LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037051.D
Acq On : 17 Aug 2023 09:59
Operator : JC/MD
Sample : 03958-06
Misc : 7.04g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 54 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB02-Z21-23

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: VX037051.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.624	85	88	95	rBV	19686	24684	1.80%	0.211%
2	4.733	582	598	611	rBV2	4512	20129	1.47%	0.172%
3	5.385	694	705	719	rBV	72507	211394	15.45%	1.808%
4	5.544	721	731	747	rVB	123670	350567	25.63%	2.998%
5	5.952	788	798	803	rBV	78596	201845	14.76%	1.726%
6	6.032	803	811	830	rVB	517588	1367823	100.00%	11.696%
7	6.757	919	930	945	rBV	201332	483394	35.34%	4.134%
8	8.647	1233	1240	1246	rBV	428835	670371	49.01%	5.732%
9	10.055	1465	1471	1485	rBV	452404	625890	45.76%	5.352%
10	10.195	1488	1494	1504	rVB	93321	122534	8.96%	1.048%
11	10.305	1504	1512	1518	rBV	13344	20884	1.53%	0.179%
12	10.640	1562	1567	1575	rBV	13648	20848	1.52%	0.178%
13	10.964	1614	1620	1625	rBV	14064	18891	1.38%	0.162%
14	11.085	1634	1640	1654	rBV	388333	535192	39.13%	4.576%
15	11.403	1684	1692	1696	rVV	11136	21823	1.60%	0.187%
16	11.610	1722	1726	1733	rBV	18742	27291	2.00%	0.233%
17	11.750	1744	1749	1755	rVB	26301	35575	2.60%	0.304%
18	12.024	1788	1794	1801	rBV	549023	707247	51.71%	6.048%
19	12.085	1801	1804	1808	rVB	20950	26813	1.96%	0.229%
20	12.244	1821	1830	1838	rVV	555619	699075	51.11%	5.978%
21	12.317	1838	1842	1849	rVB2	21052	31845	2.33%	0.272%
22	12.616	1885	1891	1894	rVB	24711	31564	2.31%	0.270%
23	12.701	1900	1905	1910	rBV	26666	41525	3.04%	0.355%
24	12.835	1910	1927	1939	rVV5	36807	219982	16.08%	1.881%
25	12.963	1944	1948	1955	rVB	14226	22000	1.61%	0.188%
26	13.170	1977	1982	1986	rVB	55156	70103	5.13%	0.599%
27	13.292	1993	2002	2007	rBV2	54959	81865	5.99%	0.700%
28	13.341	2007	2010	2014	rVB	18325	19926	1.46%	0.170%
29	13.427	2019	2024	2028	rVB	68760	90876	6.64%	0.777%
30	13.542	2040	2043	2047	rBV	11518	14694	1.07%	0.126%
31	13.676	2059	2065	2068	rBV3	10721	18675	1.37%	0.160%
32	13.774	2072	2081	2089	rVV	939277	1155832	84.50%	9.884%
33	13.865	2093	2096	2101	rVV	19505	28478	2.08%	0.244%
34	13.920	2102	2105	2111	rVB2	12582	18071	1.32%	0.155%
35	14.128	2136	2139	2148	rVV7	13092	31135	2.28%	0.266%
36	14.219	2149	2154	2157	rVV2	18974	28815	2.11%	0.246%

LSC Area Percent Report

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Data File : VX037051.D
Acq On : 17 Aug 2023 09:59
Operator : JC/MD
Sample : 03958-06
Misc : 7.04g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 54 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB02-Z21-23

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	14.317	2163	2170	2176	rBV	19196	33166	2.42%	0.284%
38	14.634	2217	2222	2233	rVB	526475	662648	48.45%	5.666%
39	14.780	2240	2246	2255	rVV	374166	502388	36.73%	4.296%
40	15.207	2308	2316	2320	rBV	64908	94216	6.89%	0.806%
41	15.249	2320	2323	2331	rVV5	10004	21145	1.55%	0.181%
42	15.371	2331	2343	2347	rVV	129951	210963	15.42%	1.804%
43	15.408	2347	2349	2354	rVV	27437	34126	2.49%	0.292%
44	15.475	2354	2360	2371	rVV	174216	303464	22.19%	2.595%
45	15.566	2371	2375	2376	rVV3	11243	18428	1.35%	0.158%
46	15.609	2377	2382	2386	rVV	219821	358494	26.21%	3.066%
47	15.646	2386	2388	2396	rVV	101953	144468	10.56%	1.235%
48	15.737	2398	2403	2409	rVV2	20208	37600	2.75%	0.322%
49	15.835	2409	2419	2430	rVB2	65094	193233	14.13%	1.652%
50	15.987	2437	2444	2454	rBV	43779	82053	6.00%	0.702%
51	16.085	2454	2460	2468	rBV	66978	117140	8.56%	1.002%
52	16.194	2473	2478	2484	rVB	24780	42689	3.12%	0.365%
53	16.322	2484	2499	2511	rBV2	210104	484583	35.43%	4.144%
54	16.469	2519	2523	2528	rVB2	13393	21795	1.59%	0.186%
55	16.554	2528	2537	2539	rVV7	21288	45040	3.29%	0.385%
56	16.591	2539	2543	2548	rVV2	38879	82581	6.04%	0.706%
57	16.652	2548	2553	2570	rVB2	39765	106512	7.79%	0.911%

