LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090921\
Data File : VX024144.D
Acq On : 09 Sep 2021 16:43
Operator : JC/MD
Sample : M3694-01 10X
Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : S-1

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\82X081721W.M
Title : SW846 8260

Signal : TIC: VX024144.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	23	26	35	rVB3	4807	9910	1.30%	0.090%
2	1.618	82	87	95	rVB6	6657	18686	2.45%	0.169%
3	2.953	297	306	319	rVB	22479	53431	7.02%	0.483%
4	4.605	567	577	589	rVB2	3155	10421	1.37%	0.094%
5	5.397	696	707	722	rBV	86308	252882	33.21%	2.288%
6	5.556	722	733	747	rBV	142032	411721	54.06%	3.725%
7	5.964	788	800	817	rBV2	96626	256716	33.71%	2.323%
8	6.769	922	932	943	rBV	230253	549235	72.12%	4.970%
9	8.653	1234	1241	1250	rVB	498292	761556	100.00%	6.891%
10	10.055	1466	1471	1478	rVB	520537	682393	89.61%	6.175%
11	10.323	1510	1515	1518	rVV3	6555	12422	1.63%	0.112%
12	10.586	1552	1558	1566	rBV6	9737	17885	2.35%	0.162%
13	10.671	1566	1572	1577	rBV5	5526	9763	1.28%	0.088%
14	10.781	1587	1590	1594	rVB2	17731	23525	3.09%	0.213%
15	10.860	1594	1603	1606	rBV4	15803	27391	3.60%	0.248%
16	10.897	1606	1609	1614	rVB2	10421	14548	1.91%	0.132%
17	11.085	1634	1640	1645	rBV	443488	565030	74.19%	5.113%
18	11.195	1654	1658	1660	rBV2	13930	17463	2.29%	0.158%
19	11.226	1660	1663	1667	rVB2	15385	18975	2.49%	0.172%
20	11.342	1678	1682	1686	rBV6	8113	13866	1.82%	0.125%
21	11.390	1686	1690	1694	rVV4	10085	14768	1.94%	0.134%
22	11.433	1694	1697	1701	rVV	22850	31177	4.09%	0.282%
23	11.482	1701	1705	1710	rVB3	14982	25815	3.39%	0.234%
24	11.634	1723	1730	1734	rBV6	16979	37897	4.98%	0.343%
25	11.683	1734	1738	1741	rBV2	17596	24917	3.27%	0.225%
26	11.720	1741	1744	1747	rVV	59948	63718	8.37%	0.577%
27	11.841	1759	1764	1767	rBV2	21026	34513	4.53%	0.312%
28	11.890	1769	1772	1777	rVV3	35579	56007	7.35%	0.507%
29	11.945	1777	1781	1784	rVV3	49342	73854	9.70%	0.668%
30	11.976	1784	1786	1789	rVV4	19396	22452	2.95%	0.203%
31	12.024	1789	1794	1800	rVV	476445	638936	83.90%	5.781%
32	12.079	1800	1803	1807	rVB2	24032	30038	3.94%	0.272%
33	12.152	1812	1815	1817	rBV3	9009	9663	1.27%	0.087%
34	12.250	1826	1831	1836	rBV3	41858	66703	8.76%	0.604%
35	12.311	1836	1841	1848	rBV7	61670	115962	15.23%	1.049%
36	12.421	1848	1859	1864	rBV5	34400	102732	13.49%	0.930%

LSC Area Percent Report

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Operator : JC/MD
Sample : M3694-01 10X
Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : S-1

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

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Title : SW846 8260

37	12.469	1864	1867	1873	rVB3	55983	90743	11.92%	0.821%
38	12.555	1876	1881	1883	rBV4	31522	58122	7.63%	0.526%
39	12.585	1883	1886	1888	rVV3	27934	42087	5.53%	0.381%
40	12.616	1888	1891	1894	rVB	65172	71900	9.44%	0.651%
41	12.689	1899	1903	1913	rVB4	42892	111278	14.61%	1.007%
42	12.768	1913	1916	1920	rBV6	7232	14051	1.85%	0.127%
43	12.823	1920	1925	1927	rBV2	57963	81638	10.72%	0.739%
44	12.890	1932	1936	1939	rVV2	71213	109364	14.36%	0.990%
45	12.921	1939	1941	1948	rVB	83461	118016	15.50%	1.068%
46	12.988	1948	1952	1955	rBV3	51677	64453	8.46%	0.583%
47	13.024	1955	1958	1966	rVB3	40743	84269	11.07%	0.763%
48	13.097	1966	1970	1972	rBV3	22127	35728	4.69%	0.323%
49	13.140	1975	1977	1979	rVV2	14872	14490	1.90%	0.131%
50	13.170	1979	1982	1985	rVB	23494	24369	3.20%	0.221%
51	13.262	1994	1997	1998	rBV2	17448	17652	2.32%	0.160%
52	13.292	1998	2002	2008	rVV4	121569	207340	27.23%	1.876%
53	13.384	2013	2017	2020	rVV2	54654	108317	14.22%	0.980%
54	13.420	2020	2023	2032	rVB8	65025	159496	20.94%	1.443%
55	13.506	2034	2037	2040	rBV2	43206	62694	8.23%	0.567%
56	13.548	2040	2044	2047	rVV	57935	70984	9.32%	0.642%
57	13.585	2047	2050	2053	rVB2	79806	101478	13.33%	0.918%
58	13.640	2053	2059	2061	rBV6	28125	53604	7.04%	0.485%
59	13.670	2061	2064	2068	rVV2	71903	112628	14.79%	1.019%
60	13.737	2072	2075	2082	rVB4	51173	92762	12.18%	0.839%
61	13.805	2082	2086	2089	rBV2	61117	82996	10.90%	0.751%
62	13.847	2090	2093	2099	rVB4	64181	94592	12.42%	0.856%
63	13.926	2099	2106	2111	rBV6	84653	176993	23.24%	1.602%
64	13.975	2111	2114	2116	rBV2	28288	33300	4.37%	0.301%
65	14.079	2126	2131	2134	rBV	114722	152349	20.00%	1.379%
66	14.103	2134	2135	2139	rVV3	30592	30596	4.02%	0.277%
67	14.140	2139	2141	2143	rVV3	14765	18126	2.38%	0.164%
68	14.164	2143	2145	2149	rVB2	36419	38726	5.09%	0.350%
69	14.219	2149	2154	2158	rBV	140721	193579	25.42%	1.752%
70	14.323	2167	2171	2176	rBV2	79876	106659	14.01%	0.965%
71	14.378	2176	2180	2183	rVB	103508	131674	17.29%	1.191%
72	14.420	2184	2187	2193	rVB5	42348	78070	10.25%	0.706%
73	14.487	2193	2198	2201	rBV4	69469	122826	16.13%	1.111%
74	14.518	2201	2203	2206	rVB2	39022	40613	5.33%	0.367%
75	14.554	2206	2209	2211	rBV4	21444	23470	3.08%	0.212%
76	14.579	2211	2213	2216	rVB3	22530	24063	3.16%	0.218%

