LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022924\
Data File : VN081269.D
Acq On : 29 Feb 2024 15:14
Operator : JC\MD
Sample : P1587-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1823-A

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\82N021624W.M
Title : SW846 8260

Signal : TIC: VN081269.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.283	49	56	63	rBV	152079	206904	11.82%	1.085%
2	2.483	83	90	100	rBV3	25522	48489	2.77%	0.254%
3	2.665	114	121	128	rBV	63424	122424	6.99%	0.642%
4	2.754	132	136	141	rVV2	13961	27806	1.59%	0.146%
5	2.818	142	147	154	rVB2	16657	34015	1.94%	0.178%
6	3.789	303	312	324	rBV	162835	426688	24.37%	2.238%
7	4.430	411	421	435	rBV	50244	151831	8.67%	0.796%
8	4.712	458	469	470	rBV4	9158	18479	1.06%	0.097%
9	7.430	919	931	939	rBV2	83386	241270	13.78%	1.265%
10	8.165	1046	1056	1060	rBV2	239973	539014	30.79%	2.827%
11	8.224	1061	1066	1078	rVB	480333	1043732	59.62%	5.474%
12	8.577	1110	1126	1141	rBV	266905	702438	40.13%	3.684%
13	9.100	1204	1215	1231	rBV	690746	1430771	81.73%	7.504%
14	10.447	1435	1444	1452	rBV2	34940	67864	3.88%	0.356%
15	10.571	1456	1465	1470	rBV	935710	1750558	100.00%	9.182%
16	10.630	1470	1475	1486	rVB	570825	1059716	60.54%	5.558%
17	11.200	1564	1572	1580	rBV2	19738	35512	2.03%	0.186%
18	11.865	1676	1685	1695	rBV	927336	1628012	93.00%	8.539%
19	11.971	1695	1703	1709	rVB5	9995	21636	1.24%	0.113%
20	12.071	1709	1720	1728	rBV	25988	53687	3.07%	0.282%
21	12.400	1766	1776	1781	rBV3	29260	62307	3.56%	0.327%
22	12.459	1781	1786	1796	rVV2	24978	41267	2.36%	0.216%
23	12.853	1843	1853	1861	rBV	590488	1033414	59.03%	5.420%
24	13.035	1878	1884	1888	rBV2	16051	24421	1.40%	0.128%
25	13.100	1888	1895	1899	rBV	41841	78057	4.46%	0.409%
26	13.129	1899	1900	1904	rVV4	19838	23598	1.35%	0.124%
27	13.176	1904	1908	1914	rVB3	27108	43677	2.50%	0.229%
28	13.259	1914	1922	1931	rBV	677857	1101948	62.95%	5.780%
29	13.335	1931	1935	1941	rVB	34898	60078	3.43%	0.315%
30	13.506	1955	1964	1973	rVV2	279229	620963	35.47%	3.257%
31	13.612	1976	1982	1990	rVV4	90170	167698	9.58%	0.880%
32	13.794	2006	2013	2021	rVV2	878566	1609572	91.95%	8.442%
33	13.876	2021	2027	2035	rVV	368078	711520	40.65%	3.732%
34	13.953	2035	2040	2042	rVV4	34126	65301	3.73%	0.343%
35	13.994	2042	2047	2062	rVB4	107466	295848	16.90%	1.552%
36	14.118	2062	2068	2073	rBV4	21421	34399	1.97%	0.180%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022924\
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Operator : JC\MD
Sample : P1587-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1823-A

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\82N021624W.M
Title : SW846 8260

37	14.182	2075	2079	2084	rVB2	15328	22393	1.28%	0.117%
38	14.241	2084	2089	2093	rBV4	39187	72603	4.15%	0.381%
39	14.276	2093	2095	2099	rVV2	26755	33925	1.94%	0.178%
40	14.329	2099	2104	2111	rVB	61340	100026	5.71%	0.525%
41	14.400	2111	2116	2119	rBV4	23324	46337	2.65%	0.243%
42	14.447	2119	2124	2129	rVB3	90720	160205	9.15%	0.840%
43	14.576	2139	2146	2151	rVB3	29287	54918	3.14%	0.288%
44	14.653	2151	2159	2163	rBV	67013	122933	7.02%	0.645%
45	14.694	2163	2166	2170	rVV3	49340	71848	4.10%	0.377%
46	14.882	2190	2198	2201	rBV7	17403	39627	2.26%	0.208%
47	14.929	2201	2206	2218	rVB5	76523	165724	9.47%	0.869%
48	15.053	2218	2227	2235	rBV3	201010	482298	27.55%	2.530%
49	15.106	2235	2236	2244	rVB6	17091	28071	1.60%	0.147%
50	15.212	2248	2254	2262	rBV	165942	301855	17.24%	1.583%
51	15.323	2262	2273	2277	rVV5	55059	145257	8.30%	0.762%
52	15.365	2277	2280	2286	rVV2	40803	82764	4.73%	0.434%
53	15.435	2286	2292	2302	rVB5	68700	181298	10.36%	0.951%
54	15.594	2314	2319	2322	rBV5	22709	38878	2.22%	0.204%
55	15.641	2322	2327	2333	rVV	102193	203725	11.64%	1.069%
56	15.700	2333	2337	2342	rVV4	37179	71045	4.06%	0.373%
57	15.747	2342	2345	2346	rVV3	28052	29386	1.68%	0.154%
58	15.782	2347	2351	2371	rVB7	59560	194029	11.08%	1.018%
59	15.947	2371	2379	2385	rBV2	35580	76399	4.36%	0.401%
60	16.029	2387	2393	2397	rBV9	12362	26744	1.53%	0.140%
61	16.129	2402	2410	2411	rBV8	33719	66628	3.81%	0.349%
62	16.170	2412	2417	2427	rVB4	73504	166687	9.52%	0.874%
63	16.253	2427	2431	2439	rBV7	20175	47762	2.73%	0.251%
64	16.353	2439	2448	2451	rBV9	19194	50427	2.88%	0.264%
65	16.506	2466	2474	2480	rBV5	93724	220012	12.57%	1.154%
66	16.612	2489	2492	2498	rVB6	13869	21966	1.25%	0.115%
67	16.717	2498	2510	2514	rBV8	26202	66353	3.79%	0.348%
68	16.782	2515	2521	2522	rBV	65974	88476	5.05%	0.464%

