LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037045.D
Acq On : 17 Aug 2023 07:35
Operator : JC/MD
Sample : 03975-04 10X
Misc : 6.31g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB03-Z82-83

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\82X072123W.M
Title : SW846 8260

Signal : TIC: VX037045.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.385	693	705	720	rBV	92195	267320	9.36%	1.471%
2	5.550	720	732	747	rVB	148271	423736	14.84%	2.332%
3	5.952	787	798	807	rBV	96593	258008	9.03%	1.420%
4	6.037	807	812	828	rVB2	10557	29386	1.03%	0.162%
5	6.757	917	930	949	rBV	245824	591169	20.70%	3.253%
6	8.647	1234	1240	1250	rBV	525729	814524	28.52%	4.482%
7	10.055	1465	1471	1482	rBV	566378	771084	27.00%	4.243%
8	10.195	1488	1494	1504	rBV	192746	258999	9.07%	1.425%
9	10.299	1504	1511	1518	rVV	70740	99372	3.48%	0.547%
10	10.640	1562	1567	1575	rBV	51251	69232	2.42%	0.381%
11	10.963	1614	1620	1628	rBV	44627	59443	2.08%	0.327%
12	11.079	1634	1639	1652	rBV	481610	622681	21.80%	3.427%
13	11.378	1683	1688	1696	rVV	209149	403257	14.12%	2.219%
14	11.451	1696	1700	1713	rVB	58688	86566	3.03%	0.476%
15	11.610	1721	1726	1734	rBV	42697	56007	1.96%	0.308%
16	11.750	1740	1749	1754	rBV	185676	234345	8.21%	1.290%
17	11.811	1754	1759	1765	rVB	28397	36270	1.27%	0.200%
18	11.969	1781	1785	1788	rBV	36087	40920	1.43%	0.225%
19	12.018	1788	1793	1799	rVV	626447	810120	28.37%	4.458%
20	12.085	1799	1804	1808	rVV	62724	77715	2.72%	0.428%
21	12.128	1808	1811	1816	rVB	25650	30606	1.07%	0.168%
22	12.244	1824	1830	1837	rBV	547878	714475	25.02%	3.932%
23	12.317	1837	1842	1848	rVV2	152867	197252	6.91%	1.086%
24	12.414	1853	1858	1863	rBV2	43736	69722	2.44%	0.384%
25	12.555	1878	1881	1885	rVB	35671	44043	1.54%	0.242%
26	12.609	1885	1890	1894	rBV	148902	183298	6.42%	1.009%
27	12.695	1900	1904	1910	rBV2	44007	77875	2.73%	0.429%
28	12.750	1910	1913	1917	rVB	43232	49326	1.73%	0.271%
29	12.792	1917	1920	1924	rBV	35997	44853	1.57%	0.247%
30	12.920	1937	1941	1944	rVB	29597	33290	1.17%	0.183%
31	12.963	1944	1948	1953	rVB	70442	87175	3.05%	0.480%
32	13.164	1977	1981	1986	rVB	85922	109278	3.83%	0.601%
33	13.286	1992	2001	2006	rBV3	100470	187232	6.56%	1.030%
34	13.341	2006	2010	2014	rVB	199871	229983	8.05%	1.266%
35	13.420	2019	2023	2028	rVB	278921	358099	12.54%	1.971%
36	13.499	2033	2036	2039	rVV2	30217	39231	1.37%	0.216%

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Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB03-Z82-83

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\82X072123W.M
Title : SW846 8260

37	13.542	2039	2043	2047	rVV	50378	74484	2.61%	0.410%
38	13.579	2047	2049	2057	rVV2	17929	34963	1.22%	0.192%
39	13.676	2060	2065	2068	rVV2	18934	32746	1.15%	0.180%
40	13.774	2072	2081	2088	rVV	2251349	2855759	100.00%	15.716%
41	13.865	2088	2096	2100	rVV3	33133	81929	2.87%	0.451%
42	13.926	2102	2106	2111	rVB4	20972	33209	1.16%	0.183%
43	14.036	2120	2124	2127	rBV	26146	30498	1.07%	0.168%
44	14.097	2131	2134	2137	rVV	60215	73662	2.58%	0.405%
45	14.133	2137	2140	2145	rVB2	33042	56967	1.99%	0.313%
46	14.219	2150	2154	2157	rVV2	81831	115748	4.05%	0.637%
47	14.255	2157	2160	2164	rVV2	41726	59379	2.08%	0.327%
48	14.316	2164	2170	2177	rVV	83413	159546	5.59%	0.878%
49	14.408	2181	2185	2191	rVB	30101	40314	1.41%	0.222%
50	14.469	2191	2195	2200	rBV5	14274	29194	1.02%	0.161%
51	14.518	2200	2203	2210	rVV2	41973	67147	2.35%	0.370%
52	14.597	2212	2216	2217	rVV	24655	29847	1.05%	0.164%
53	14.633	2217	2222	2233	rVB	1263738	1551564	54.33%	8.539%
54	14.780	2240	2246	2259	rVB	1241404	1591517	55.73%	8.758%
55	15.206	2307	2316	2320	rBV	131731	187791	6.58%	1.033%
56	15.371	2331	2343	2347	rBV	335954	497394	17.42%	2.737%
57	15.475	2354	2360	2365	rBV	276684	432791	15.16%	2.382%
58	15.609	2377	2382	2386	rVV	342244	540162	18.91%	2.973%
59	15.645	2386	2388	2395	rVB	179142	240245	8.41%	1.322%
60	15.834	2409	2419	2423	rBV	89009	235962	8.26%	1.299%
61	15.987	2437	2444	2453	rVB	55440	103221	3.61%	0.568%
62	16.084	2453	2460	2467	rBV2	37177	65082	2.28%	0.358%
63	16.322	2491	2499	2509	rBV	231024	446367	15.63%	2.456%
64	16.651	2549	2553	2565	rVB3	15254	37951	1.33%	0.209%

