LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010224\
Data File : VN080629.D
Acq On : 02 Jan 2024 16:54
Operator : JC\MD
Sample : 06038-01
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
T-402

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_N\methods\82N122723W.M
Title : SW846 8260

Signal : TIC: VN080629.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.859	136	154	155	rBV6	31738	94936	1.25%	0.289%
2	8.165	1045	1056	1060	rBV2	236316	542907	7.14%	1.653%
3	8.223	1060	1066	1077	rVB	421097	950413	12.51%	2.893%
4	8.576	1115	1126	1142	rBV2	221825	541119	7.12%	1.647%
5	9.100	1205	1215	1229	rBV	656438	1341470	17.65%	4.084%
6	10.565	1455	1464	1473	rBV	889318	1661459	21.86%	5.058%
7	11.870	1678	1686	1695	rBV	1005057	1829551	24.08%	5.569%
8	11.964	1695	1702	1710	rVV	406425	676661	8.90%	2.060%
9	12.070	1712	1720	1731	rVV	152719	308787	4.06%	0.940%
10	12.400	1766	1776	1786	rBV	105856	195726	2.58%	0.596%
11	12.694	1821	1826	1835	rVB	85053	151468	1.99%	0.461%
12	12.853	1846	1853	1863	rVB	730719	1253509	16.50%	3.816%
13	13.100	1889	1895	1897	rVV	112456	171573	2.26%	0.522%
14	13.129	1897	1900	1904	rVV	131572	241555	3.18%	0.735%
15	13.170	1904	1907	1920	rVB2	128667	239186	3.15%	0.728%
16	13.335	1927	1935	1942	rBV	125508	253617	3.34%	0.772%
17	13.482	1950	1960	1966	rBV	412973	704512	9.27%	2.145%
18	13.676	1985	1993	1997	rBV3	68655	146671	1.93%	0.446%
19	13.729	1997	2002	2007	rVV	64170	145210	1.91%	0.442%
20	13.794	2007	2013	2022	rVV2	1143162	2194329	28.88%	6.680%
21	13.858	2022	2024	2032	rVB	73549	100120	1.32%	0.305%
22	13.953	2033	2040	2042	rBV	138779	216624	2.85%	0.659%
23	13.994	2042	2047	2060	rVV	1606908	3016558	39.70%	9.183%
24	14.105	2061	2066	2072	rVV4	67193	122218	1.61%	0.372%
25	14.276	2092	2095	2099	rVV2	68218	97263	1.28%	0.296%
26	14.329	2099	2104	2111	rVB	197858	298889	3.93%	0.910%
27	14.447	2118	2124	2134	rBV	197351	391051	5.15%	1.190%
28	14.658	2151	2160	2163	rVV3	82413	183062	2.41%	0.557%
29	14.694	2163	2166	2170	rVV	114433	158040	2.08%	0.481%
30	14.735	2170	2173	2178	rVB2	60919	79483	1.05%	0.242%
31	14.800	2179	2184	2188	rBV4	59015	102991	1.36%	0.314%
32	14.929	2200	2206	2218	rVB	423473	801523	10.55%	2.440%
33	15.052	2218	2227	2233	rBV3	385693	922487	12.14%	2.808%
34	15.117	2233	2238	2247	rVB3	161583	326943	4.30%	0.995%
35	15.205	2247	2253	2261	rBV3	348951	660523	8.69%	2.011%
36	15.317	2261	2272	2279	rBV3	140490	339601	4.47%	1.034%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010224\
Data File : VN080629.D
Acq On : 02 Jan 2024 16:54
Operator : JC\MD
Sample : 06038-01
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
T-402

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_N\methods\82N122723W.M
Title : SW846 8260

37	15.435	2287	2292	2299	rVB6	52179	121052	1.59%	0.369%
38	15.641	2320	2327	2338	rVB	3954194	7598960	100.00%	23.132%
39	15.747	2340	2345	2350	rBV3	70529	134864	1.77%	0.411%
40	15.947	2372	2379	2383	rBV6	37555	100015	1.32%	0.304%
41	16.146	2407	2413	2418	rBV2	74936	163130	2.15%	0.497%
42	16.276	2428	2435	2452	rVB6	89000	379349	4.99%	1.155%
43	16.570	2482	2485	2500	rVB4	38531	121651	1.60%	0.370%
44	16.782	2512	2521	2522	rBV	1799522	2768849	36.44%	8.429%

