LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082721\
Data File : VX023998.D
Acq On : 27 Aug 2021 17:31
Operator : JC/MD
Sample : M3561-15
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : VE4-7

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: VX023998.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	23	28	47	rBV	204975	999176	97.93%	6.085%
2	2.392	208	214	224	rBV2	8913	17627	1.73%	0.107%
3	2.550	231	240	248	rBV2	10400	24053	2.36%	0.146%
4	5.397	694	707	722	rBV	98590	288901	28.32%	1.759%
5	5.562	722	734	749	rVB	171290	479022	46.95%	2.917%
6	5.964	790	800	812	rBV2	112715	296626	29.07%	1.806%
7	6.769	922	932	943	rBV	272346	642401	62.96%	3.912%
8	8.653	1234	1241	1249	rBV	564944	869038	85.18%	5.292%
9	8.720	1249	1252	1258	rVB2	6497	10628	1.04%	0.065%
10	10.055	1465	1471	1481	rBV	603582	800799	78.49%	4.877%
11	10.299	1504	1511	1518	rVB	24800	36510	3.58%	0.222%
12	11.085	1635	1640	1646	rBV	499720	615493	60.33%	3.748%
13	11.189	1651	1657	1659	rBV6	7917	15641	1.53%	0.095%
14	12.024	1789	1794	1801	rBV	627186	766465	75.12%	4.668%
15	12.091	1801	1805	1808	rVV	8368	10440	1.02%	0.064%
16	12.244	1826	1830	1834	rBV2	53957	77083	7.56%	0.469%
17	12.317	1839	1842	1848	rVB3	24050	42854	4.20%	0.261%
18	12.421	1854	1859	1862	rBV7	8341	14788	1.45%	0.090%
19	12.463	1864	1866	1873	rVB6	12953	26121	2.56%	0.159%
20	12.536	1875	1878	1879	rBV	11852	12027	1.18%	0.073%
21	12.585	1883	1886	1888	rVV2	11666	13627	1.34%	0.083%
22	12.616	1888	1891	1894	rVV	28840	37122	3.64%	0.226%
23	12.646	1894	1896	1899	rVV3	17468	22223	2.18%	0.135%
24	12.701	1900	1905	1914	rVB6	43292	113824	11.16%	0.693%
25	12.823	1918	1925	1926	rBV6	17623	32918	3.23%	0.200%
26	12.927	1938	1942	1945	rVB	54542	72695	7.13%	0.443%
27	12.963	1945	1948	1954	rVB	46484	62149	6.09%	0.378%
28	13.030	1955	1959	1960	rBV	22430	27866	2.73%	0.170%
29	13.170	1974	1982	1986	rBV7	68117	185344	18.17%	1.129%
30	13.256	1993	1996	1998	rBV3	20748	30165	2.96%	0.184%
31	13.292	1998	2002	2008	rVB3	176580	273824	26.84%	1.667%
32	13.353	2009	2012	2013	rBV3	14864	16462	1.61%	0.100%
33	13.390	2014	2018	2021	rBV2	44685	56131	5.50%	0.342%
34	13.420	2021	2023	2025	rBV3	16491	17089	1.67%	0.104%
35	13.506	2033	2037	2040	rBV4	43695	68048	6.67%	0.414%
36	13.548	2040	2044	2046	rVV	48724	62119	6.09%	0.378%

LSC Area Percent Report

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Operator : JC/MD
Sample : M3561-15
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ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : VE4-7

