LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082274.D
Acq On : 22 May 2024 05:33
Operator : JC\MD
Sample : P2494-14 40X
Misc : 5.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
14

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: VN082274.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.165	1047	1056	1061	rBV	152329	370213	12.04%	2.233%
2	8.224	1061	1066	1079	rVB	282781	636212	20.70%	3.837%
3	8.583	1117	1127	1140	rBV	187029	458381	14.91%	2.765%
4	9.100	1206	1215	1226	rBV	411796	868960	28.27%	5.241%
5	10.565	1454	1464	1471	rBV	660155	1240261	40.35%	7.481%
6	10.630	1471	1475	1484	rVB	69211	126031	4.10%	0.760%
7	11.865	1677	1685	1696	rBV	619641	1108332	36.06%	6.685%
8	11.965	1696	1702	1708	rBV	26924	44594	1.45%	0.269%
9	12.065	1712	1719	1729	rBV	142053	264499	8.61%	1.595%
10	12.400	1764	1776	1785	rBV	131426	253937	8.26%	1.532%
11	12.624	1802	1814	1823	rBV3	20177	100396	3.27%	0.606%
12	12.847	1846	1852	1862	rVB	510891	875200	28.47%	5.279%
13	13.100	1889	1895	1902	rBV2	52030	118406	3.85%	0.714%
14	13.176	1902	1908	1914	rVB2	111265	207284	6.74%	1.250%
15	13.335	1920	1935	1942	rBV4	66778	247534	8.05%	1.493%
16	13.482	1953	1960	1965	rBV	190837	314918	10.25%	1.900%
17	13.529	1965	1968	1973	rVB2	26104	38881	1.26%	0.235%
18	13.676	1973	1993	2006	rBV5	126389	712316	23.18%	4.297%
19	13.794	2006	2013	2022	rVB2	598946	1157930	37.67%	6.984%
20	14.012	2033	2050	2060	rBV6	206441	788758	25.66%	4.758%
21	14.106	2060	2066	2073	rVV3	144458	365920	11.91%	2.207%
22	14.176	2074	2078	2083	rVB2	129410	220720	7.18%	1.331%
23	14.247	2085	2090	2091	rBV2	23245	33434	1.09%	0.202%
24	14.329	2100	2104	2108	rVB	29956	41380	1.35%	0.250%
25	14.441	2117	2123	2127	rBV6	33802	72372	2.35%	0.437%
26	14.570	2138	2145	2151	rVB4	54126	144822	4.71%	0.874%
27	14.629	2151	2155	2157	rBV5	30488	43631	1.42%	0.263%
28	14.659	2157	2160	2163	rVV3	38776	58249	1.90%	0.351%
29	14.694	2163	2166	2170	rVB	45273	60116	1.96%	0.363%
30	14.841	2187	2191	2202	rVB7	31812	98522	3.21%	0.594%
31	14.959	2202	2211	2217	rVB3	77858	152315	4.96%	0.919%
32	15.041	2218	2225	2234	rBV6	76731	273586	8.90%	1.650%
33	15.206	2248	2253	2260	rVB5	34072	71591	2.33%	0.432%
34	15.317	2268	2272	2280	rVB7	27838	63441	2.06%	0.383%
35	15.429	2287	2291	2299	rVB4	26910	60426	1.97%	0.364%
36	15.517	2302	2306	2314	rVB8	25644	68092	2.22%	0.411%

LSC Area Percent Report

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Operator : JC\MD
Sample : P2494-14 40X
Misc : 5.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
14

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	15.641	2315	2327	2339	rBV	1552082	3073617	100.00%	18.539%
38	15.747	2339	2345	2350	rVB3	41482	79840	2.60%	0.482%
39	15.829	2356	2359	2371	rVB6	50380	110998	3.61%	0.670%
40	15.947	2371	2379	2386	rBV8	24548	82848	2.70%	0.500%
41	16.023	2386	2392	2397	rBV8	17112	43768	1.42%	0.264%
42	16.112	2400	2407	2414	rVB9	19911	70034	2.28%	0.422%
43	16.253	2429	2431	2439	rVB6	26537	49310	1.60%	0.297%
44	16.711	2503	2509	2513	rBV4	20745	48000	1.56%	0.290%
45	16.782	2513	2521	2522	rBV	779831	1258881	40.96%	7.593%