Sum of corrected areas: 19065513

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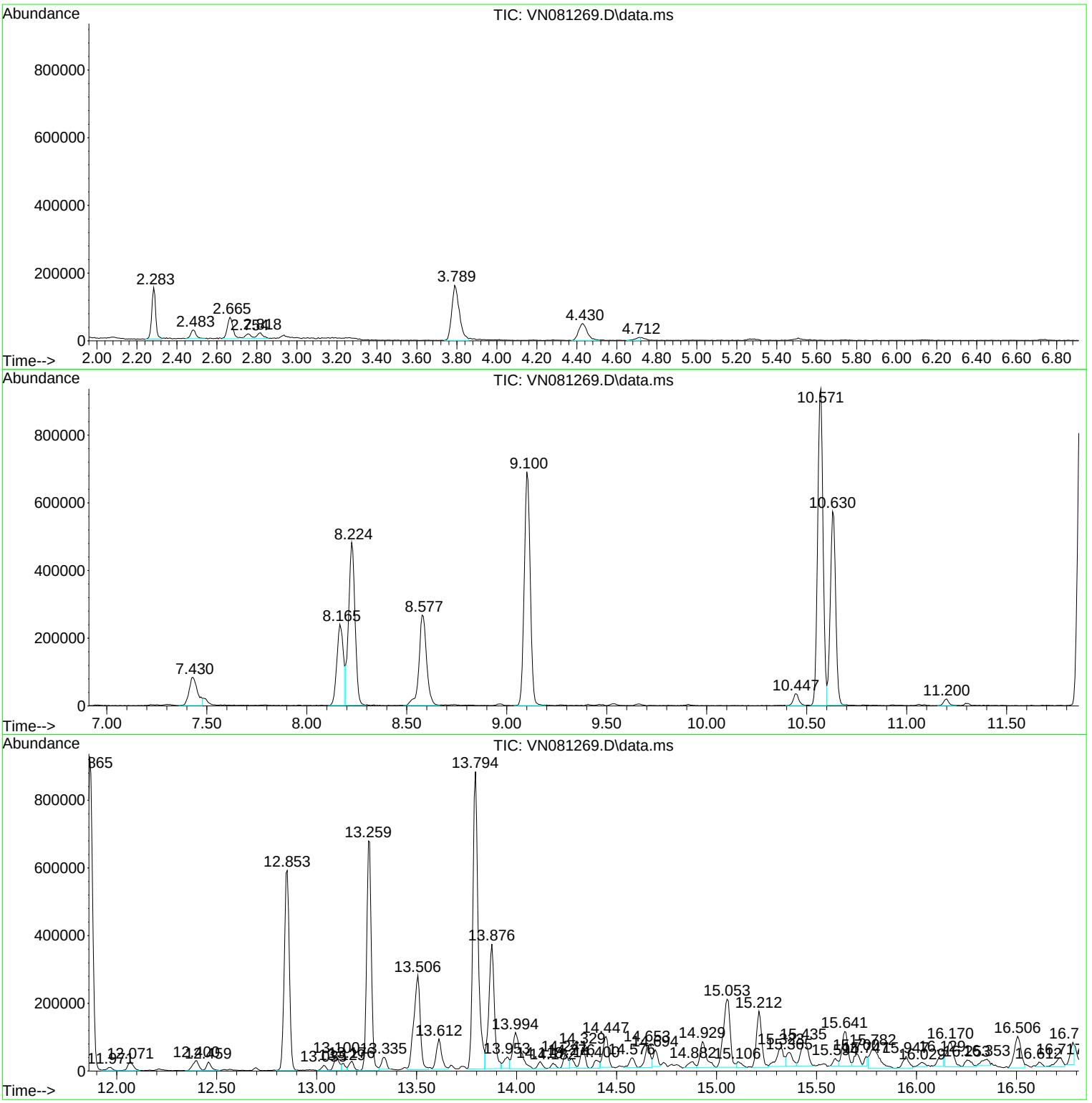
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1823-A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022924\
Data File : VN081269.D
Acq On : 29 Feb 2024 15:14
Operator : JC\MD
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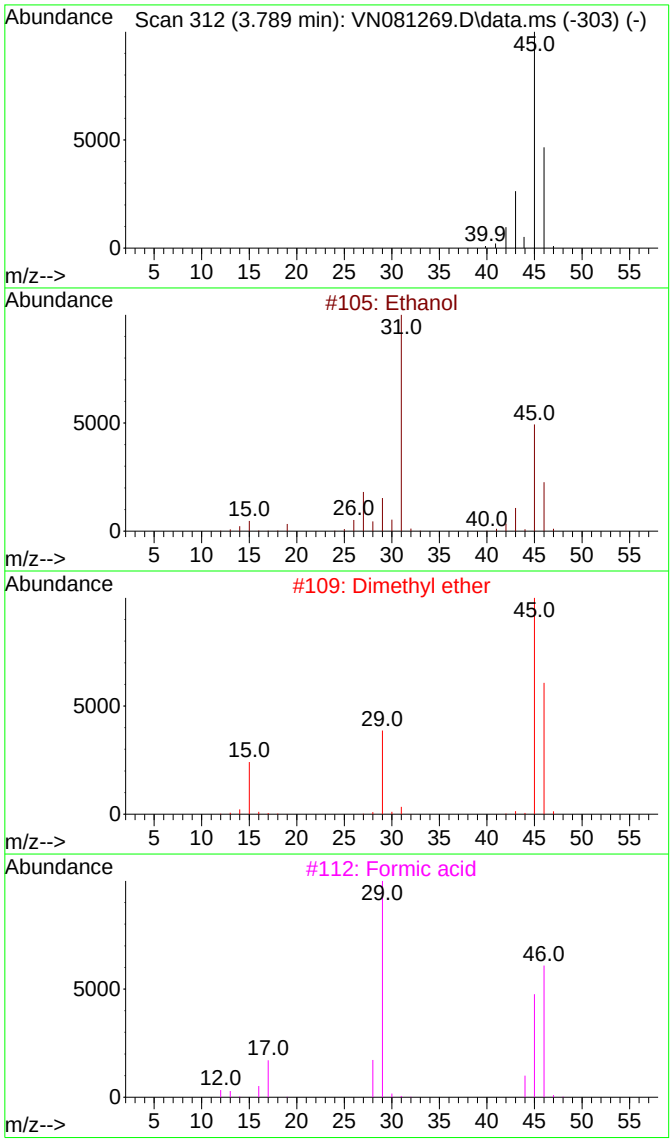
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