Sum of corrected areas: 32849905

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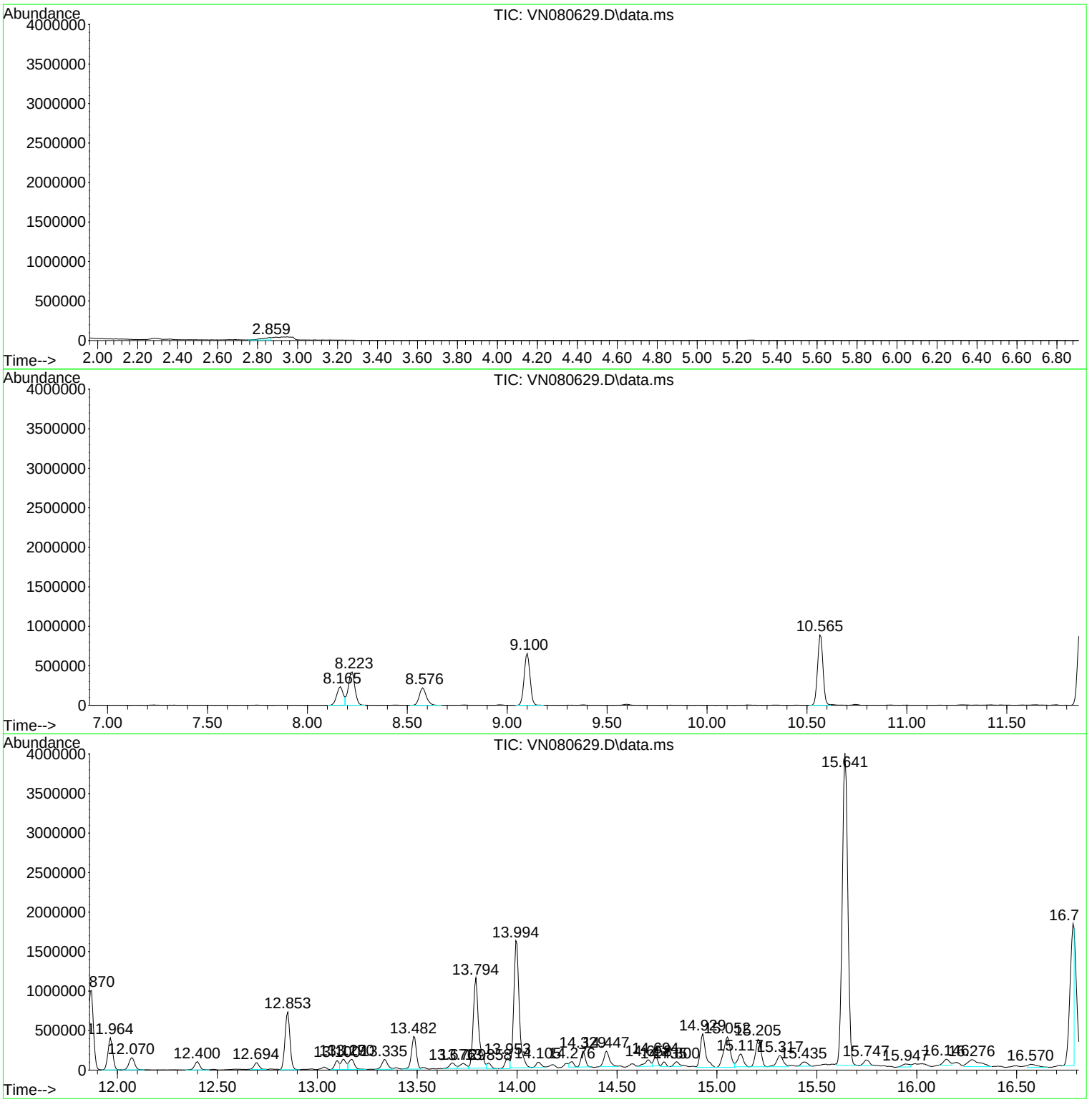
Instrument :
MSVOA_N
ClientSampleId :
T-402

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122723W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010224\
Data File : VN080629.D
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Operator : JC\MD
Sample : 06038-01
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
T-402

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122723W.M
Quant Title : SW846 8260

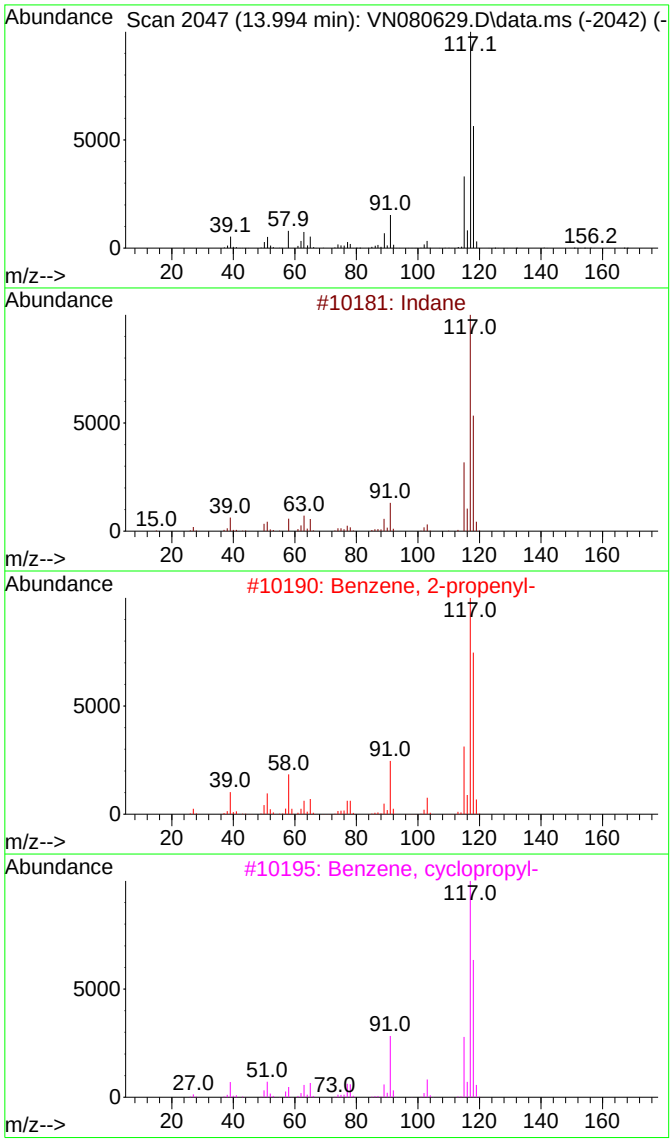
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

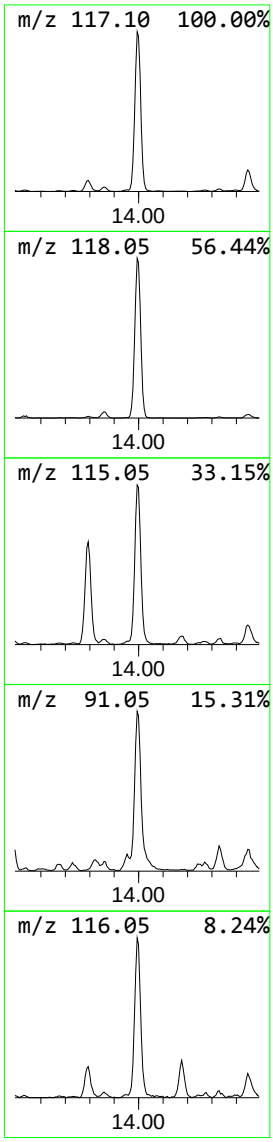
****

Peak Number 1 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	68.74 ug/l	3016560	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	93
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	72
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	72
4	7-Methylenecycloocta-1,3,5-triene	118	C9H10	002570-13-0	59
5	Indan, 1-methyl-	132	C10H12	000767-58-8	59





