LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082273.D
Acq On : 22 May 2024 05:09
Operator : JC\MD
Sample : P2494-13 40X
Misc : 5.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
13

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\82N051524W.M
Title : SW846 8260

Signal : TIC: VN082273.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.171	1046	1057	1061	rBV	160032	386682	8.94%	1.963%
2	8.224	1061	1066	1079	rVB	300520	675654	15.62%	3.429%
3	8.582	1117	1127	1140	rBV	201056	483617	11.18%	2.455%
4	9.100	1206	1215	1227	rBV	449377	918780	21.24%	4.663%
5	10.571	1456	1465	1471	rBV	686940	1290149	29.83%	6.548%
6	10.629	1471	1475	1486	rVB	89721	165818	3.83%	0.842%
7	11.865	1678	1685	1696	rBV	638093	1139928	26.36%	5.786%
8	11.965	1696	1702	1708	rBV	36011	62374	1.44%	0.317%
9	12.065	1713	1719	1730	rVB	193002	363441	8.40%	1.845%
10	12.400	1764	1776	1783	rBV	189695	353737	8.18%	1.795%
11	12.623	1796	1814	1817	rBV7	26335	110420	2.55%	0.560%
12	12.847	1846	1852	1863	rVB	503944	892634	20.64%	4.531%
13	13.100	1889	1895	1899	rBV	75187	142086	3.29%	0.721%
14	13.170	1902	1907	1914	rVB2	154893	285865	6.61%	1.451%
15	13.335	1921	1935	1943	rBV4	84185	295992	6.84%	1.502%
16	13.482	1954	1960	1965	rBV	268928	427937	9.90%	2.172%
17	13.529	1965	1968	1973	rVB2	34376	52255	1.21%	0.265%
18	13.670	1973	1992	2007	rBV3	147776	790852	18.29%	4.014%
19	13.794	2007	2013	2023	rBV2	611812	1223584	28.29%	6.210%
20	14.017	2033	2051	2059	rBV5	233111	901027	20.83%	4.573%
21	14.106	2060	2066	2073	rVV2	174564	422295	9.76%	2.143%
22	14.176	2073	2078	2085	rVB2	185493	336957	7.79%	1.710%
23	14.247	2085	2090	2091	rBV	34221	44670	1.03%	0.227%
24	14.329	2100	2104	2108	rVB2	40041	58208	1.35%	0.295%
25	14.441	2117	2123	2127	rBV4	45477	95736	2.21%	0.486%
26	14.629	2151	2155	2157	rBV3	39084	58762	1.36%	0.298%
27	14.659	2157	2160	2163	rVV2	50725	80184	1.85%	0.407%
28	14.694	2163	2166	2170	rVB	65557	83515	1.93%	0.424%
29	14.794	2177	2183	2187	rBV6	23806	51459	1.19%	0.261%
30	14.847	2187	2192	2202	rVB6	36280	110568	2.56%	0.561%
31	14.958	2202	2211	2217	rVB3	95128	185854	4.30%	0.943%
32	15.035	2218	2224	2234	rBV5	102072	344748	7.97%	1.750%
33	15.206	2248	2253	2260	rVB4	46104	88155	2.04%	0.447%
34	15.317	2267	2272	2280	rVV6	38963	90081	2.08%	0.457%
35	15.435	2287	2292	2298	rVB7	36670	83515	1.93%	0.424%
36	15.641	2314	2327	2338	rBV	2222764	4324698	100.00%	21.950%

LSC Area Percent Report

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Sample : P2494-13 40X
Misc : 5.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
13

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\82N051524W.M
Title : SW846 8260

37	15.747	2339	2345	2350	rVB2	55633	112103	2.59%	0.569%
38	15.829	2356	2359	2370	rVB6	50751	115637	2.67%	0.587%
39	15.947	2371	2379	2384	rBV7	29732	82205	1.90%	0.417%
40	16.111	2400	2407	2414	rVB8	22204	68158	1.58%	0.346%
41	16.253	2423	2431	2441	rVB10	30364	84057	1.94%	0.427%
42	16.494	2463	2472	2477	rBV10	21480	63007	1.46%	0.320%
43	16.717	2503	2510	2512	rBV4	26873	54864	1.27%	0.278%
44	16.782	2513	2521	2522	rBV	1080632	1700482	39.32%	8.631%

