LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062822\
Data File : VX029839.D
Acq On : 28 Jun 2022 19:26
Operator : JC/MD
Sample : N3494-04
Misc : 6.77g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SP-EXC-3-GR

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\82X062822W.M
Title : SW846 8260

Signal : TIC: VX029839.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.636	78	90	93	rBV	28597	53861	1.26%	0.067%
2	1.910	132	135	141	rBV	73883	89121	2.09%	0.112%
3	3.416	374	382	396	rVB2	52690	120113	2.82%	0.150%
4	5.391	692	706	719	rBV3	123085	386077	9.06%	0.484%
5	5.550	722	732	749	rVB	241220	700820	16.44%	0.878%
6	5.958	788	799	806	rBV	147149	391828	9.19%	0.491%
7	6.031	806	811	823	rVB	54010	143283	3.36%	0.180%
8	6.604	896	905	915	rBV2	41955	100915	2.37%	0.126%
9	6.763	921	931	950	rBV	370090	915142	21.46%	1.147%
10	7.379	1021	1032	1041	rBV2	25874	60275	1.41%	0.076%
11	8.647	1234	1240	1247	rVV	737081	1181997	27.72%	1.481%
12	8.720	1247	1252	1258	rVB	63344	93868	2.20%	0.118%
13	8.909	1279	1283	1289	rBV	46319	68230	1.60%	0.085%
14	10.055	1466	1471	1479	rBV	662132	992499	23.28%	1.243%
15	10.195	1487	1494	1500	rBV	58454	95900	2.25%	0.120%
16	10.305	1500	1512	1518	rBV2	162718	324524	7.61%	0.407%
17	10.360	1518	1521	1532	rVB4	46533	78119	1.83%	0.098%
18	10.457	1532	1537	1542	rBV2	52262	83424	1.96%	0.105%
19	10.567	1551	1555	1557	rBV	60295	80843	1.90%	0.101%
20	10.781	1582	1590	1593	rBV3	96100	168922	3.96%	0.212%
21	10.817	1593	1596	1599	rVV4	45109	67036	1.57%	0.084%
22	10.854	1599	1602	1605	rVV4	54603	86587	2.03%	0.108%
23	10.890	1605	1608	1613	rVV2	120623	185868	4.36%	0.233%
24	10.945	1613	1617	1623	rVB3	81633	134916	3.16%	0.169%
25	11.006	1623	1627	1630	rBV2	93064	138676	3.25%	0.174%
26	11.085	1635	1640	1645	rBV	511548	732725	17.19%	0.918%
27	11.128	1645	1647	1651	rVB2	82954	91518	2.15%	0.115%
28	11.220	1651	1662	1668	rBV	780631	1356164	31.81%	1.699%
29	11.311	1672	1677	1680	rBV2	217885	402267	9.44%	0.504%
30	11.396	1684	1691	1694	rBV5	202744	372590	8.74%	0.467%
31	11.433	1694	1697	1702	rBV4	127108	209675	4.92%	0.263%
32	11.482	1702	1705	1709	rBV2	310848	403637	9.47%	0.506%
33	11.524	1709	1712	1718	rVB2	287121	471987	11.07%	0.591%
34	11.604	1718	1725	1727	rBV3	80856	152756	3.58%	0.191%
35	11.634	1727	1730	1734	rVB3	144380	166751	3.91%	0.209%
36	11.689	1735	1739	1742	rBV6	265102	324079	7.60%	0.406%

LSC Area Percent Report

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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SP-EXC-3-GR

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\82X062822W.M
Title : SW846 8260

37	11.750	1742	1749	1759	rBV5	720674	1552450	36.41%	1.945%
38	11.847	1759	1765	1768	rBV3	234581	464701	10.90%	0.582%
39	11.890	1768	1772	1776	rVB5	367750	626532	14.70%	0.785%
40	11.933	1776	1779	1782	rBV4	197018	243939	5.72%	0.306%
41	11.975	1782	1786	1790	rVB6	212990	327502	7.68%	0.410%
42	12.024	1790	1794	1805	rBV2	770649	1471897	34.52%	1.844%
43	12.110	1805	1808	1810	rBV2	160826	202711	4.75%	0.254%
44	12.158	1812	1816	1821	rVB2	1341736	1889818	44.33%	2.368%
45	12.201	1821	1823	1826	rVB3	208746	222916	5.23%	0.279%
46	12.256	1826	1832	1835	rBV5	635258	1280912	30.04%	1.605%
47	12.335	1838	1845	1849	rBV3	1081380	2203281	51.68%	2.760%
48	12.475	1860	1868	1876	rBV7	1629980	3654308	85.71%	4.578%
49	12.579	1880	1885	1886	rBV4	424956	677360	15.89%	0.849%
50	12.628	1891	1893	1897	rVB2	279964	304144	7.13%	0.381%
51	12.689	1897	1903	1907	rBV5	678966	1444544	33.88%	1.810%
52	12.738	1907	1911	1913	rBV4	295935	459920	10.79%	0.576%
53	12.768	1913	1916	1920	rVB5	460554	648193	15.20%	0.812%
54	12.823	1920	1925	1930	rVB2	2162310	3357822	78.76%	4.207%
55	12.920	1934	1941	1945	rBV4	1278538	2328168	54.61%	2.917%
56	12.987	1948	1952	1957	rVB2	3571337	4263509	100.00%	5.342%
57	13.042	1958	1961	1965	rVB5	511565	668658	15.68%	0.838%
58	13.103	1965	1971	1975	rBV7	482163	1130967	26.53%	1.417%
59	13.189	1982	1985	1987	rBV3	298322	427563	10.03%	0.536%
60	13.237	1990	1993	1998	rVV3	608544	929698	21.81%	1.165%
61	13.292	1998	2002	2008	rVB2	2070769	3301753	77.44%	4.137%
62	13.347	2008	2011	2013	rBV2	493721	618941	14.52%	0.775%
63	13.414	2018	2022	2025	rVV3	2198632	3439210	80.67%	4.309%
64	13.445	2025	2027	2034	rVB4	1625266	2326933	54.58%	2.915%
65	13.506	2034	2037	2042	rBV4	398486	541215	12.69%	0.678%
66	13.676	2062	2065	2066	rBV2	656862	679253	15.93%	0.851%
67	13.707	2067	2070	2074	rVV	2507914	3049311	71.52%	3.820%
68	13.768	2078	2080	2083	rVV3	441574	553412	12.98%	0.693%
69	13.804	2083	2086	2090	rVV2	2021301	2559738	60.04%	3.207%
70	13.847	2090	2093	2096	rVV2	1043696	1298914	30.47%	1.627%
71	13.896	2096	2101	2109	rVB7	1396251	3599819	84.43%	4.510%
72	13.993	2115	2117	2119	rBV2	392241	416822	9.78%	0.522%
73	14.067	2125	2129	2132	rBV3	764726	1161819	27.25%	1.456%
74	14.103	2132	2135	2138	rVV	1383249	1618149	37.95%	2.027%
75	14.140	2138	2141	2145	rVV	1678472	2051342	48.11%	2.570%
76	14.274	2161	2163	2166	rVB2	720184	717742	16.83%	0.899%