Sum of corrected areas: 16578956

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Operator : JC\MD
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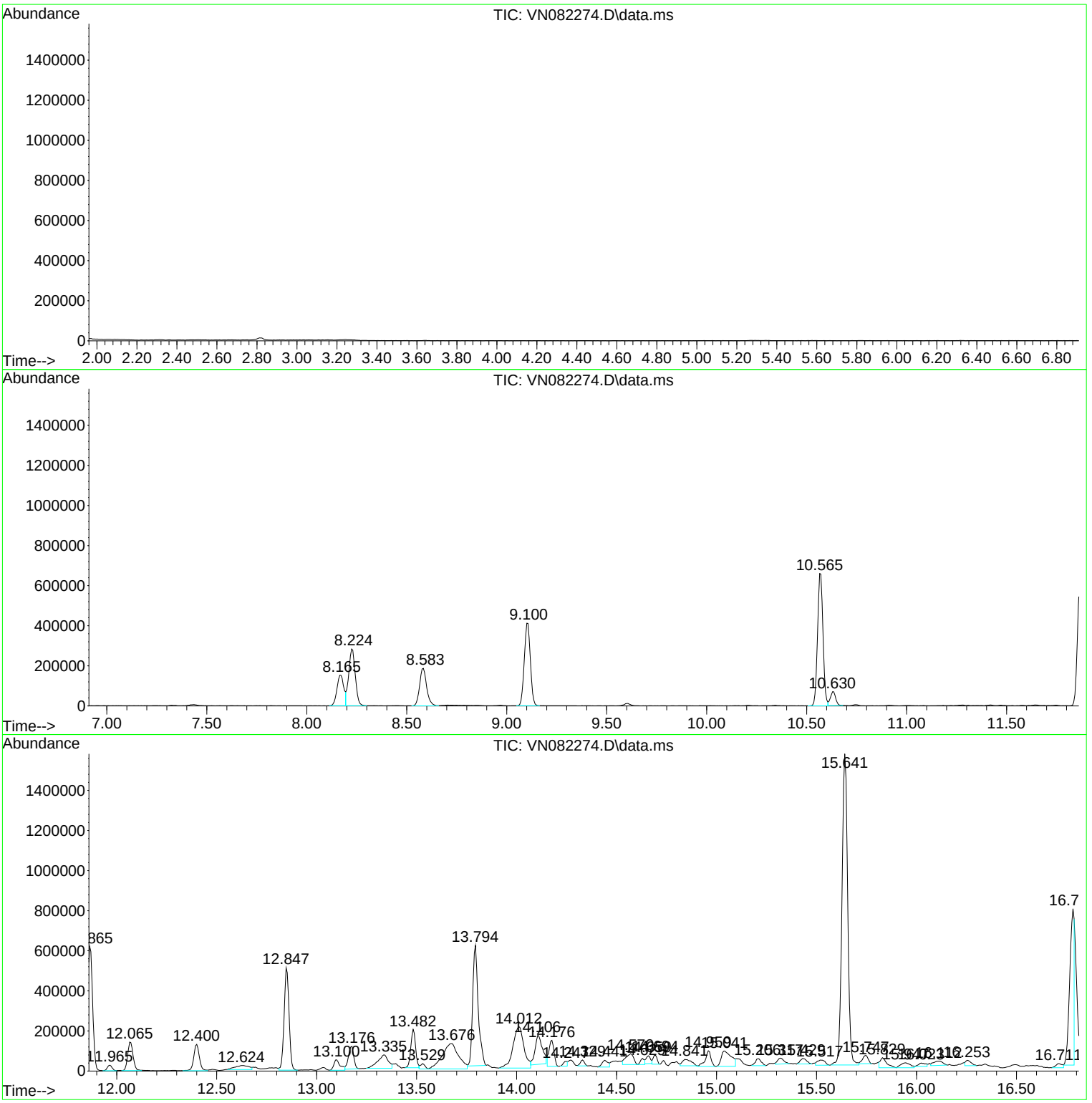
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
14

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 : VN082274.D
Acq On : 22 May 2024 05:33
Operator : JC\MD
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Misc : 5.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
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Instrument :
MSVOA_N
ClientSampleId :
14

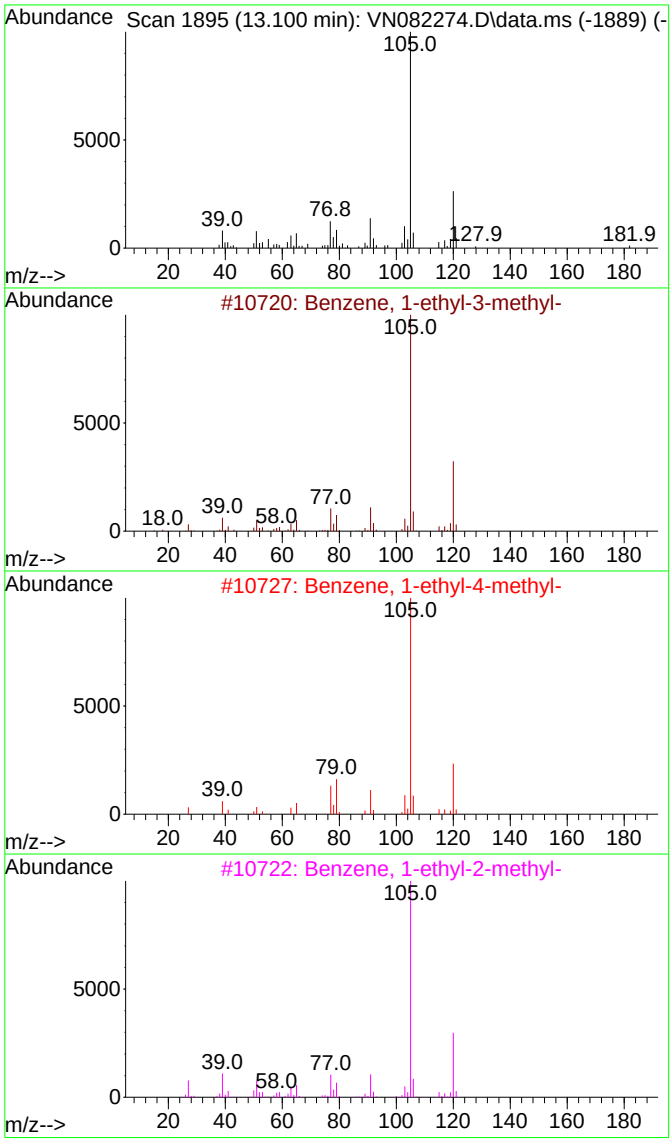
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

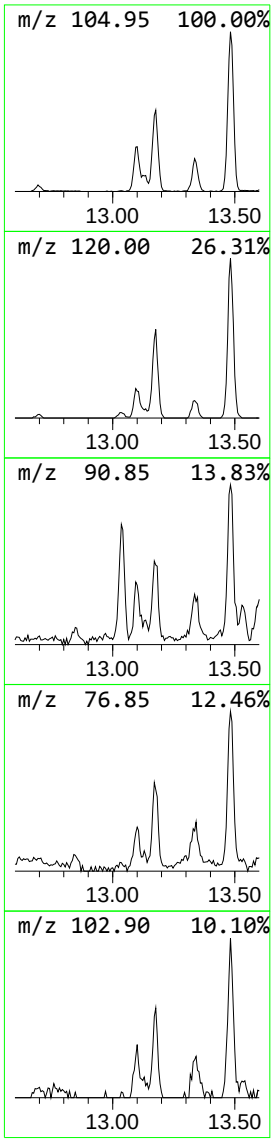
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Benzene, 1-ethyl-3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.100	5.11 ug/l	118406	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	94
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90
3	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	87
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	83
5	Benzene, (1-methylethyl)-	120	C9H12	000098-82-8	68