Sum of corrected areas: 18171331

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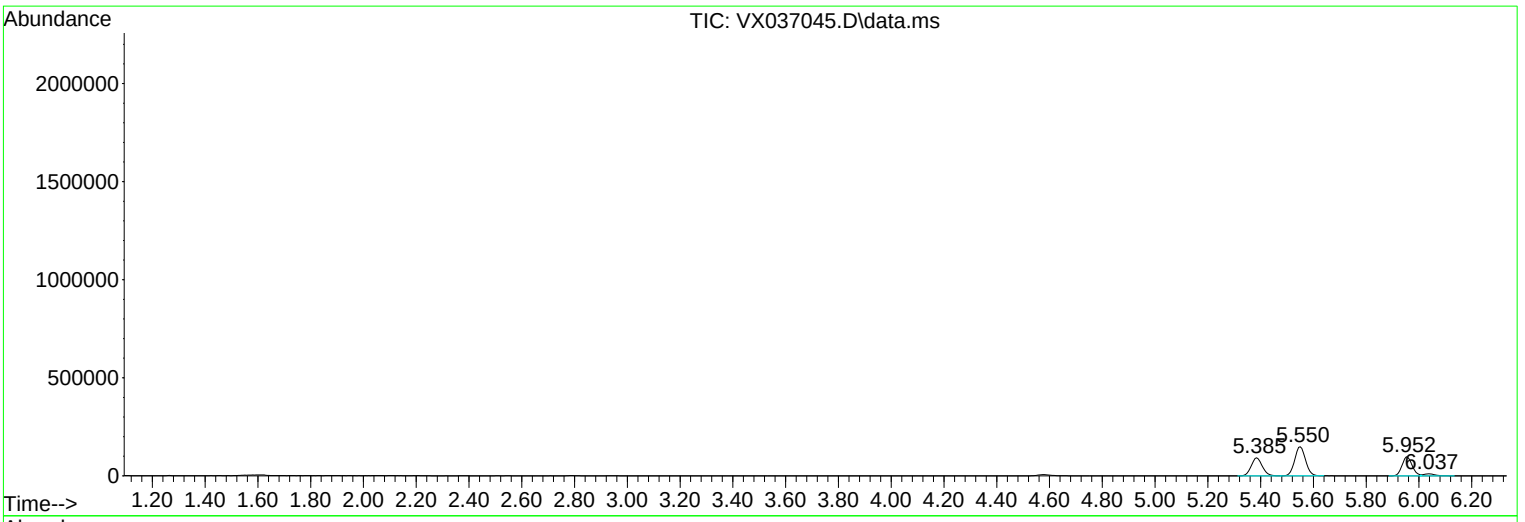
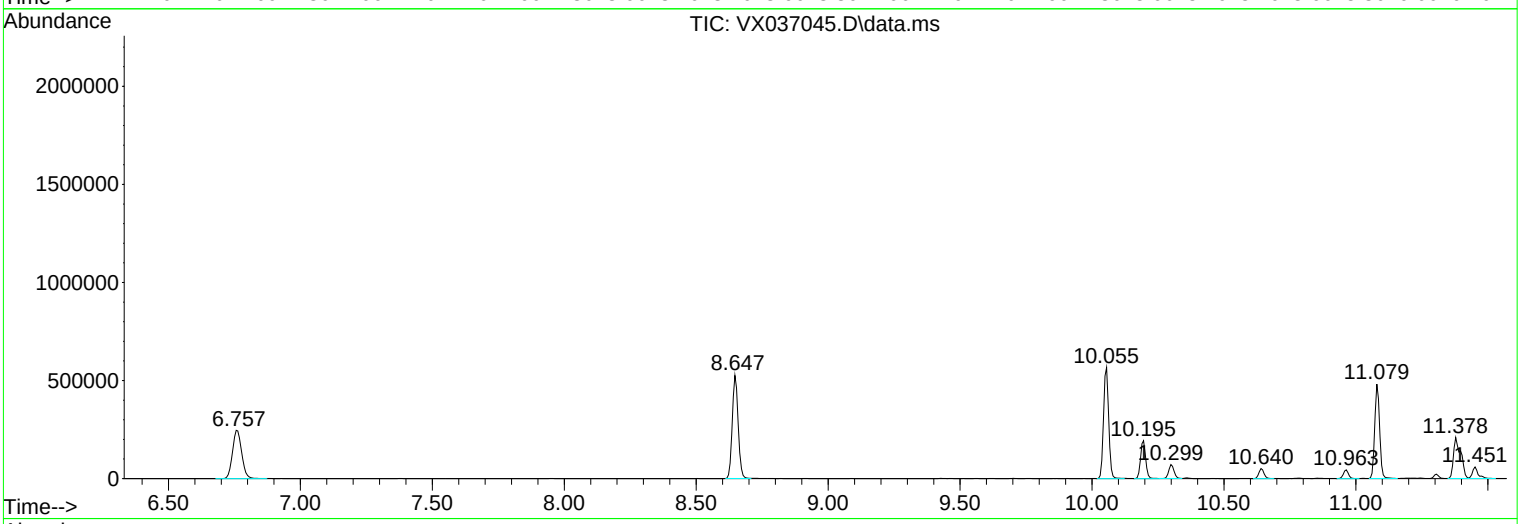
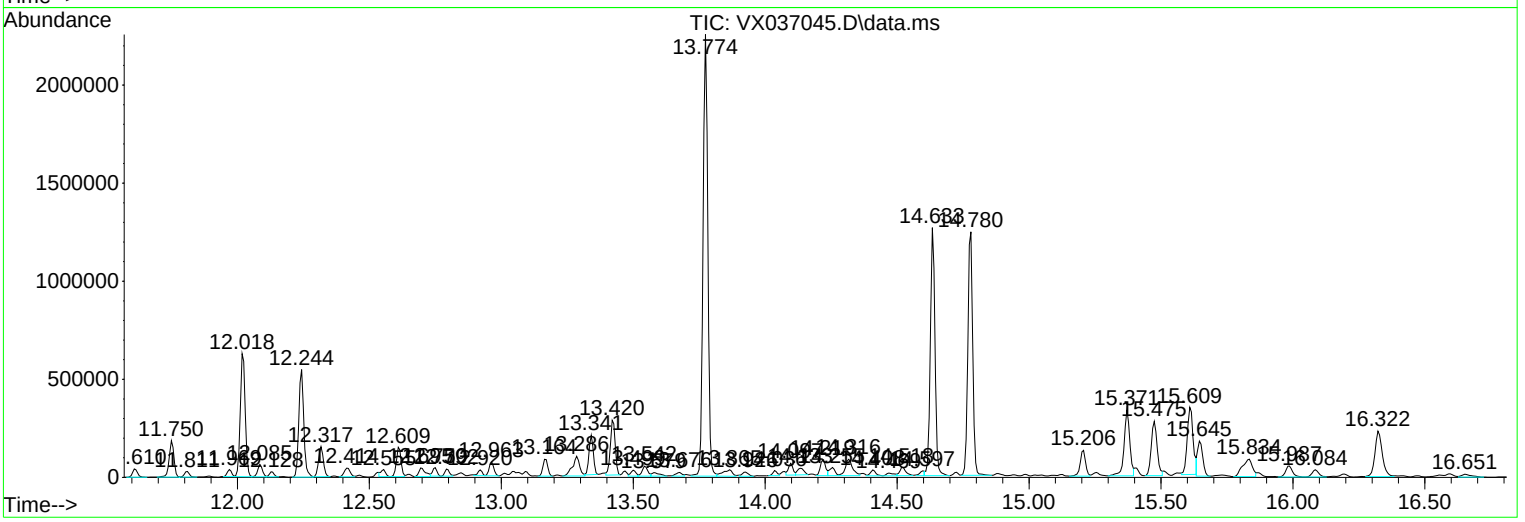
ClientSampleId :
NEVINS-SB03-Z82-83