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Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : S-1

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
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Title : SW846 8260

77	14.615	2216	2219	2223	rBV3	81064	99853	13.11%	0.904%
78	14.676	2226	2229	2233	rVB2	51034	71168	9.35%	0.644%
79	14.731	2234	2238	2240	rBV3	44934	62958	8.27%	0.570%
80	14.756	2240	2242	2244	rVV2	30540	30221	3.97%	0.273%
81	14.786	2244	2247	2251	rVV4	87679	134520	17.66%	1.217%
82	14.853	2255	2258	2264	rVB4	40777	59276	7.78%	0.536%
83	15.054	2287	2291	2293	rBV4	19243	24318	3.19%	0.220%
84	15.188	2307	2313	2320	rBV2	73710	152707	20.05%	1.382%
85	15.377	2340	2344	2347	rBV2	90132	124440	16.34%	1.126%
86	15.420	2347	2351	2356	rVV3	72550	126564	16.62%	1.145%
87	15.481	2356	2361	2373	rVB	207206	340781	44.75%	3.084%
88	15.615	2378	2383	2387	rBV	247030	392424	51.53%	3.551%
89	15.652	2387	2389	2398	rVB2	98907	159454	20.94%	1.443%
90	15.743	2400	2404	2409	rVV3	57920	99571	13.07%	0.901%
91	15.841	2411	2420	2430	rVB3	62898	228117	29.95%	2.064%
92	15.993	2441	2445	2456	rVB3	48309	105300	13.83%	0.953%
93	16.091	2457	2461	2465	rBV4	18652	29990	3.94%	0.271%
94	16.267	2486	2490	2492	rBV3	17360	28309	3.72%	0.256%
95	16.353	2500	2504	2512	rVB	63423	120546	15.83%	1.091%
96	16.426	2513	2516	2520	rVB3	12480	16018	2.10%	0.145%
97	16.475	2521	2524	2531	rVB2	21132	35739	4.69%	0.323%
98	16.566	2534	2539	2540	rVV3	20518	34556	4.54%	0.313%
99	16.603	2540	2545	2550	rVV2	76535	143975	18.91%	1.303%
100	16.658	2550	2554	2560	rVB	58909	97766	12.84%	0.885%

Sum of corrected areas: 11051637

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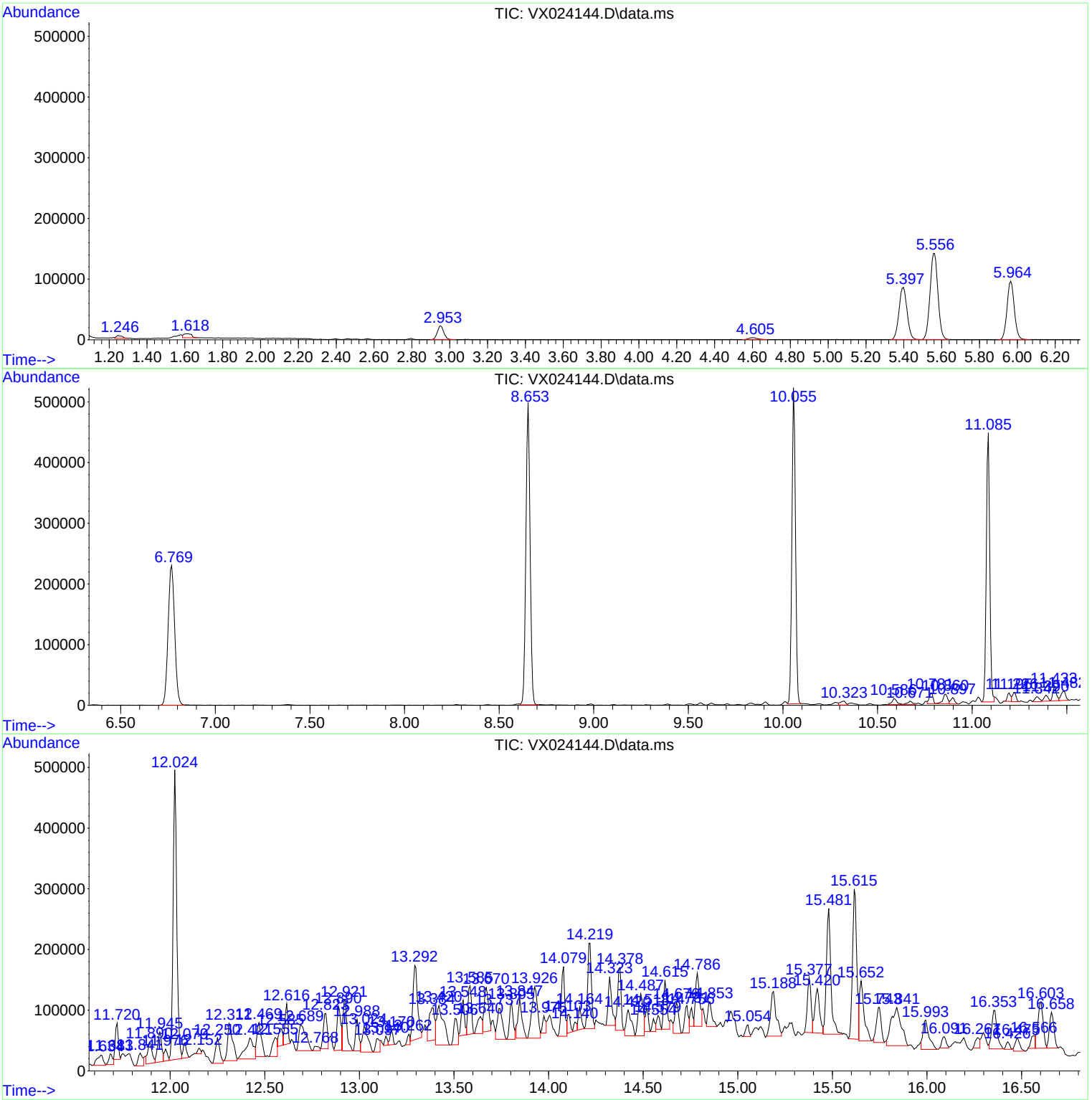
Instrument :
MSVOA_X
ClientSampleId :
S-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