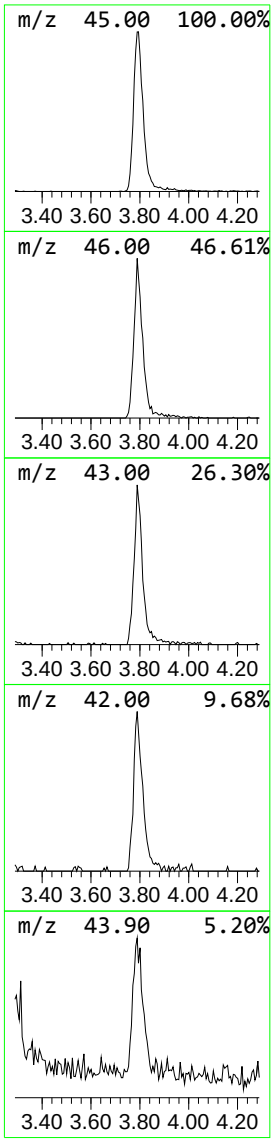
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.789	20.44 ug/l	426688	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	64
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Formic acid	46	CH2O2	000064-18-6	5
4	Oxalic acid	90	C2H2O4	000144-62-7	4
5	Methane, nitroso-	45	CH3NO	000865-40-7	3





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022924\
Data File : VN081269.D
Acq On : 29 Feb 2024 15:14
Operator : JC\MD
Sample : P1587-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1823-A

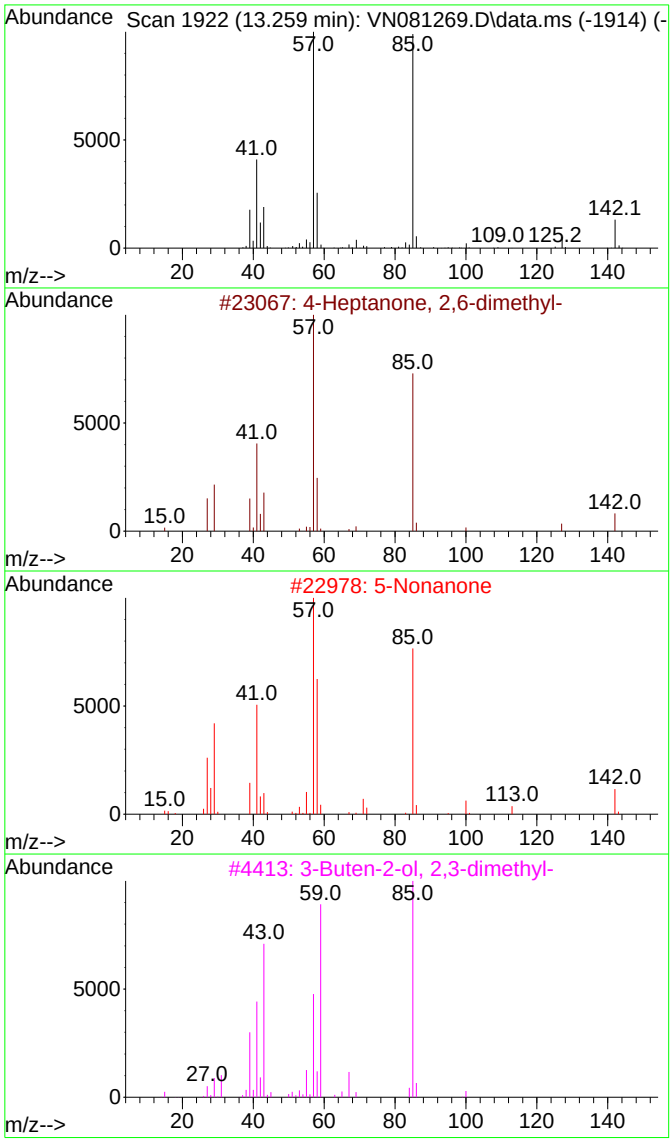
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