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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SP-EXC-3-GR

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\82X062822W.M
Title : SW846 8260

77	14.359	2174	2177	2182	rVB3	687168	1071239	25.13%	1.342%
78	14.426	2184	2188	2195	rVB4	977335	1919217	45.01%	2.405%
79	14.615	2216	2219	2222	rBV	956331	1091703	25.61%	1.368%
80	14.755	2239	2242	2246	rBV2	933346	1115018	26.15%	1.397%
81	14.847	2255	2257	2261	rVB3	402124	390854	9.17%	0.490%
82	14.932	2268	2271	2274	rBV2	835667	1140495	26.75%	1.429%
83	15.420	2347	2351	2356	rVB	1069533	1522438	35.71%	1.907%
84	15.743	2400	2404	2410	rVB	820857	1423240	33.38%	1.783%

Sum of corrected areas: 79817083

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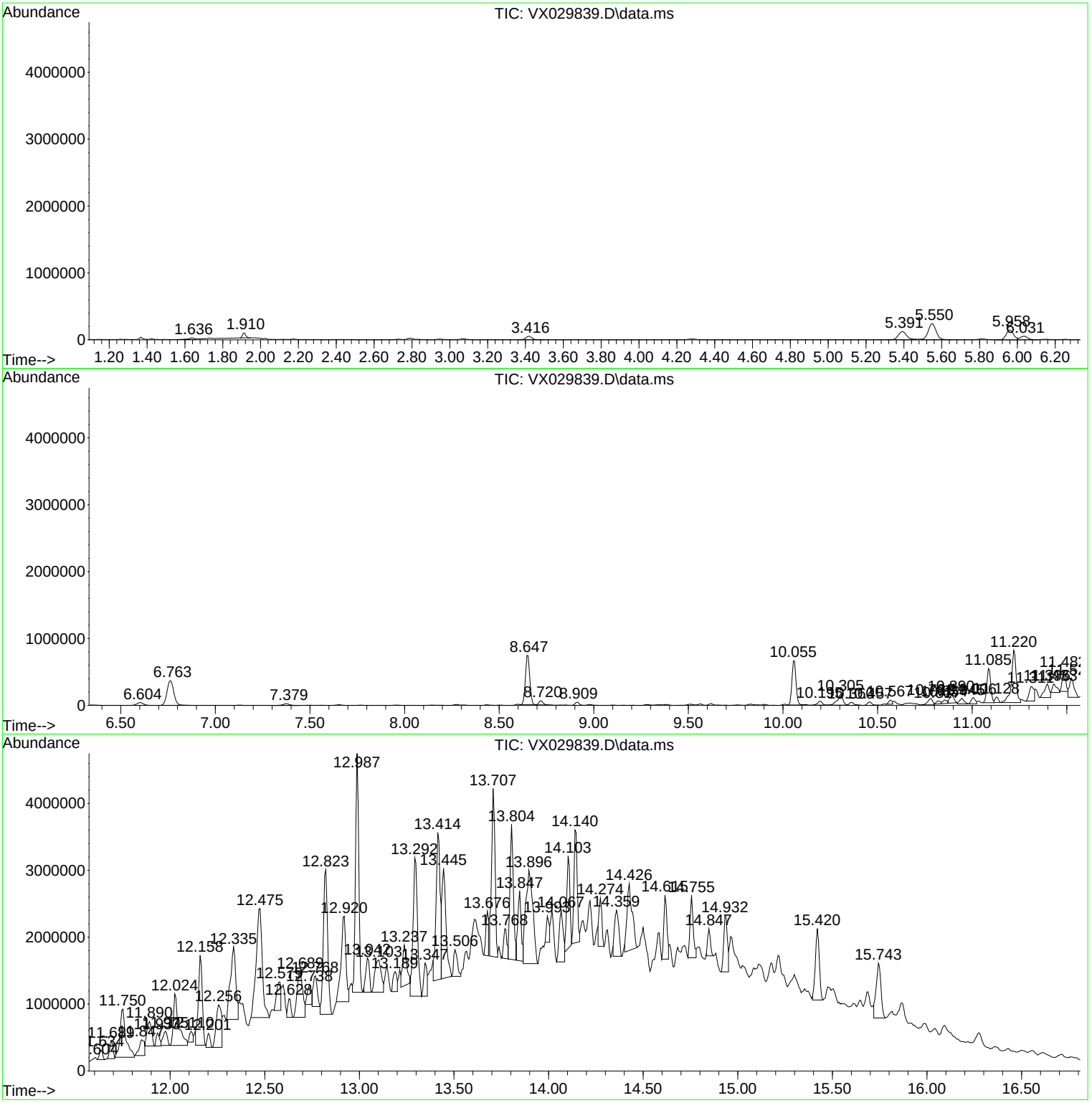
Instrument :
MSVOA_X
ClientSampleId :
SP-EXC-3-GR

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062822\
Data File : VX029839.D
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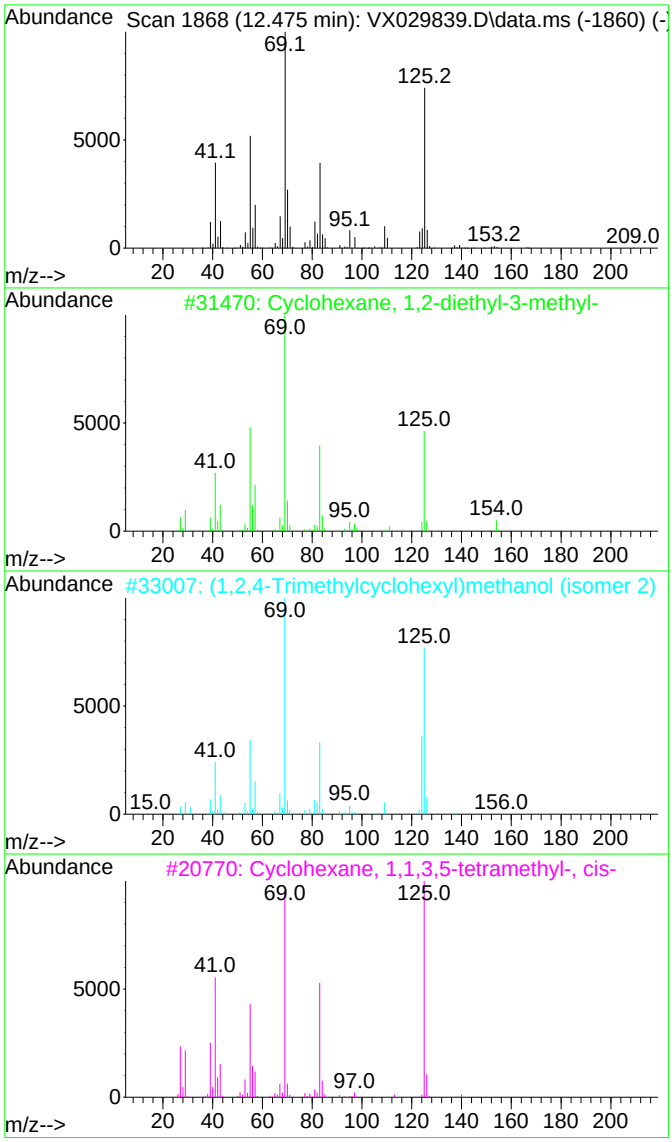
Quant Title : SW846 8260