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082274.D
Acq On : 22 May 2024 05:33
Operator : JC\MD
Sample : P2494-14 40X
Misc : 5.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
14

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

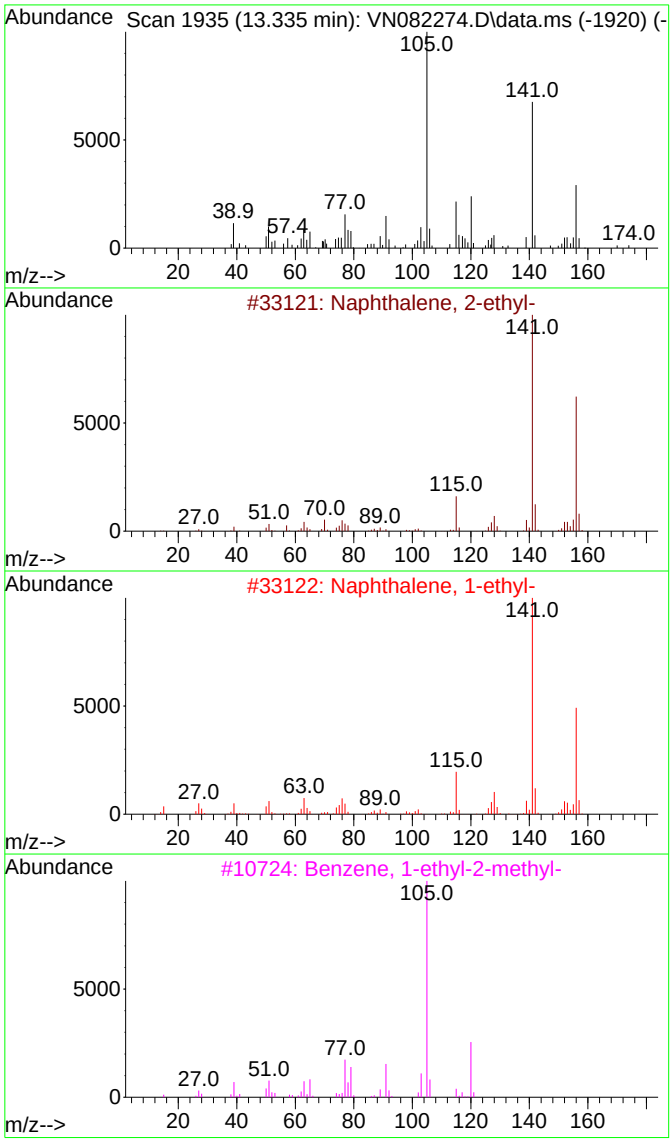
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

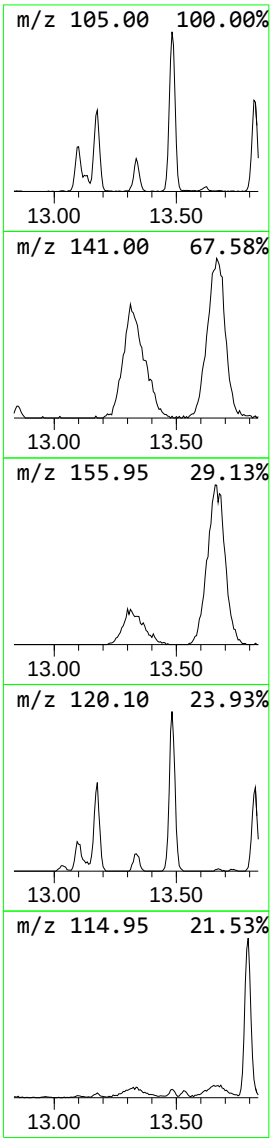
****

Peak Number 2 unknown13.335 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	10.69 ug/l	247534	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-ethyl-	156	C12H12	000939-27-5	49
2	Naphthalene, 1-ethyl-	156	C12H12	001127-76-0	43
3	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	42
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	42
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	42





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Data File : VN082274.D
Acq On : 22 May 2024 05:33
Operator : JC\MD
Sample : P2494-14 40X
Misc : 5.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
14

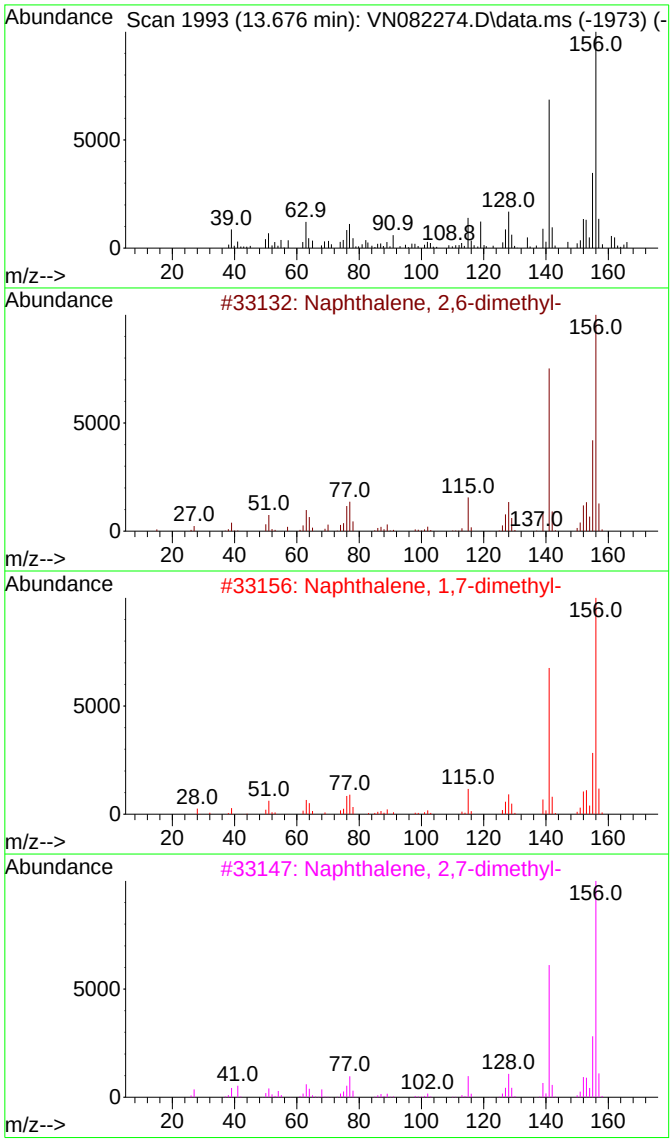
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