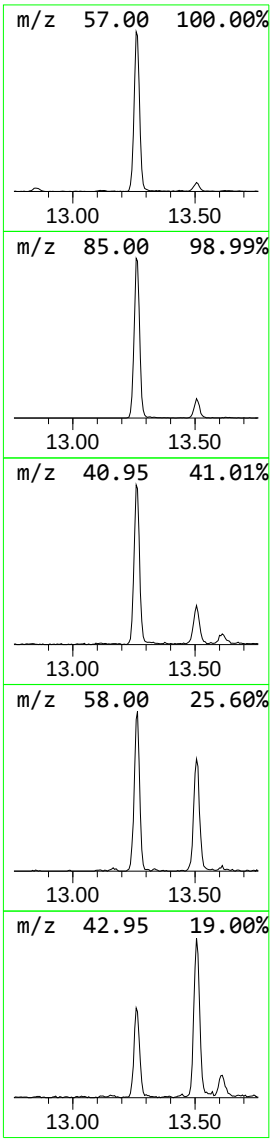
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 4-Heptanone, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.259	34.23 ug/l	1101950	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	94
2	5-Nonanone	142	C9H18O	000502-56-7	64
3	3-Buten-2-ol, 2,3-dimethyl-	100	C6H12O	010473-13-9	53
4	t-Butyl isobutyl ketone	142	C9H18O	014705-50-1	50
5	4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022924\
Data File : VN081269.D
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Operator : JC\MD
Sample : P1587-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1823-A

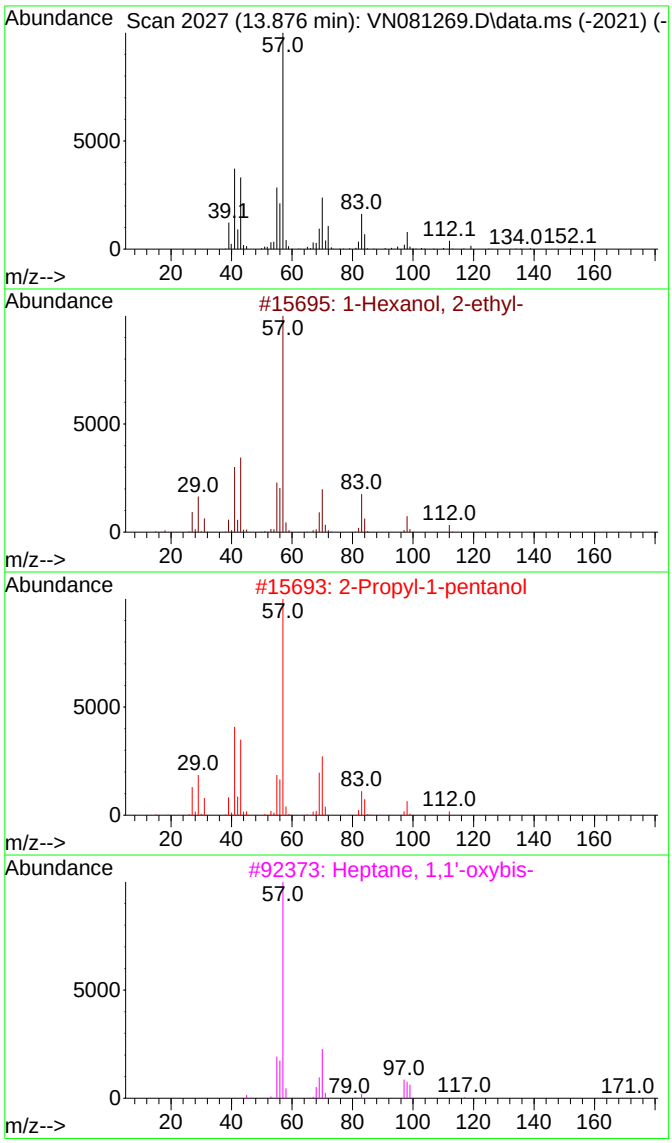
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