Sum of corrected areas: 19702750

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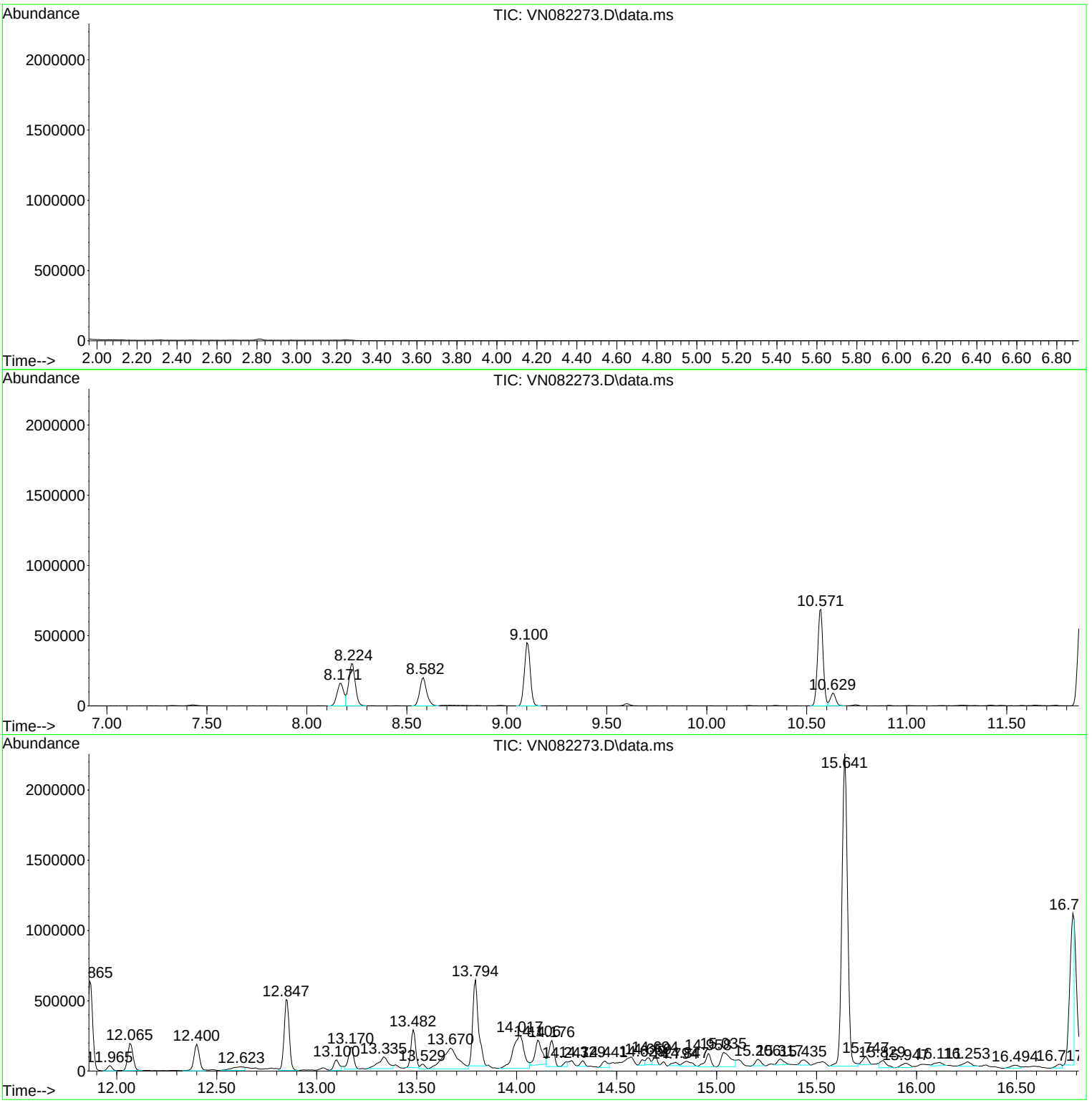
MSVOA_N
ClientSampleId :
13

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082273.D
Acq On : 22 May 2024 05:09
Operator : JC\MD
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Misc : 5.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
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Instrument :
MSVOA_N
ClientSampleId :
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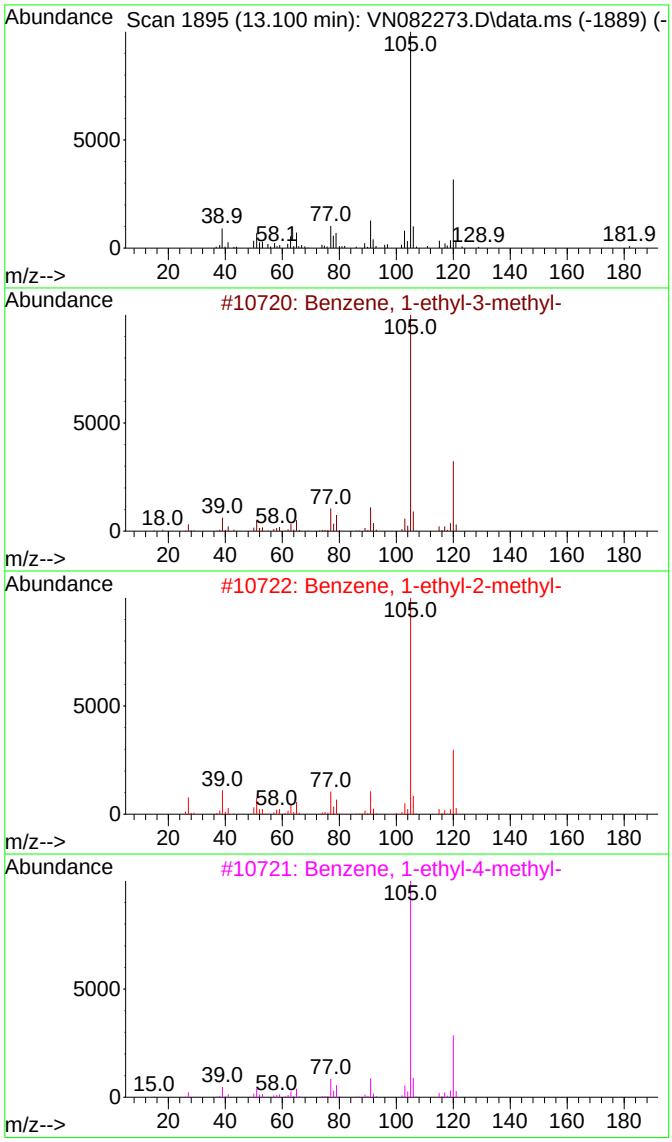
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