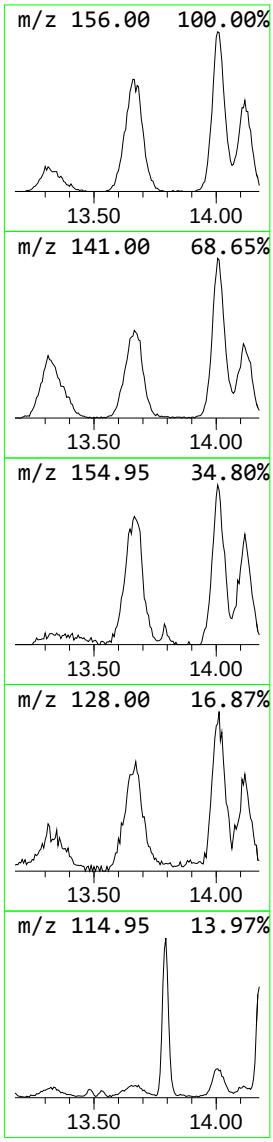
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Naphthalene, 2,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.676	30.76 ug/l	712316	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
2	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
3	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	96
4	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
5	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082274.D
Acq On : 22 May 2024 05:33
Operator : JC\MD
Sample : P2494-14 40X
Misc : 5.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
14

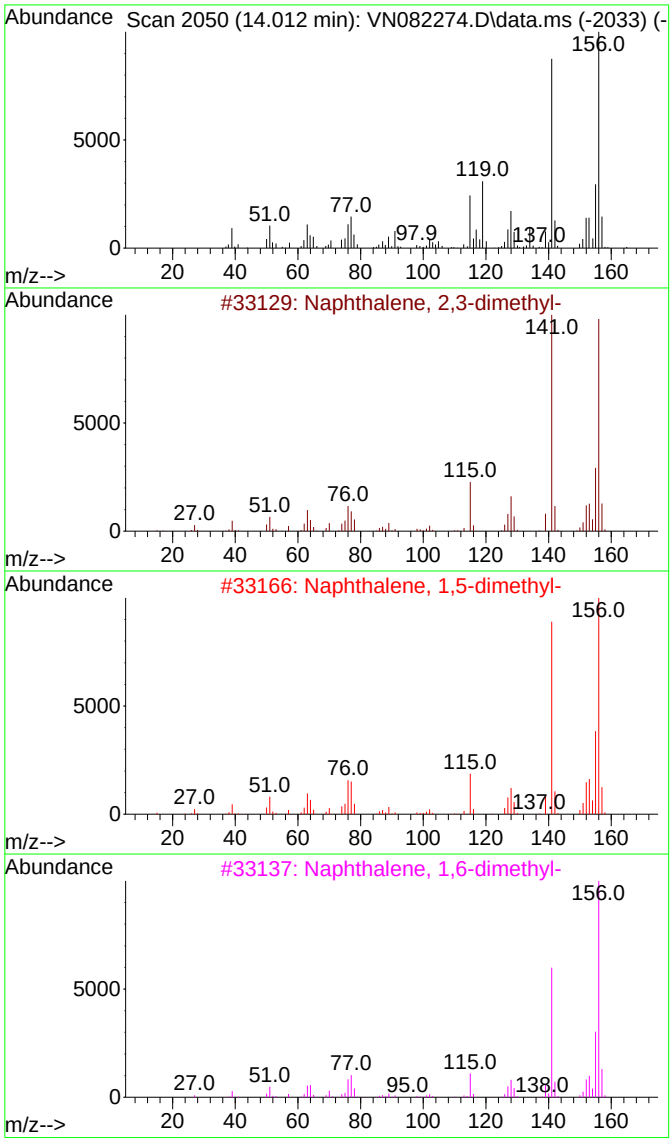
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

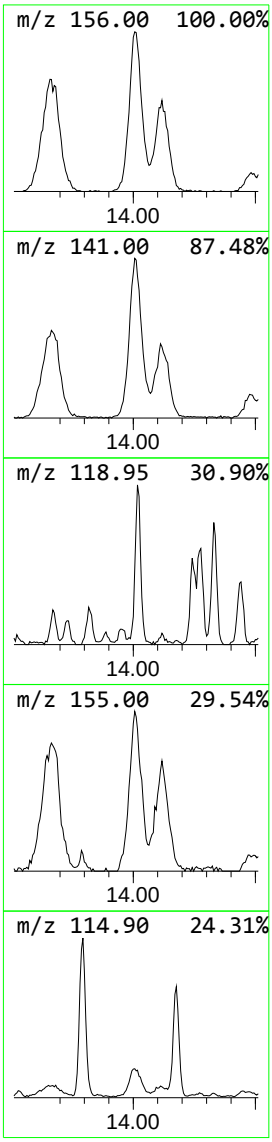
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.012	34.06 ug/l	788758	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, 1,5-dimethyl-	156	C12H12	000571-61-9	96
3	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
4	Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	96
5	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	96





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082274.D
Acq On : 22 May 2024 05:33
Operator : JC\MD
Sample : P2494-14 40X
Misc : 5.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
14