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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







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Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB03-Z82-83

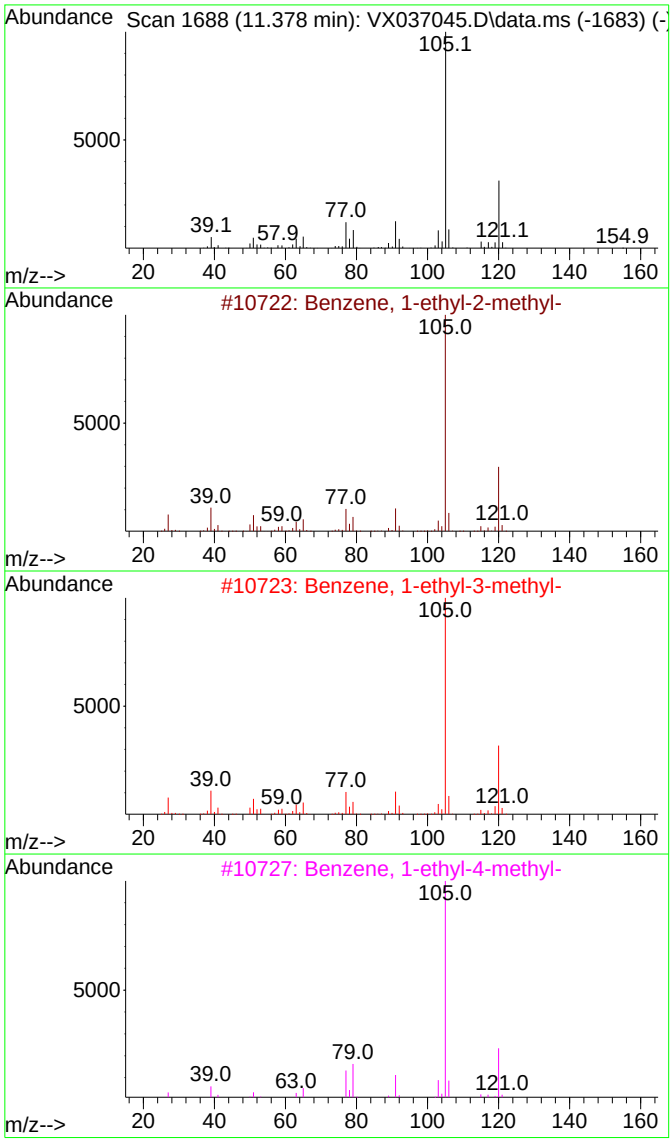
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

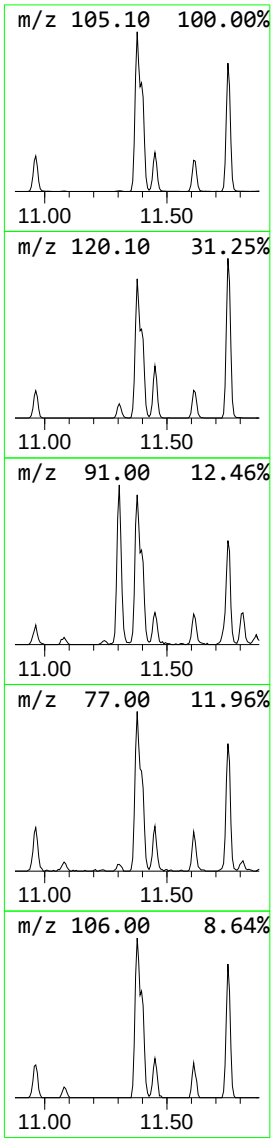
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Benzene, 1-ethyl-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	24.89 ug/l	403257	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
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	91





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Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB03-Z82-83

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

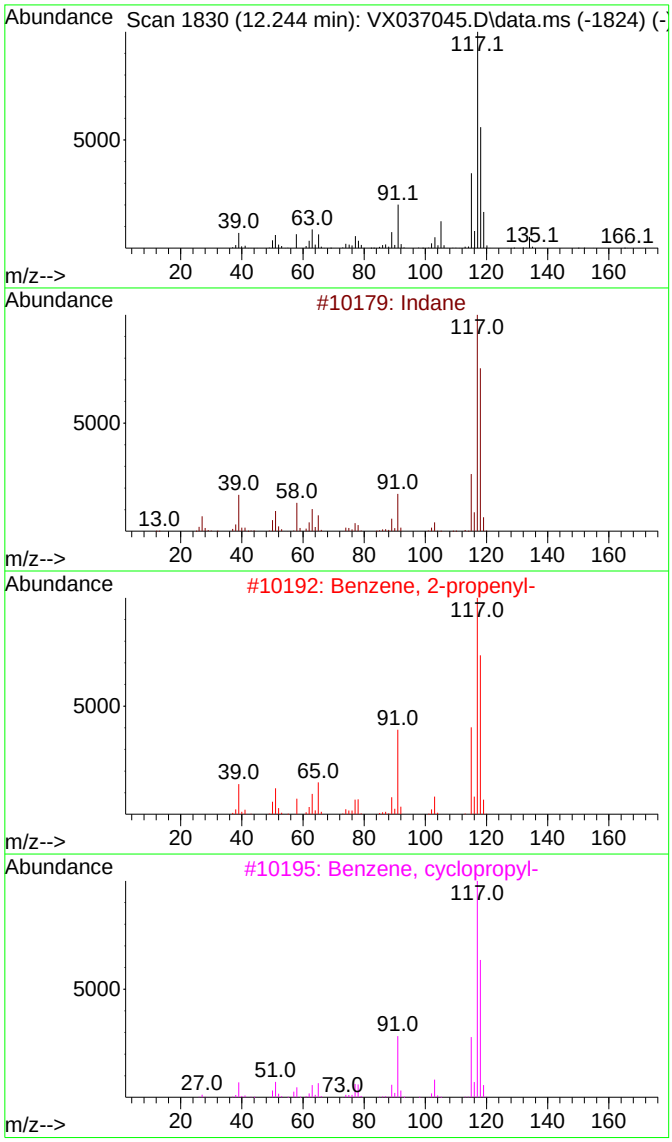
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