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Data File : VN080629.D
Acq On : 02 Jan 2024 16:54
Operator : JC\MD
Sample : 06038-01
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
T-402

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122723W.M
Quant Title : SW846 8260

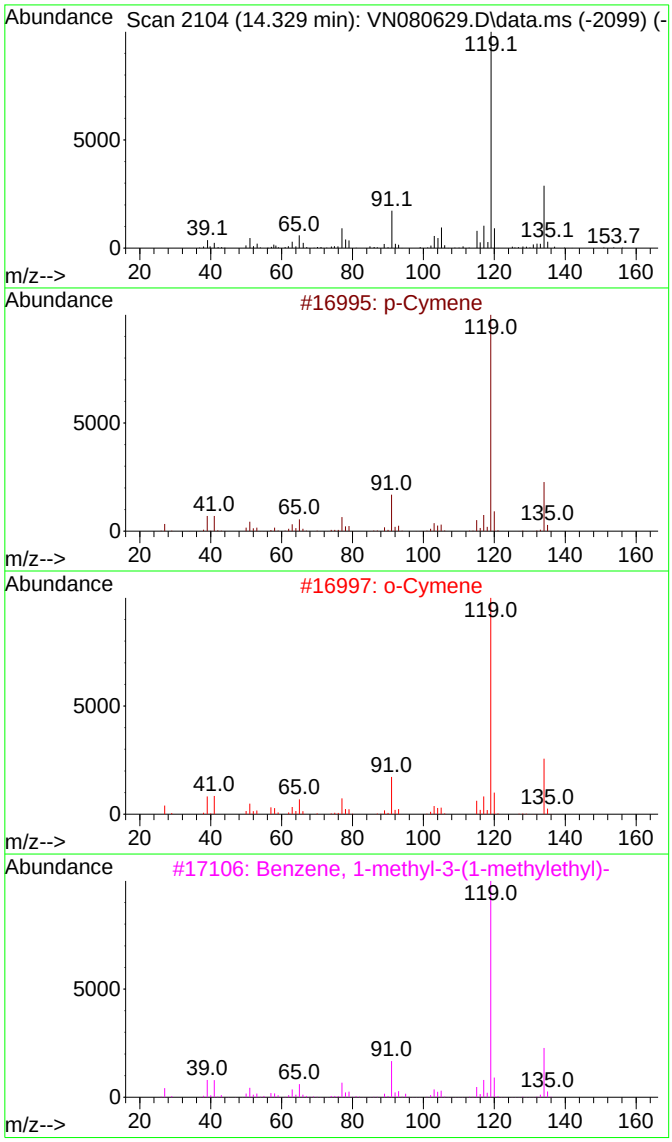
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

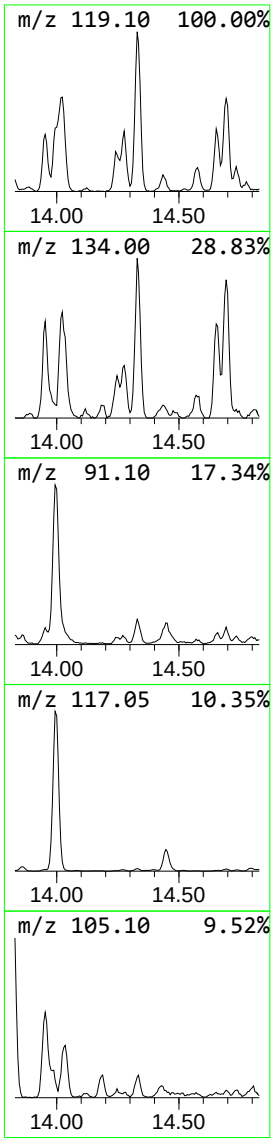
****

Peak Number 2 p-Cymene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.329	6.81 ug/l	298889	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	p-Cymene	134	C10H14	000099-87-6	95
2	o-Cymene	134	C10H14	000527-84-4	95
3	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94
4	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	93
5	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010224\
Data File : VN080629.D
Acq On : 02 Jan 2024 16:54
Operator : JC\MD
Sample : 06038-01
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
T-402

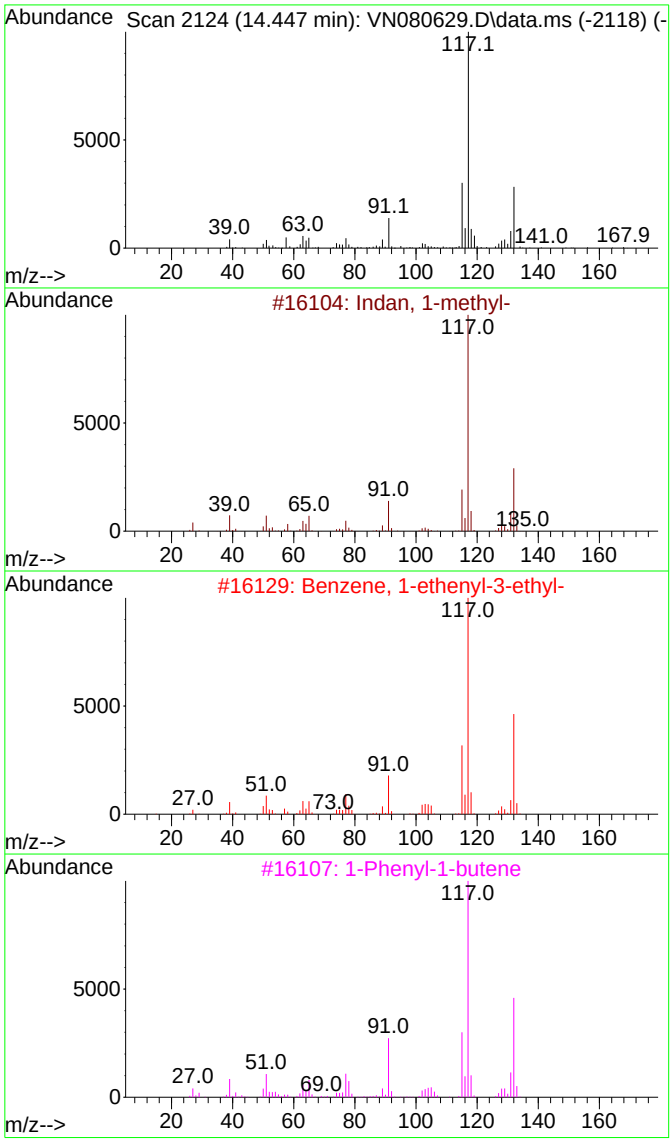
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122723W.M
Quant Title : SW846 8260