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

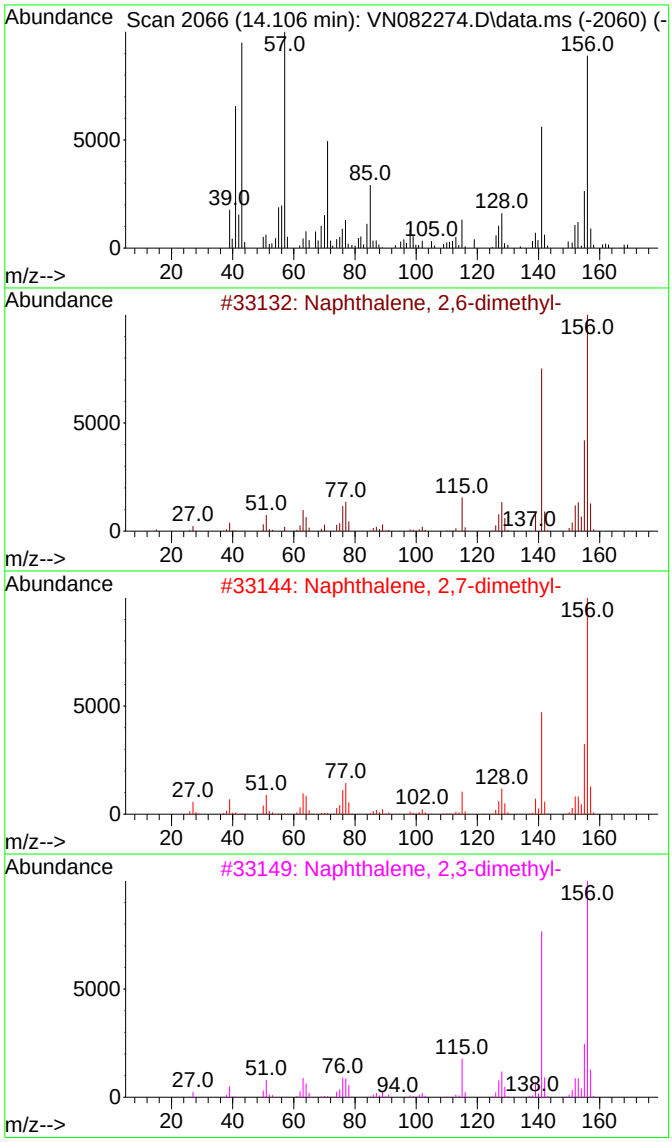
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

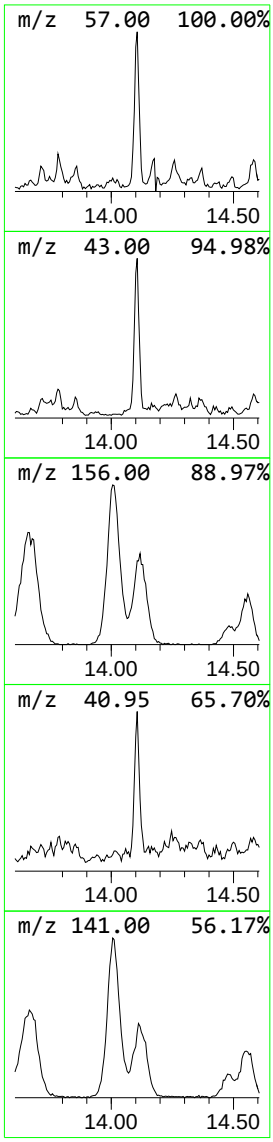
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.106	15.80 ug/l	365920	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	92
2	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	86
3	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	83
4	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	83
5	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	83





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Operator : JC\MD
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Misc : 5.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 49 Sample Multiplier: 1

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

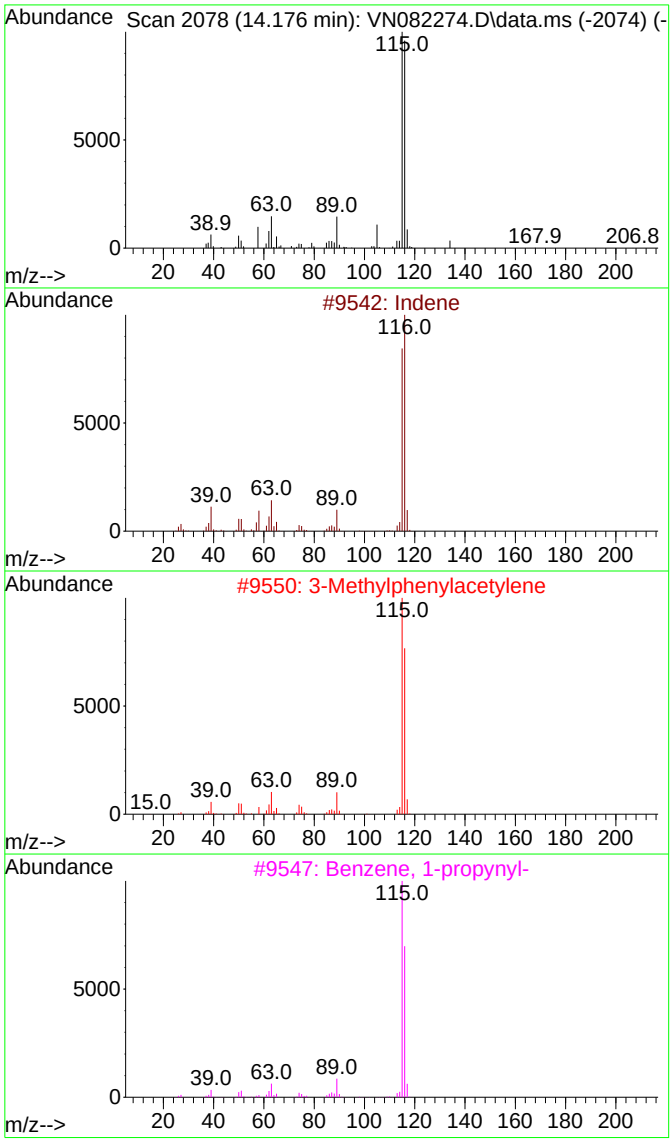
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