Sum of corrected areas: 11694388

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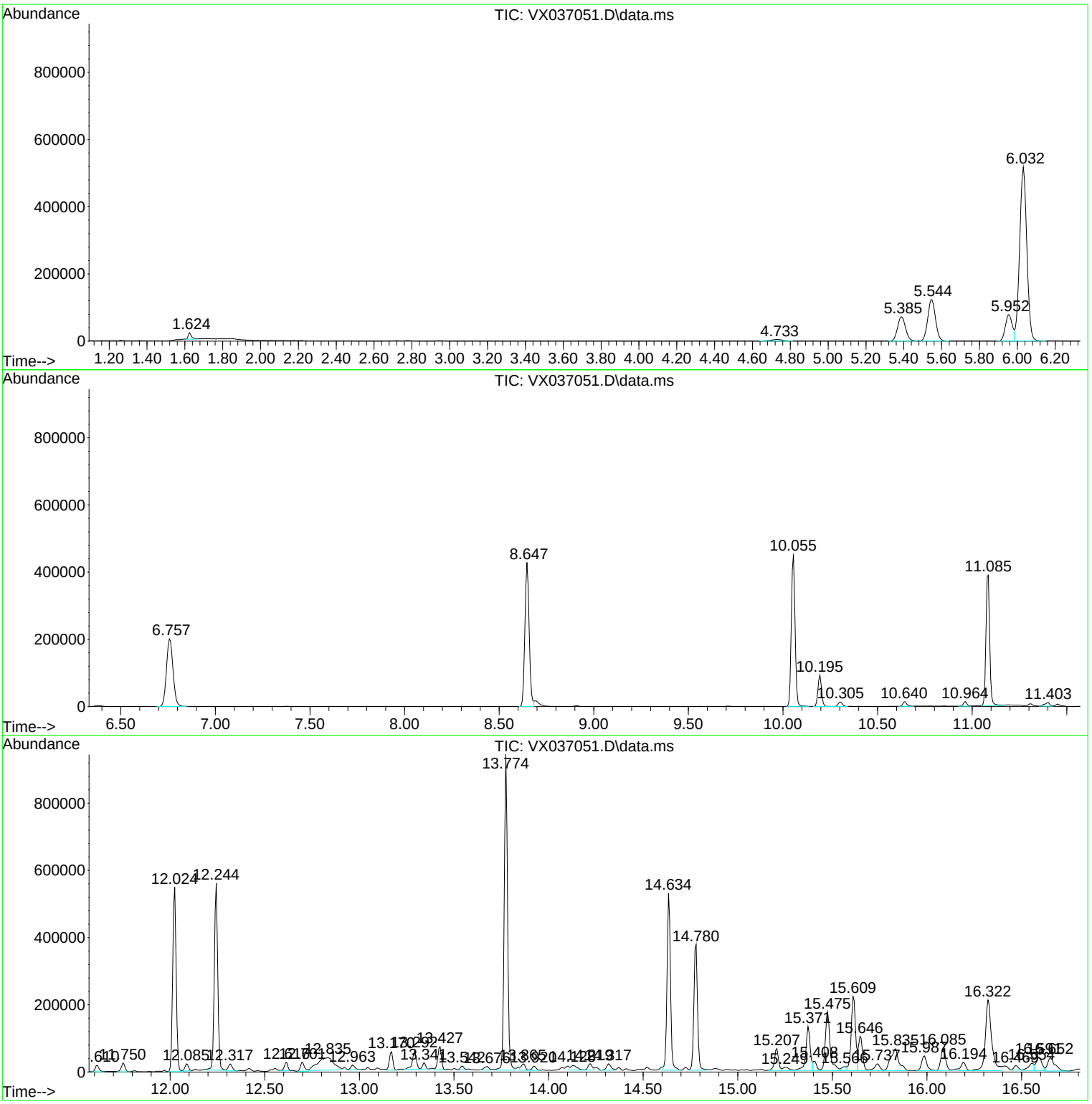
Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB02-Z21-23

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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Data File : VX037051.D
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ClientSampleId :
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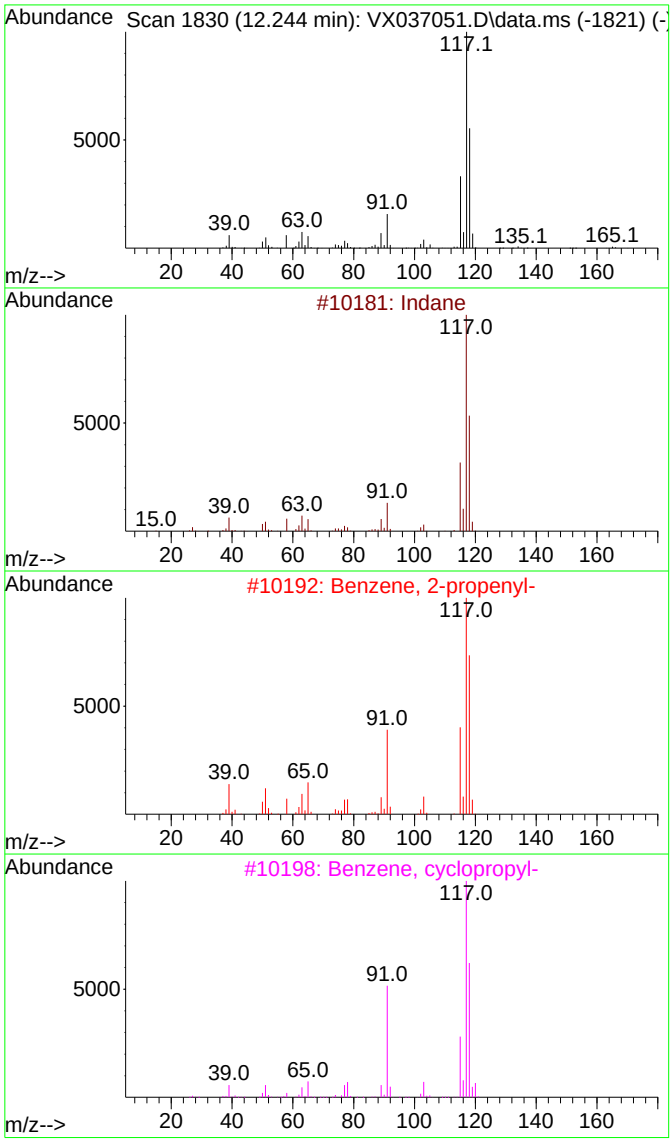
Quant Title : SW846 8260

