LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081523\
Data File : VX036995.D
Acq On : 15 Aug 2023 18:08
Operator : JC/MD
Sample : 03932-01 10X
Misc : 7.16g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB-01-Z18-20

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: VX036995.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	691	705	717	rBV2	77749	228535	1.36%	0.375%
2	5.550	721	732	752	rVB	127340	372181	2.22%	0.610%
3	5.958	789	799	806	rBV	82548	220996	1.32%	0.362%
4	6.763	920	931	956	rBV	210001	503910	3.00%	0.826%
5	8.647	1235	1240	1250	rVB	441213	693116	4.13%	1.136%
6	10.055	1466	1471	1476	rVB	456410	595063	3.55%	0.976%
7	10.195	1488	1494	1500	rBV	852392	1105282	6.59%	1.812%
8	10.963	1614	1620	1624	rBV	183172	252384	1.50%	0.414%
9	11.079	1634	1639	1650	rVB2	461338	694944	4.14%	1.139%
10	11.396	1685	1691	1694	rBV	179861	251007	1.50%	0.412%
11	11.451	1694	1700	1704	rVV	251187	334804	2.00%	0.549%
12	11.610	1722	1726	1734	rVB	377242	511788	3.05%	0.839%
13	11.750	1745	1749	1758	rVB	773617	969444	5.78%	1.590%
14	12.018	1788	1793	1799	rVV2	517920	764542	4.56%	1.254%
15	12.085	1799	1804	1809	rVV	357739	497664	2.97%	0.816%
16	12.244	1824	1830	1837	rBV	5027914	6090118	36.30%	9.986%
17	12.317	1837	1842	1848	rVV2	645262	826381	4.93%	1.355%
18	12.555	1878	1881	1885	rVV	234211	290520	1.73%	0.476%
19	12.609	1886	1890	1894	rVV	490654	579227	3.45%	0.950%
20	12.695	1899	1904	1911	rBV	391721	656130	3.91%	1.076%
21	12.963	1944	1948	1954	rVB	316793	447459	2.67%	0.734%
22	13.042	1954	1961	1964	rBV2	142376	250753	1.49%	0.411%
23	13.170	1974	1982	1986	rBV	771709	972947	5.80%	1.595%
24	13.292	1997	2002	2007	rVV2	764414	1073762	6.40%	1.761%
25	13.341	2007	2010	2014	rVB	510467	553132	3.30%	0.907%
26	13.426	2019	2024	2029	rVB	1305964	1702505	10.15%	2.792%
27	13.542	2039	2043	2047	rBV	191320	259308	1.55%	0.425%
28	13.676	2060	2065	2068	rBV2	163698	244141	1.46%	0.400%
29	13.780	2076	2082	2089	rVB	12663947	16775405	100.00%	27.506%
30	13.865	2090	2096	2100	rVV	174198	282151	1.68%	0.463%
31	13.926	2100	2106	2111	rVB3	190004	311093	1.85%	0.510%
32	14.073	2125	2130	2132	rBV2	149315	213085	1.27%	0.349%
33	14.097	2132	2134	2137	rVV	171869	188334	1.12%	0.309%
34	14.127	2137	2139	2147	rVB3	107178	198041	1.18%	0.325%
35	14.219	2149	2154	2158	rBV3	330138	537165	3.20%	0.881%
36	14.316	2163	2170	2176	rVV	275903	478265	2.85%	0.784%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081523\
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Operator : JC/MD
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Misc : 7.16g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB-01-Z18-20

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	14.640	2217	2223	2228	rBV	6168224	7658582	45.65%	12.558%
38	14.780	2240	2246	2255	rVB	4125785	5031823	30.00%	8.251%
39	15.207	2308	2316	2320	rBV	284142	422731	2.52%	0.693%
40	15.371	2331	2343	2347	rBV	1011720	1520189	9.06%	2.493%
41	15.408	2347	2349	2353	rVV	177365	205567	1.23%	0.337%
42	15.475	2354	2360	2371	rVV	759885	1289772	7.69%	2.115%
43	15.615	2372	2383	2386	rVV	879599	1457369	8.69%	2.390%
44	15.646	2386	2388	2394	rVB	468937	660085	3.93%	1.082%
45	15.835	2409	2419	2424	rBV	207460	554098	3.30%	0.909%
46	15.987	2438	2444	2454	rVB	135103	230506	1.37%	0.378%
47	16.328	2491	2500	2510	rBV2	488709	1031430	6.15%	1.691%