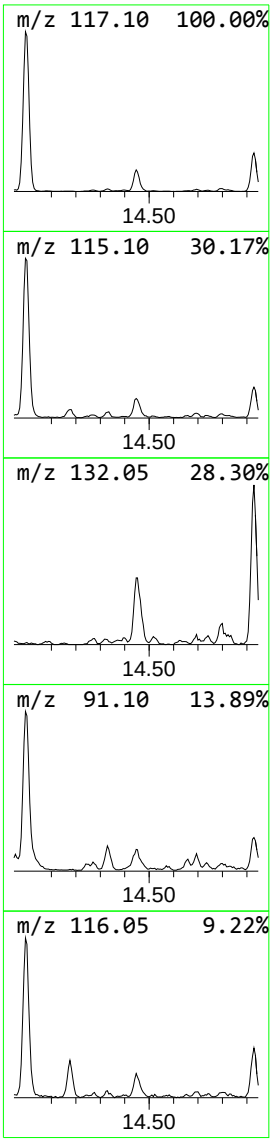
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Indan, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.447	8.91 ug/l	391051	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indan, 1-methyl-	132	C10H12	000767-58-8	87
2	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	86
3	1-Phenyl-1-butene	132	C10H12	000824-90-8	83
4	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	80
5	1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	80





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010224\
Data File : VN080629.D
Acq On : 02 Jan 2024 16:54
Operator : JC\MD
Sample : 06038-01
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
T-402

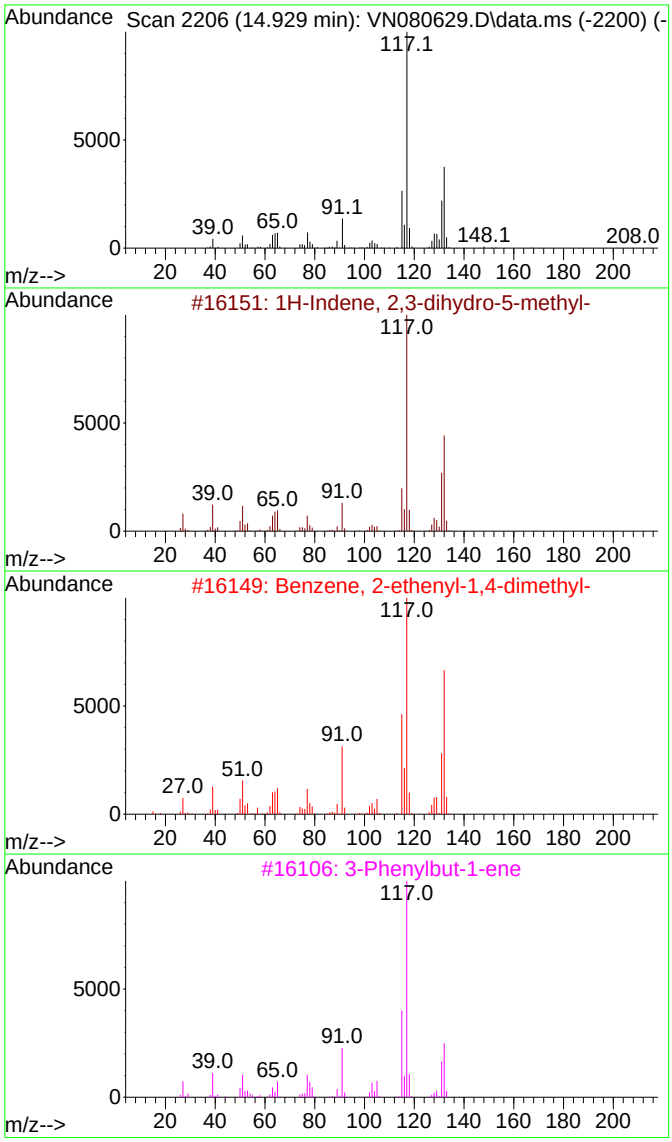
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122723W.M
Quant Title : SW846 8260

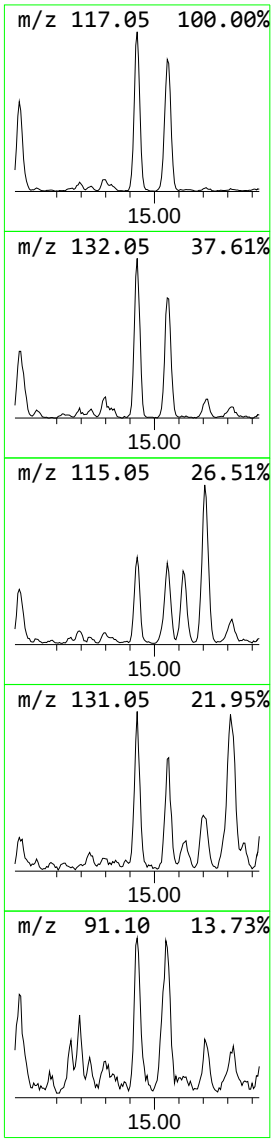
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.929	18.26 ug/l	801523	1,4-Dichlorobenzene-d4	13.794

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-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	92
3	3-Phenylbut-1-ene	132	C10H12	000934-10-1	91
4	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	90
5	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010224\
Data File : VN080629.D
Acq On : 02 Jan 2024 16:54
Operator : JC\MD
Sample : 06038-01
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
T-402