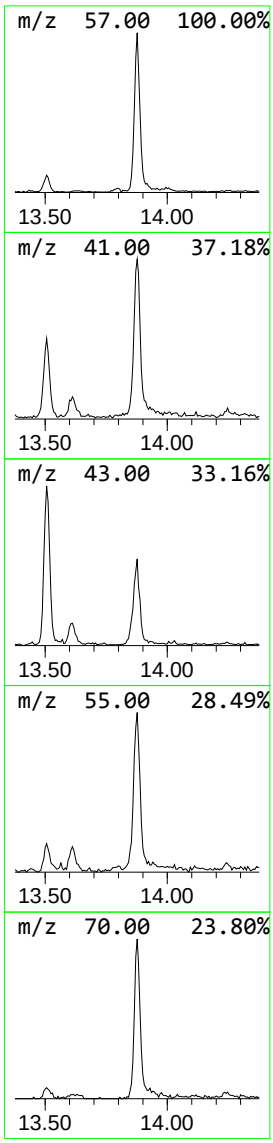
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	22.10 ug/l	711520	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	86
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
4	Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	50
5	Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022924\
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Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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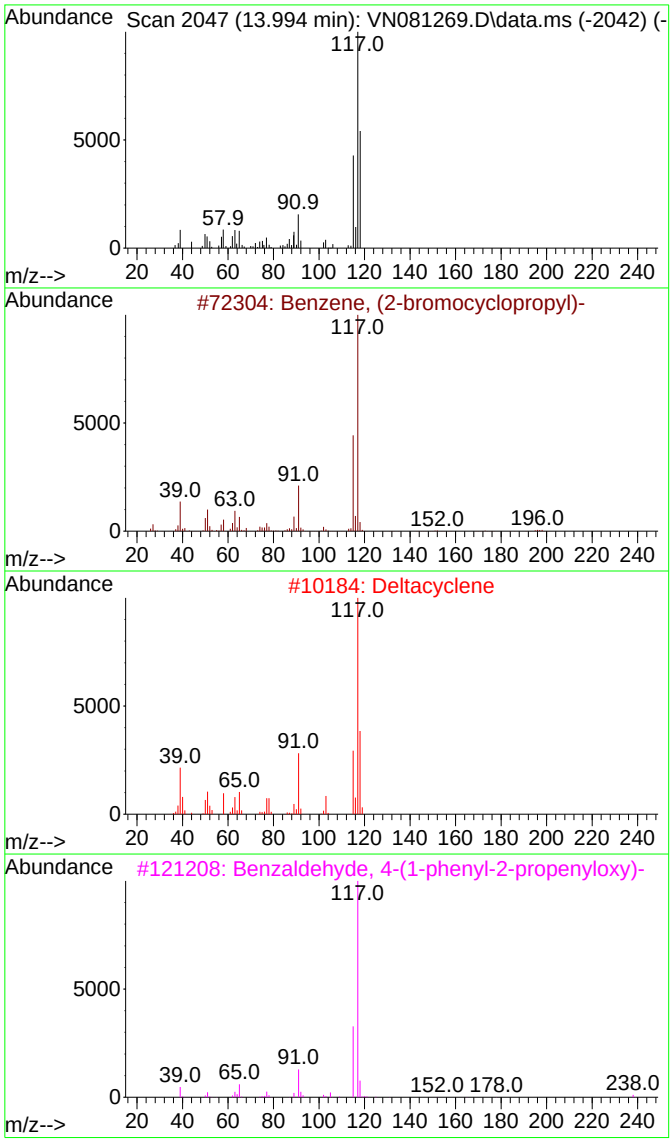
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

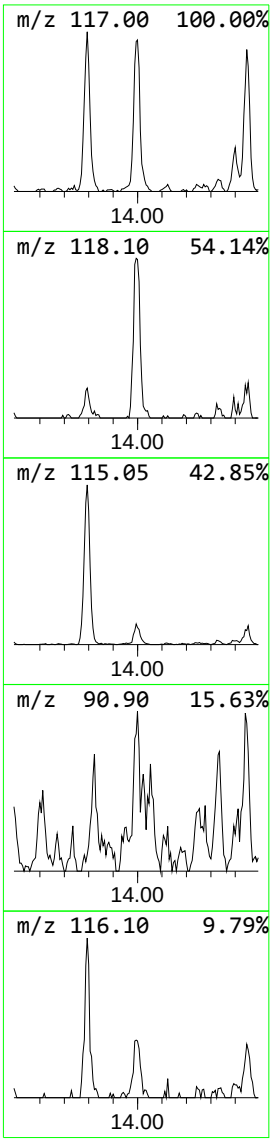
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, (2-bromocyclopropyl)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	9.19 ug/l	295848	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	53
2	Deltacyclene	118	C9H10	007785-10-6	53
3	Benzaldehyde, 4-(1-phenyl-2-prop...	238	C16H14O2	1000277-56-1	50
4	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	47
5	Indole	117	C8H7N	000120-72-9	43