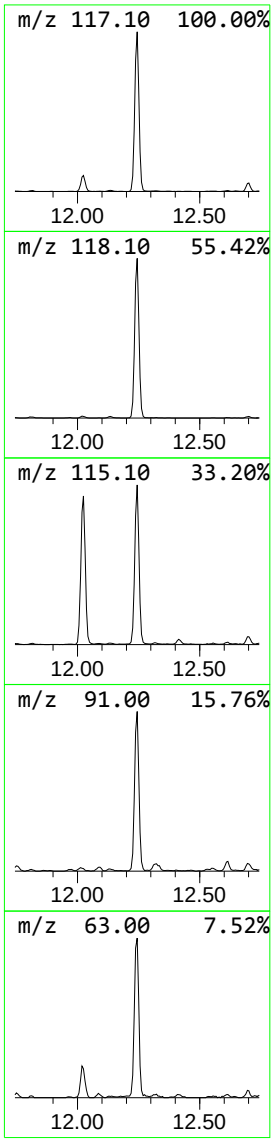
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	49.42 ug/l	699075	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	93
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	83
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	83
4	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	80
5	Deltacyclene	118	C9H10	007785-10-6	74





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Operator : JC/MD
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ALS Vial : 54 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB02-Z21-23

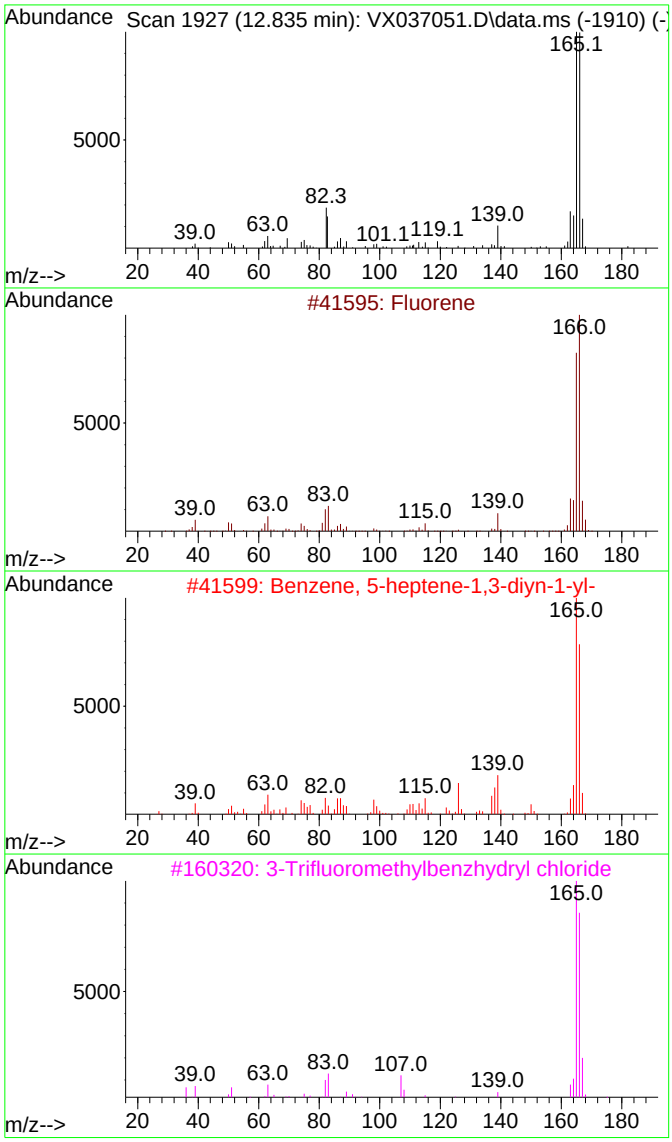
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

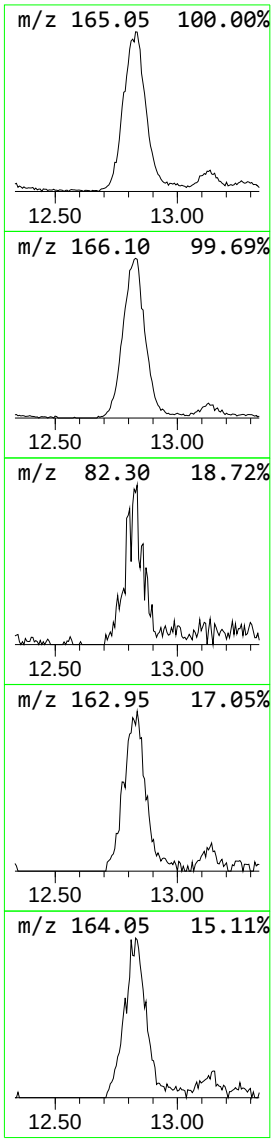
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Fluorene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.835	15.55 ug/l	219982	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluorene	166	C13H10	000086-73-7	94
2	Benzene, 5-heptene-1,3-diyn-1-yl-	166	C13H10	013678-98-3	64
3	3-Trifluoromethylbenzhydryl chlo...	270	C14H10ClF3	067240-79-3	53
4	1H-Phenalene	166	C13H10	000203-80-5	46
5	Benzaldehyde, 2,4-dihydroxy-3,6-...	166	C9H10O3	034883-14-2	45