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

37	13.585	2046	2050	2055	rVV4	79561	133923	13.13%	0.816%
38	13.670	2061	2064	2068	rVB2	70872	107170	10.50%	0.653%
39	13.707	2068	2070	2075	rBV4	20947	34060	3.34%	0.207%
40	13.798	2082	2085	2089	rBV3	51403	66756	6.54%	0.407%
41	13.847	2089	2093	2099	rBV3	165880	258383	25.32%	1.573%
42	13.926	2100	2106	2111	rBV5	105573	186697	18.30%	1.137%
43	13.975	2111	2114	2118	rBV4	49004	87159	8.54%	0.531%
44	14.079	2126	2131	2134	rBV3	146430	218710	21.44%	1.332%
45	14.140	2139	2141	2143	rVV2	39428	41465	4.06%	0.253%
46	14.170	2143	2146	2147	rVV3	30296	35303	3.46%	0.215%
47	14.213	2150	2153	2159	rVB	173655	256029	25.09%	1.559%
48	14.323	2167	2171	2176	rBV	114616	170024	16.66%	1.035%
49	14.378	2176	2180	2184	rVB	155669	200078	19.61%	1.218%
50	14.420	2184	2187	2190	rBV	58425	69785	6.84%	0.425%
51	14.481	2193	2197	2202	rBV2	146274	251415	24.64%	1.531%
52	14.579	2211	2213	2215	rBV3	32919	37685	3.69%	0.229%
53	14.615	2215	2219	2226	rVV3	346572	511880	50.17%	3.117%
54	14.676	2226	2229	2233	rVB3	94898	126294	12.38%	0.769%
55	14.731	2234	2238	2240	rBV3	82932	119430	11.71%	0.727%
56	14.780	2242	2246	2251	rVV	505557	755322	74.03%	4.600%
57	14.847	2255	2257	2261	rVB3	71900	92808	9.10%	0.565%
58	14.963	2273	2276	2283	rVB5	106441	224115	21.97%	1.365%
59	15.188	2309	2313	2315	rBV	135558	191920	18.81%	1.169%
60	15.213	2315	2317	2321	rVB	260885	288920	28.32%	1.759%
61	15.377	2340	2344	2346	rBV2	101459	134474	13.18%	0.819%
62	15.420	2347	2351	2356	rVV2	199138	350091	34.31%	2.132%
63	15.481	2356	2361	2374	rVV	350997	675167	66.18%	4.112%
64	15.615	2378	2383	2387	rVV	623363	1020274	100.00%	6.213%
65	15.652	2387	2389	2398	rVV	247246	406255	39.82%	2.474%
66	15.749	2400	2405	2409	rVV2	124807	221024	21.66%	1.346%
67	15.841	2411	2420	2429	rVB3	203651	656415	64.34%	3.997%
68	15.987	2440	2444	2457	rVB	169853	391198	38.34%	2.382%
69	16.091	2457	2461	2465	rBV4	50492	80947	7.93%	0.493%
70	16.267	2486	2490	2492	rBV	47398	76939	7.54%	0.469%
71	16.353	2501	2504	2513	rVB2	108738	200889	19.69%	1.223%
72	16.475	2521	2524	2530	rVB	47220	78003	7.65%	0.475%
73	16.603	2541	2545	2550	rVB	176086	297152	29.12%	1.810%
74	16.658	2550	2554	2559	rBV	148393	229833	22.53%	1.400%