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Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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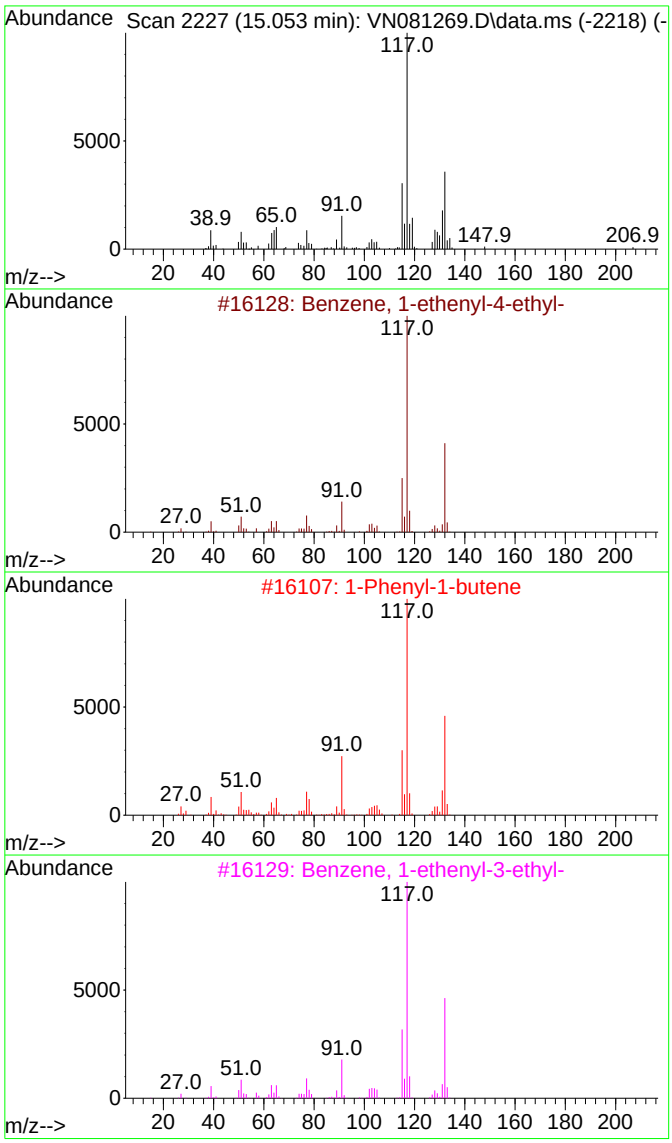
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

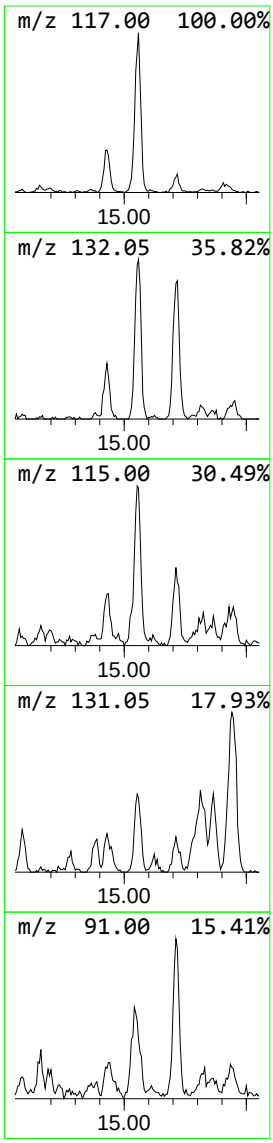
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.053	14.98 ug/l	482298	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2	1-Phenyl-1-butene	132	C10H12	000824-90-8	94
3	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	94
4	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	92
5	Benzene, 2-butenyl-	132	C10H12	001560-06-1	87





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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1823-A

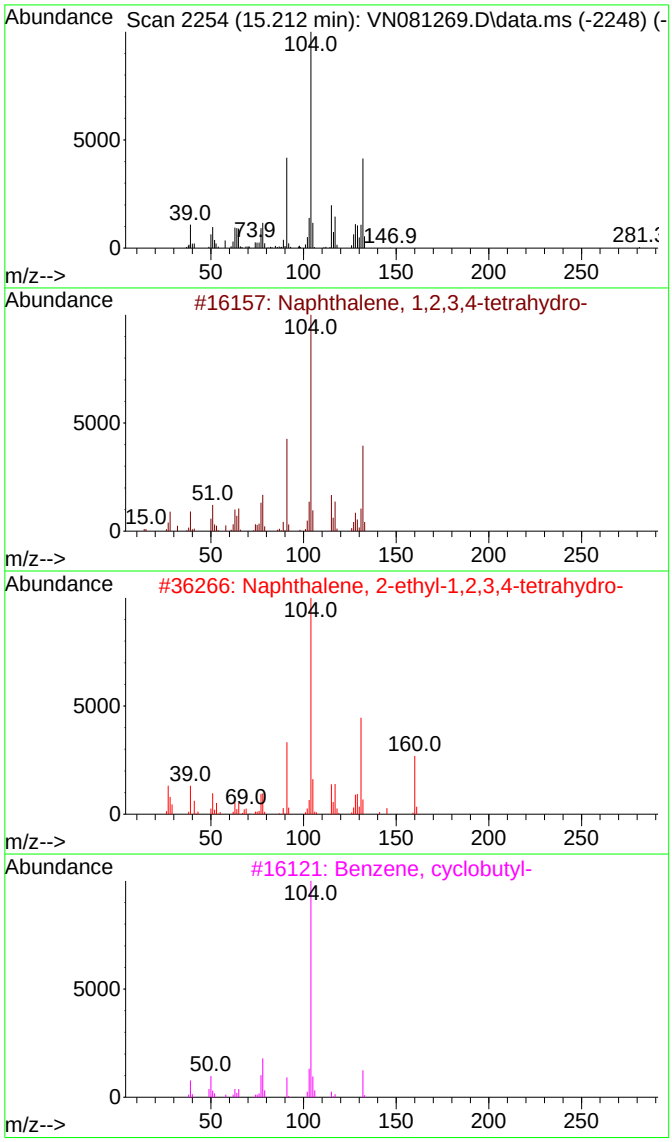
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