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Operator : JC/MD
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Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB02-Z21-23

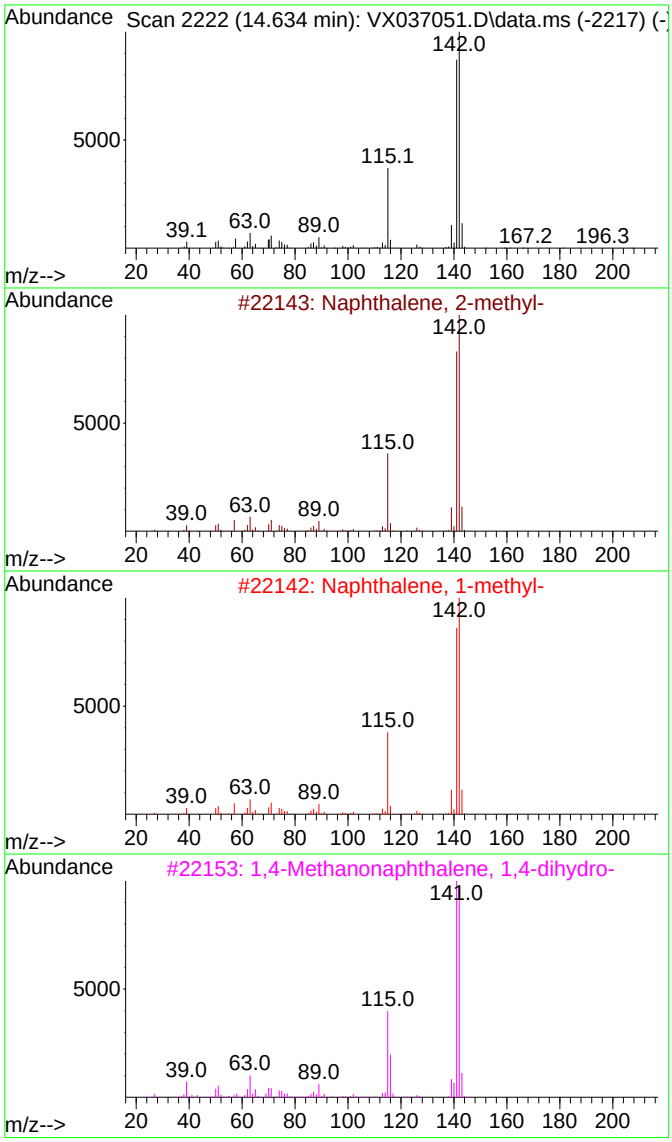
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

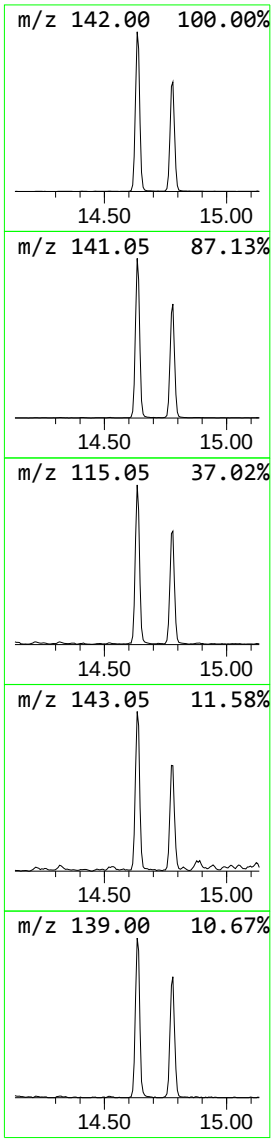
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Naphthalene, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.634	46.85 ug/l	662648	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	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037051.D
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Operator : JC/MD
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Misc : 7.04g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 54 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB02-Z21-23

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

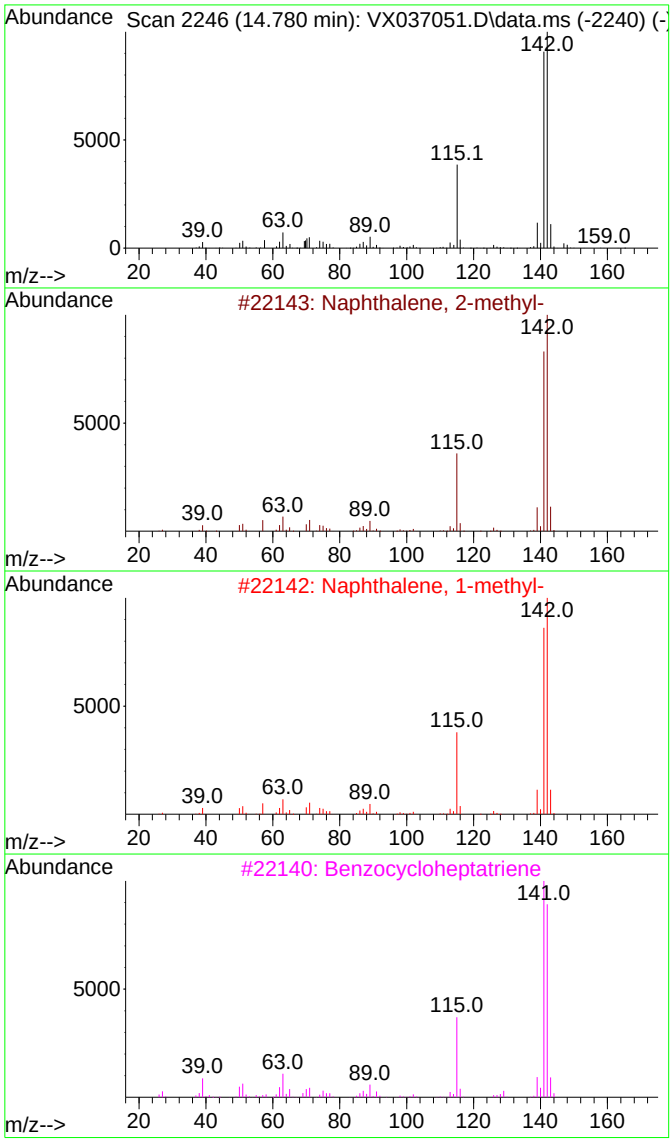
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