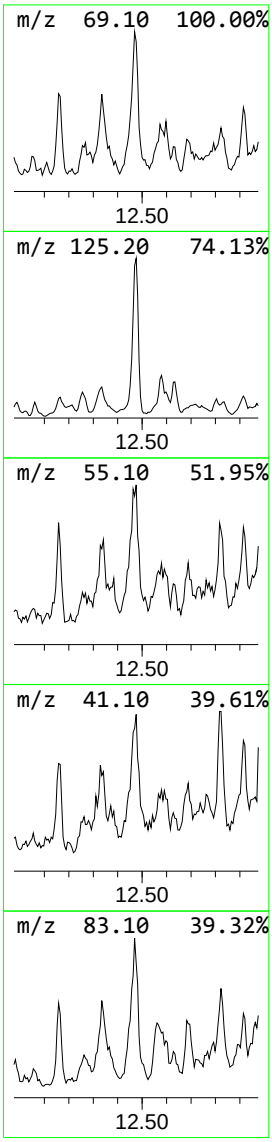
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Cyclohexane, 1,2-diethyl-3-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.475	124.14 ug/l	3654310	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,2-diethyl-3-methyl-	154	C11H22	061141-80-8	80
2	(1,2,4-Trimethylcyclohexyl)metha...	156	C10H20O	1000499-03-9	72
3	Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-32-9	64
4	Cyclohexane, 2,4-diethyl-1-methyl-	154	C11H22	061142-70-9	47
5	2-Aminothiazole-5-carbonitrile	125	C4H3N3S	051640-52-9	43





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Sample : N3494-04
Misc : 6.77g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SP-EXC-3-GR

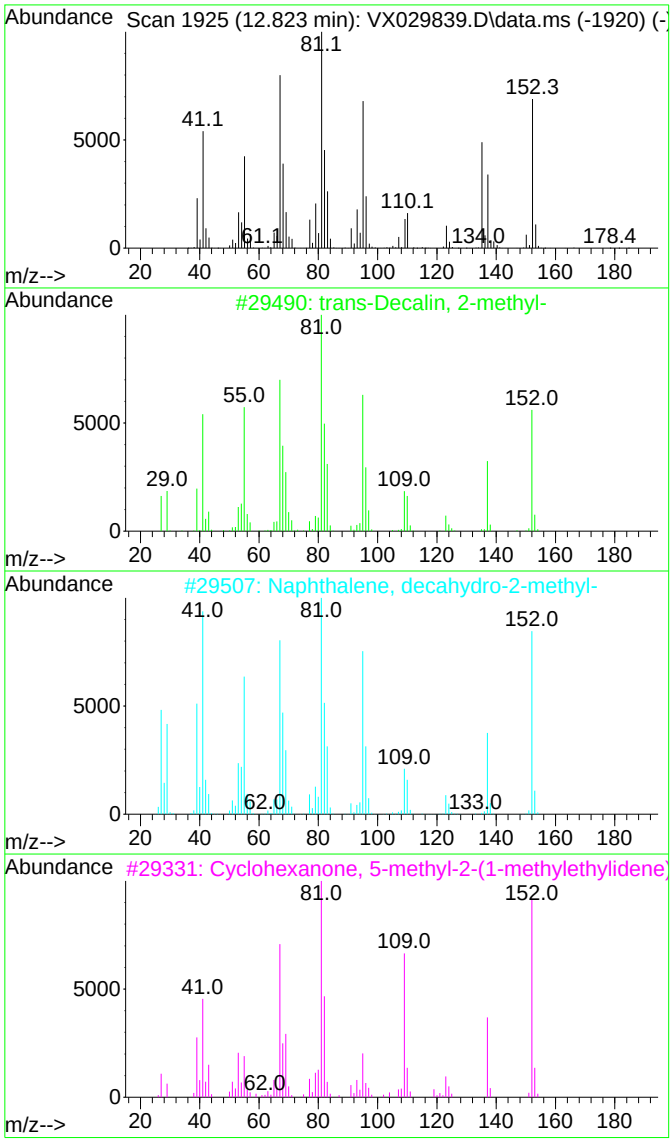
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.M
Quant Title : SW846 8260

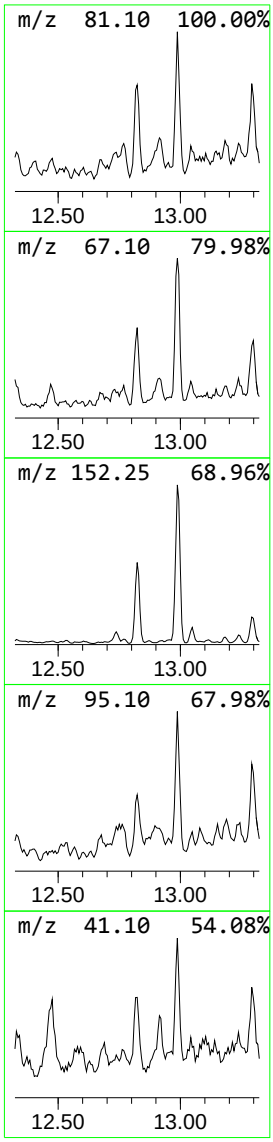
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 trans-Decalin, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.823	114.06 ug/l	3357820	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	93
2	Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	87
3	Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	76
4	Pulegone	152	C10H16O	000089-82-7	70
5	cis-Decalin, 2-syn-methyl-	152	C11H20	1000155-85-6	64





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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.M
Quant Title : SW846 8260