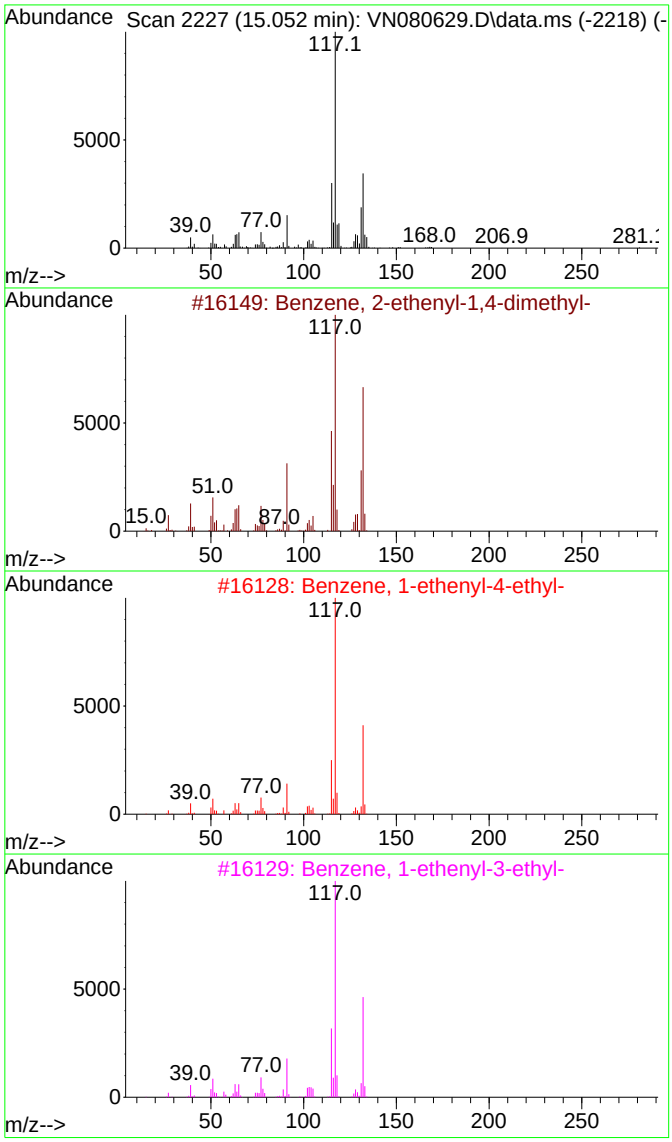
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122723W.M
Quant Title : SW846 8260

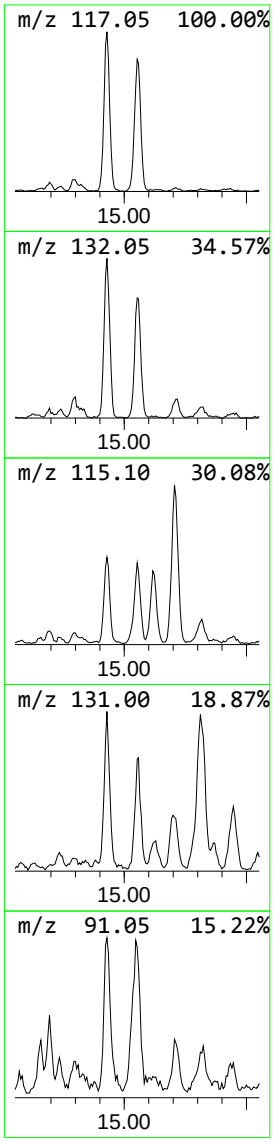
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.053	21.02 ug/l	922487	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
3	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
4	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	91
5	Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010224\
Data File : VN080629.D
Acq On : 02 Jan 2024 16:54
Operator : JC\MD
Sample : 06038-01
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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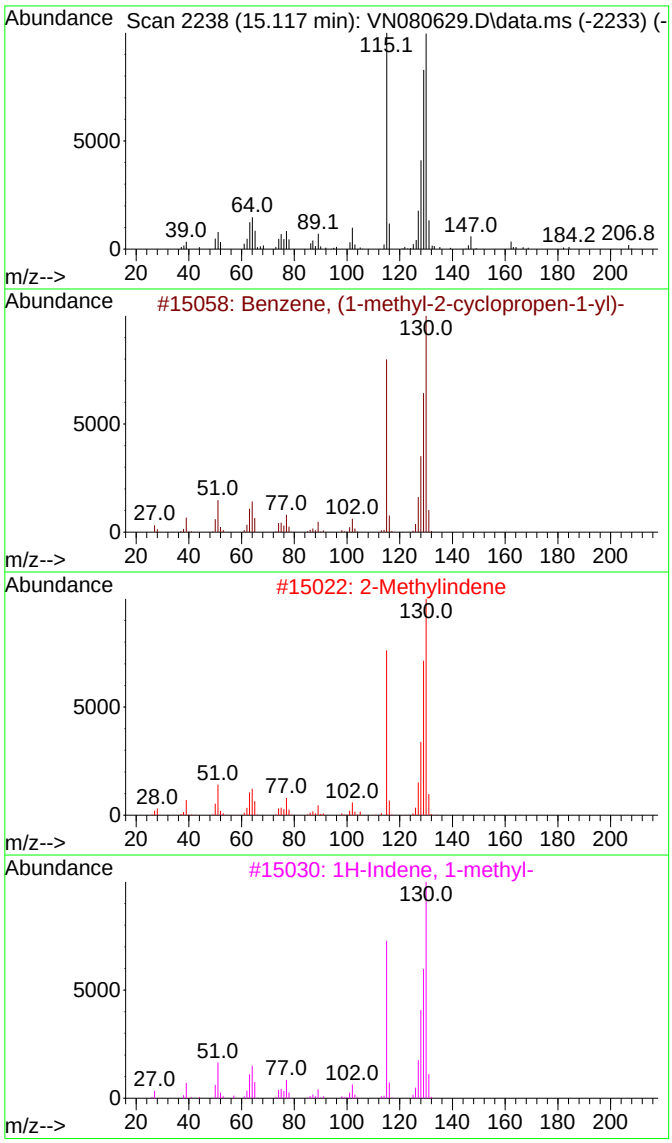
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122723W.M
Quant Title : SW846 8260