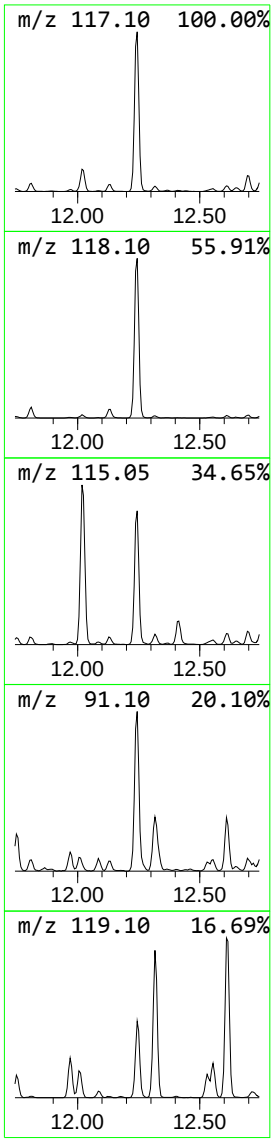
****

Peak Number 2 Indane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	44.10 ug/l	714475	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	76
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	68
4	1,4:5,8-Dimethanobiphenylene, 1,...	184	C14H16	001624-13-1	64
5	Deltacyclene	118	C9H10	007785-10-6	58





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Misc : 6.31g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB03-Z82-83

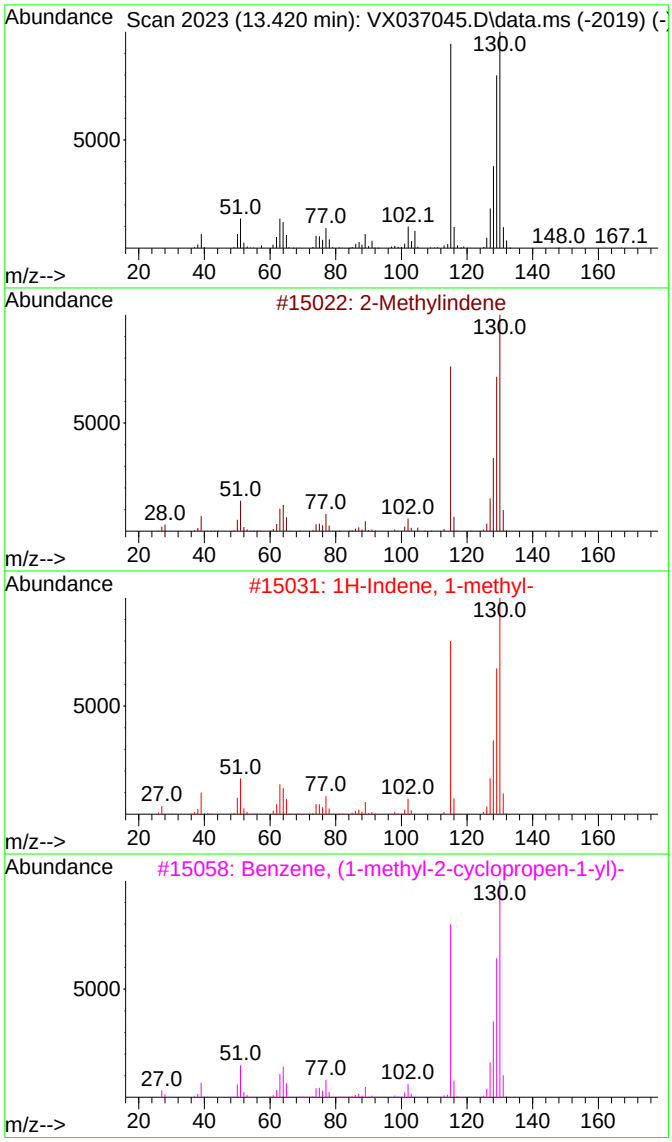
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

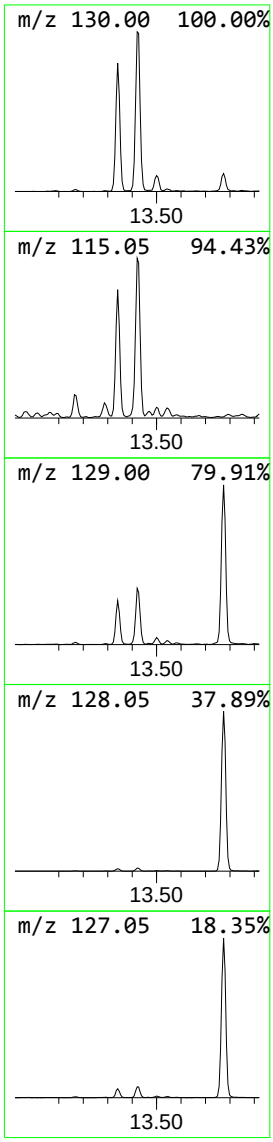
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Methylindene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.420	22.10 ug/l	358099	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methylindene	130	C10H10	002177-47-1	97
2	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	96
3	Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	96
4	Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	94
5	1H-Indene, 3-methyl-	130	C10H10	000767-60-2	94





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Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB03-Z82-83

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

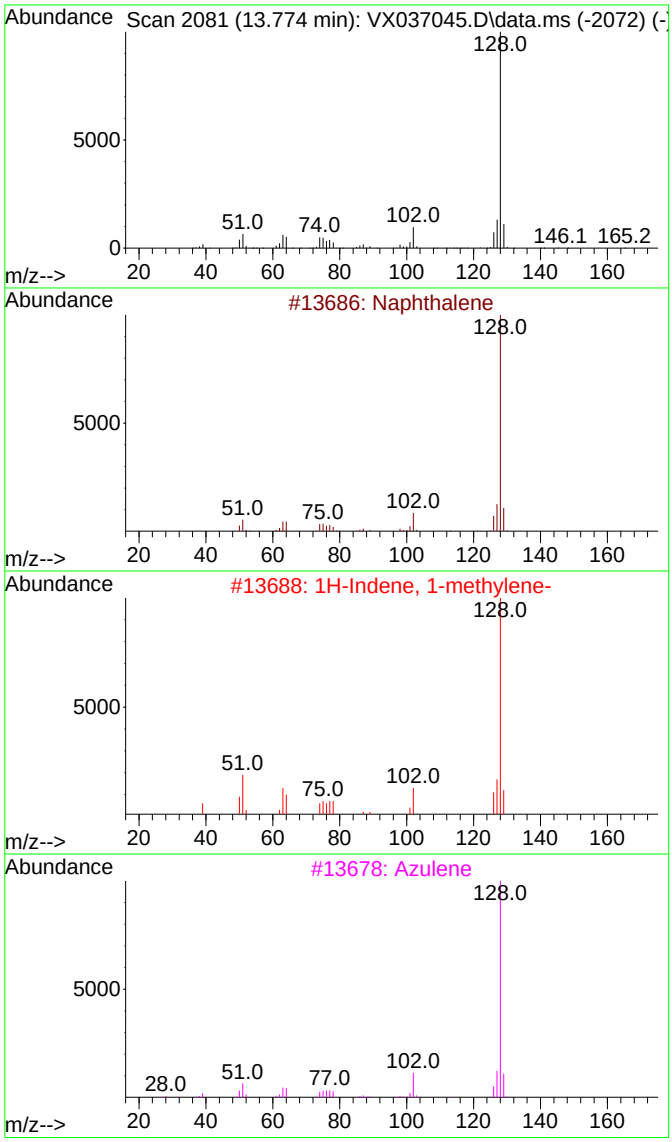
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

