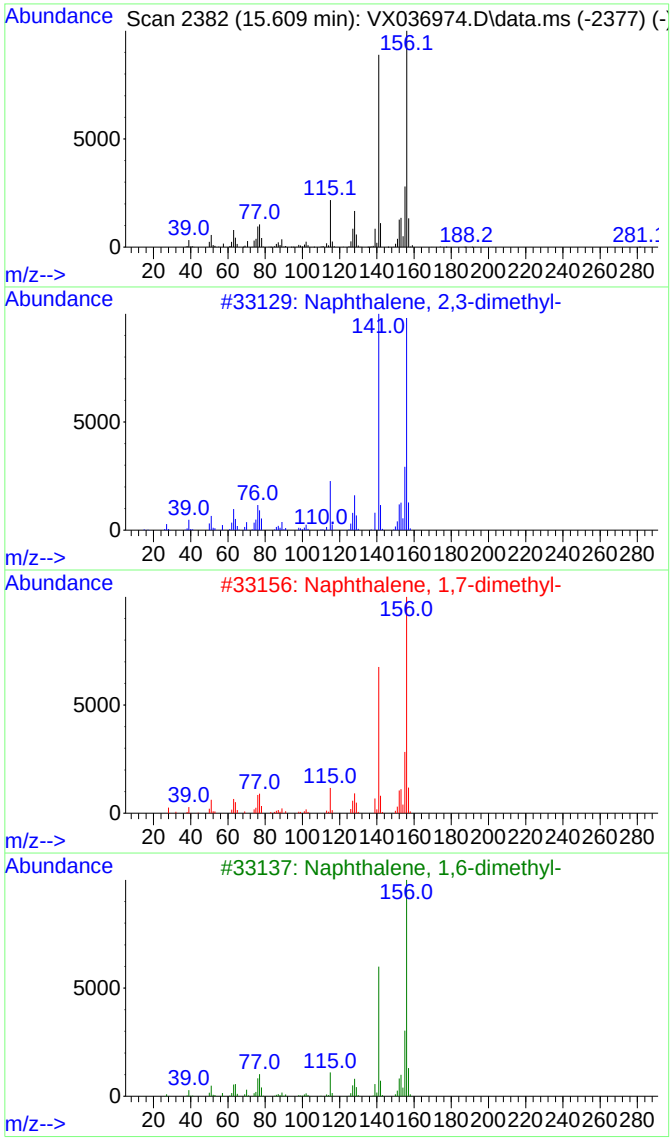
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

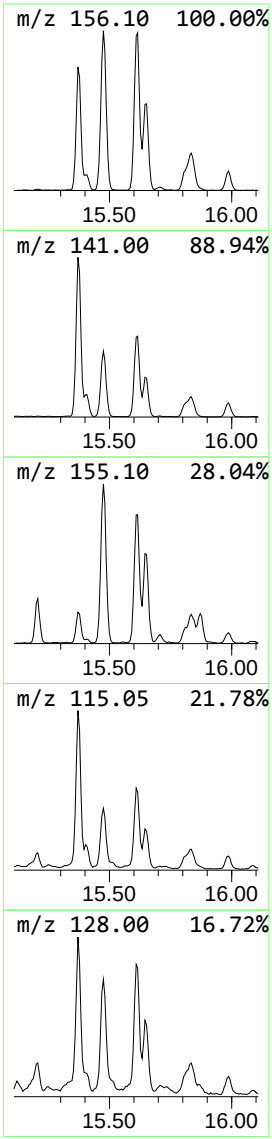
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Naphthalene, 2,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.609	54.91 ug/l	837267	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
3	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
4	Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	97
5	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	96





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081423\
Data File : VX036974.D
Acq On : 14 Aug 2023 19:00
Operator : JC/MD
Sample : 03932-03 10X
Misc : 7.14g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB-01-Z30-32