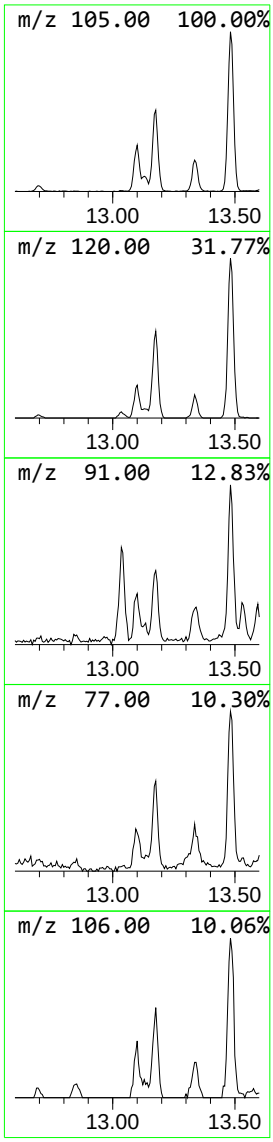
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.100	5.81 ug/l	142086	1,4-Dichlorobenzene-d4	13.794

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	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5	Mesitylene	120	C9H12	000108-67-8	90





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Data File : VN082273.D
Acq On : 22 May 2024 05:09
Operator : JC\MD
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Misc : 5.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
13

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

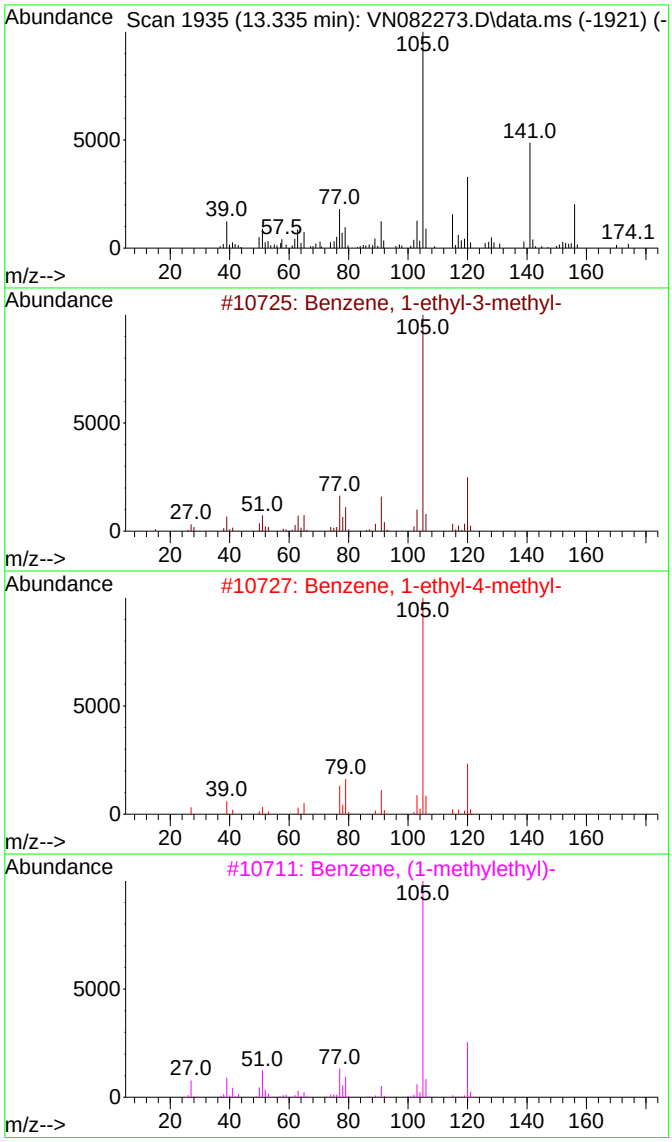
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

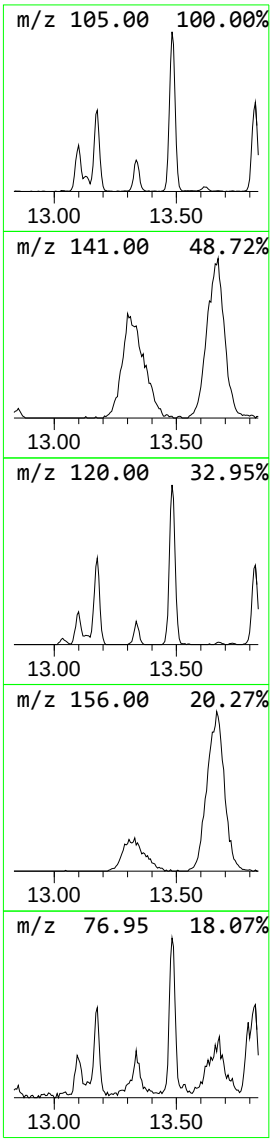
****

Peak Number 2 unknown13.335 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	12.10 ug/l	295992	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	46
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	46
3	Benzene, (1-methylethyl)-	120	C9H12	000098-82-8	42
4	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	42
5	2,4-Nonadiyne	120	C9H12	063621-15-8	38





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Data File : VN082273.D
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Operator : JC\MD
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Misc : 5.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
13