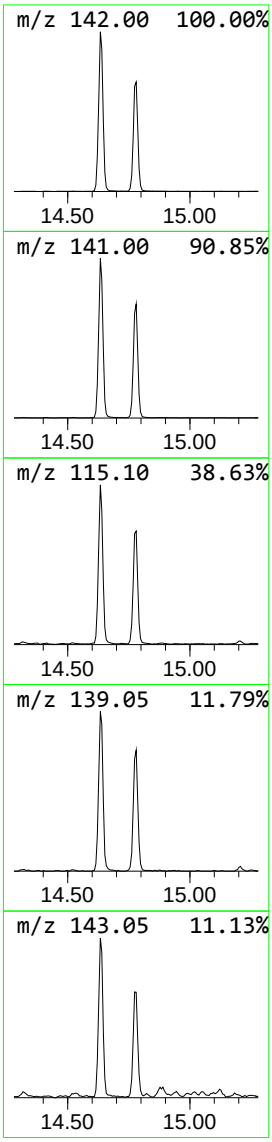
****

Peak Number 4 Benzocycloheptatriene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	35.52 ug/l	502388	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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Misc : 7.04g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 54 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB02-Z21-23

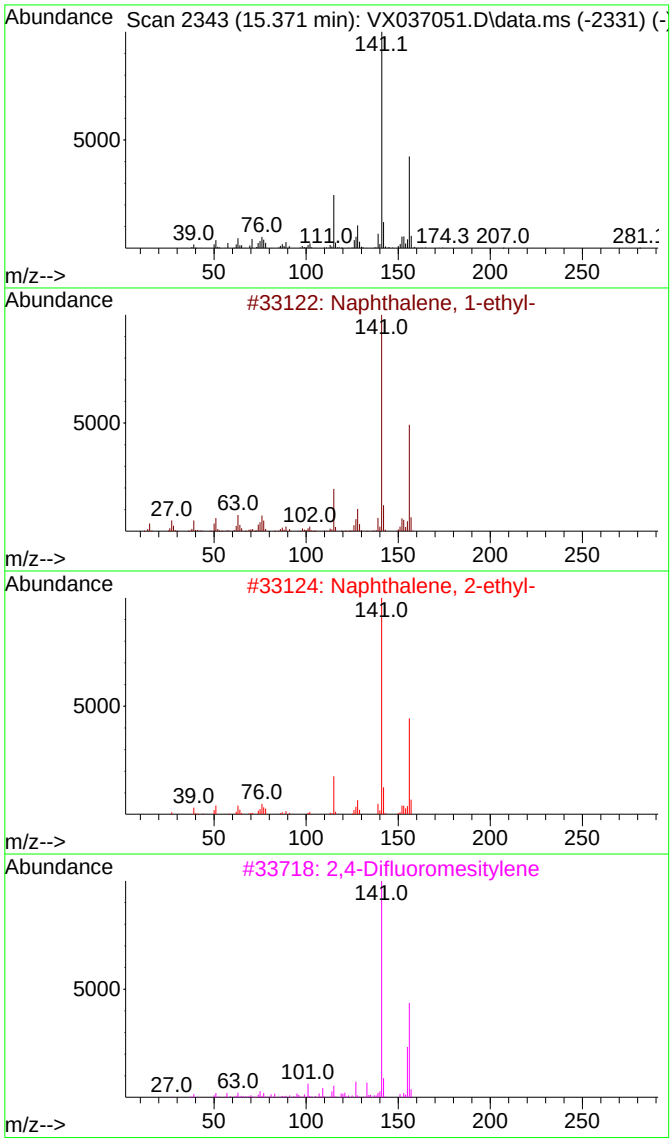
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

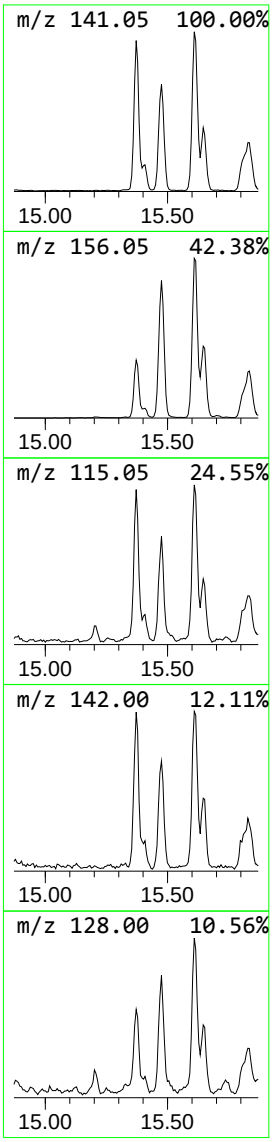
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2,4-Difluoromesitylene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.371	14.91 ug/l	210963	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-ethyl-	156	C12H12	001127-76-0	95
2	Naphthalene, 2-ethyl-	156	C12H12	000939-27-5	94
3	2,4-Difluoromesitylene	156	C9H10F2	000392-61-0	59
4	Naphthalene, 1-propyl-	170	C13H14	002765-18-6	59
5	2-Thiophenecarboxylic acid, 5-et...	156	C7H8O2S	023229-72-3	59