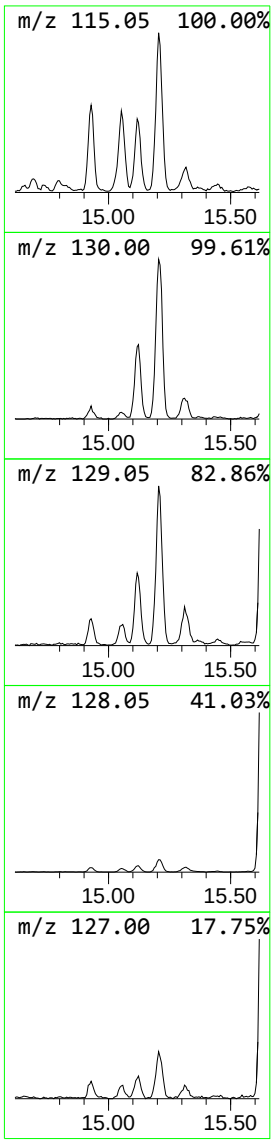
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, (1-methyl-2-cyclop... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.117	7.45 ug/l	326943	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	96
2	2-Methylindene	130	C10H10	002177-47-1	95
3	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	93
4	Benzene, 1-butynyl-	130	C10H10	000622-76-4	91
5	Tetracyclo[5.3.0.0<2,6>.0<3,10>]...	130	C10H10	034324-40-8	90





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Data File : VN080629.D
Acq On : 02 Jan 2024 16:54
Operator : JC\MD
Sample : 06038-01
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
T-402

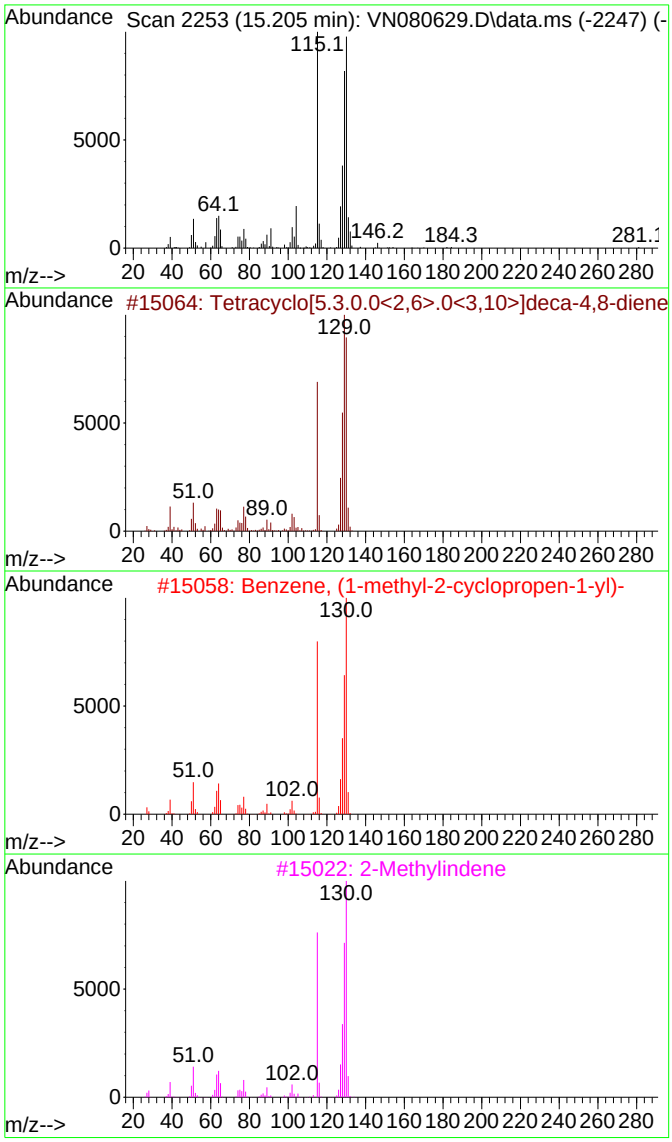
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122723W.M
Quant Title : SW846 8260

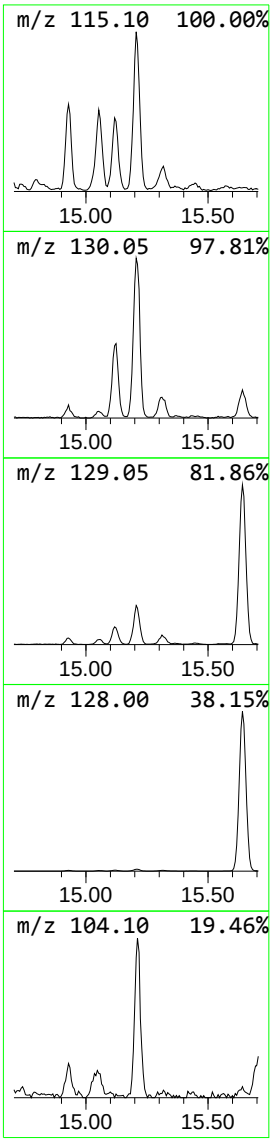
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Tetracyclo[5.3.0.0<2,6>.0<3... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.205	15.05 ug/l	660523	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracyclo[5.3.0.0<2,6>.0<3,10>]...	130	C10H10	034324-40-8	96
2	Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	96
3	2-Methylindene	130	C10H10	002177-47-1	95
4	1H-Indene, 3-methyl-	130	C10H10	000767-60-2	95
5	Benzene, 1-butynyl-	130	C10H10	000622-76-4	95





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010224\
Data File : VN080629.D
Acq On : 02 Jan 2024 16:54
Operator : JC\MD
Sample : 06038-01
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
T-402