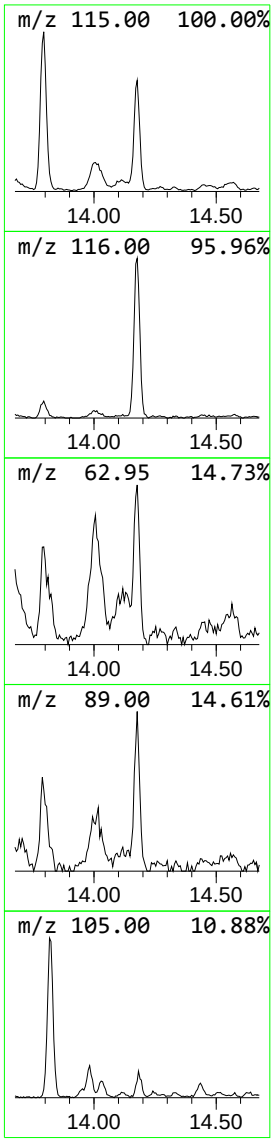
****

Peak Number 6 Indene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.176	9.53 ug/l	220720	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene	116	C9H8	000095-13-6	93
2	3-Methylphenylacetylene	116	C9H8	000766-82-5	87
3	Benzene, 1-propynyl-	116	C9H8	000673-32-5	87
4	2-Methylphenylacetylene	116	C9H8	000766-47-2	83
5	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	80





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Operator : JC\MD
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ALS Vial : 49 Sample Multiplier: 1

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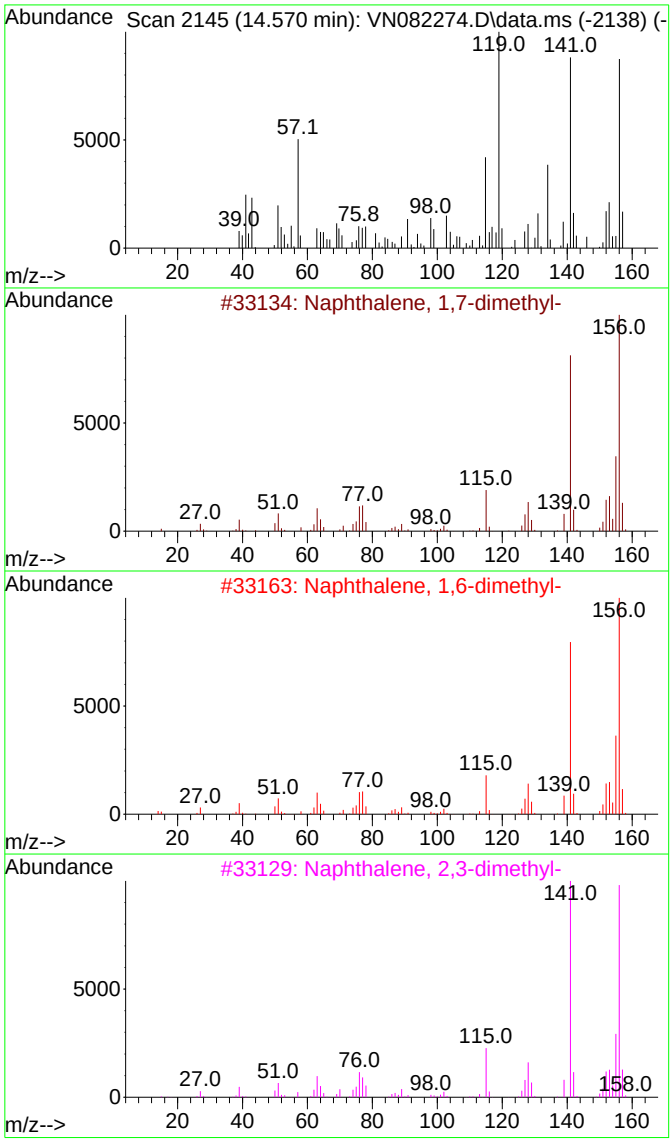
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

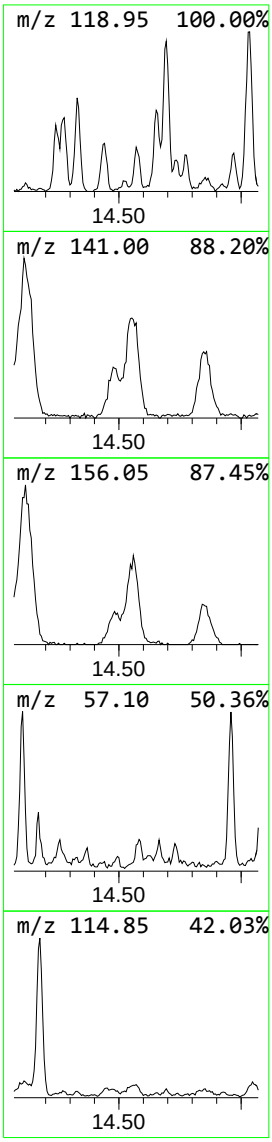
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Naphthalene, 1,7-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.570	6.25 ug/l	144822	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	64
2	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	64
3	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	64
4	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	55
5	Naphthalene, 1-ethyl-	156	C12H12	001127-76-0	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082274.D
Acq On : 22 May 2024 05:33
Operator : JC\MD
Sample : P2494-14 40X
Misc : 5.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
14