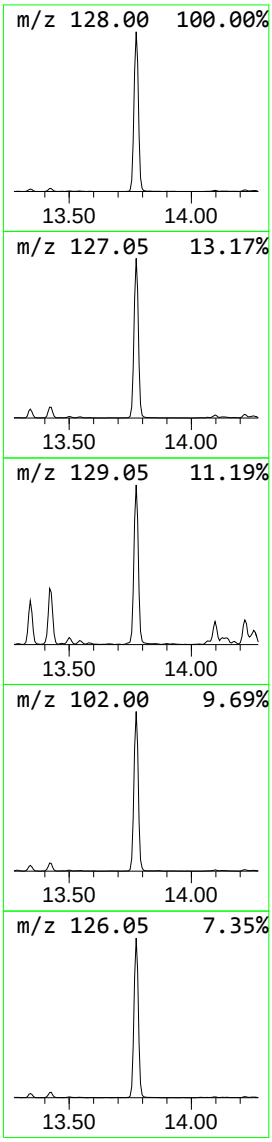
****

Peak Number 4 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	176.26 ug/l	2855760	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene	128	C10H8	000091-20-3	95
2	1H-Indene, 1-methylene-	128	C10H8	002471-84-3	95
3	Azulene	128	C10H8	000275-51-4	94
4	4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	64
5	1,3-Dicyanobenzene	128	C8H4N2	000626-17-5	53





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MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

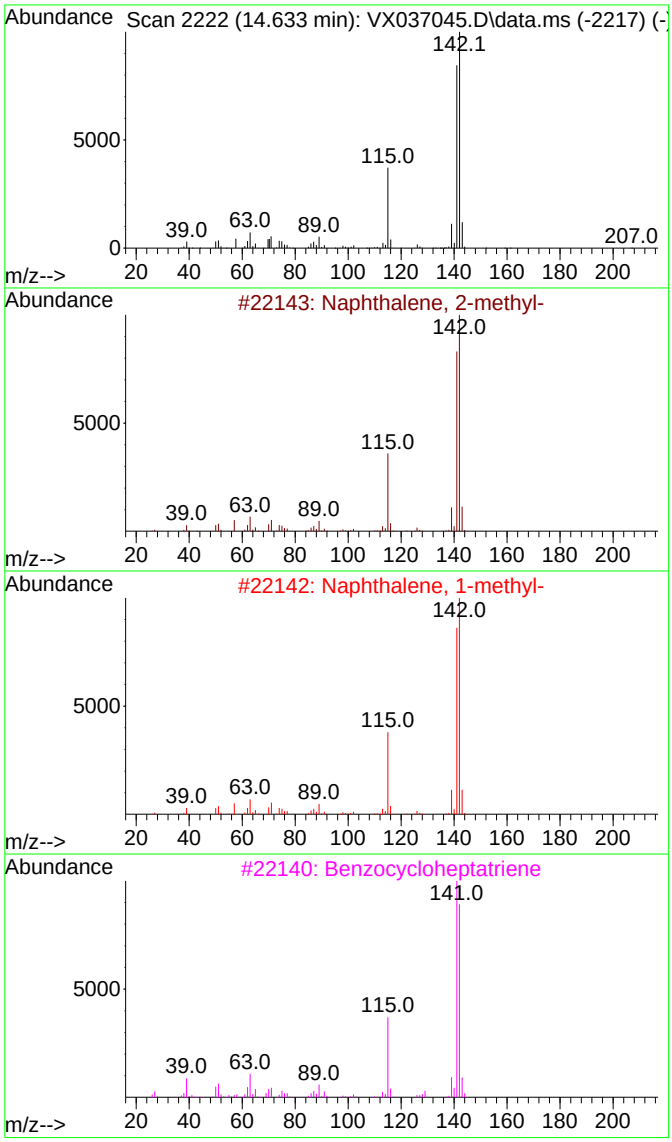
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

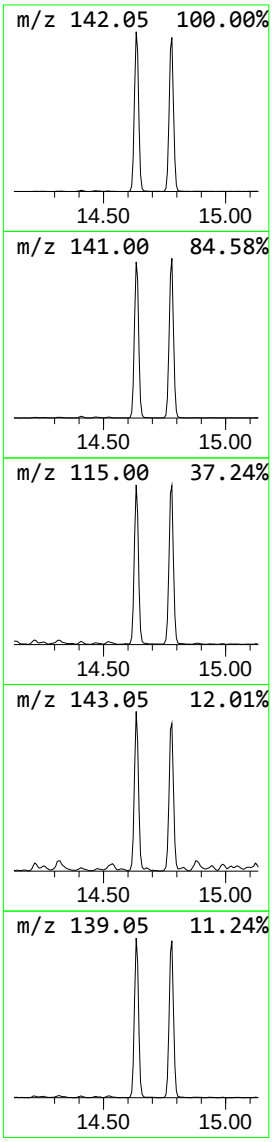
****

Peak Number 5 Benzocycloheptatriene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.633	95.76 ug/l	1551560	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3	Benzocycloheptatriene	142	C11H10	000264-09-5	91
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64





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ClientSampleId :
NEVINS-SB03-Z82-83