Sum of corrected areas: 60987734

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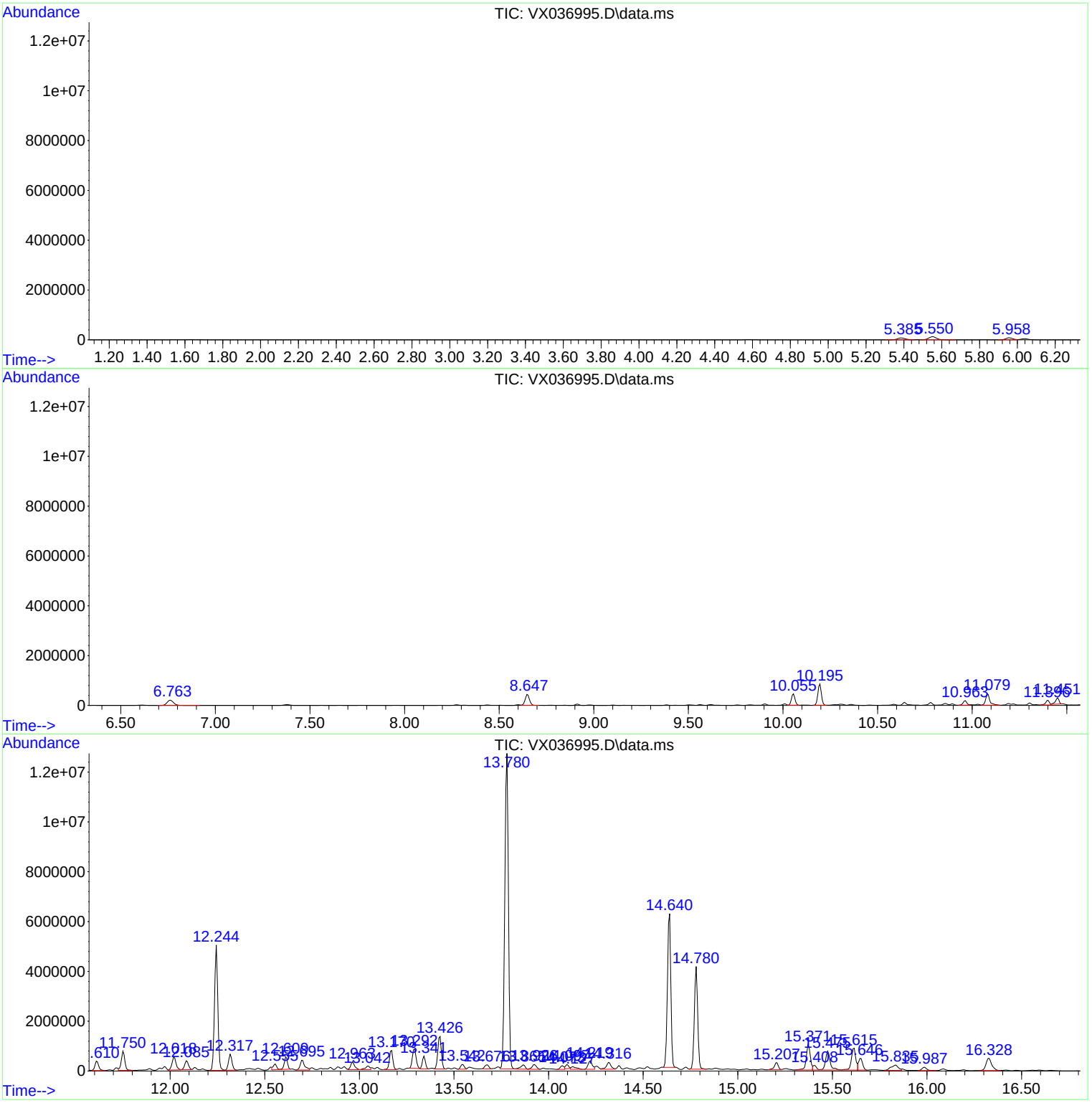
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB-01-Z18-20

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081523\
Data File : VX036995.D
Acq On : 15 Aug 2023 18:08
Operator : JC/MD
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Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB-01-Z18-20

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

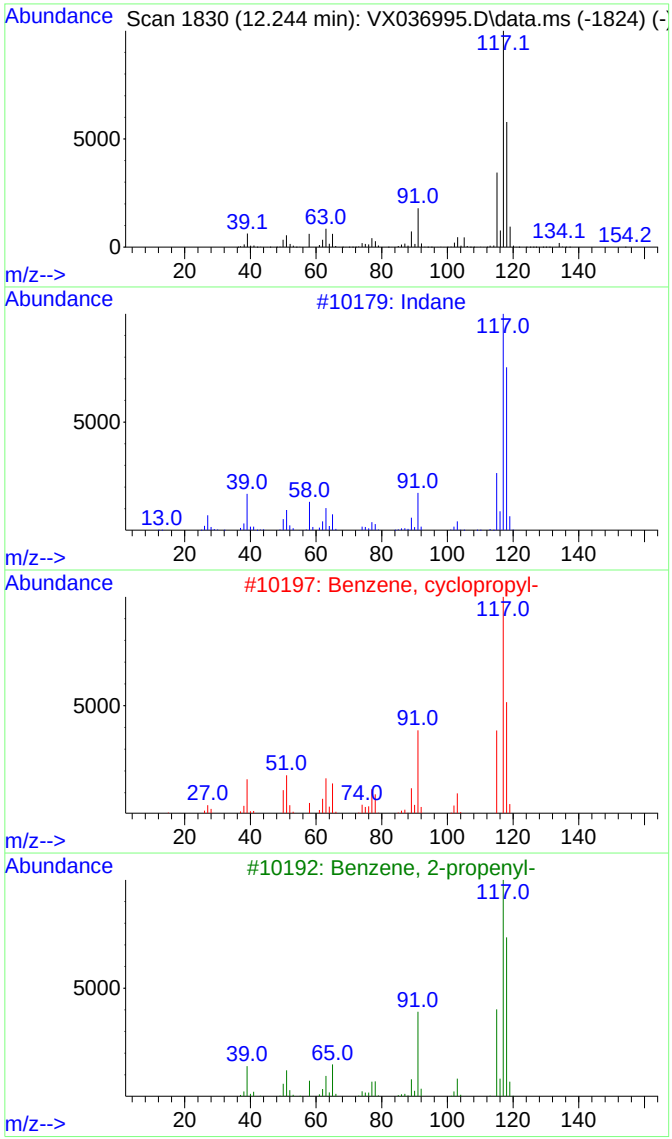
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

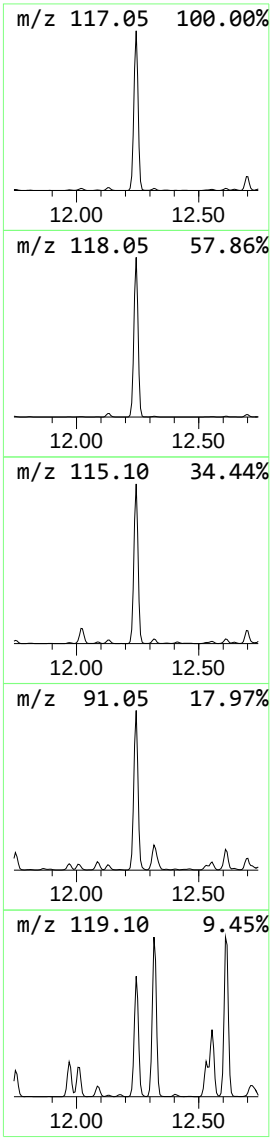
****

Peak Number 1 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	398.29 ug/l	6090120	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, cyclopropyl-	118	C9H10	000873-49-4	81
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	74
4	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	74
5	Deltacyclene	118	C9H10	007785-10-6	64