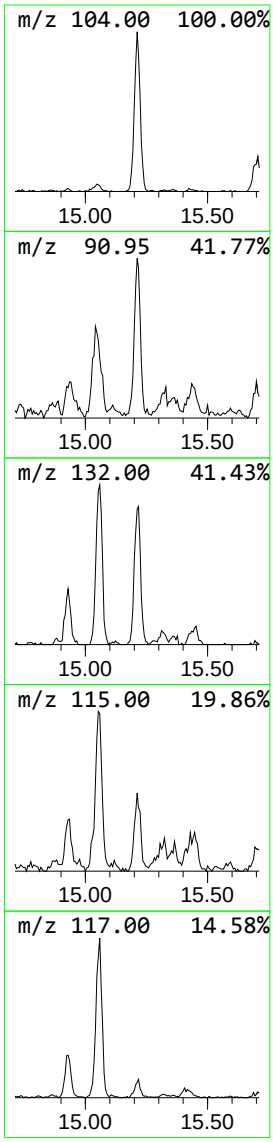
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.212	9.38 ug/l	301855	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	95
2	Naphthalene, 2-ethyl-1,2,3,4-tet...	160	C12H16	032367-54-7	53
3	Benzene, cyclobutyl-	132	C10H12	004392-30-7	50
4	Indan, epoxide	132	C9H8O	000768-22-9	49
5	2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	49





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022924\
Data File : VN081269.D
Acq On : 29 Feb 2024 15:14
Operator : JC\MD
Sample : P1587-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1823-A

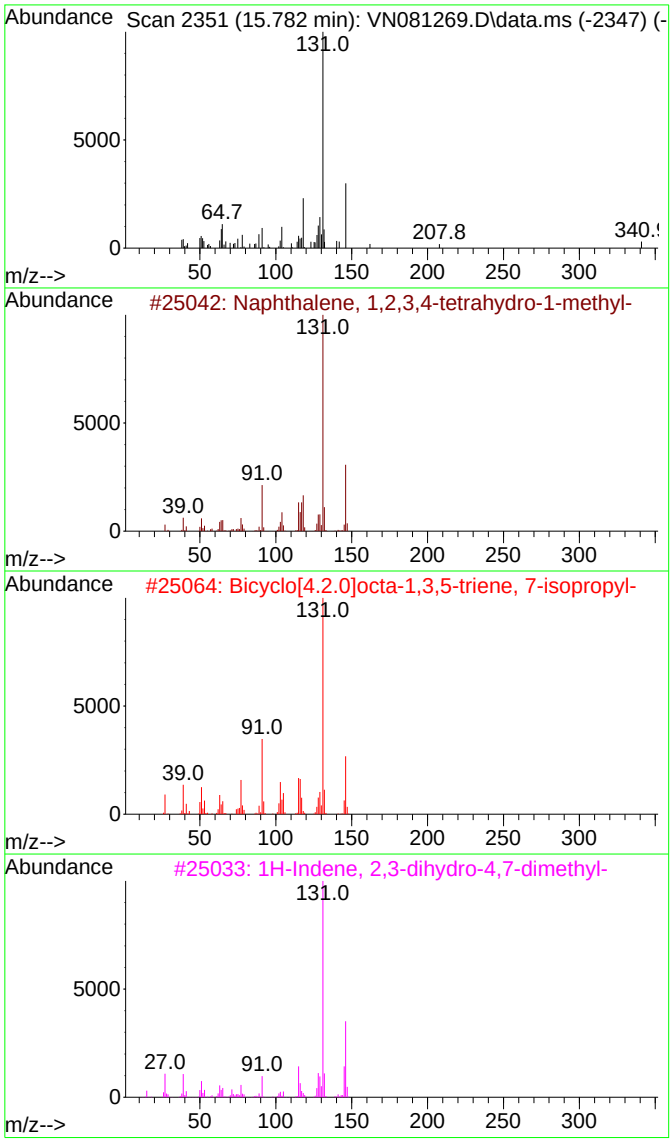
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

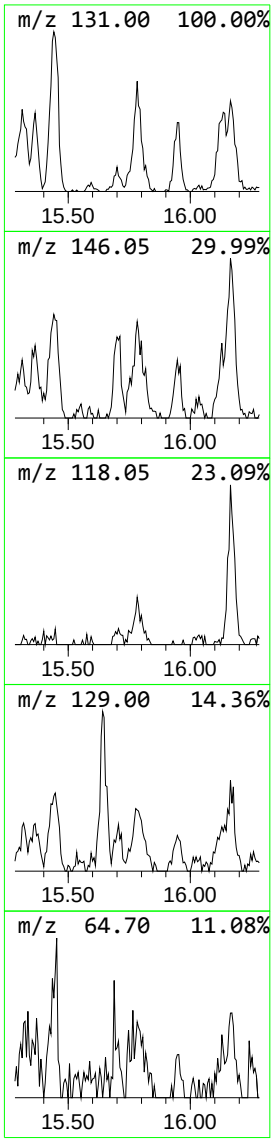
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.782	6.03 ug/l	194029	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	91
2	Bicyclo[4.2.0]octa-1,3,5-triene,...	146	C11H14	027087-54-3	80
3	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	74
4	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	74
5	Benzene, 1-methyl-4-(1-methyl-2-...	146	C11H14	097664-18-1	72