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



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Instrument :
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S-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

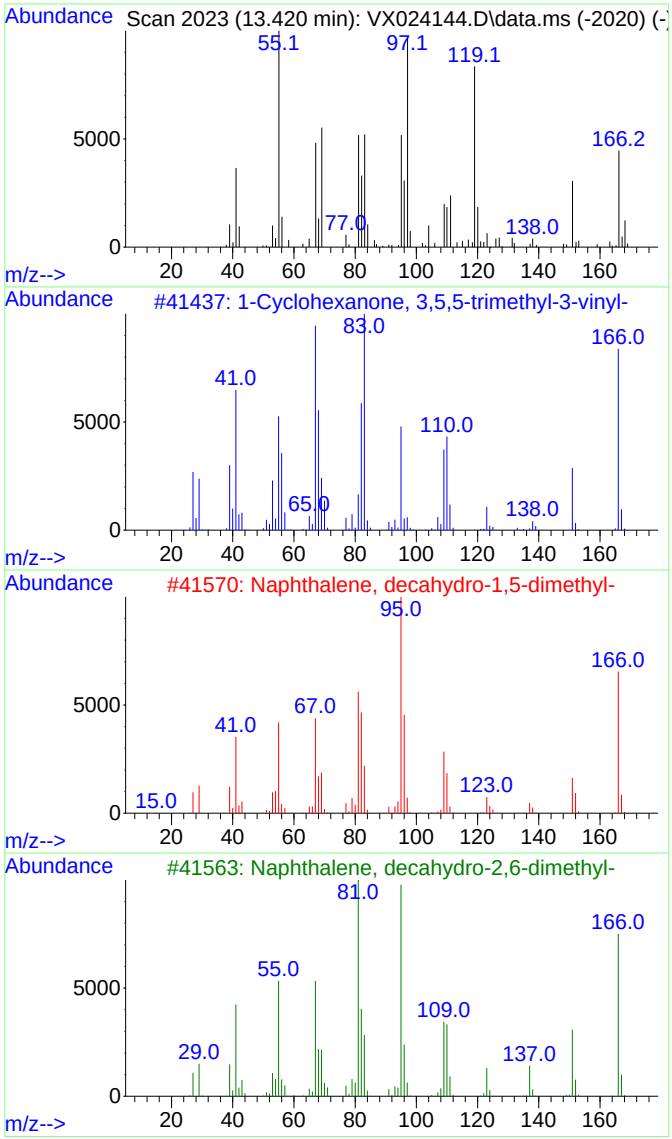
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

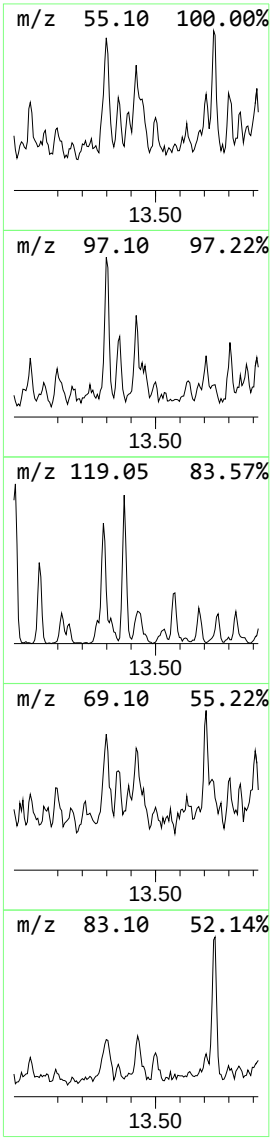
****

Peak Number 2 unknown13.420 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.420	12.48 ug/l	159496	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Cyclohexanone, 3,5,5-trimethyl...	166	C11H18O	027749-07-1	42
2	Naphthalene, decahydro-1,5-dimet...	166	C12H22	066552-62-3	38
3	Naphthalene, decahydro-2,6-dimet...	166	C12H22	001618-22-0	30
4	Naphthalene, decahydro-2,3-dimet...	166	C12H22	001008-80-6	25
5	Bicyclo[2.2.1]heptan-2-one, 1,3,...	166	C11H18O	005811-48-3	22