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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB-01-Z18-20

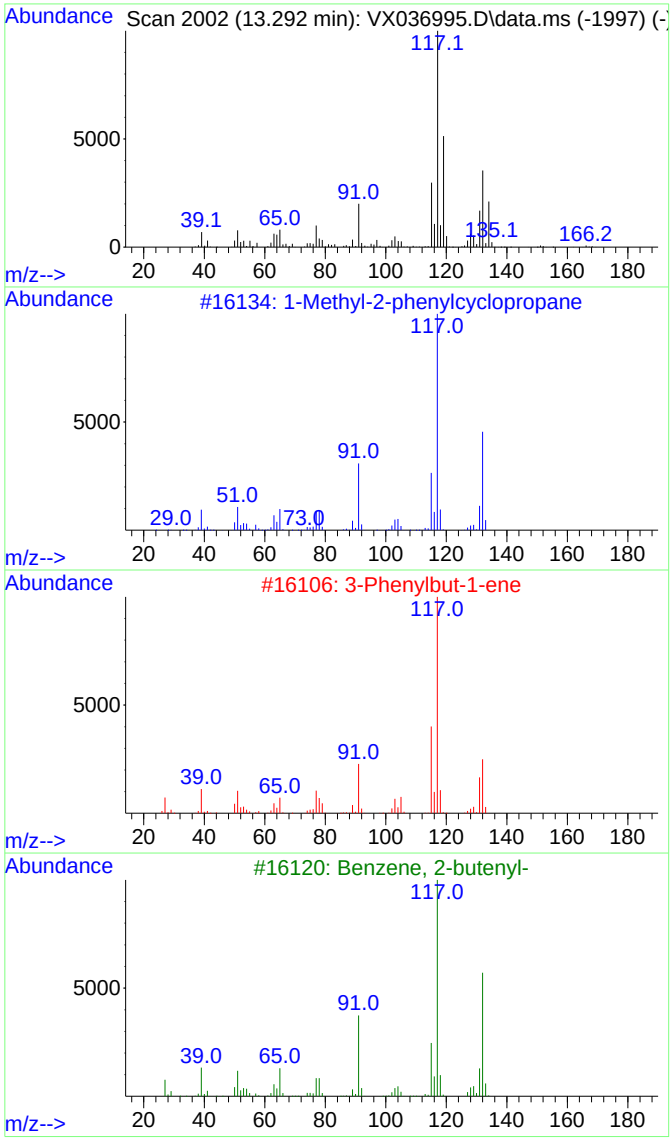
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

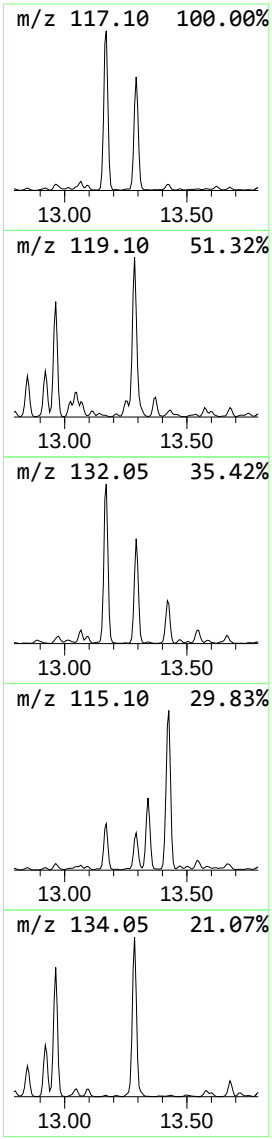
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1-Methyl-2-phenylcyclopropane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	70.22 ug/l	1073760	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	70
2	3-Phenylbut-1-ene	132	C10H12	000934-10-1	70
3	Benzene, 2-butenyl-	132	C10H12	001560-06-1	70
4	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	70
5	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081523\
Data File : VX036995.D
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Operator : JC/MD
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Misc : 7.16g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB-01-Z18-20

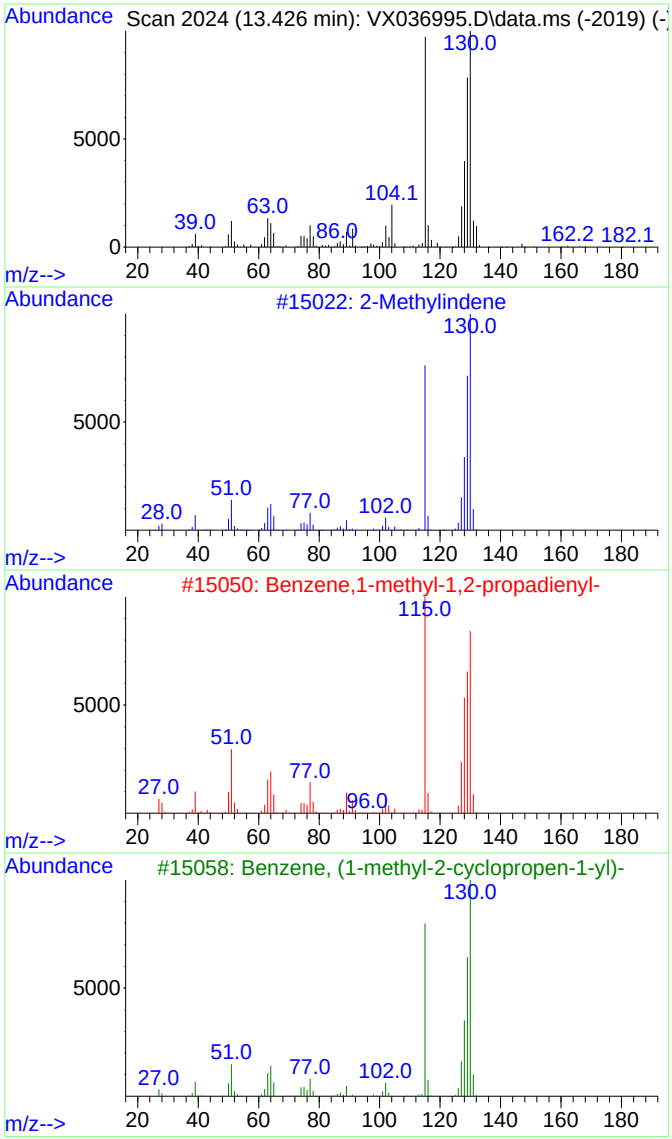
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