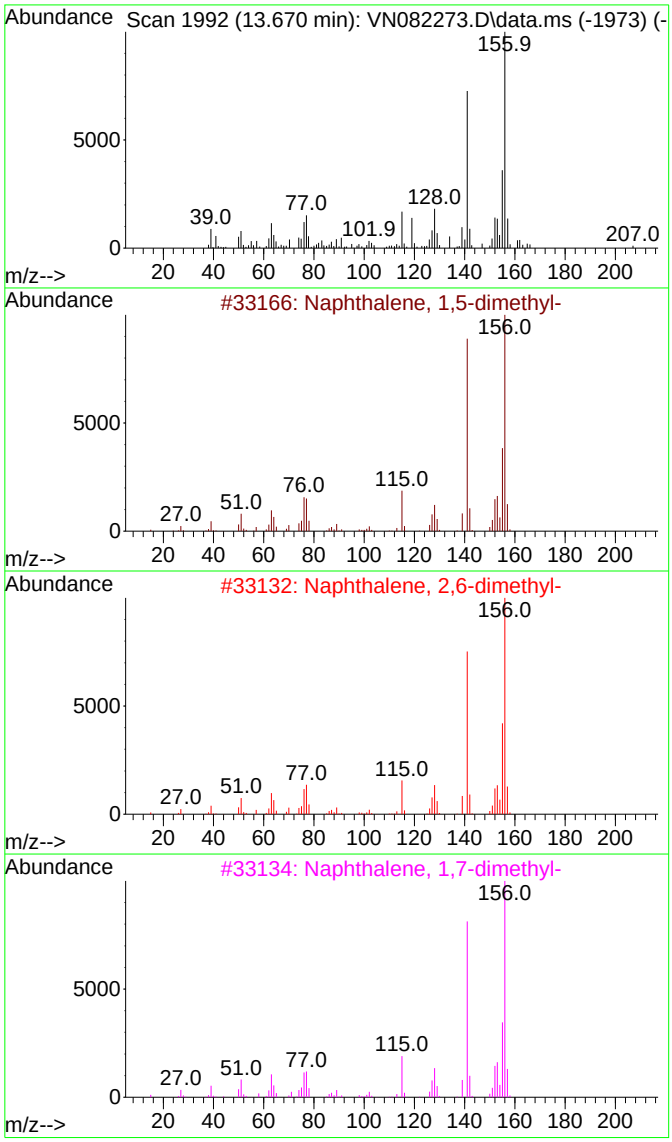
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

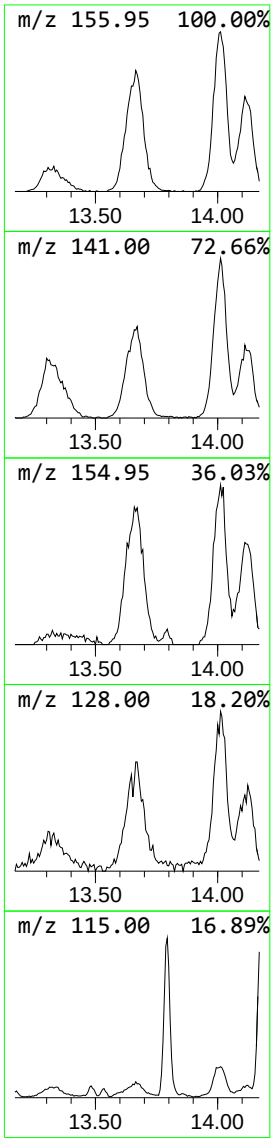
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Naphthalene, 1,5-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.670	32.32 ug/l	790852	1,4-Dichlorobenzene-d4	13.794

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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082273.D
Acq On : 22 May 2024 05:09
Operator : JC\MD
Sample : P2494-13 40X
Misc : 5.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
13

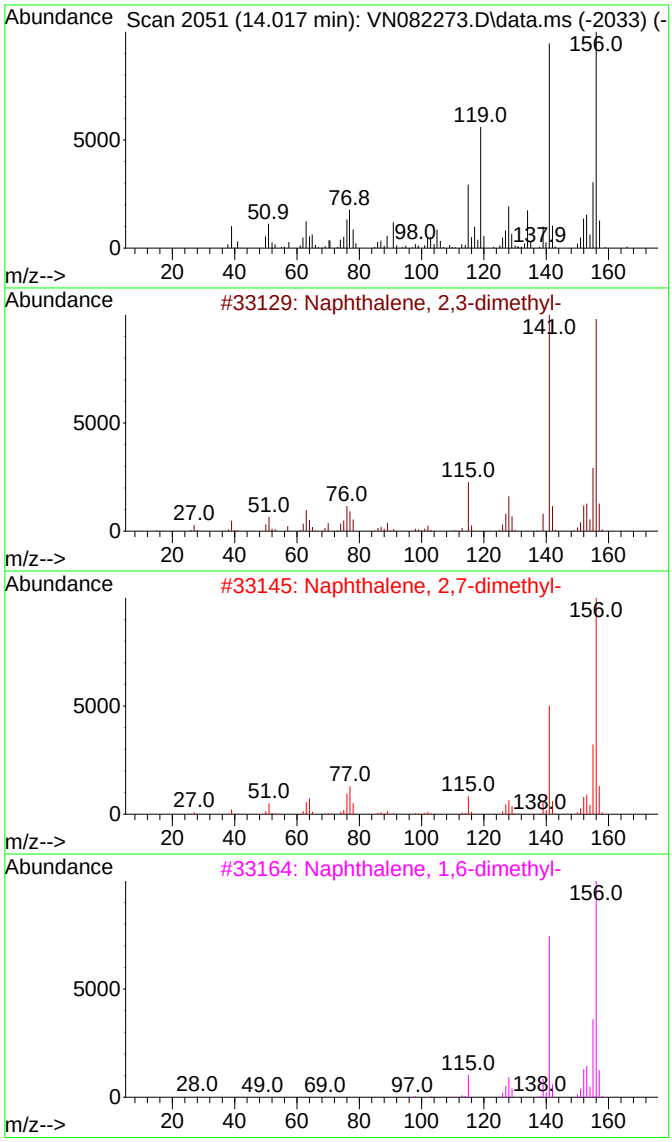
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