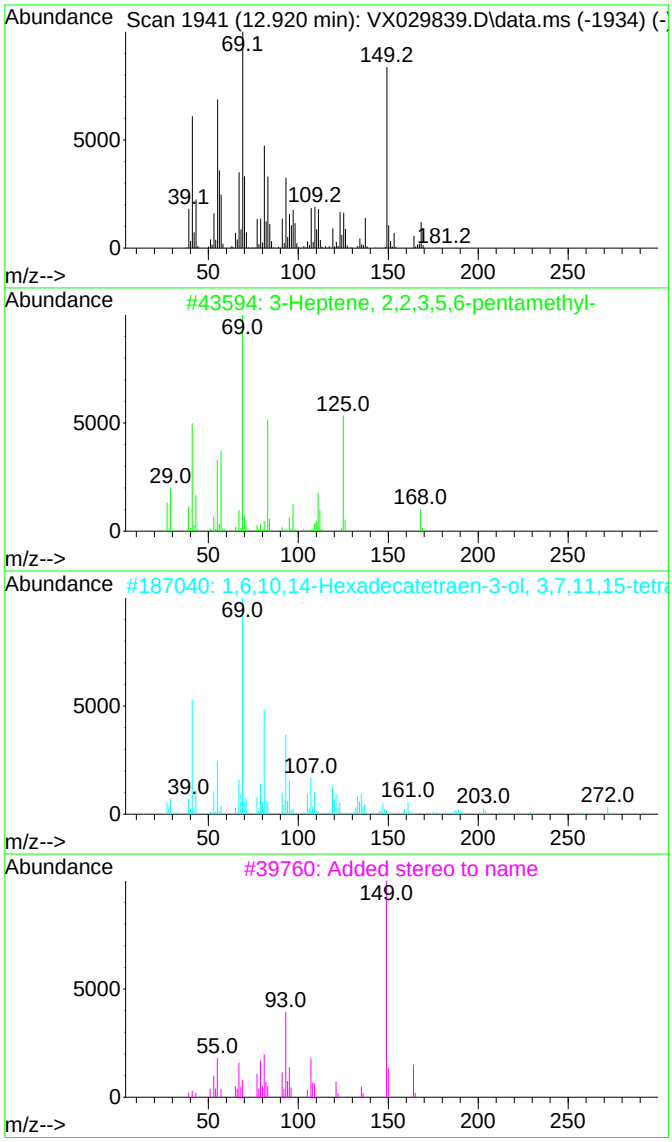
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

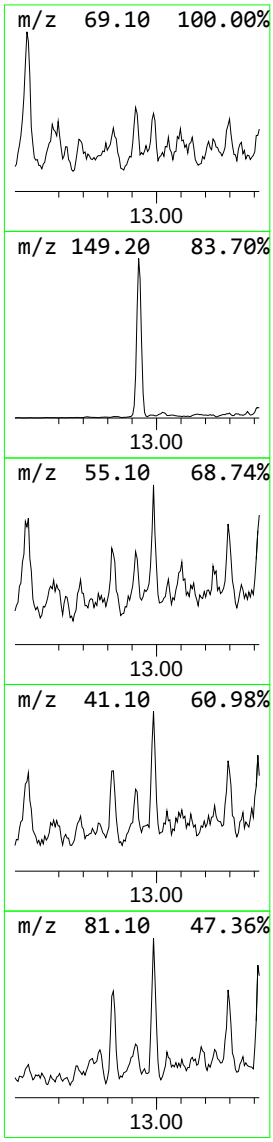
****

Peak Number 3 unknown12.920 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.920	79.09 ug/l	2328170	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Heptene, 2,2,3,5,6-pentamethyl-	168	C12H24	116164-06-8	30
2	1,6,10,14-Hexadecatetraen-3-ol, ...	290	C20H34O	001113-21-9	27
3	Added stereo to name	164	C12H20	024145-88-8	25
4	Cyclohexanone, 3,5-dimethyl-	126	C8H14O	002320-30-1	25
5	Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	25





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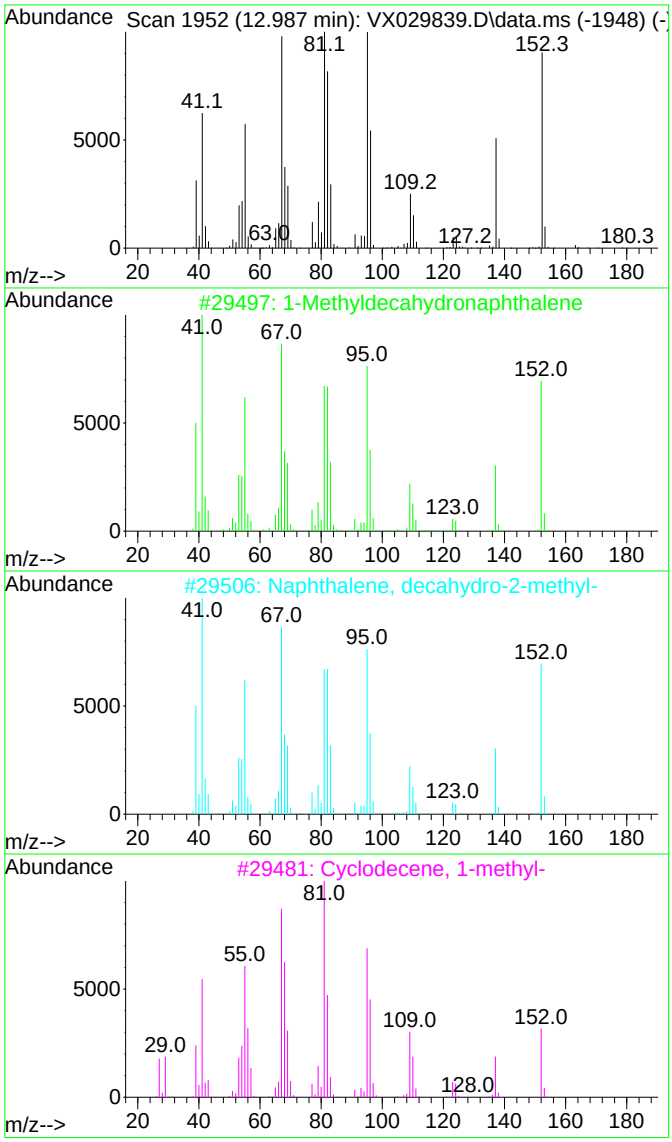
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.M
Quant Title : SW846 8260