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Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB02-Z21-23

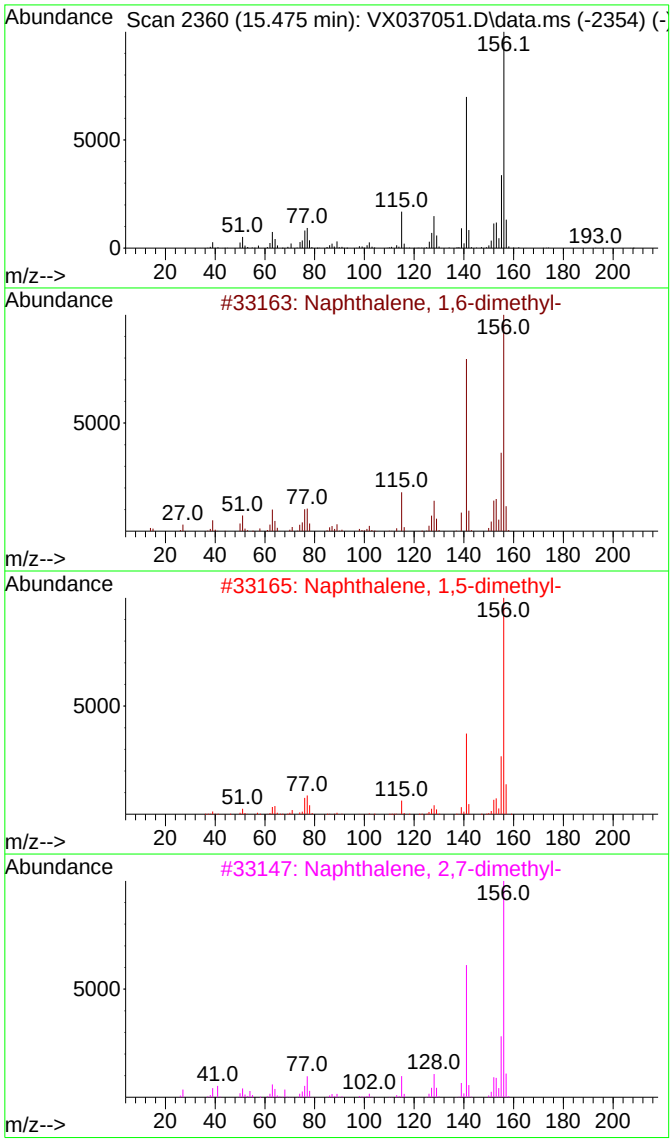
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

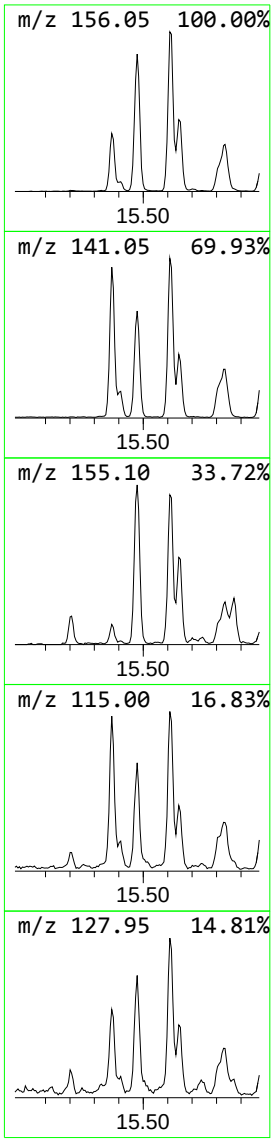
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.475	21.45 ug/l	303464	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, 1,5-dimethyl-	156	C12H12	000571-61-9	97
3	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	96
4	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96
5	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96





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Data File : VX037051.D
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Operator : JC/MD
Sample : 03958-06
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ALS Vial : 54 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB02-Z21-23

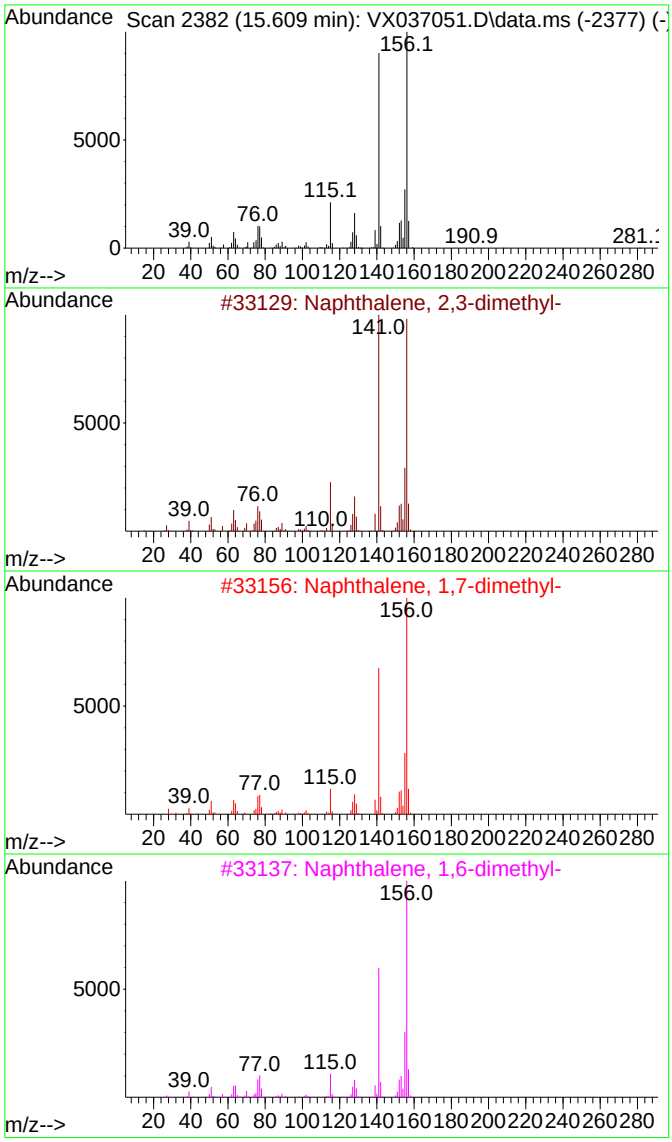
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