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

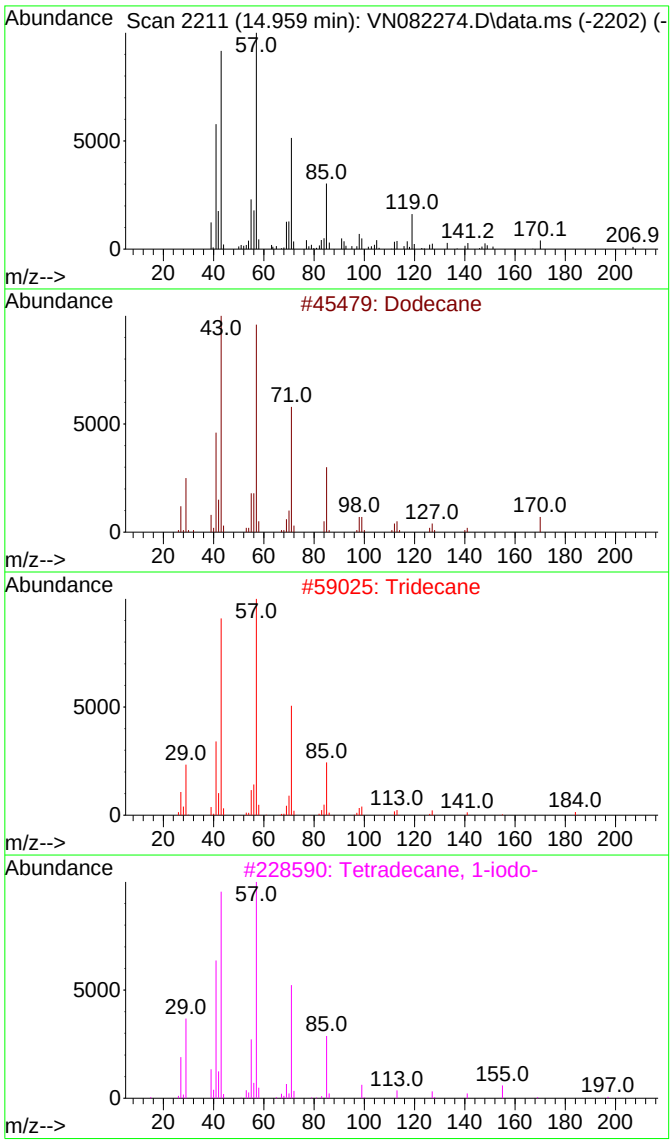
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

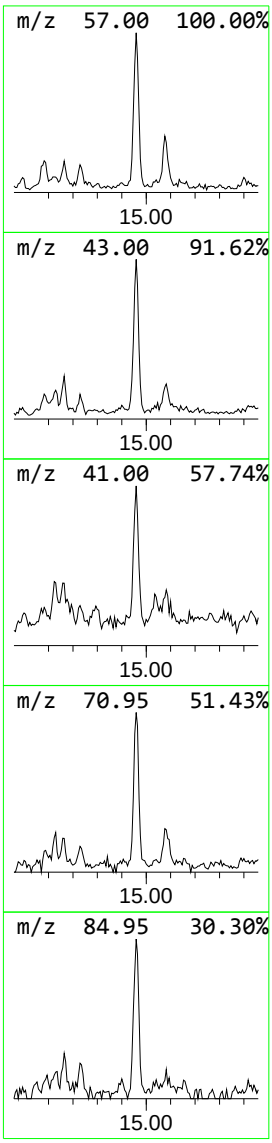
****

Peak Number 8 Dodecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.959	6.58 ug/l	152315	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	94
2	Tridecane	184	C13H28	000629-50-5	72
3	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	64
4	Hexadecane	226	C16H34	000544-76-3	64
5	Tetradecane	198	C14H30	000629-59-4	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082274.D
Acq On : 22 May 2024 05:33
Operator : JC\MD
Sample : P2494-14 40X
Misc : 5.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
14

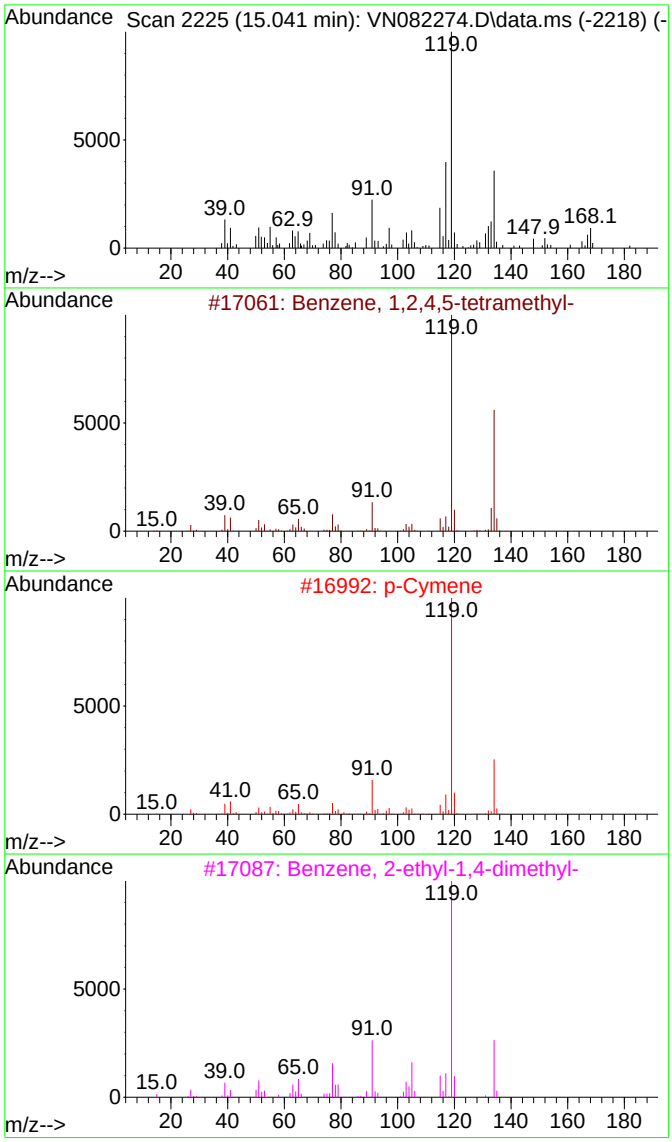
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