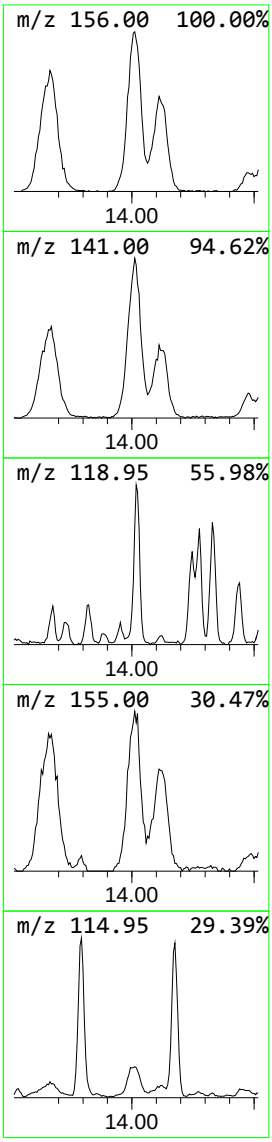
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Naphthalene, 2,3-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.017	36.82 ug/l	901027	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
3	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
4	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	96
5	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	95





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Data File : VN082273.D
Acq On : 22 May 2024 05:09
Operator : JC\MD
Sample : P2494-13 40X
Misc : 5.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
13

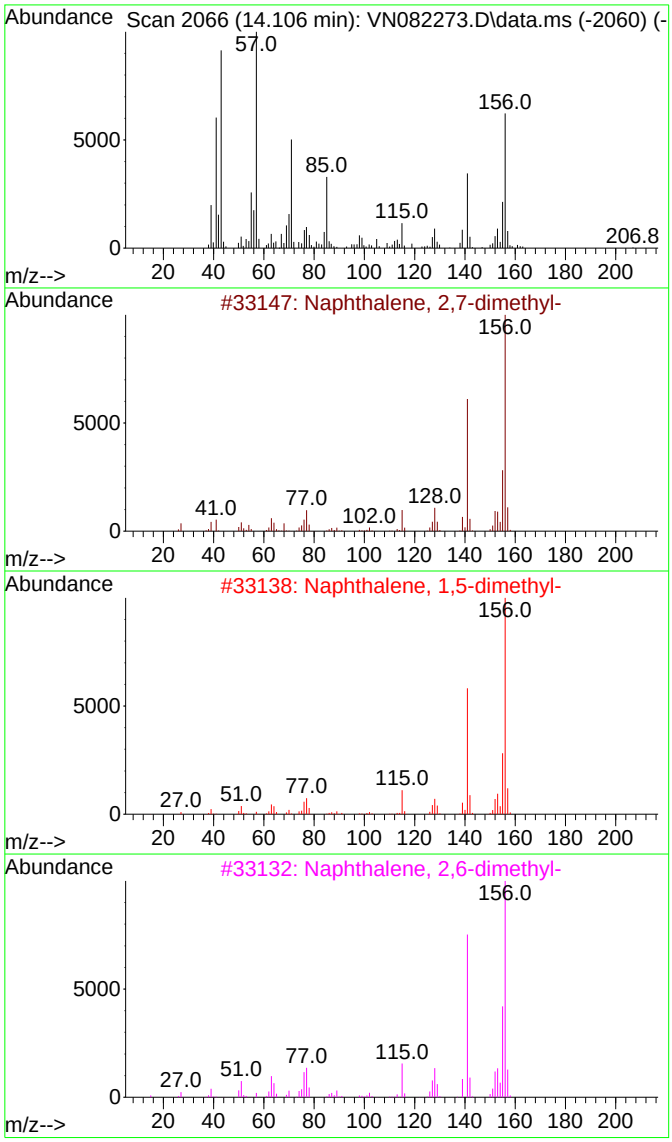
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

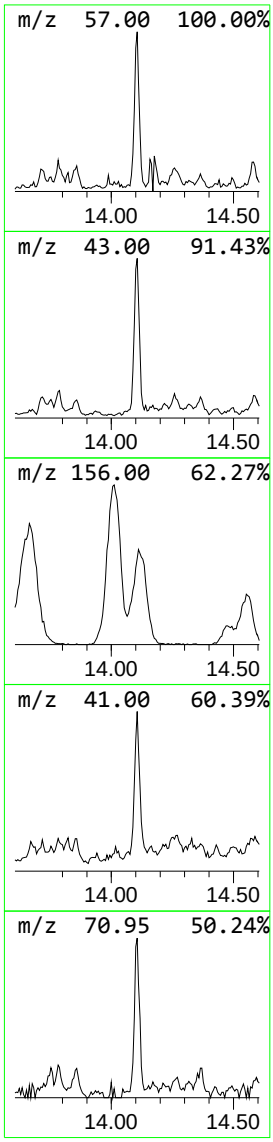
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Naphthalene, 2,7-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.106	17.26 ug/l	422295	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	91
2	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	91
3	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	90
4	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	86
5	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	86