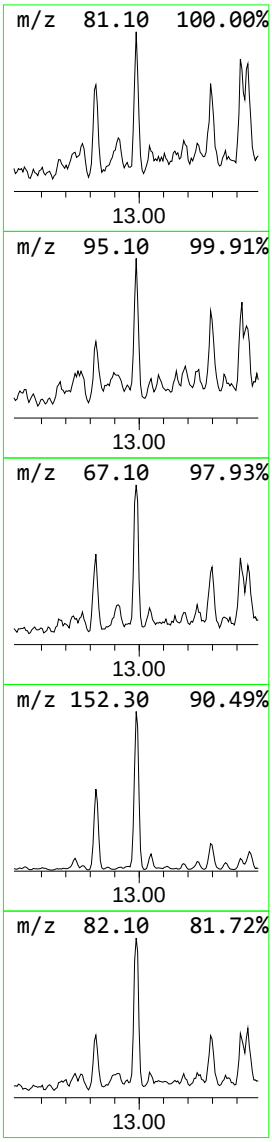
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Methyldecahydronaphthalene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.988	144.83 ug/l	4263510	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methyldecahydronaphthalene	152	C11H20	002958-75-0	96
2	Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	96
3	Cyclodecene, 1-methyl-	152	C11H20	066633-38-3	87
4	cis-Decalin, 2-syn-methyl-	152	C11H20	1000155-85-6	81
5	Decalin, syn-1-methyl-, cis-	152	C11H20	1000158-89-1	76





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Instrument :
MSVOA_X
ClientSampleId :
SP-EXC-3-GR

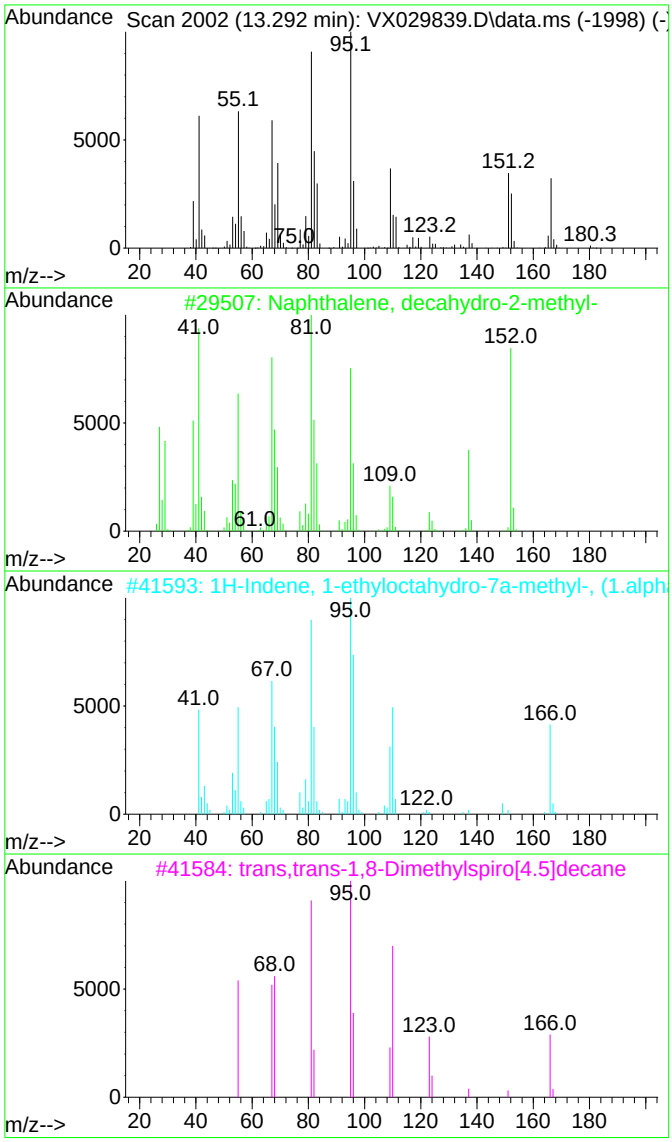
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.M
Quant Title : SW846 8260

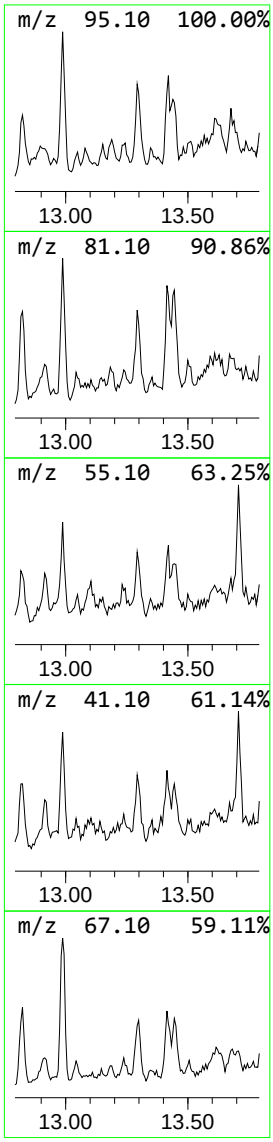
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Naphthalene, decahydro-2-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	112.16 ug/l	3301750	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	90
2	1H-Indene, 1-ethyloctahydro-7a-m...	166	C12H22	056324-71-1	81
3	trans,trans-1,8-Dimethylspiro[4....	166	C12H22	1000111-72-8	76
4	trans,cis-1,8-Dimethylspiro[4.5]...	166	C12H22	1000111-72-9	76
5	trans,trans-1,6-Dimethylspiro[4....	166	C12H22	1000111-72-1	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062822\
Data File : VX029839.D
Acq On : 28 Jun 2022 19:26
Operator : JC/MD
Sample : N3494-04
Misc : 6.77g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SP-EXC-3-GR

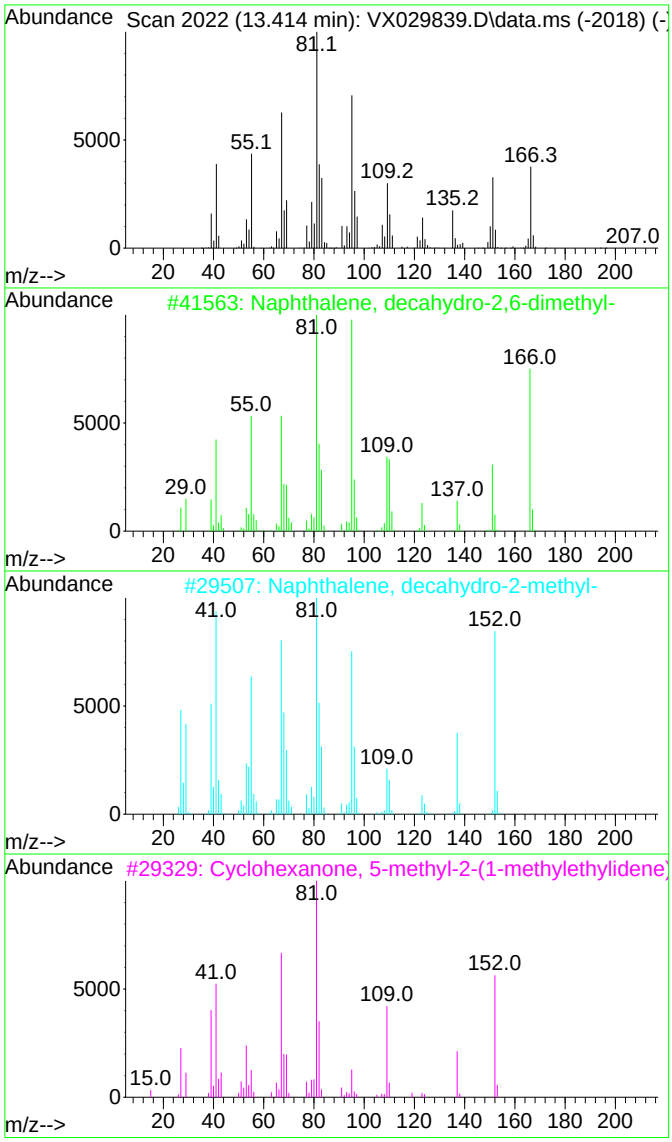
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.M
Quant Title : SW846 8260