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Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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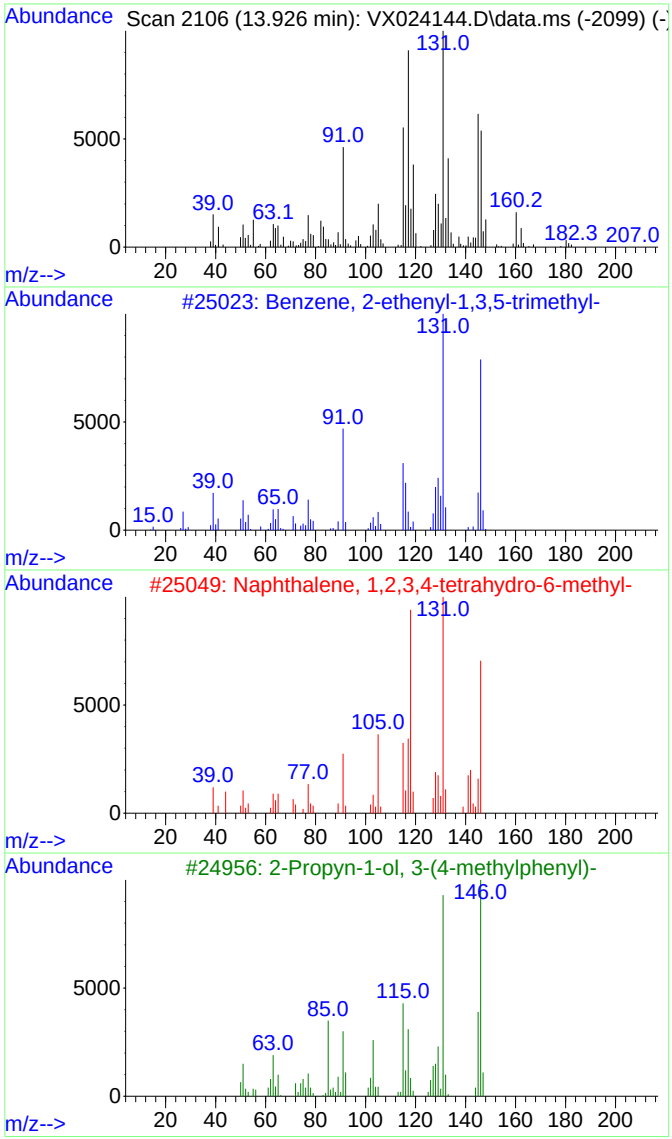
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

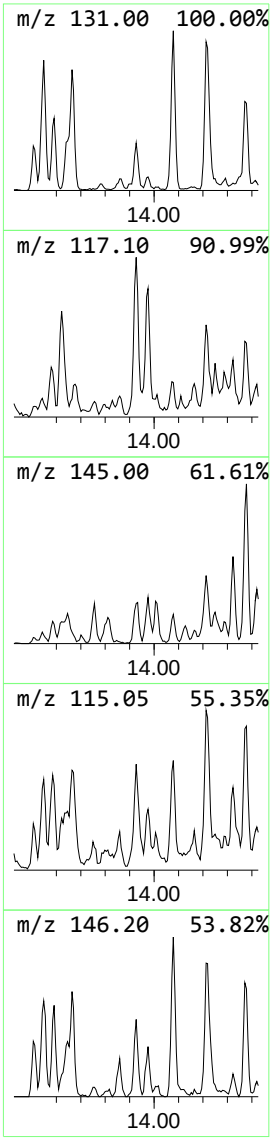
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzene, 2-ethenyl-1,3,5-tr... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.926	13.85 ug/l	176993	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	50
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	49
3	2-Propyn-1-ol, 3-(4-methylphenyl)-	146	C10H10O	016017-24-6	49
4	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	46
5	Benzene, (1-ethyl-1-propenyl)-	146	C11H14	004701-36-4	46





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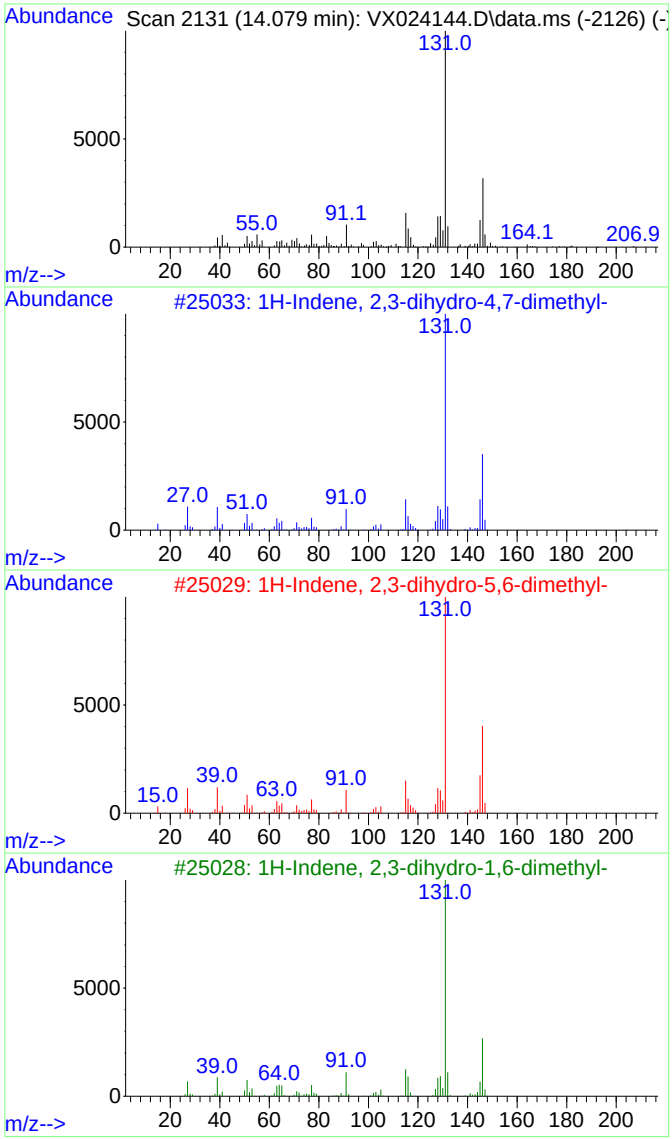
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

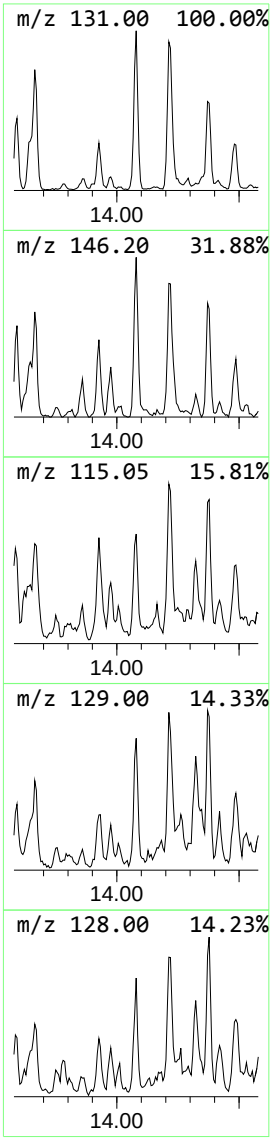
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1H-Indene, 2,3-dihydro-4,7-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.079	11.92 ug/l	152349	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	97
2	1H-Indene, 2,3-dihydro-5,6-dimet...	146	C11H14	001075-22-5	96
3	1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	94
4	1H-Indene, 2,3-dihydro-4,6-dimet...	146	C11H14	001685-82-1	93
5	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	91