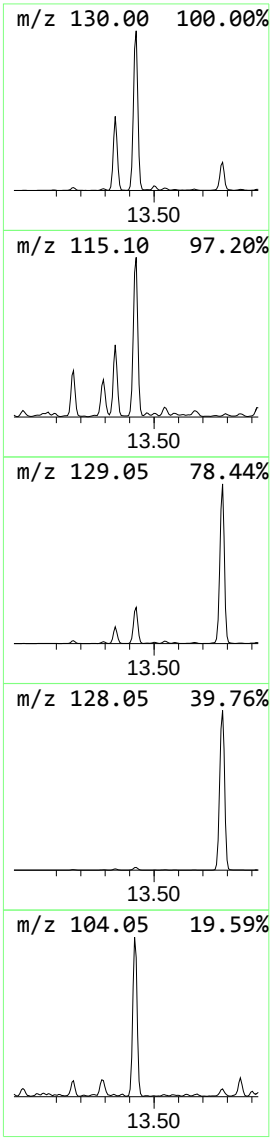
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Methylindene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.426	111.34 ug/l	1702510	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	Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	94
3	Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	94
4	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	94
5	1H-Indene, 3-methyl-	130	C10H10	000767-60-2	94





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081523\
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Misc : 7.16g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB-01-Z18-20

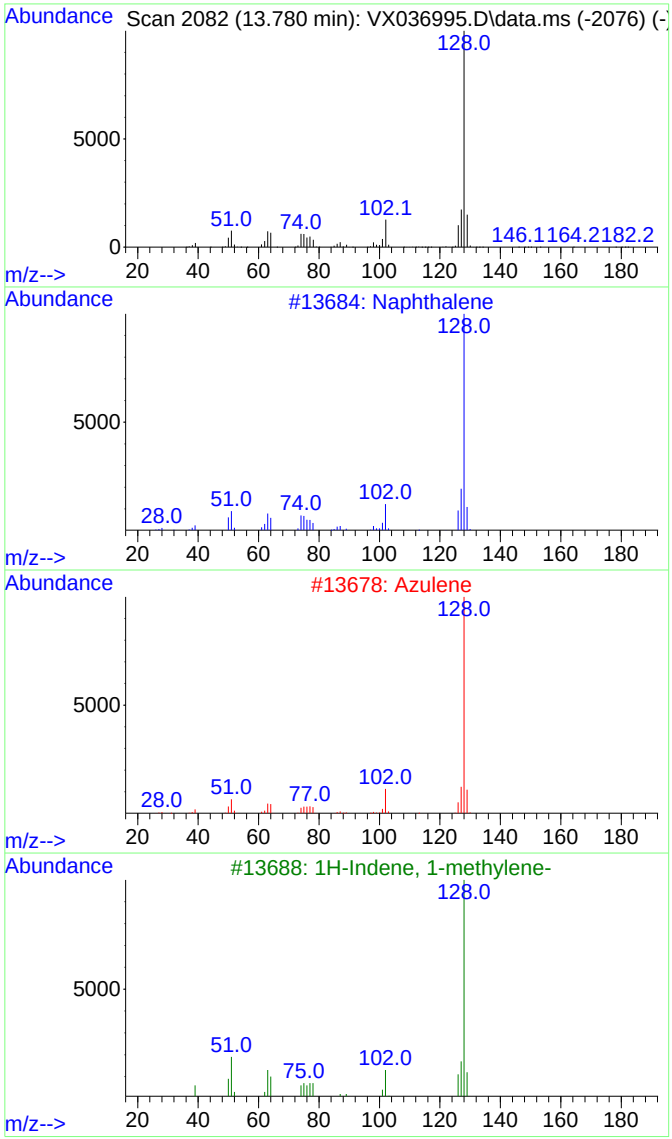
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

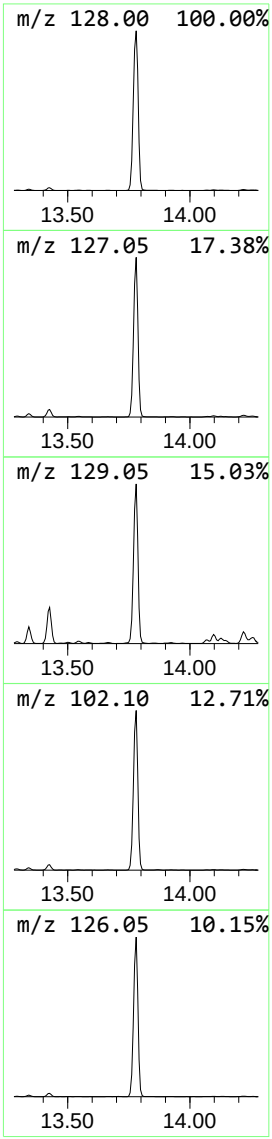
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.780	1097.09 ug/l	16775400	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	56
5	1,3-Dicyanobenzene	128	C8H4N2	000626-17-5	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081523\
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Misc : 7.16g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB-01-Z18-20