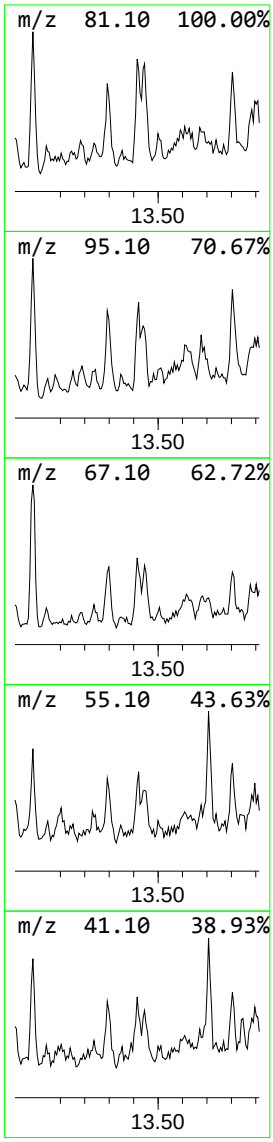
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Naphthalene, decahydro-2,6-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.414	116.83 ug/l	3439210	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-2,6-dimet...	166	C12H22	001618-22-0	83
2	Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	68
3	Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	60
4	Cyclohexene,3-hexyl-	166	C12H22	015232-78-7	58
5	Bicyclo[4.1.0]heptane, 3-methyl-	110	C8H14	041977-47-3	58





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062822\
Data File : VX029839.D
Acq On : 28 Jun 2022 19:26
Operator : JC/MD
Sample : N3494-04
Misc : 6.77g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SP-EXC-3-GR

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.M
Quant Title : SW846 8260

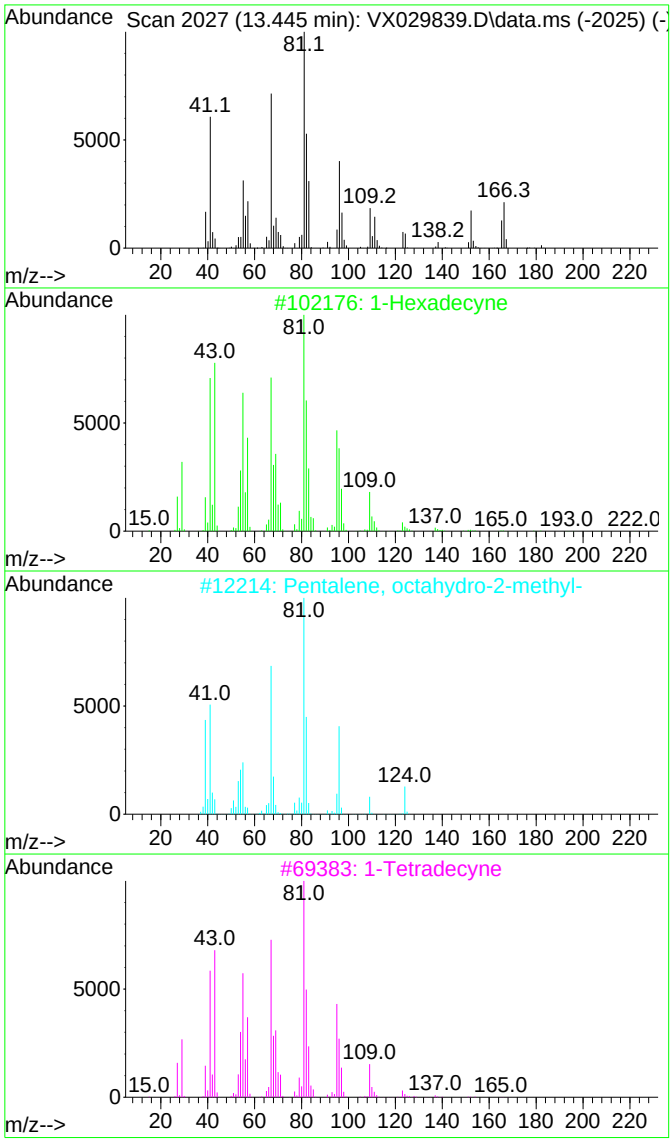
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

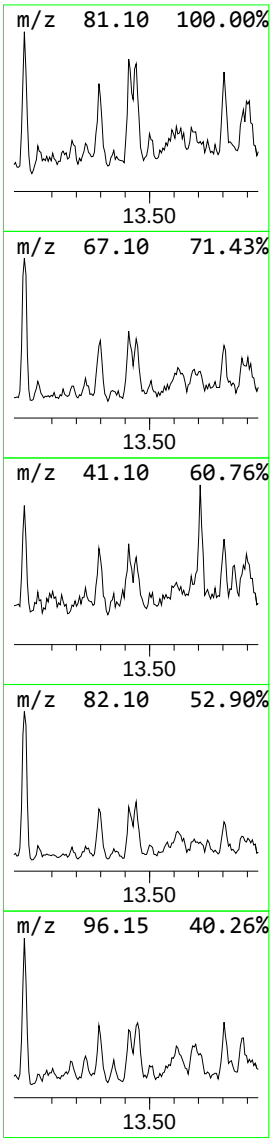
****

Peak Number 7 1-Hexadecyne Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.445	79.05 ug/l	2326930	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecyne	222	C16H30	000629-74-3	72
2	Pentalene, octahydro-2-methyl-	124	C9H16	003868-64-2	68
3	1-Tetradecyne	194	C14H26	000765-10-6	59
4	Cyclohexane, ethenyl-	110	C8H14	000695-12-5	49
5	Cyclododecene	166	C12H22	001501-82-2	49





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062822\
Data File : VX029839.D
Acq On : 28 Jun 2022 19:26
Operator : JC/MD
Sample : N3494-04
Misc : 6.77g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SP-EXC-3-GR