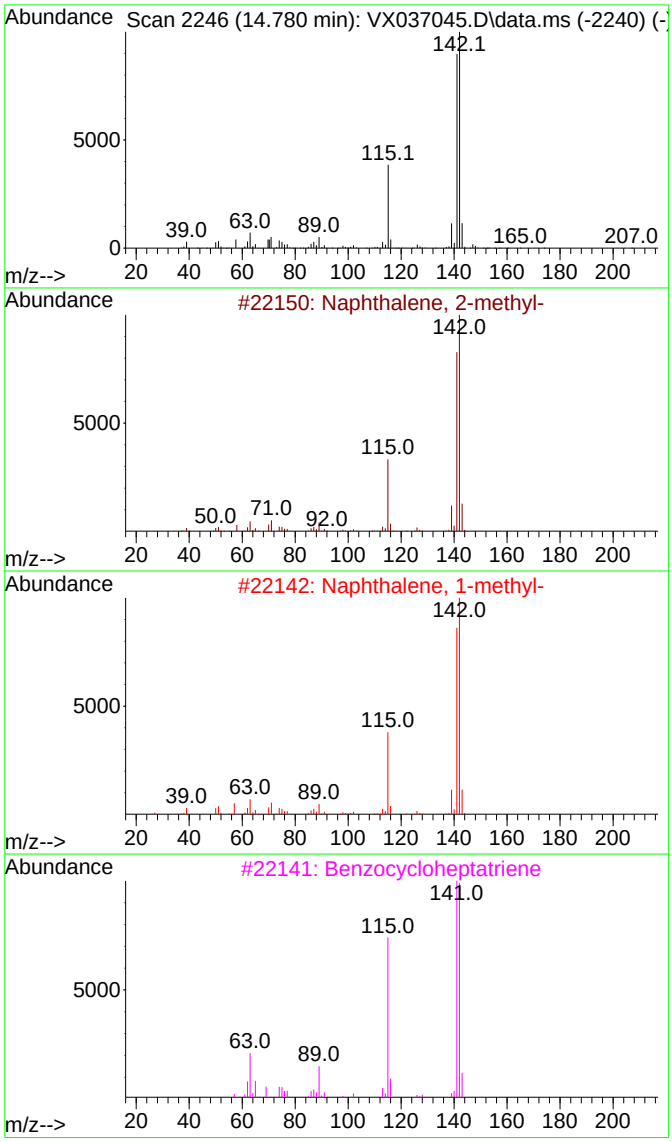
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

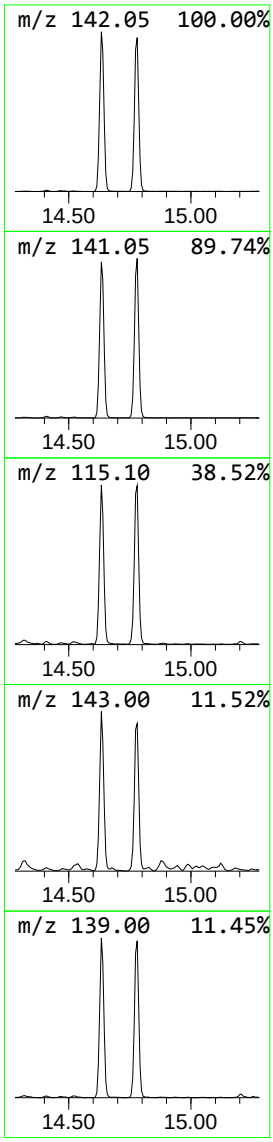
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1,4-Methanonaphthalene, 1,4... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	98.23 ug/l	1591520	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3	Benzocycloheptatriene	142	C11H10	000264-09-5	91
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64





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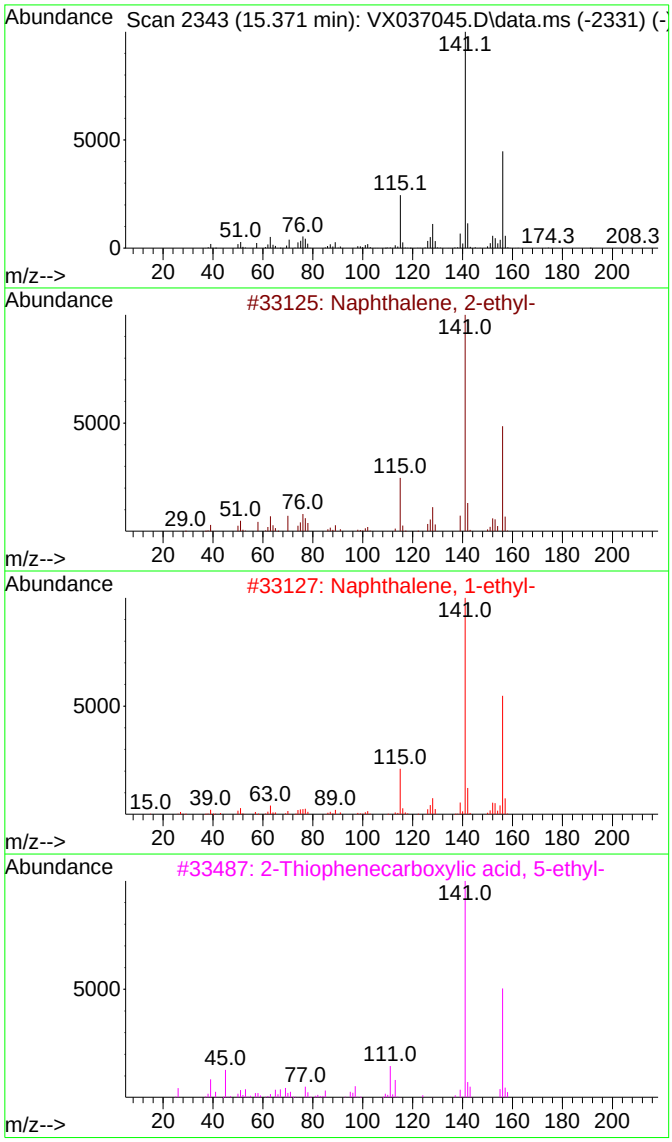
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

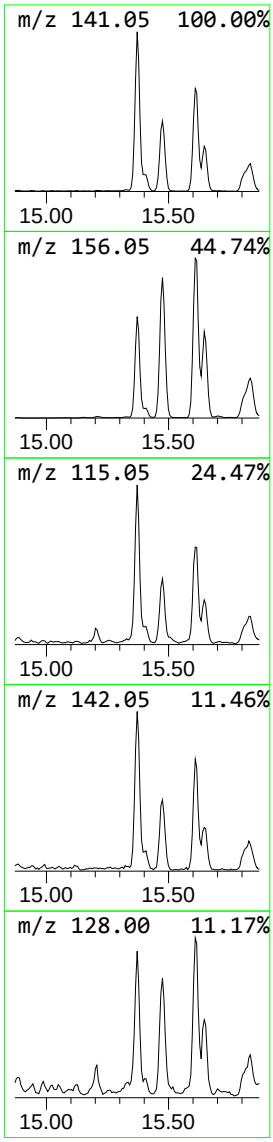
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.371	30.70 ug/l	497394	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-ethyl-	156	C12H12	000939-27-5	96
2	Naphthalene, 1-ethyl-	156	C12H12	001127-76-0	95
3	2-Thiophenecarboxylic acid, 5-et...	156	C7H8O2S	023229-72-3	64
4	2,4-Difluoromesitylene	156	C9H10F2	000392-61-0	59
5	7-Methyl-trans-8-thiabicyclo[4.3...	156	C9H16S	060133-10-0	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037045.D
Acq On : 17 Aug 2023 07:35
Operator : JC/MD
Sample : 03975-04 10X
Misc : 6.31g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB03-Z82-83