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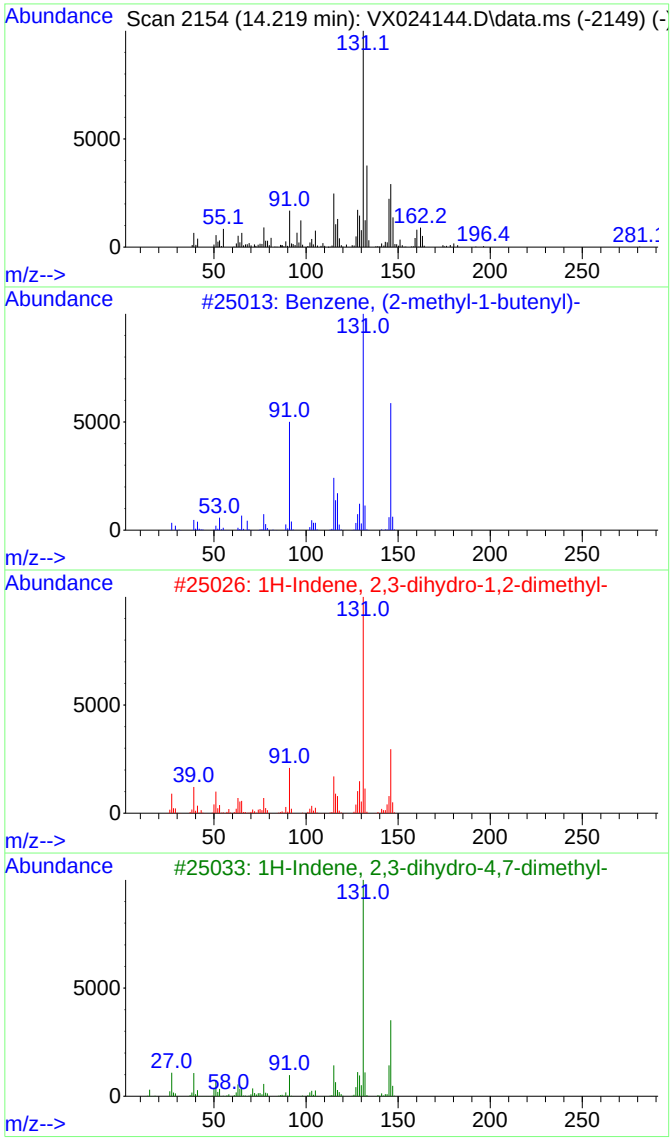
Quant Title : SW846 8260

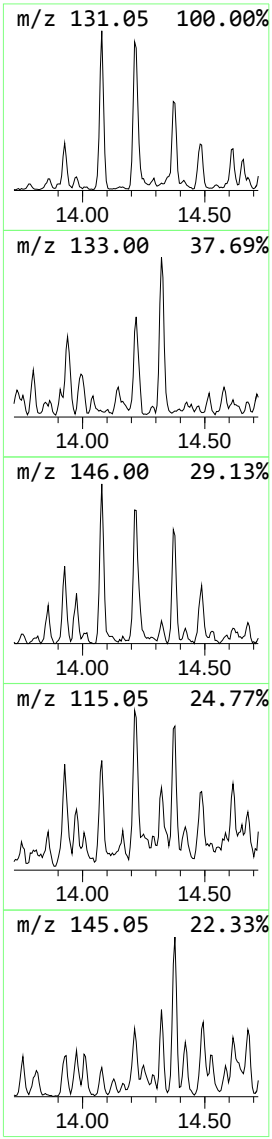
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, (2-methyl-1-butenyl)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.219	15.15 ug/l	193579	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	76
2	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	72
3	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	68
4	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	68
5	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	64





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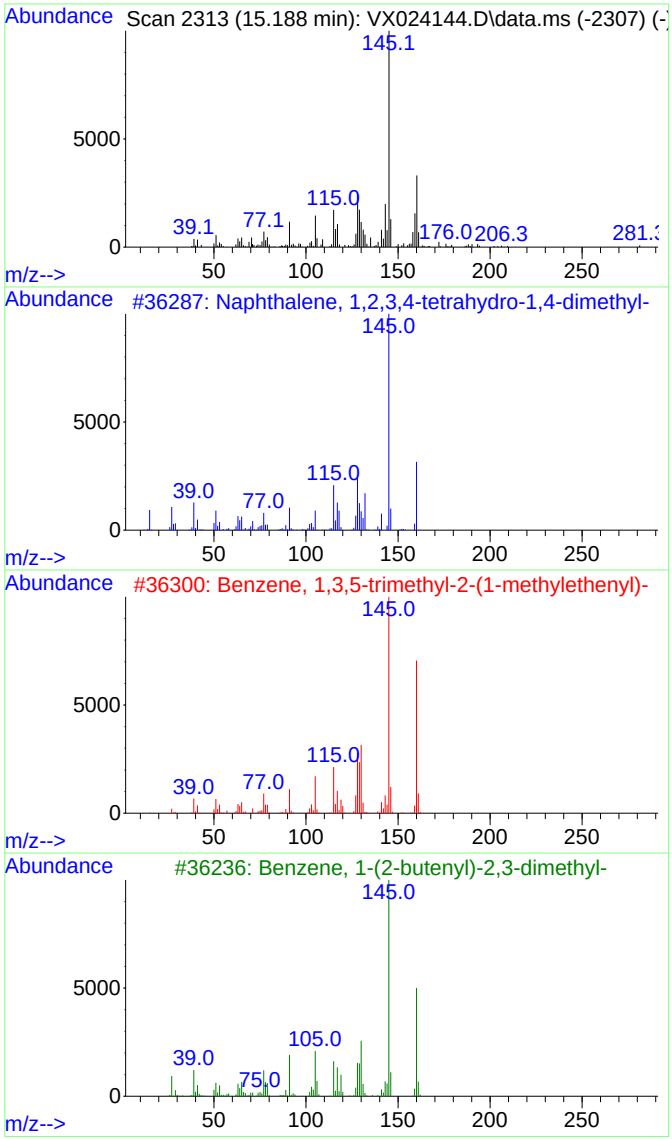
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