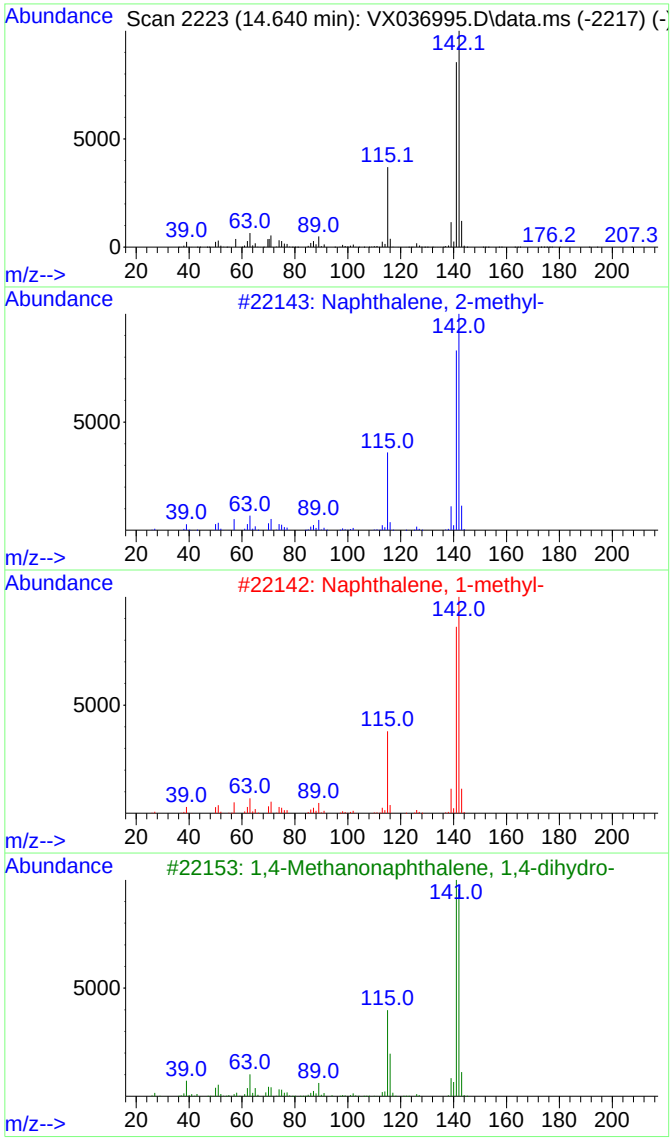
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

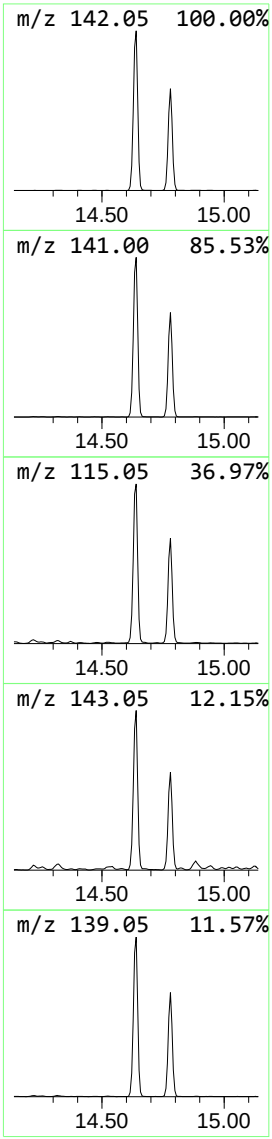
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	500.86 ug/l	7658580	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	91
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64





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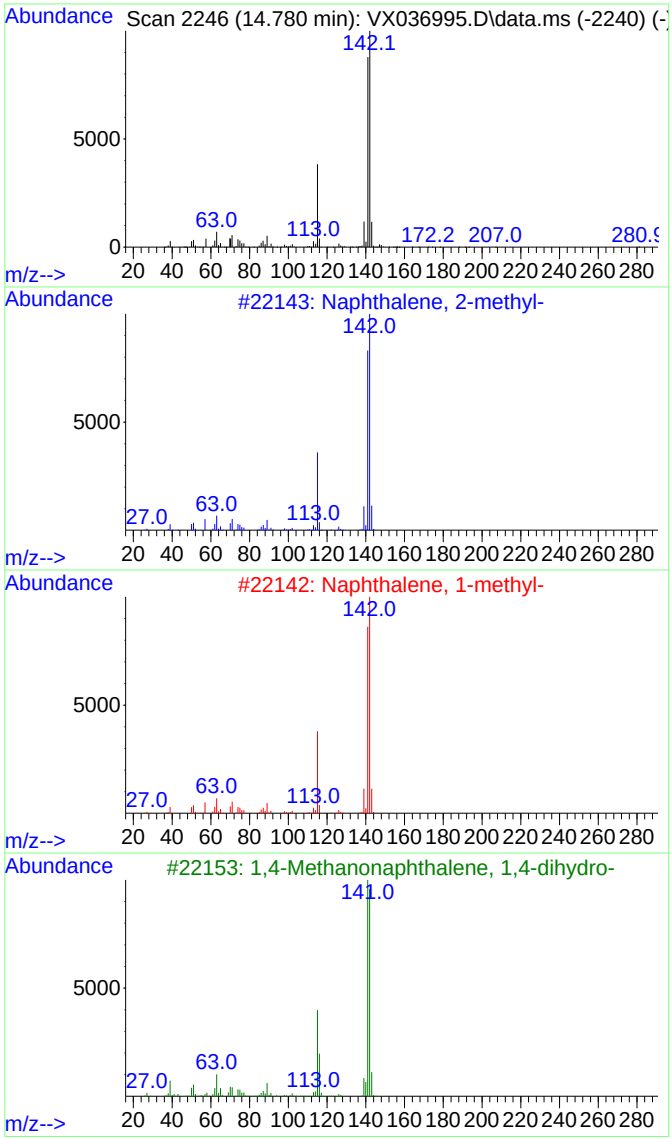
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