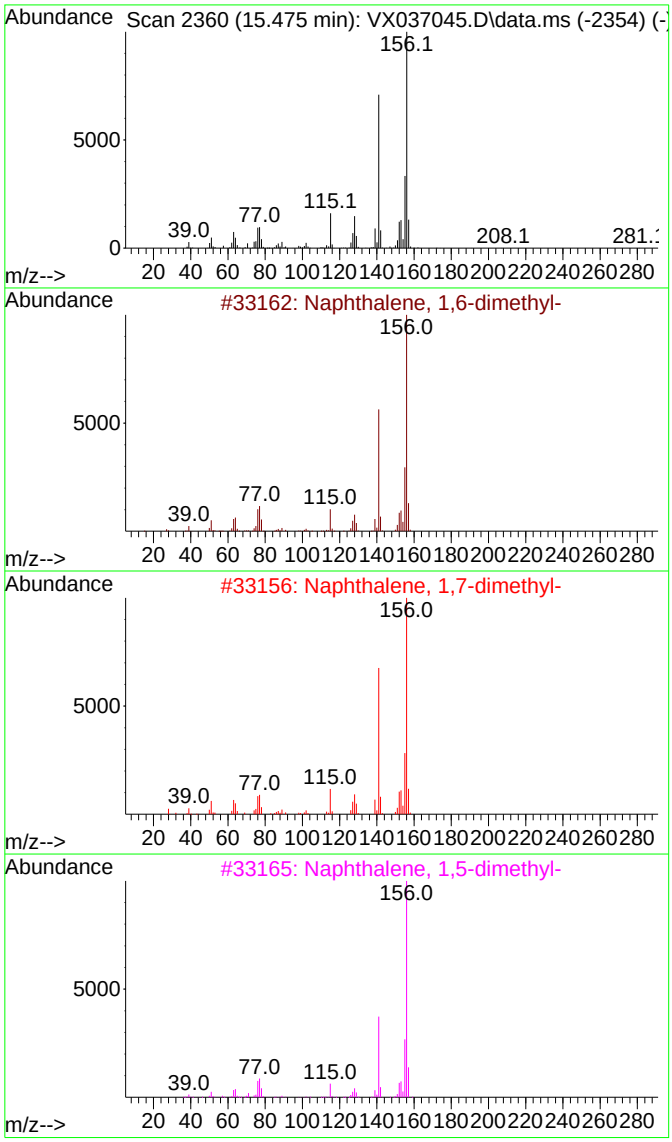
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

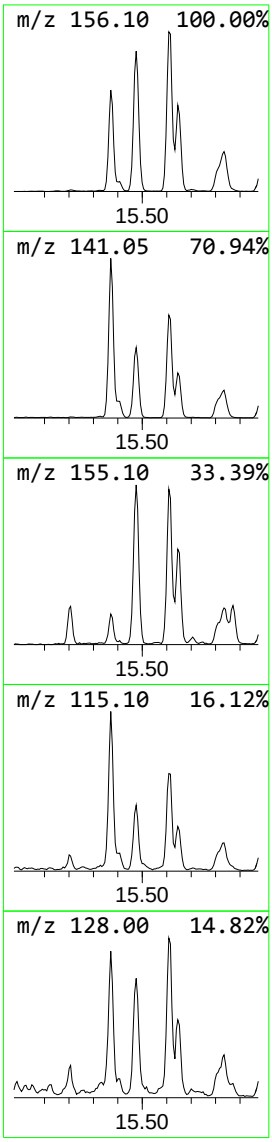
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Naphthalene, 1,6-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.475	26.71 ug/l	432791	1,4-Dichlorobenzene-d4	12.024

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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037045.D
Acq On : 17 Aug 2023 07:35
Operator : JC/MD
Sample : 03975-04 10X
Misc : 6.31g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB03-Z82-83

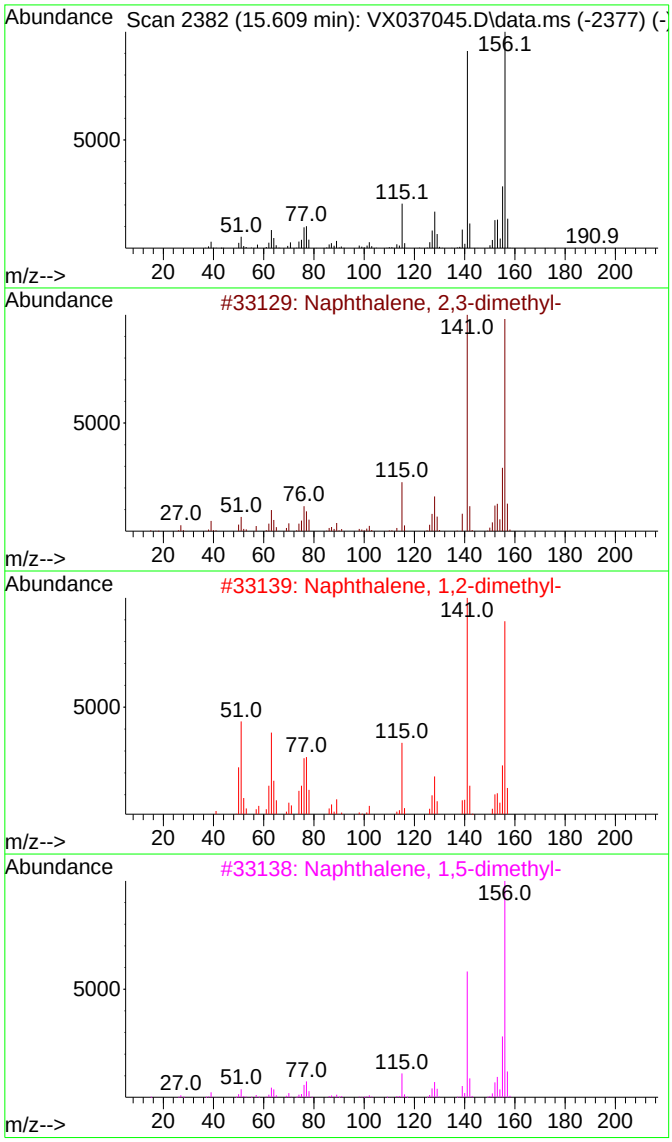
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