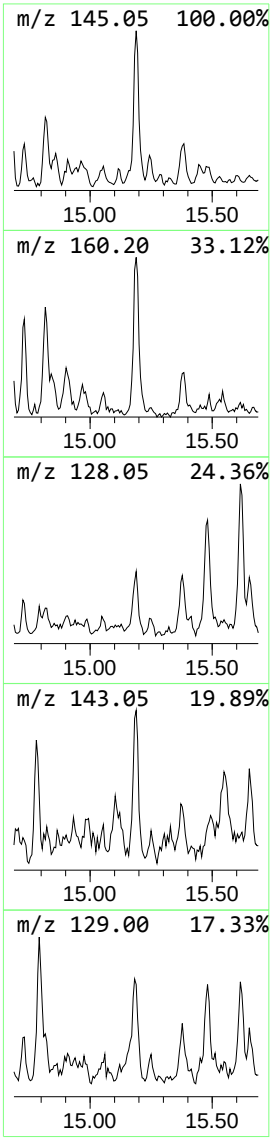
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.188	11.95 ug/l	152707	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	90
2	Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	81
3	Benzene, 1-(2-butenyl)-2,3-dimet...	160	C12H16	054340-85-1	76
4	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	001076-61-5	70
5	1H-Indene, 2,3-dihydro-1,1,3-tri...	160	C12H16	002613-76-5	68





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090921\
Data File : VX024144.D
Acq On : 09 Sep 2021 16:43
Operator : JC/MD
Sample : M3694-01 10X
Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
S-1

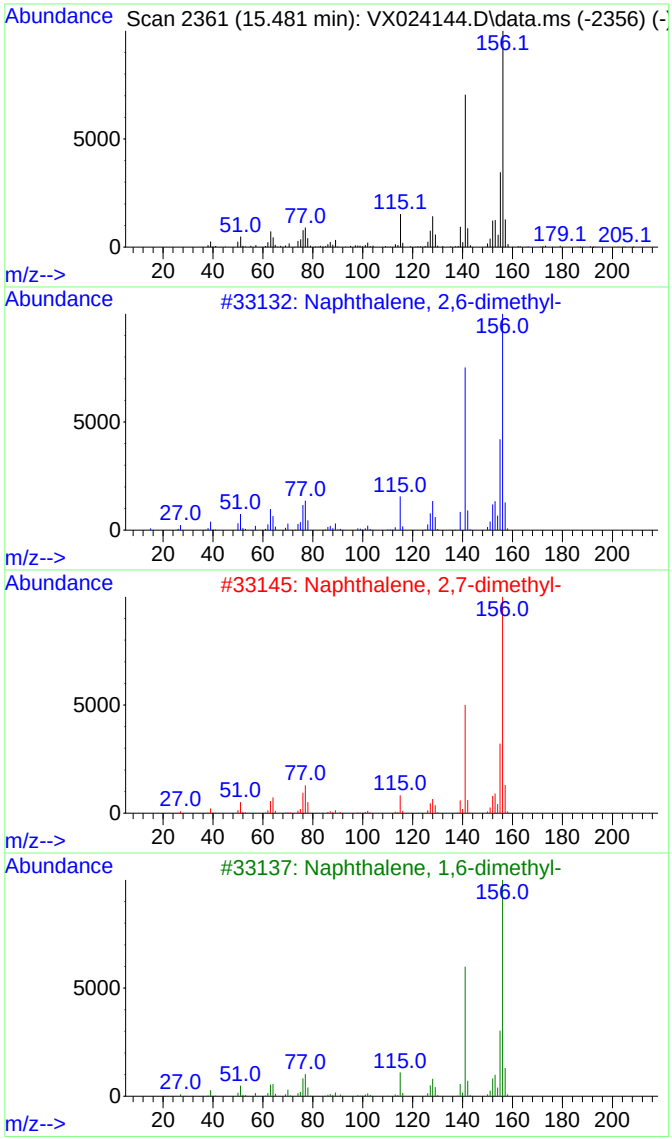
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

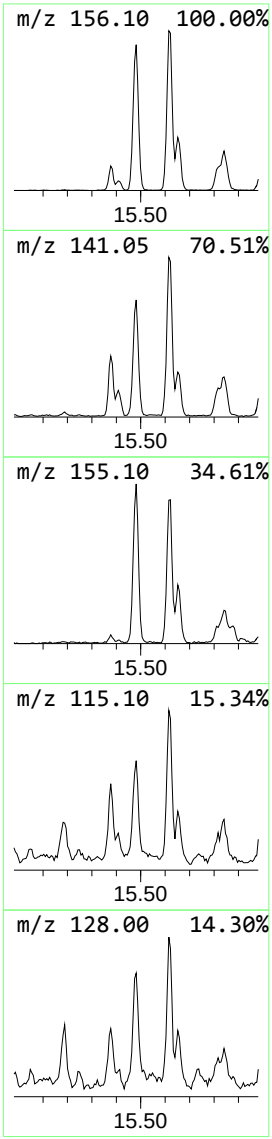
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Naphthalene, 2,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.481	26.67 ug/l	340781	1,4-Dichlorobenzene-d4	12.024

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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090921\
Data File : VX024144.D
Acq On : 09 Sep 2021 16:43
Operator : JC/MD
Sample : M3694-01 10X
Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
S-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