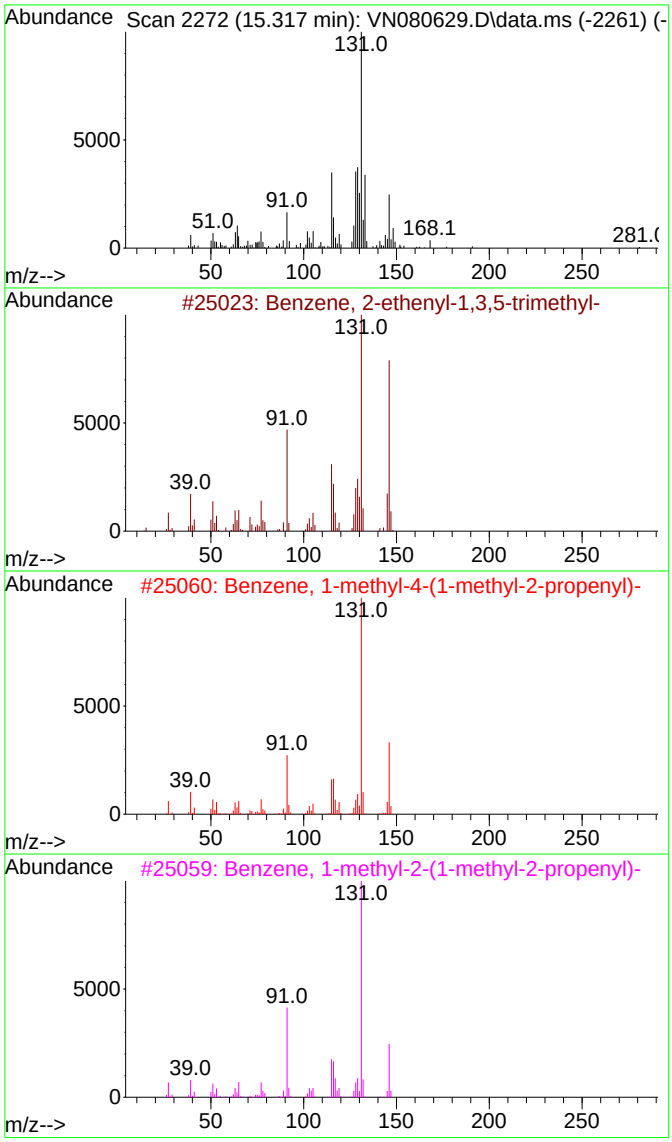
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122723W.M
Quant Title : SW846 8260

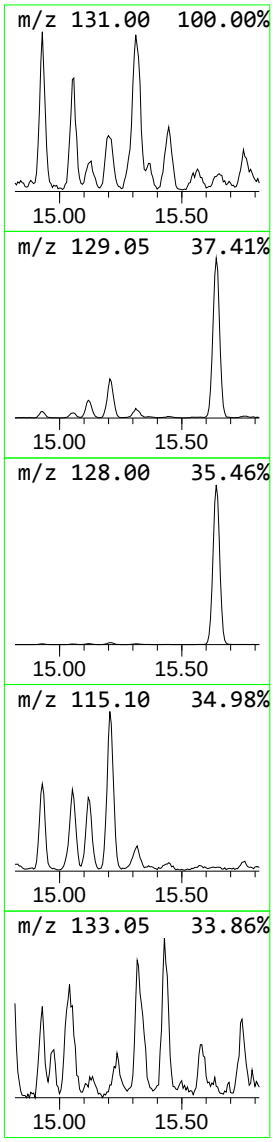
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 2-ethenyl-1,3,5-tr... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.317	7.74 ug/l	339601	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	64
2	Benzene, 1-methyl-4-(1-methyl-2-...	146	C11H14	097664-18-1	60
3	Benzene, 1-methyl-2-(1-methyl-2-...	146	C11H14	097664-19-2	53
4	Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	53
5	Benzene, 1,3-bis(1-buten-3-yl-)-	186	C14H18	158117-62-5	50





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Data File : VN080629.D
Acq On : 02 Jan 2024 16:54
Operator : JC\MD
Sample : 06038-01
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
T-402

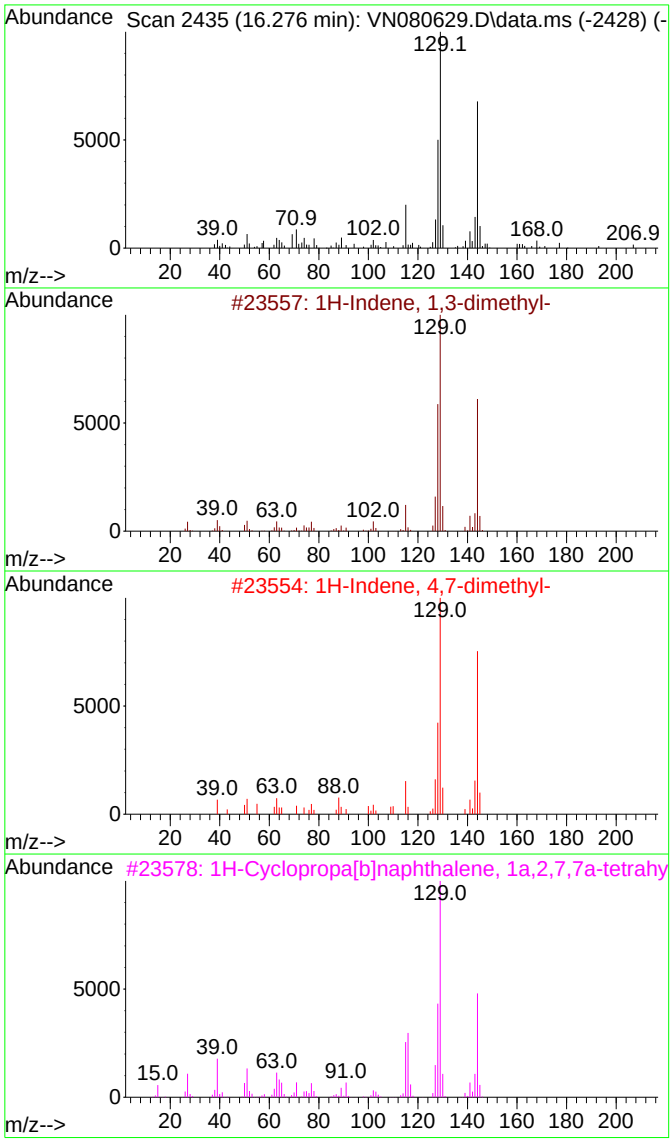
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122723W.M
Quant Title : SW846 8260