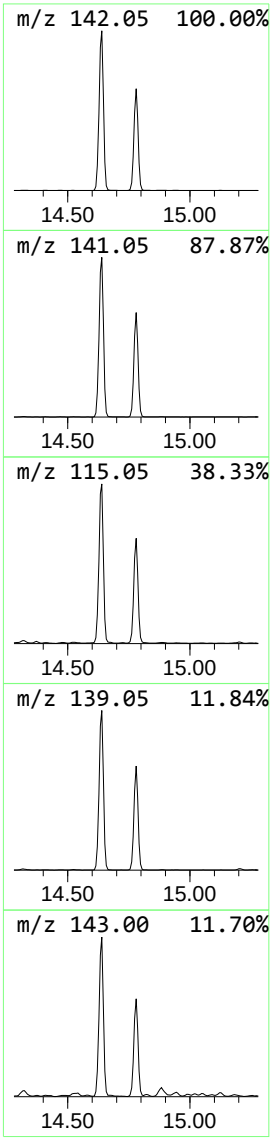
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzocycloheptatriene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	329.07 ug/l	5031820	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	91
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	64





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Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB-01-Z18-20

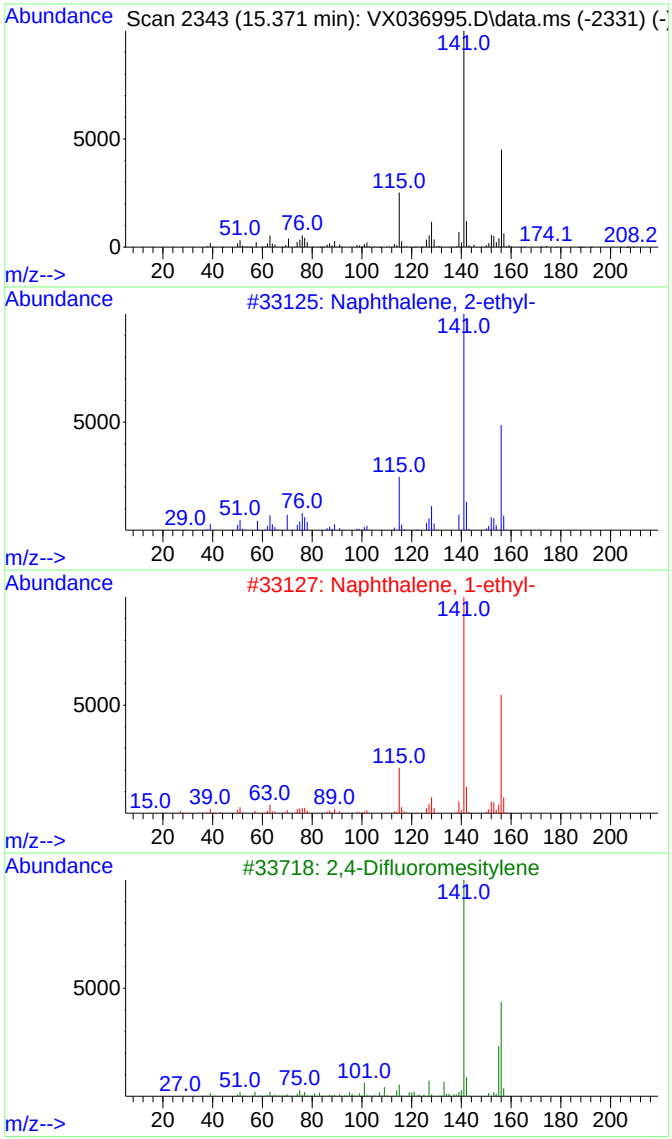
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

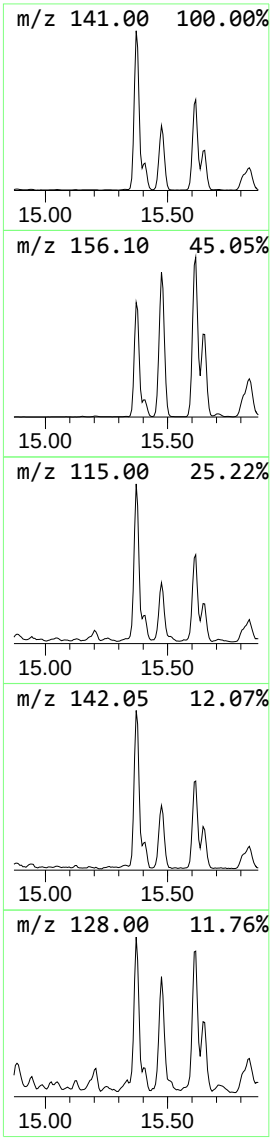
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2,4-Difluoromesitylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.371	99.42 ug/l	1520190	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	2,4-Difluoromesitylene	156	C9H10F2	000392-61-0	59
4	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	58
5	5-Acetyl-2-amino-4-methylthiazole	156	C6H8N2OS	030748-47-1	53





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Data File : VX036995.D
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Operator : JC/MD
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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB-01-Z18-20