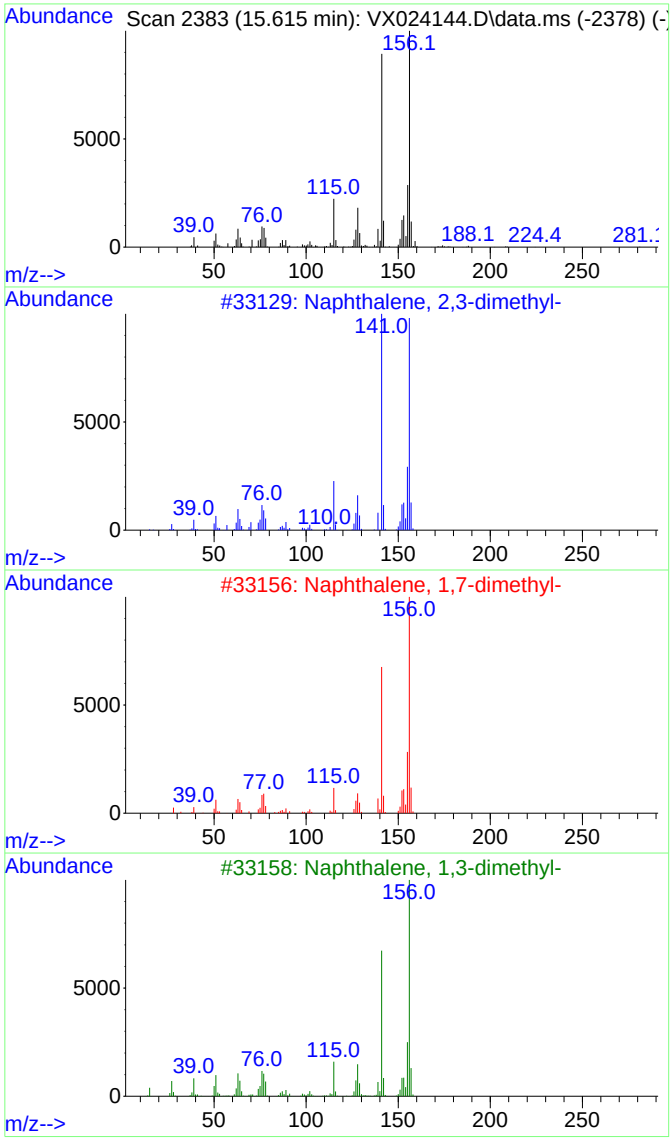
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

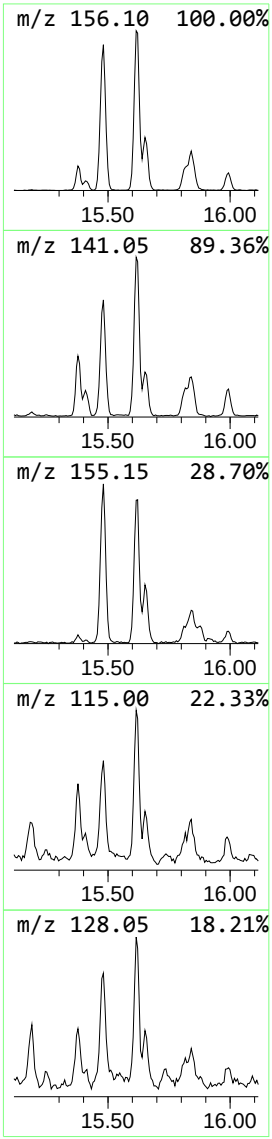
****

Peak Number 8 Naphthalene, 2,3-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	30.71 ug/l	392424	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, 1,7-dimethyl-	156	C12H12	000575-37-1	97
3	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
4	Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	97
5	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	96





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090921\
Data File : VX024144.D
Acq On : 09 Sep 2021 16:43
Operator : JC/MD
Sample : M3694-01 10X
Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
S-1

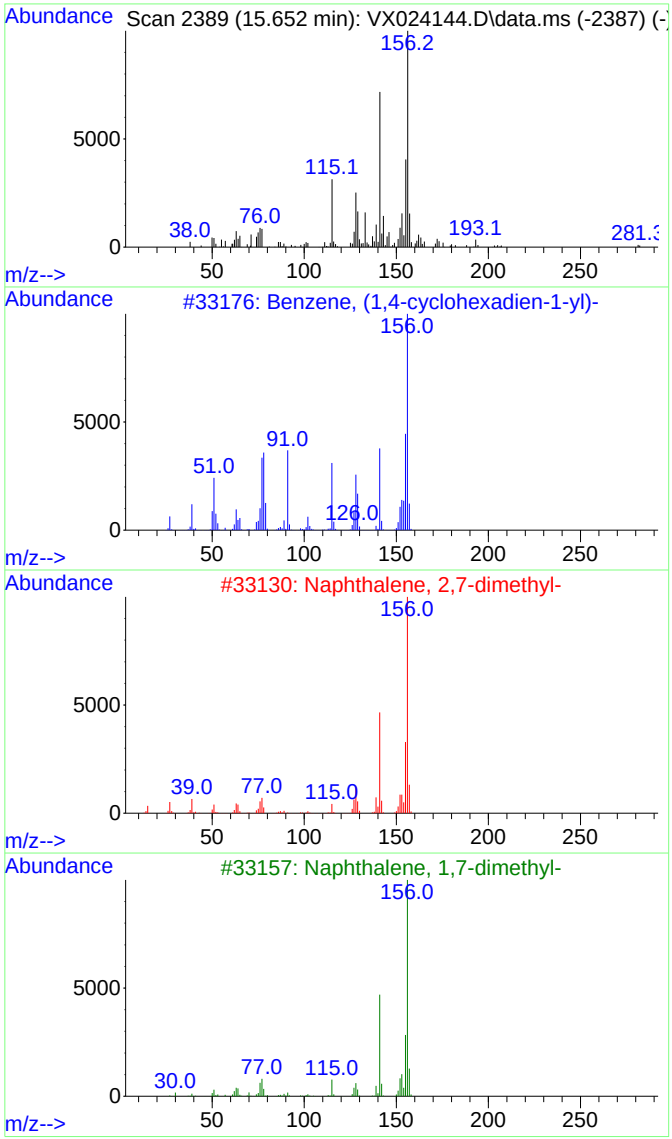
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