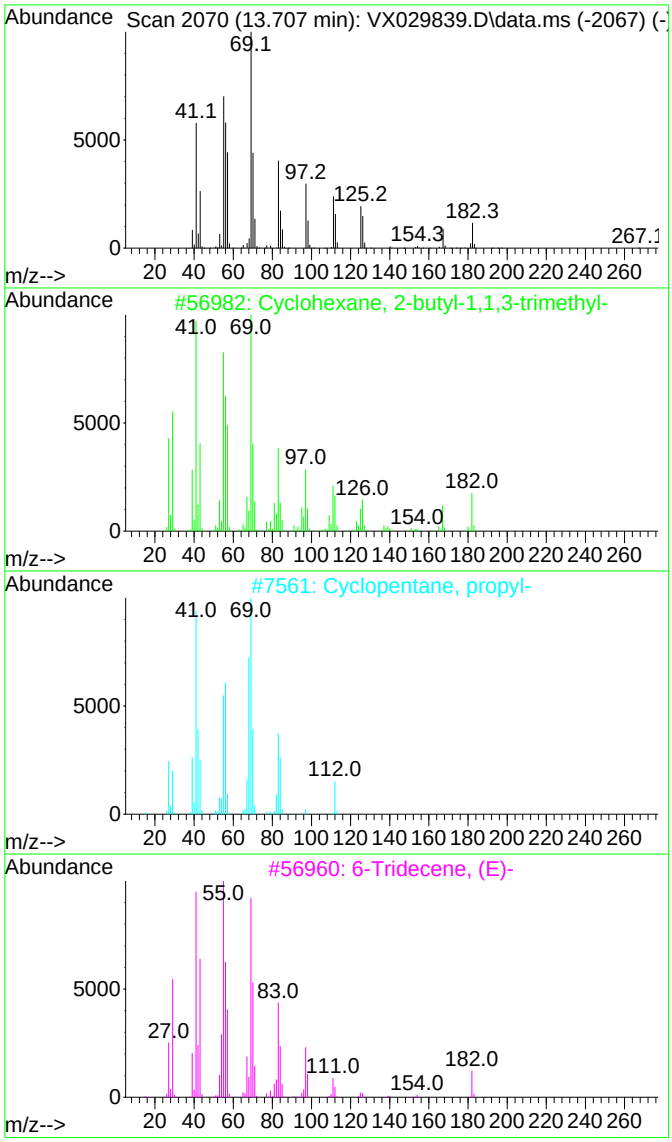
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.M
Quant Title : SW846 8260

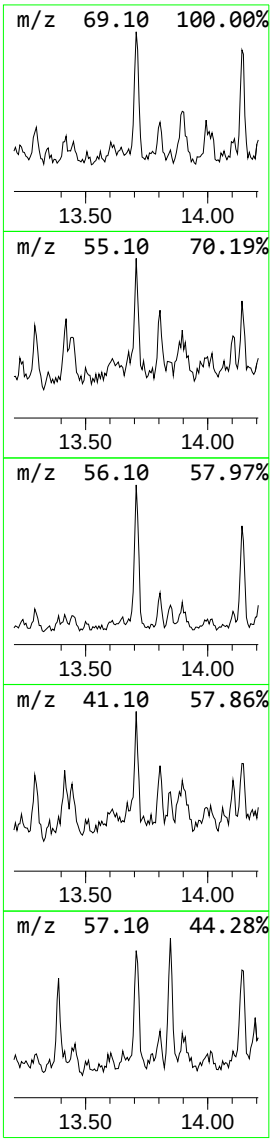
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Cyclohexane, 2-butyl-1,1,3-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.707	103.58 ug/l	3049310	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 2-butyl-1,1,3-trime...	182	C13H26	054676-39-0	96
2	Cyclopentane, propyl-	112	C8H16	002040-96-2	58
3	6-Tridecene, (E)-	182	C13H26	006434-76-0	55
4	2-Tridecene, (E)-	182	C13H26	041446-58-6	49
5	Cyclodecane, methyl-	154	C11H22	013151-43-4	49





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062822\
Data File : VX029839.D
Acq On : 28 Jun 2022 19:26
Operator : JC/MD
Sample : N3494-04
Misc : 6.77g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SP-EXC-3-GR

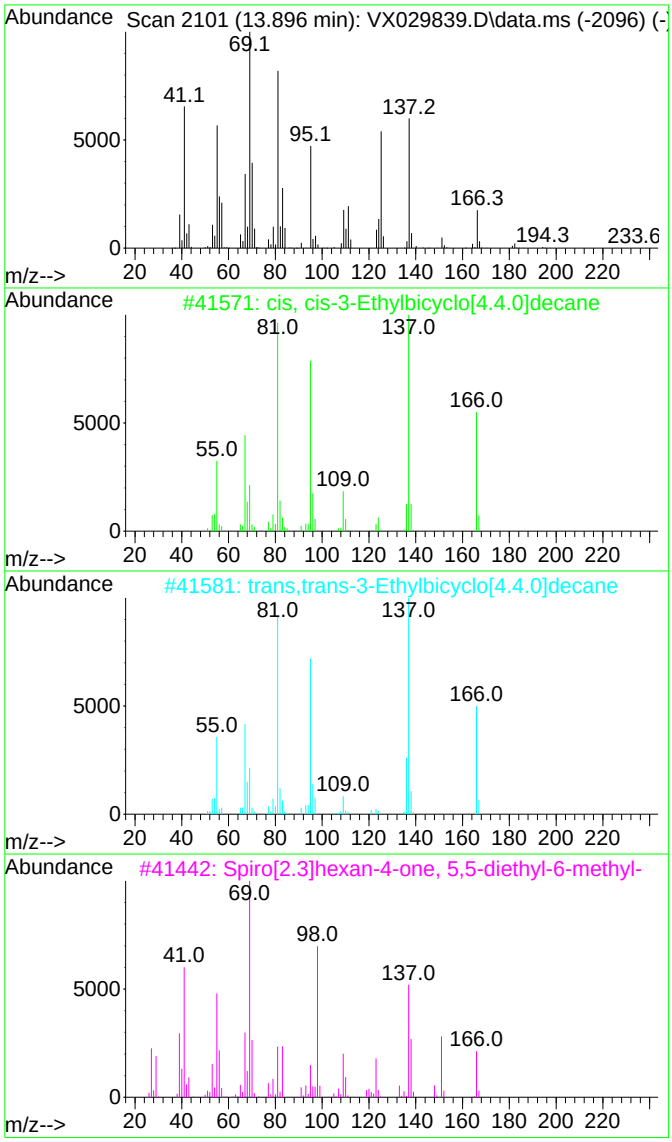
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.M
Quant Title : SW846 8260