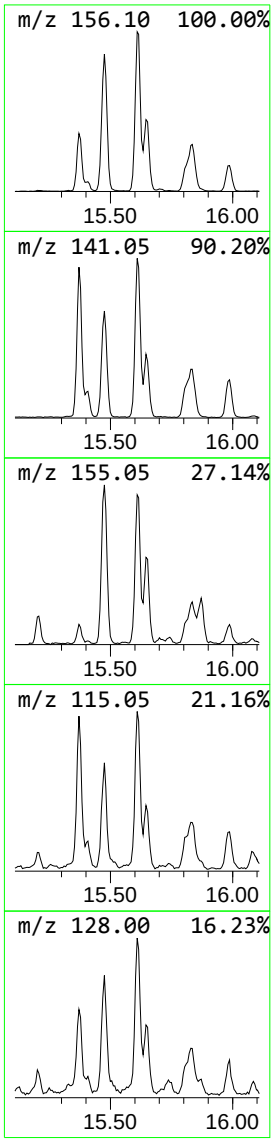
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Naphthalene, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.609	25.34 ug/l	358494	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, 1,6-dimethyl-	156	C12H12	000575-43-9	97
4	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
5	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97





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Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB02-Z21-23

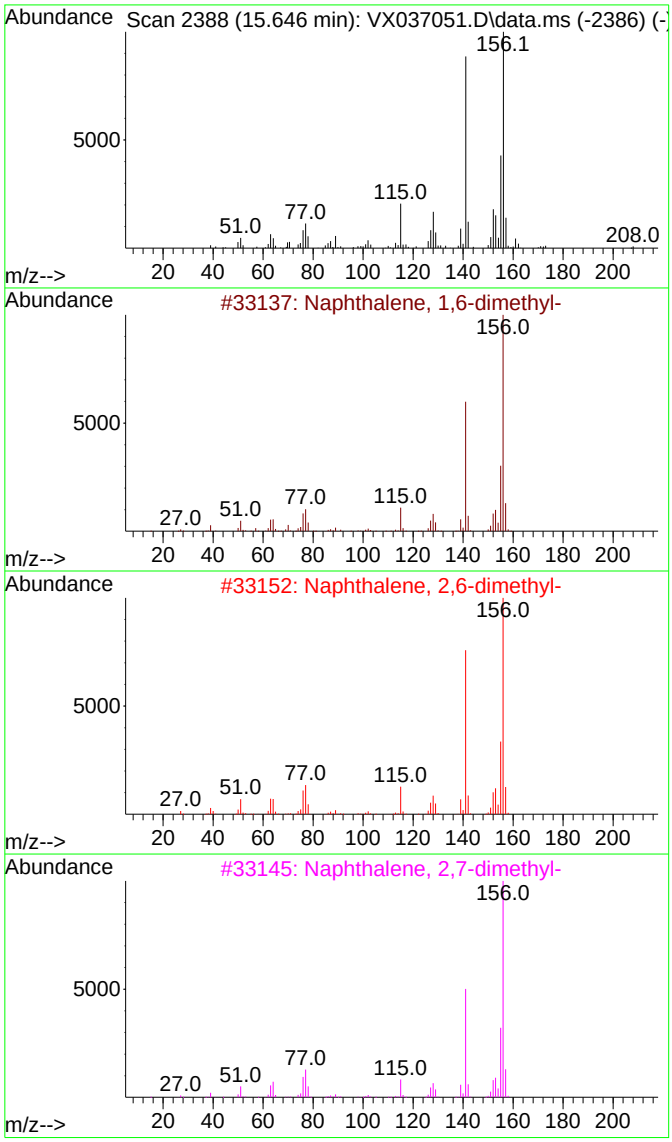
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

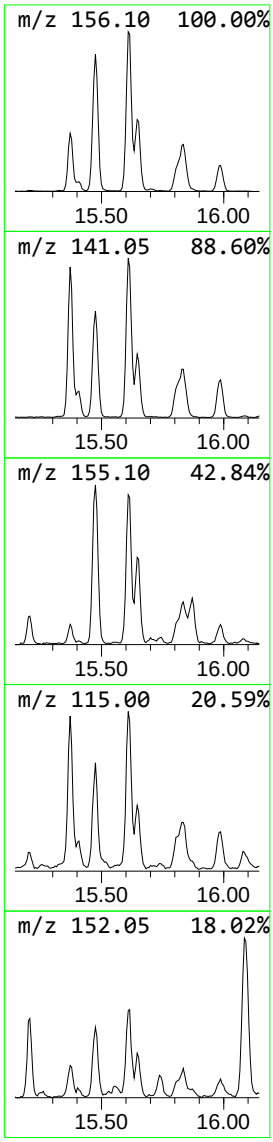
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Naphthalene, 2,7-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.646	10.21 ug/l	144468	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, 2,6-dimethyl-	156	C12H12	000581-42-0	96
3	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	96
4	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	95
5	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	95