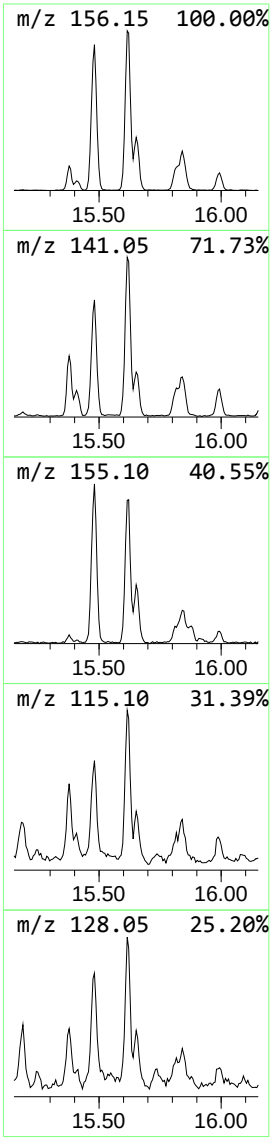
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, (1,4-cyclohexadien... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.652	12.48 ug/l	159454	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1,4-cyclohexadien-1-yl)-	156	C12H12	013703-52-1	89
2	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	87
3	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	87
4	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	83
5	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	83





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090921\
Data File : VX024144.D
Acq On : 09 Sep 2021 16:43
Operator : JC/MD
Sample : M3694-01 10X
Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
S-1

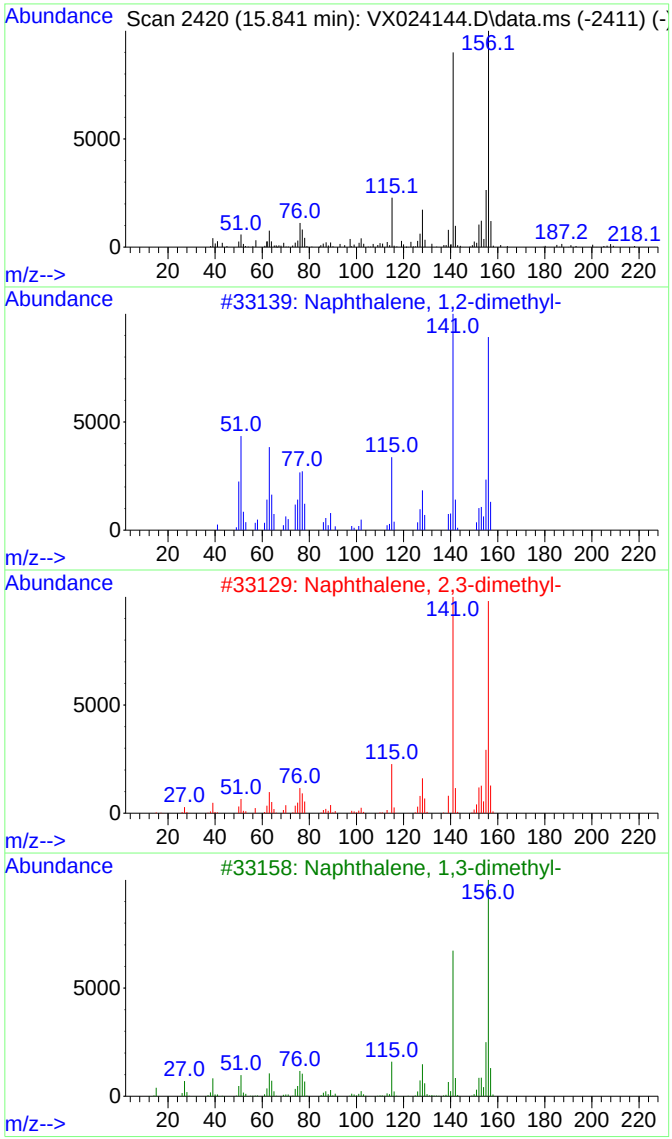
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

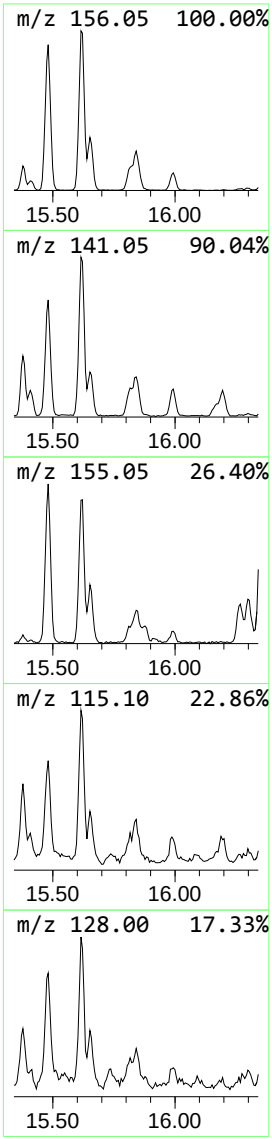
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, 1,2-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.841	17.85 ug/l	228117	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	95
2	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	94
3	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	94
4	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	93
5	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090921\
Data File : VX024144.D
Acq On : 09 Sep 2021 16:43
Operator : JC/MD
Sample : M3694-01 10X
Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : S-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.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
unknown13.420	13.420	12.5	ug/l	159496	4	12.024	638936	50.0
Benzene, 2-ethe...	13.926	13.9	ug/l	176993	4	12.024	638936	50.0
1H-Indene, 2,3-...	14.079	11.9	ug/l	152349	4	12.024	638936	50.0
Benzene, (2-met...	14.219	15.2	ug/l	193579	4	12.024	638936	50.0
Naphthalene, 1,...	15.188	11.9	ug/l	152707	4	12.024	638936	50.0
Naphthalene, 2,...	15.481	26.7	ug/l	340781	4	12.024	638936	50.0
Naphthalene, 2,...	15.615	30.7	ug/l	392424	4	12.024	638936	50.0
Benzene, (1,4-c...	15.652	12.5	ug/l	159454	4	12.024	638936	50.0
Naphthalene, 1,...	15.841	17.9	ug/l	228117	4	12.024	638936	50.0