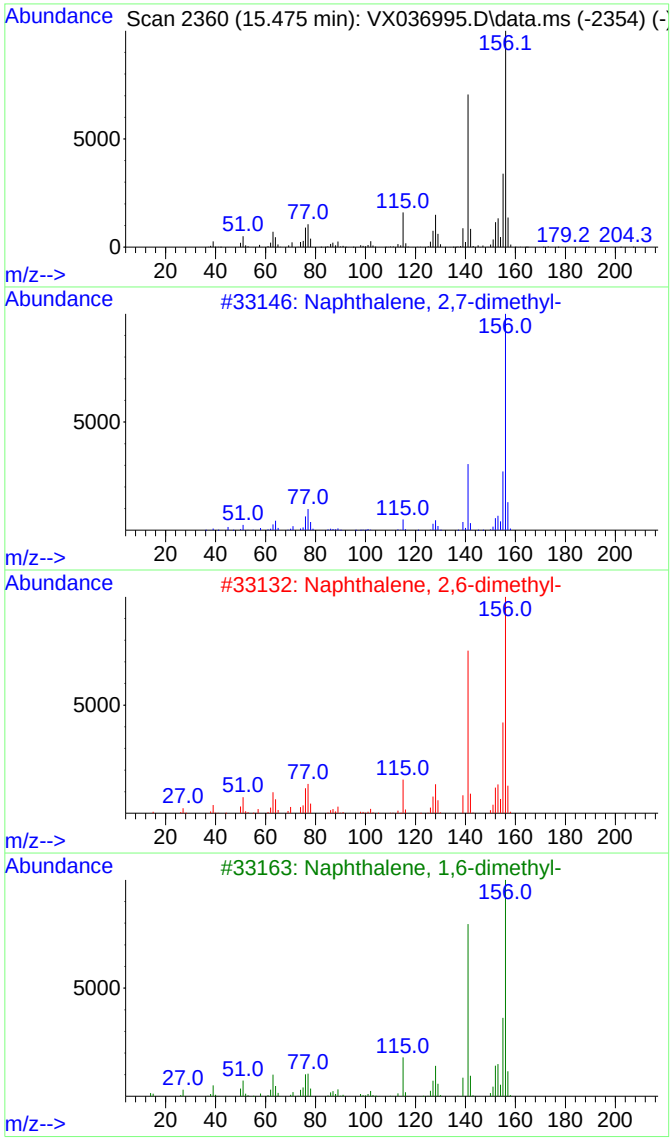
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

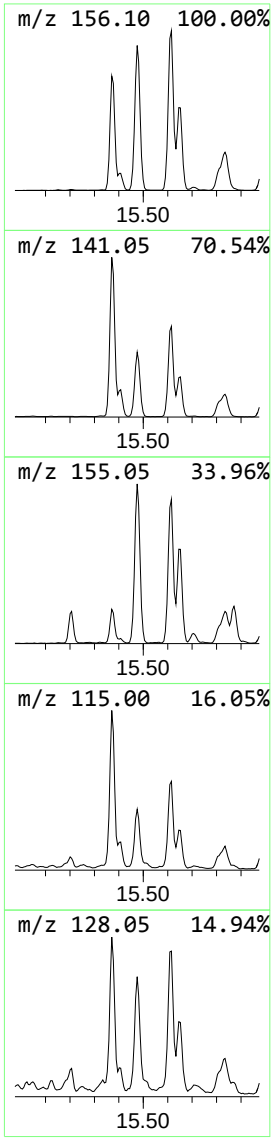
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.475	84.35 ug/l	1289770	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, 2,6-dimethyl-	156	C12H12	000581-42-0	97
3	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
4	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97
5	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081523\
Data File : VX036995.D
Acq On : 15 Aug 2023 18:08
Operator : JC/MD
Sample : 03932-01 10X
Misc : 7.16g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB-01-Z18-20

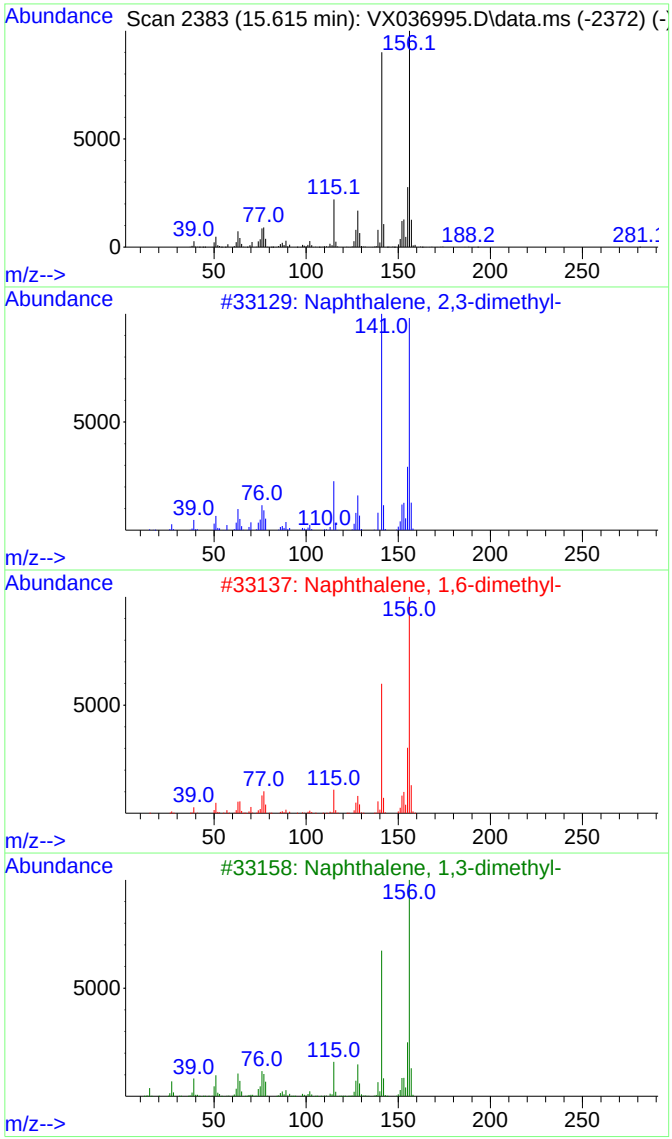
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