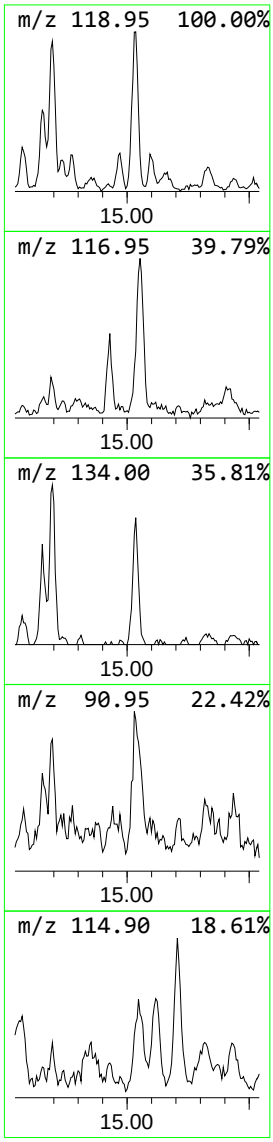
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 unknown15.041 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.041	11.81 ug/l	273586	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	49
2	p-Cymene	134	C10H14	000099-87-6	47
3	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	46
4	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	46
5	o-Cymene	134	C10H14	000527-84-4	46





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082274.D
Acq On : 22 May 2024 05:33
Operator : JC\MD
Sample : P2494-14 40X
Misc : 5.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
14

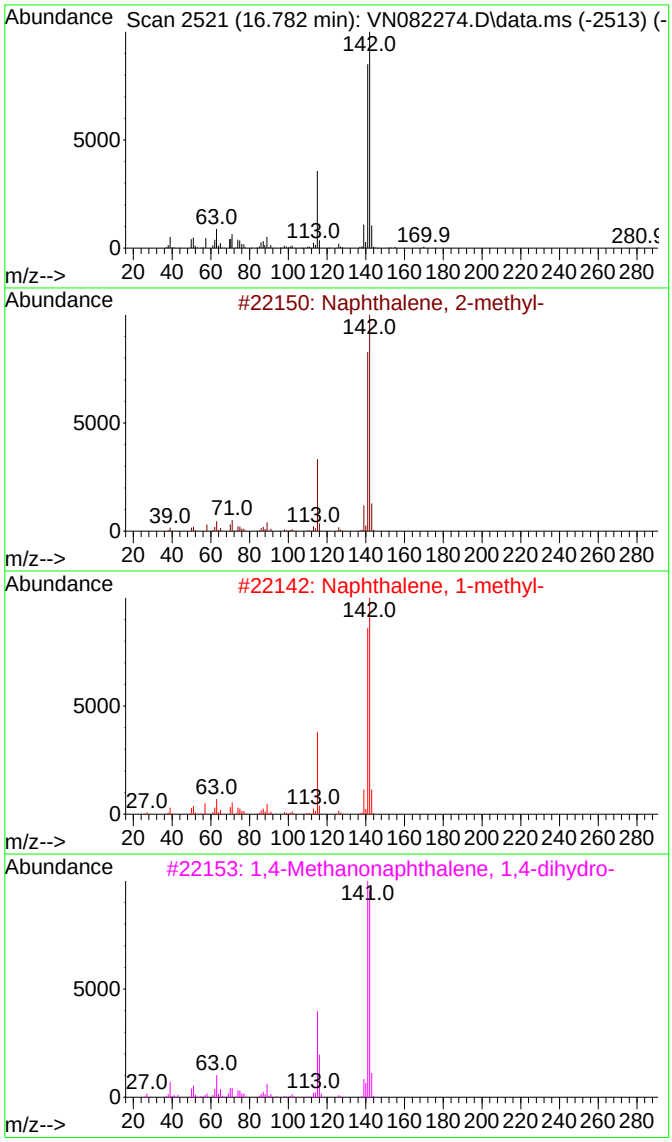
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

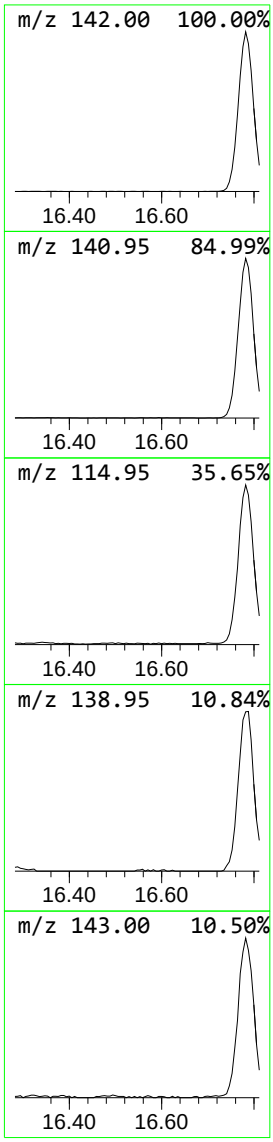
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.782	54.36 ug/l	1258880	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	97
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





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082274.D
Acq On : 22 May 2024 05:33
Operator : JC\MD
Sample : P2494-14 40X
Misc : 5.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
14

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	5.1	ug/l	118406	4	13.794	1157930	50.0
unknown13.335	13.335	10.7	ug/l	247534	4	13.794	1157930	50.0
Naphthalene, 2,...	13.676	30.8	ug/l	712316	4	13.794	1157930	50.0
Naphthalene, 2,...	14.012	34.1	ug/l	788758	4	13.794	1157930	50.0
Naphthalene, 2,...	14.106	15.8	ug/l	365920	4	13.794	1157930	50.0
Indene	14.176	9.5	ug/l	220720	4	13.794	1157930	50.0
Naphthalene, 1,...	14.570	6.3	ug/l	144822	4	13.794	1157930	50.0
Dodecane	14.959	6.6	ug/l	152315	4	13.794	1157930	50.0
unknown15.041	15.041	11.8	ug/l	273586	4	13.794	1157930	50.0
Naphthalene, 2-...	16.782	54.4	ug/l	1258880	4	13.794	1157930	50.0