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Data File : VN081269.D
Acq On : 29 Feb 2024 15:14
Operator : JC\MD
Sample : P1587-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1823-A

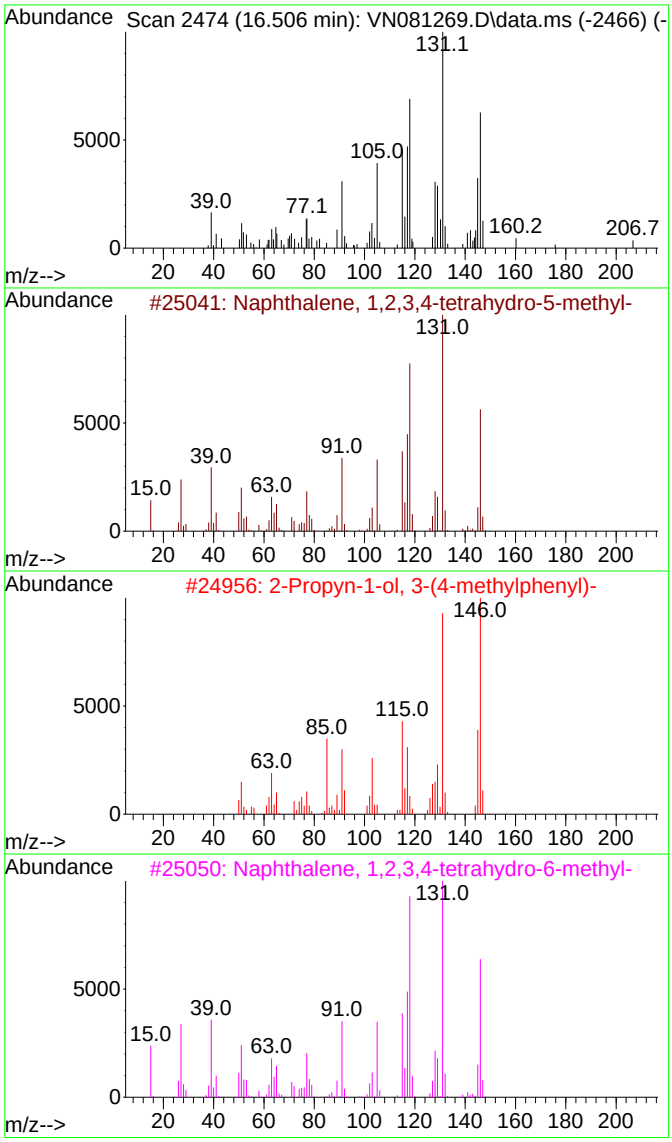
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

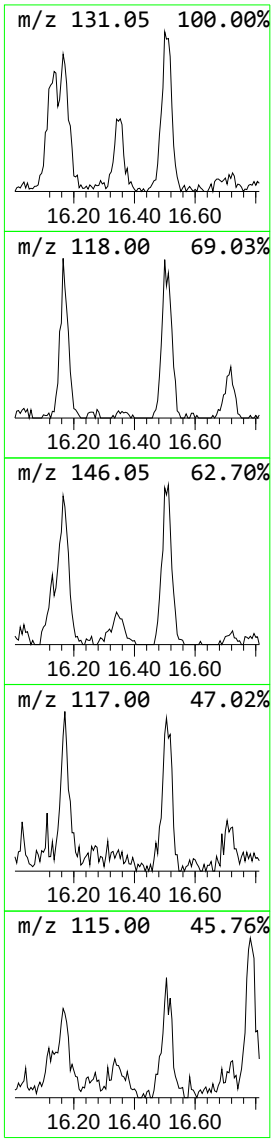
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.506	6.83 ug/l	220012	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	91
2	2-Propyn-1-ol, 3-(4-methylphenyl)-	146	C10H10O	016017-24-6	90
3	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	76
4	Naphth[1,2-b]oxirene, 1a,2,3,7b-...	146	C10H10O	002461-34-9	58
5	1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022924\
Data File : VN081269.D
Acq On : 29 Feb 2024 15:14
Operator : JC\MD
Sample : P1587-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1823-A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.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
Ethanol	3.789	20.4	ug/l	426688	1	8.224	1043730	50.0
4-Heptanone, 2,...	13.259	34.2	ug/l	1101950	4	13.794	1609570	50.0
1-Hexanol, 2-et...	13.876	22.1	ug/l	711520	4	13.794	1609570	50.0
Benzene, (2-bro...	13.994	9.2	ug/l	295848	4	13.794	1609570	50.0
Benzene, 1-ethe...	15.053	15.0	ug/l	482298	4	13.794	1609570	50.0
Naphthalene, 1,...	15.212	9.4	ug/l	301855	4	13.794	1609570	50.0
Naphthalene, 1,...	15.782	6.0	ug/l	194029	4	13.794	1609570	50.0
Naphthalene, 1,...	16.506	6.8	ug/l	220012	4	13.794	1609570	50.0