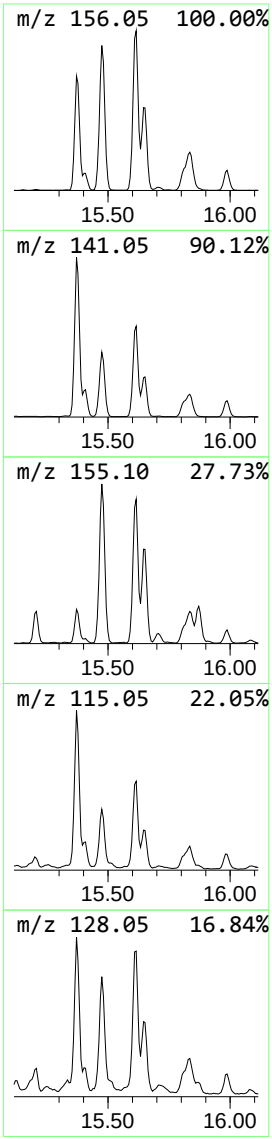
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	95.31 ug/l	1457370	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, 1,6-dimethyl-	156	C12H12	000575-43-9	97
3	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
4	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
5	Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	97





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081523\
Data File : VX036995.D
Acq On : 15 Aug 2023 18:08
Operator : JC/MD
Sample : 03932-01 10X
Misc : 7.16g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB-01-Z18-20

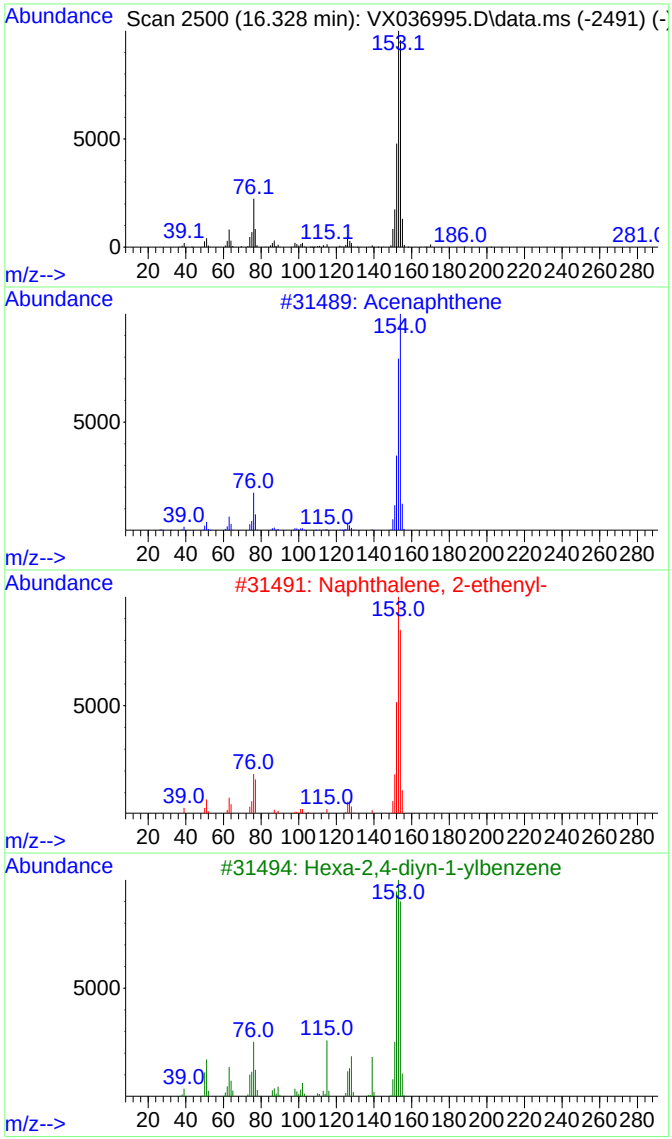
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

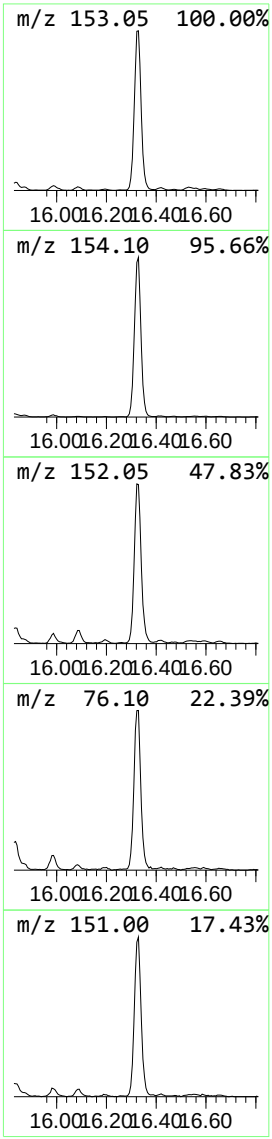
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, 2-ethenyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.328	67.45 ug/l	1031430	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acenaphthene	154	C12H10	000083-32-9	93
2	Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	68
3	Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	59
4	3-Fluoro-para-anisaldehyde	154	C8H7FO2	000351-54-2	50
5	Biphenyl	154	C12H10	000092-52-4	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081523\
Data File : VX036995.D
Acq On : 15 Aug 2023 18:08
Operator : JC/MD
Sample : 03932-01 10X
Misc : 7.16g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB-01-Z18-20

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	398.3	ug/l	6090120	4	12.024	764542	50.0
1-Methyl-2-phen...	13.292	70.2	ug/l	1073760	4	12.024	764542	50.0
2-Methylindene	13.426	111.3	ug/l	1702510	4	12.024	764542	50.0
Azulene	13.780	1097.1	ug/l	16775400	4	12.024	764542	50.0
1,4-Methanonaph...	14.640	500.9	ug/l	7658580	4	12.024	764542	50.0
Benzocyclohepta...	14.780	329.1	ug/l	5031820	4	12.024	764542	50.0
2,4-Difluoromes...	15.371	99.4	ug/l	1520190	4	12.024	764542	50.0
Naphthalene, 2,...	15.475	84.3	ug/l	1289770	4	12.024	764542	50.0
Naphthalene, 2,...	15.615	95.3	ug/l	1457370	4	12.024	764542	50.0
Naphthalene, 2-...	16.328	67.5	ug/l	1031430	4	12.024	764542	50.0