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ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

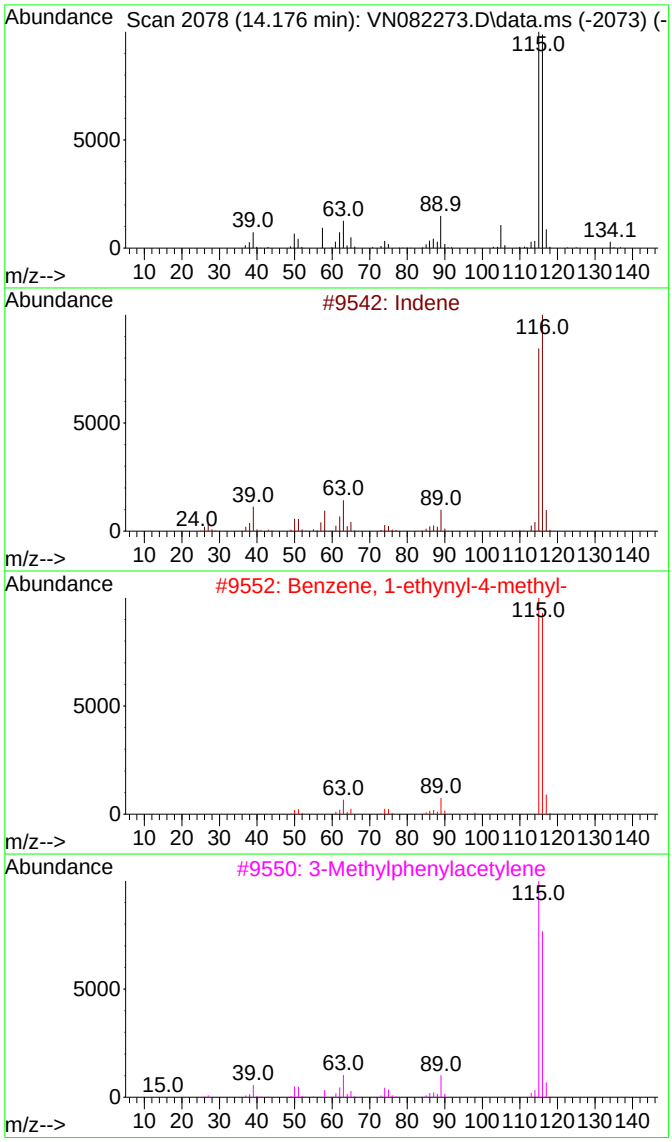
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

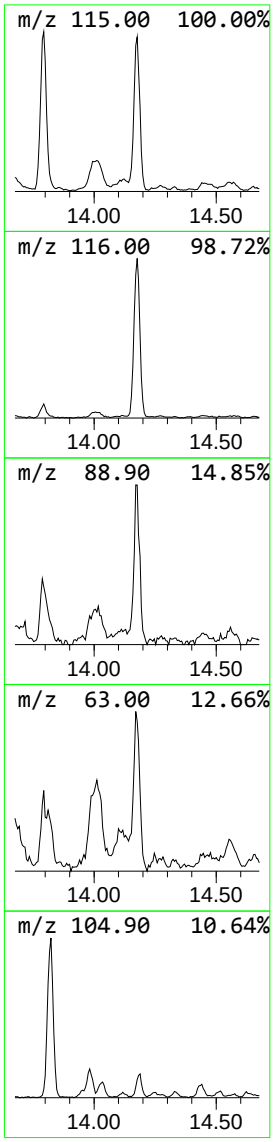
****

Peak Number 6 Indene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.176	13.77 ug/l	336957	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene	116	C9H8	000095-13-6	95
2	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	91
3	3-Methylphenylacetylene	116	C9H8	000766-82-5	91
4	Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91
5	Benzene, 1-propynyl-	116	C9H8	000673-32-5	90





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MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

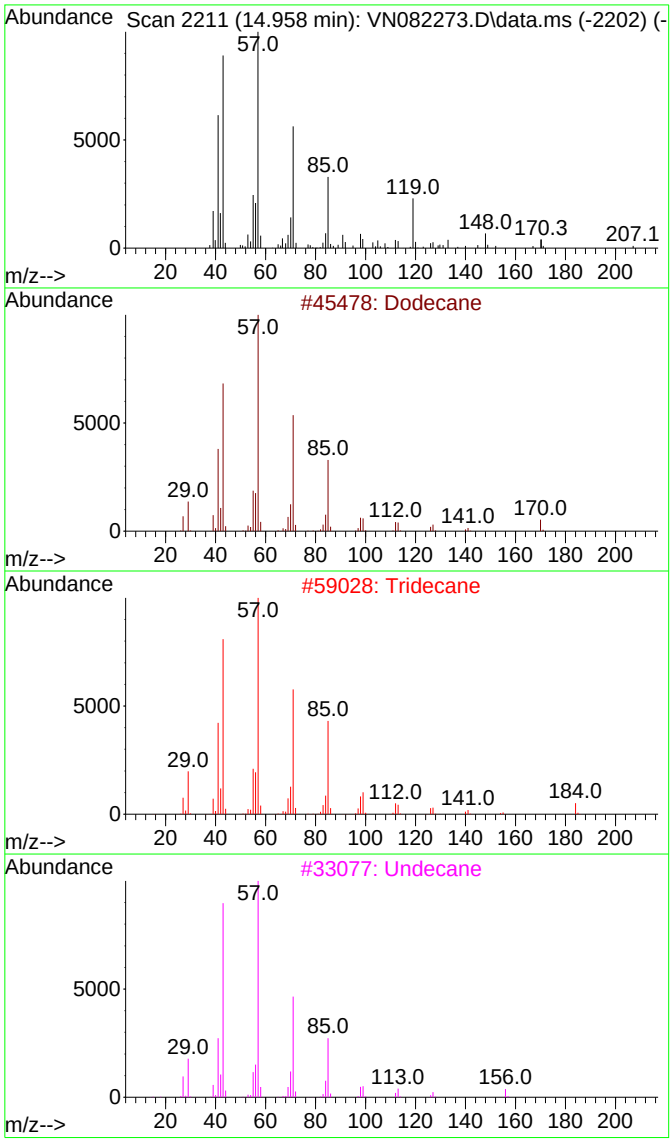
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