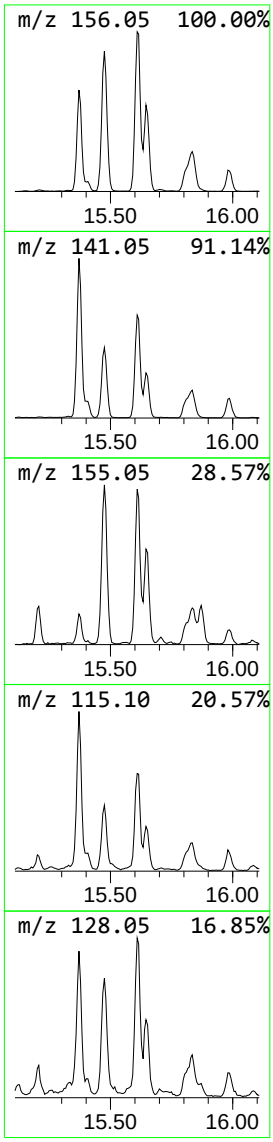
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Naphthalene, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.609	33.34 ug/l	540162	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, 1,2-dimethyl-	156	C12H12	000573-98-8	97
3	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	97
4	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
5	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037045.D
Acq On : 17 Aug 2023 07:35
Operator : JC/MD
Sample : 03975-04 10X
Misc : 6.31g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB03-Z82-83

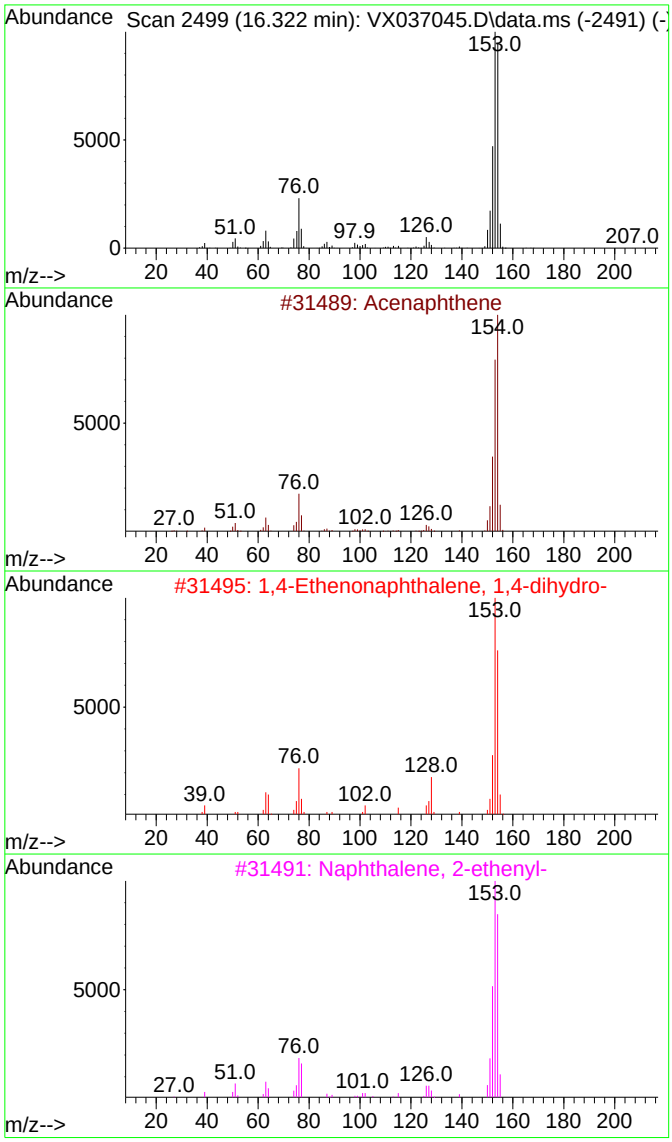
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

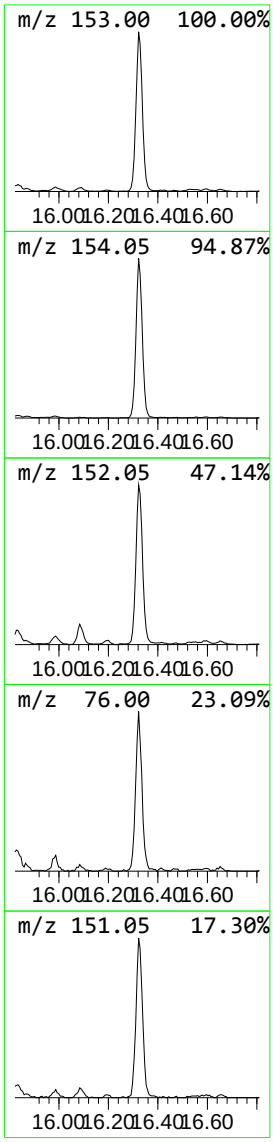
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1,4-Ethenonaphthalene, 1,4-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.322	27.55 ug/l	446367	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acenaphthene	154	C12H10	000083-32-9	93
2	1,4-Ethenonaphthalene, 1,4-dihydro-	154	C12H10	007322-47-6	72
3	Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	64
4	Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	59
5	Biphenyl	154	C12H10	000092-52-4	52





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037045.D
Acq On : 17 Aug 2023 07:35
Operator : JC/MD
Sample : 03975-04 10X
Misc : 6.31g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB03-Z82-83

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.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...	11.378	24.9	ug/l	403257	4	12.024	810120	50.0
Indane	12.244	44.1	ug/l	714475	4	12.024	810120	50.0
2-Methylindene	13.420	22.1	ug/l	358099	4	12.024	810120	50.0
Azulene	13.774	176.3	ug/l	2855760	4	12.024	810120	50.0
Benzocyclohepta...	14.633	95.8	ug/l	1551560	4	12.024	810120	50.0
1,4-Methanonaph...	14.780	98.2	ug/l	1591520	4	12.024	810120	50.0
Naphthalene, 2-...	15.371	30.7	ug/l	497394	4	12.024	810120	50.0
Naphthalene, 1,...	15.475	26.7	ug/l	432791	4	12.024	810120	50.0
Naphthalene, 2,...	15.609	33.3	ug/l	540162	4	12.024	810120	50.0
1,4-Ethenonapht...	16.322	27.6	ug/l	446367	4	12.024	810120	50.0