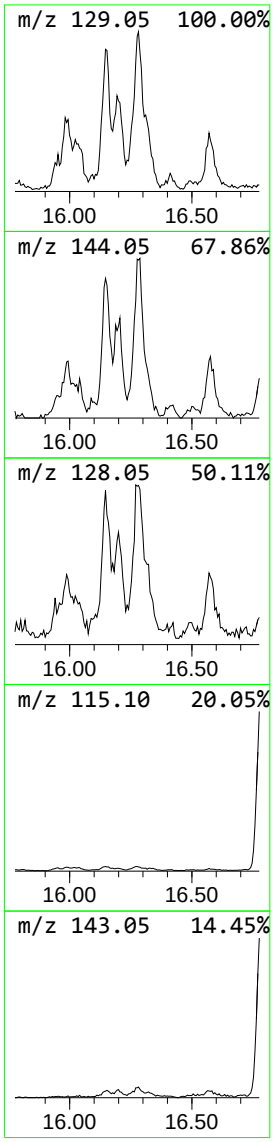
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1H-Indene, 1,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.276	8.64 ug/l	379349	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 1,3-dimethyl-	144	C11H12	002177-48-2	95
2	1H-Indene, 4,7-dimethyl-	144	C11H12	006974-97-6	93
3	1H-Cyclopropa[b]naphthalene, 1a,...	144	C11H12	006571-72-8	91
4	Naphthalene, 1,2-dihydro-4-methyl-	144	C11H12	004373-13-1	90
5	1H-Indene, 1-ethenyl-2,3-dihydro-	144	C11H12	051783-46-1	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010224\
Data File : VN080629.D
Acq On : 02 Jan 2024 16:54
Operator : JC\MD
Sample : 06038-01
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
T-402

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122723W.M
Quant Title : SW846 8260

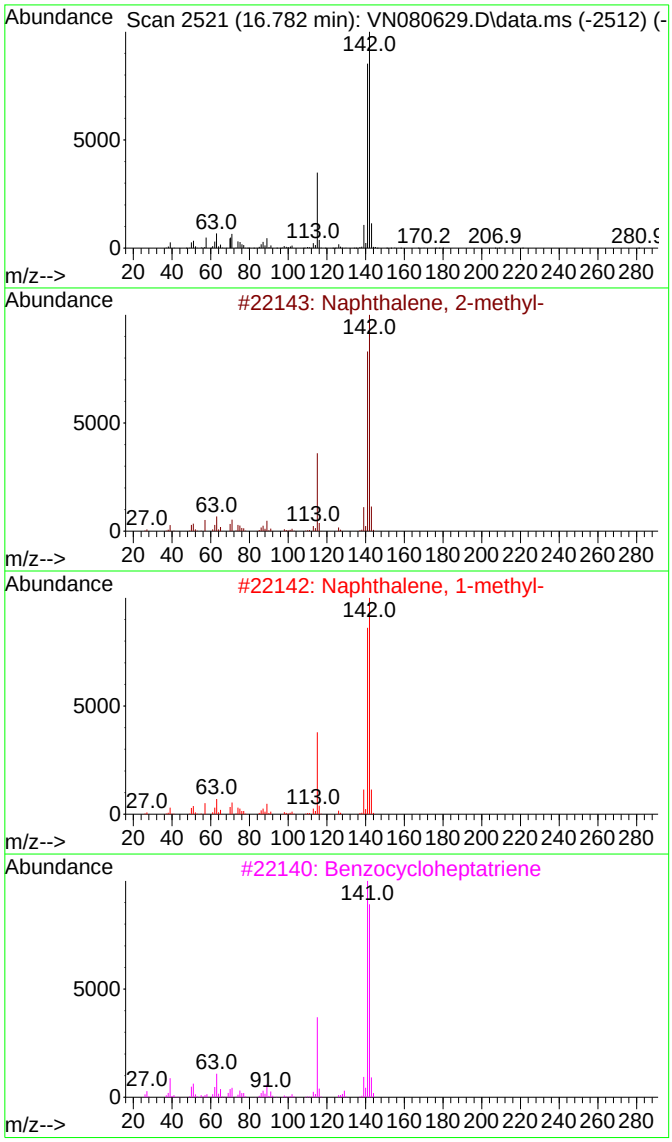
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

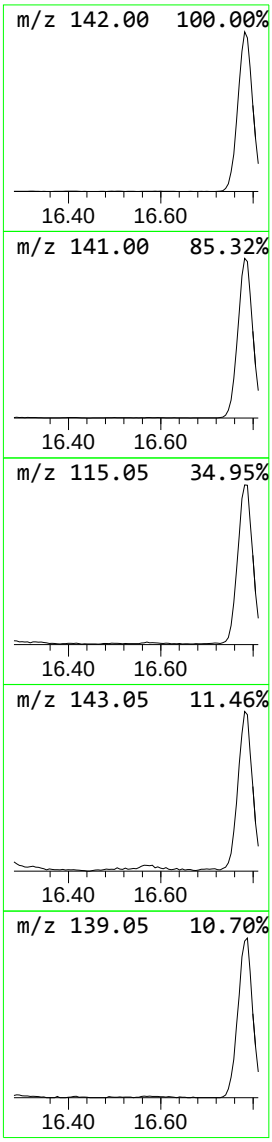
****

Peak Number 10 Naphthalene, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.782	63.09 ug/l	2768850	1,4-Dichlorobenzene-d4	13.794

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	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	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010224\
Data File : VN080629.D
Acq On : 02 Jan 2024 16:54
Operator : JC\MD
Sample : 06038-01
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
T-402

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122723W.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	13.994	68.7	ug/l	3016560	4	13.794	2194330	50.0
p-Cymene	14.329	6.8	ug/l	298889	4	13.794	2194330	50.0
Indan, 1-methyl-	14.447	8.9	ug/l	391051	4	13.794	2194330	50.0
1H-Indene, 2,3-...	14.929	18.3	ug/l	801523	4	13.794	2194330	50.0
Benzene, 2-ethe...	15.053	21.0	ug/l	922487	4	13.794	2194330	50.0
Benzene, (1-met...	15.117	7.5	ug/l	326943	4	13.794	2194330	50.0
Tetracyclo[5.3....	15.205	15.1	ug/l	660523	4	13.794	2194330	50.0
Benzene, 2-ethe...	15.317	7.7	ug/l	339601	4	13.794	2194330	50.0
1H-Indene, 1,3-...	16.276	8.6	ug/l	379349	4	13.794	2194330	50.0
Naphthalene, 2-...	16.782	63.1	ug/l	2768850	4	13.794	2194330	50.0