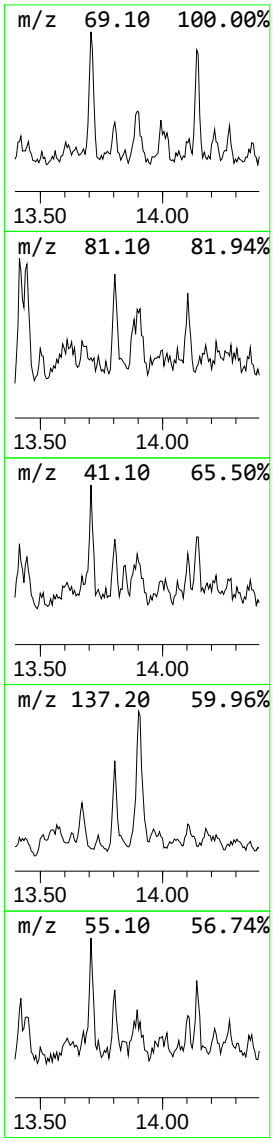
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 cis, cis-3-Ethylbicyclo[4.4... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.896	122.29 ug/l	3599820	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis, cis-3-Ethylbicyclo[4.4.0]de...	166	C12H22	066660-42-2	50
2	trans,trans-3-Ethylbicyclo[4.4.0...	166	C12H22	058462-32-1	46
3	Spiro[2.3]hexan-4-one, 5,5-dieth...	166	C11H18O	1000152-25-2	46
4	Trans, trans-2-ethylbicyclo[4.4....	166	C12H22	066660-37-5	46
5	trans, cis-3-Ethylbicyclo[4.4.0]...	166	C12H22	066660-43-3	43





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Data File : VX029839.D
Acq On : 28 Jun 2022 19:26
Operator : JC/MD
Sample : N3494-04
Misc : 6.77g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SP-EXC-3-GR

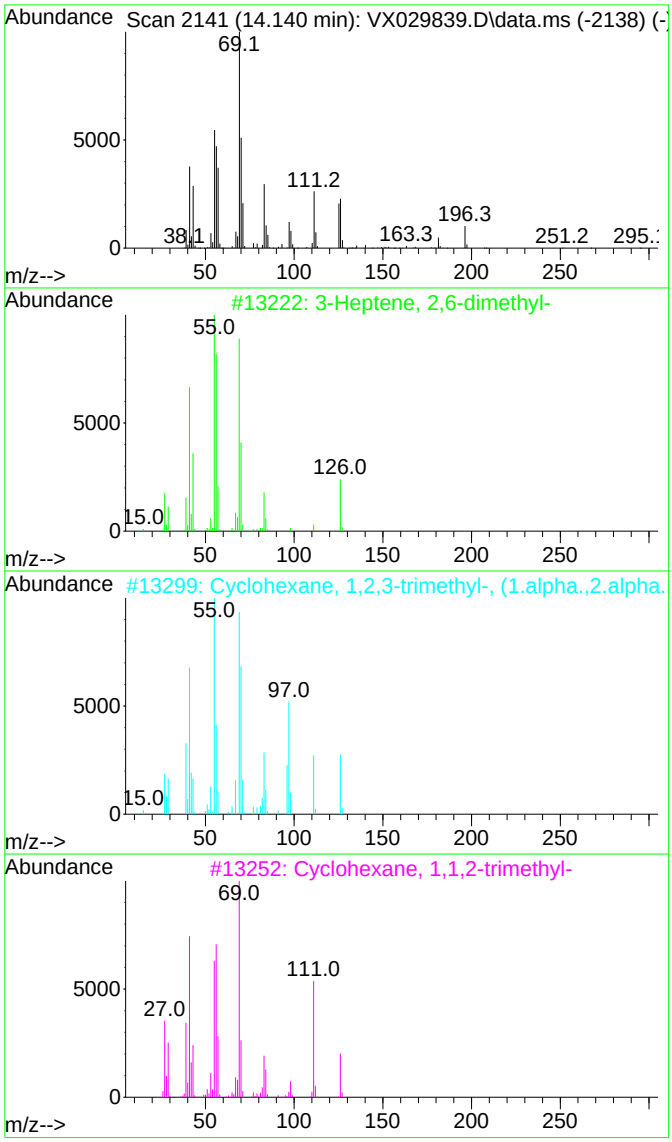
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.M
Quant Title : SW846 8260

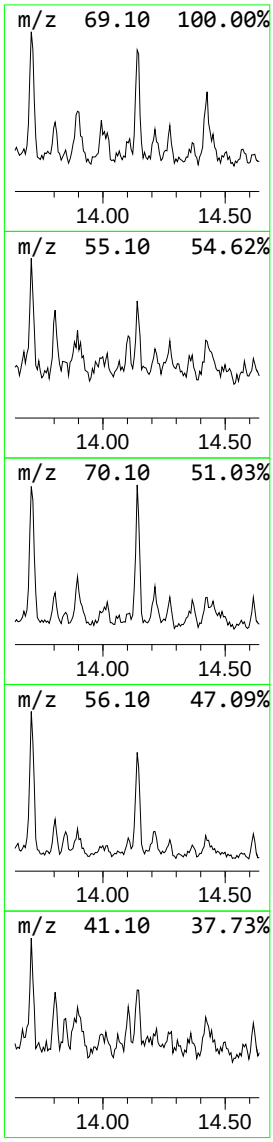
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 3-Heptene, 2,6-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.140	69.68 ug/l	2051340	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Heptene, 2,6-dimethyl-	126	C9H18	002738-18-3	72
2	Cyclohexane, 1,2,3-trimethyl-, (...	126	C9H18	007667-55-2	64
3	Cyclohexane, 1,1,2-trimethyl-	126	C9H18	007094-26-0	50
4	Cyclopentane, ethyl-	98	C7H14	001640-89-7	47
5	1-Hexene, 3,3-dimethyl-	112	C8H16	003404-77-1	45





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062822\
Data File : VX029839.D
Acq On : 28 Jun 2022 19:26
Operator : JC/MD
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MSVOA_X
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062822W.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
Cyclohexane, 1,...	12.475	124.1	ug/l	3654310	4	12.024	1471900	50.0
trans-Decalin, ...	12.823	114.1	ug/l	3357820	4	12.024	1471900	50.0
unknown12.920	12.920	79.1	ug/l	2328170	4	12.024	1471900	50.0
1-Methyldecahyd...	12.988	144.8	ug/l	4263510	4	12.024	1471900	50.0
Naphthalene, de...	13.292	112.2	ug/l	3301750	4	12.024	1471900	50.0
Naphthalene, de...	13.414	116.8	ug/l	3439210	4	12.024	1471900	50.0
1-Hexadecyne	13.445	79.0	ug/l	2326930	4	12.024	1471900	50.0
Cyclohexane, 2-...	13.707	103.6	ug/l	3049310	4	12.024	1471900	50.0
cis, cis-3-Ethy...	13.896	122.3	ug/l	3599820	4	12.024	1471900	50.0
3-Heptene, 2,6-...	14.140	69.7	ug/l	2051340	4	12.024	1471900	50.0