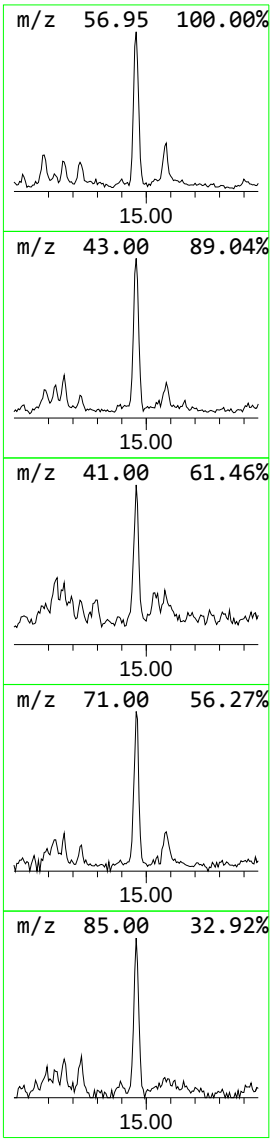
****

Peak Number 7 Dodecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.959	7.59 ug/l	185854	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	92
2	Tridecane	184	C13H28	000629-50-5	58
3	Undecane	156	C11H24	001120-21-4	50
4	Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	50
5	3,5-Dimethyldodecane	198	C14H30	107770-99-0	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082273.D
Acq On : 22 May 2024 05:09
Operator : JC\MD
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ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
13

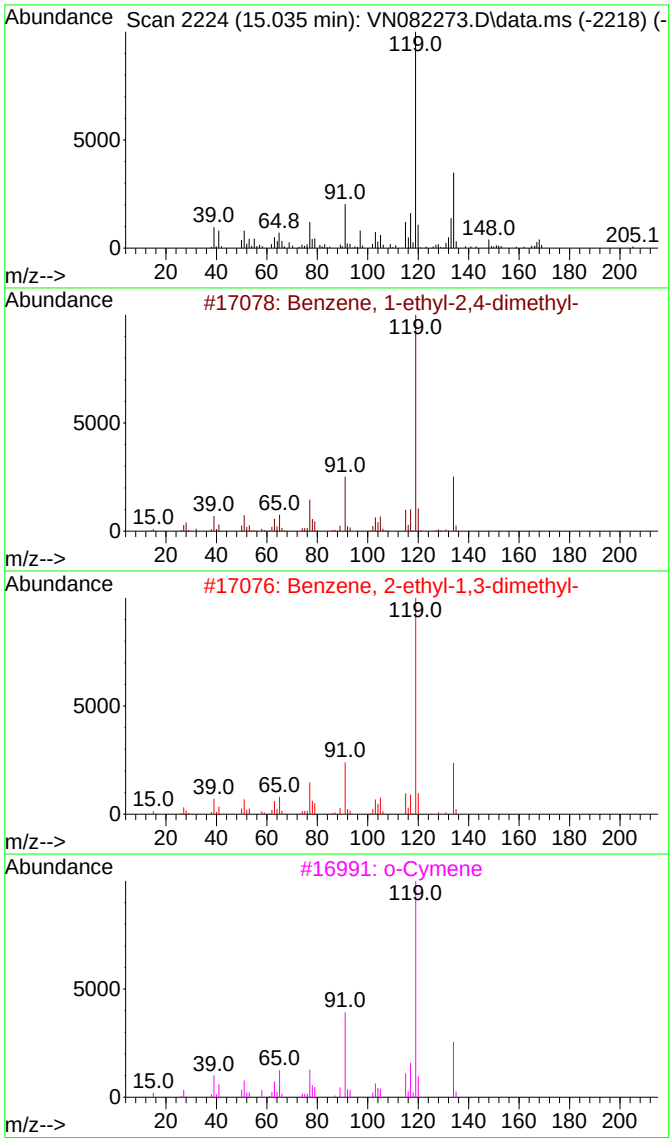
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