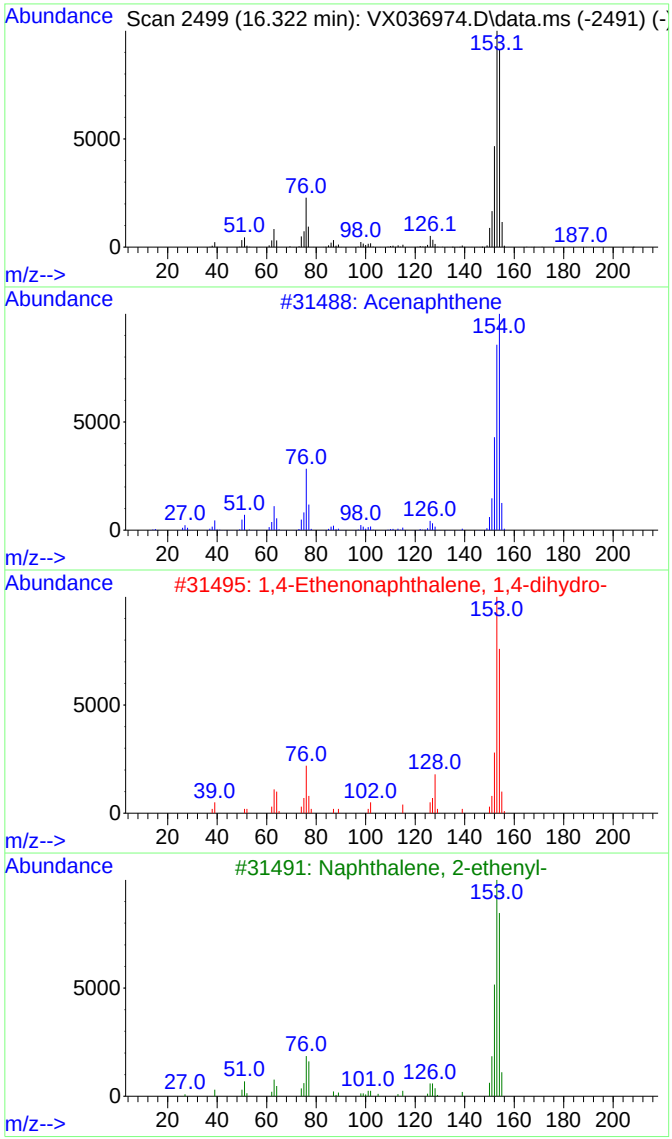
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

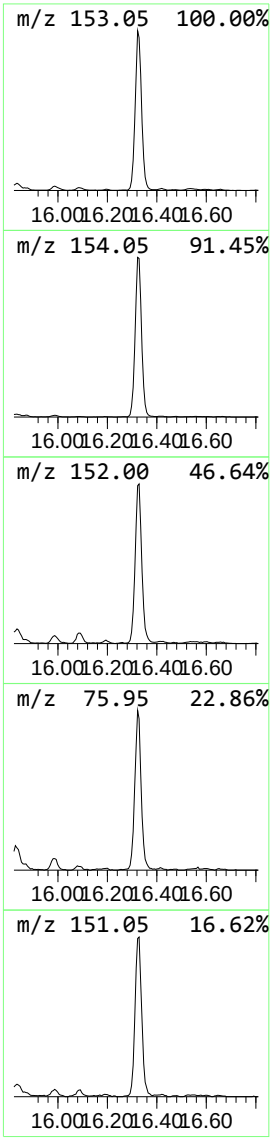
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1,4-Ethenonaphthalene, 1,4-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.322	42.49 ug/l	647880	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acenaphthene	154	C12H10	000083-32-9	94
2	1,4-Ethenonaphthalene, 1,4-dihydro-	154	C12H10	007322-47-6	64
3	Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	59
4	Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	58
5	3-Fluoro-para-anisaldehyde	154	C8H7FO2	000351-54-2	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081423\
Data File : VX036974.D
Acq On : 14 Aug 2023 19:00
Operator : JC/MD
Sample : 03932-03 10X
Misc : 7.14g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB-01-Z30-32

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
Indane	12.244	234.4	ug/l	3574620	4	12.024	762342	50.0
Benzene, 1,2,3,...	13.286	41.8	ug/l	637946	4	12.024	762342	50.0
1H-Indene, 1-me...	13.420	77.6	ug/l	1183610	4	12.024	762342	50.0
1H-Indene, 1-me...	13.780	1102.8	ug/l	16813900	4	12.024	762342	50.0
1,4-Methanonaph...	14.634	377.8	ug/l	5760460	4	12.024	762342	50.0
Benzocyclohepta...	14.780	251.2	ug/l	3830450	4	12.024	762342	50.0
2-Thiophenecarb...	15.371	59.2	ug/l	902363	4	12.024	762342	50.0
Naphthalene, 2,...	15.475	51.3	ug/l	782727	4	12.024	762342	50.0
Naphthalene, 2,...	15.609	54.9	ug/l	837267	4	12.024	762342	50.0
1,4-Ethenonapht...	16.322	42.5	ug/l	647880	4	12.024	762342	50.0