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037051.D
Acq On : 17 Aug 2023 09:59
Operator : JC/MD
Sample : 03958-06
Misc : 7.04g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 54 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB02-Z21-23

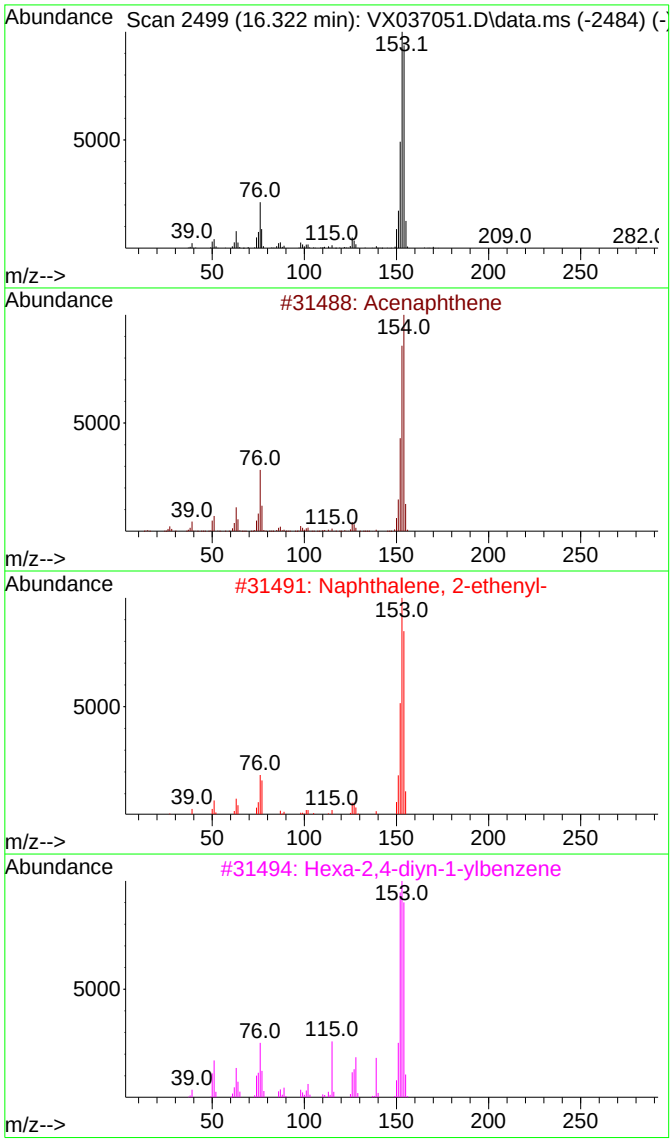
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

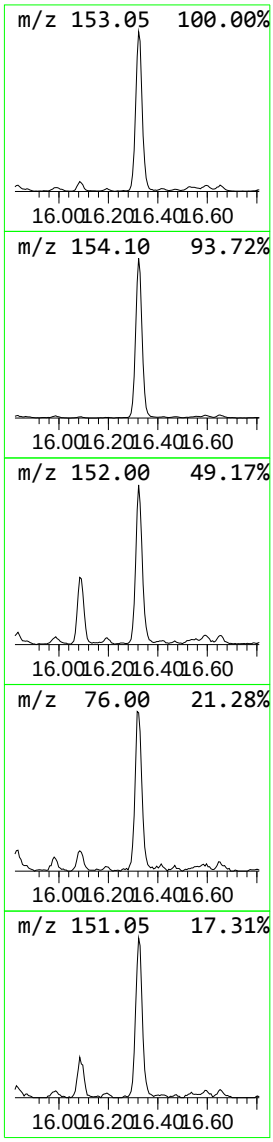
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Hexa-2,4-diyn-1-ylbenzene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.322	34.26 ug/l	484583	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acenaphthene	154	C12H10	000083-32-9	94
2	Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	72
3	Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	64
4	3-Fluoro-para-anisaldehyde	154	C8H7FO2	000351-54-2	50
5	2,4,6-Trihydroxybenzaldehyde	154	C7H6O4	000487-70-7	40





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081623\
Data File : VX037051.D
Acq On : 17 Aug 2023 09:59
Operator : JC/MD
Sample : 03958-06
Misc : 7.04g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 54 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NEVINS-SB02-Z21-23

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
Indane	12.244	49.4	ug/l	699075	4	12.024	707247	50.0
Fluorene	12.835	15.6	ug/l	219982	4	12.024	707247	50.0
Naphthalene, 1-...	14.634	46.9	ug/l	662648	4	12.024	707247	50.0
Benzocyclohepta...	14.780	35.5	ug/l	502388	4	12.024	707247	50.0
2,4-Difluoromes...	15.371	14.9	ug/l	210963	4	12.024	707247	50.0
Naphthalene, 1,...	15.475	21.4	ug/l	303464	4	12.024	707247	50.0
Naphthalene, 2,...	15.609	25.3	ug/l	358494	4	12.024	707247	50.0
Naphthalene, 2,...	15.646	10.2	ug/l	144468	4	12.024	707247	50.0
Hexa-2,4-diyn-1...	16.322	34.3	ug/l	484583	4	12.024	707247	50.0