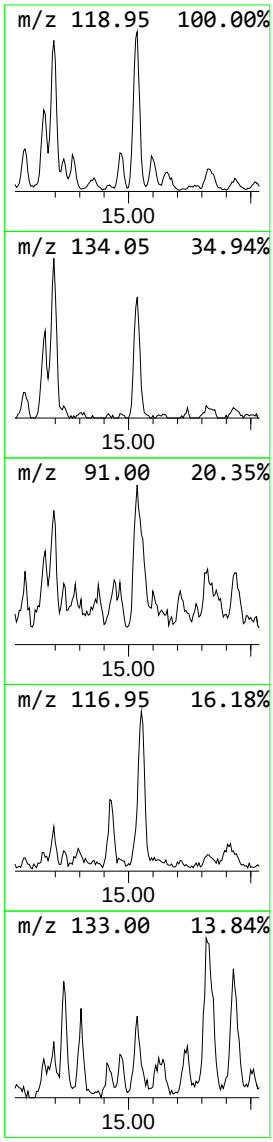
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.035	14.09 ug/l	344748	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	95
2	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	93
3	o-Cymene	134	C10H14	000527-84-4	87
4	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	87
5	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	87





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082273.D
Acq On : 22 May 2024 05:09
Operator : JC\MD
Sample : P2494-13 40X
Misc : 5.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
13

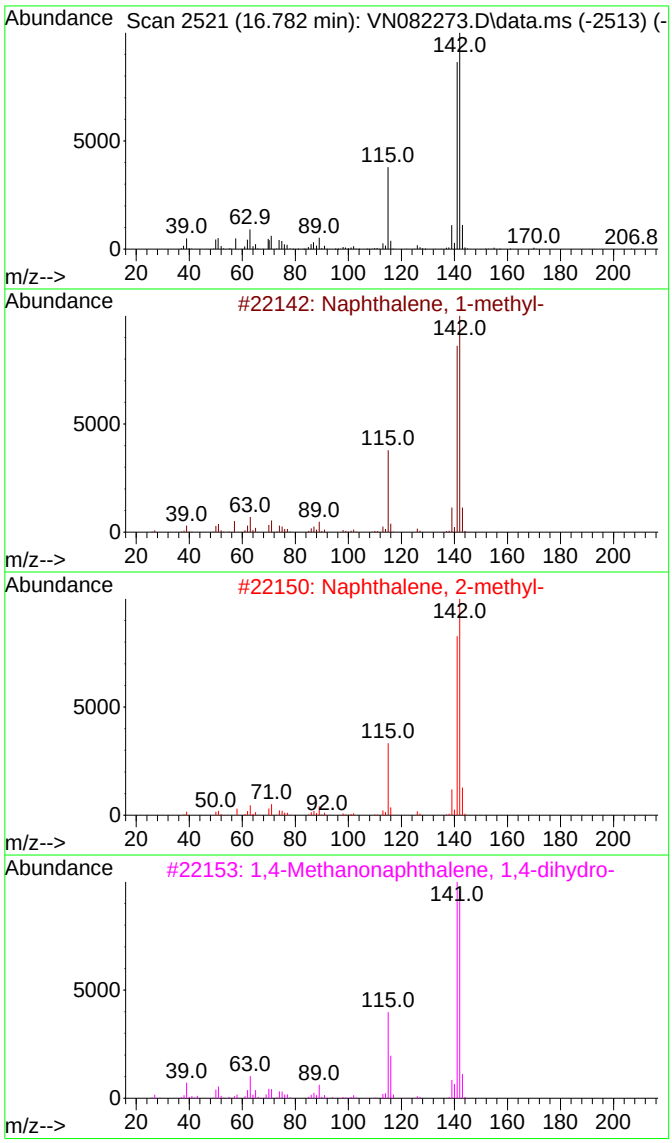
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

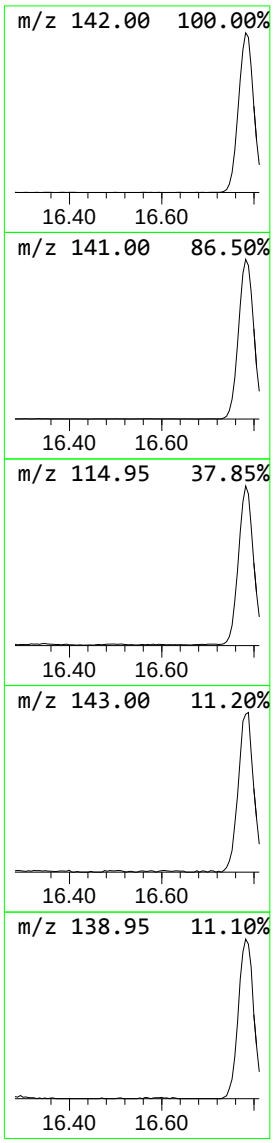
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.782	69.49 ug/l	1700480	1,4-Dichlorobenzene-d4	13.794

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	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	94
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	3,4-Difluorobenzaldehyde	142	C7H4F2O	034036-07-2	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082273.D
Acq On : 22 May 2024 05:09
Operator : JC\MD
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Misc : 5.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
13

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.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...	13.100	5.8	ug/l	142086	4	13.794	1223580	50.0
unknown13.335	13.335	12.1	ug/l	295992	4	13.794	1223580	50.0
Naphthalene, 1,...	13.670	32.3	ug/l	790852	4	13.794	1223580	50.0
Naphthalene, 2,...	14.017	36.8	ug/l	901027	4	13.794	1223580	50.0
Naphthalene, 2,...	14.106	17.3	ug/l	422295	4	13.794	1223580	50.0
Indene	14.176	13.8	ug/l	336957	4	13.794	1223580	50.0
Dodecane	14.959	7.6	ug/l	185854	4	13.794	1223580	50.0
Benzene, 1-ethy...	15.035	14.1	ug/l	344748	4	13.794	1223580	50.0
Naphthalene, 1-...	16.782	69.5	ug/l	1700480	4	13.794	1223580	50.0