Sum of corrected areas: 16421291

Instrument :
MSVOA_X
ClientSampleId :
VE4-7

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Operator : JC/MD
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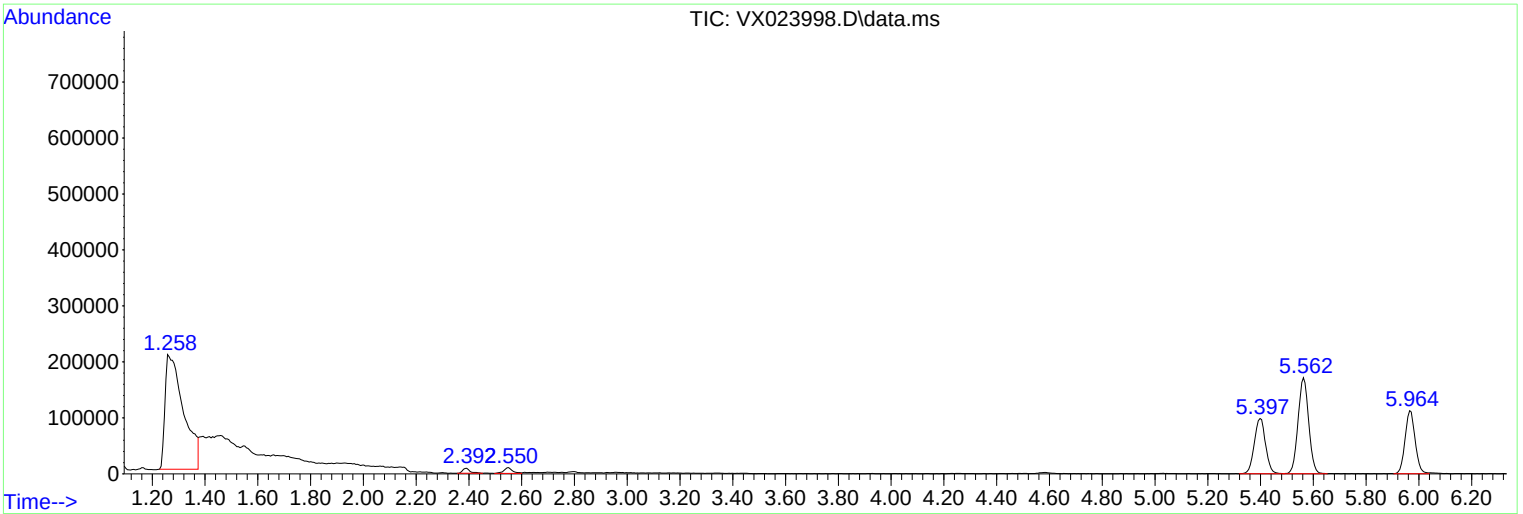
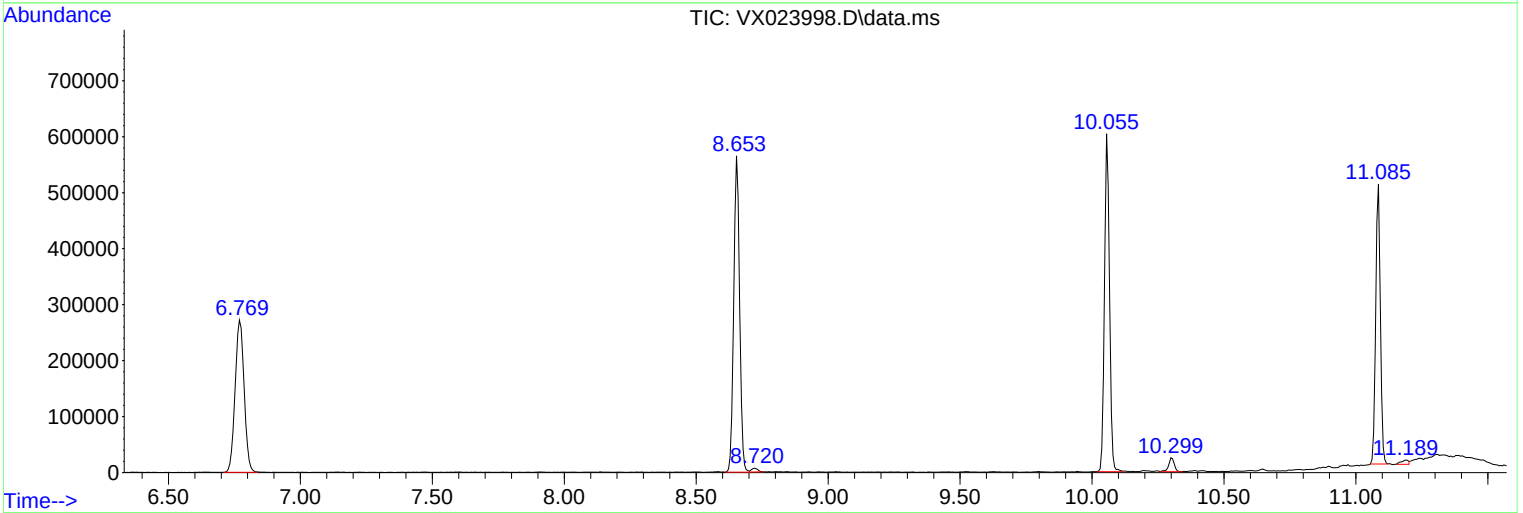
ALS Vial : 22 Sample Multiplier: 1

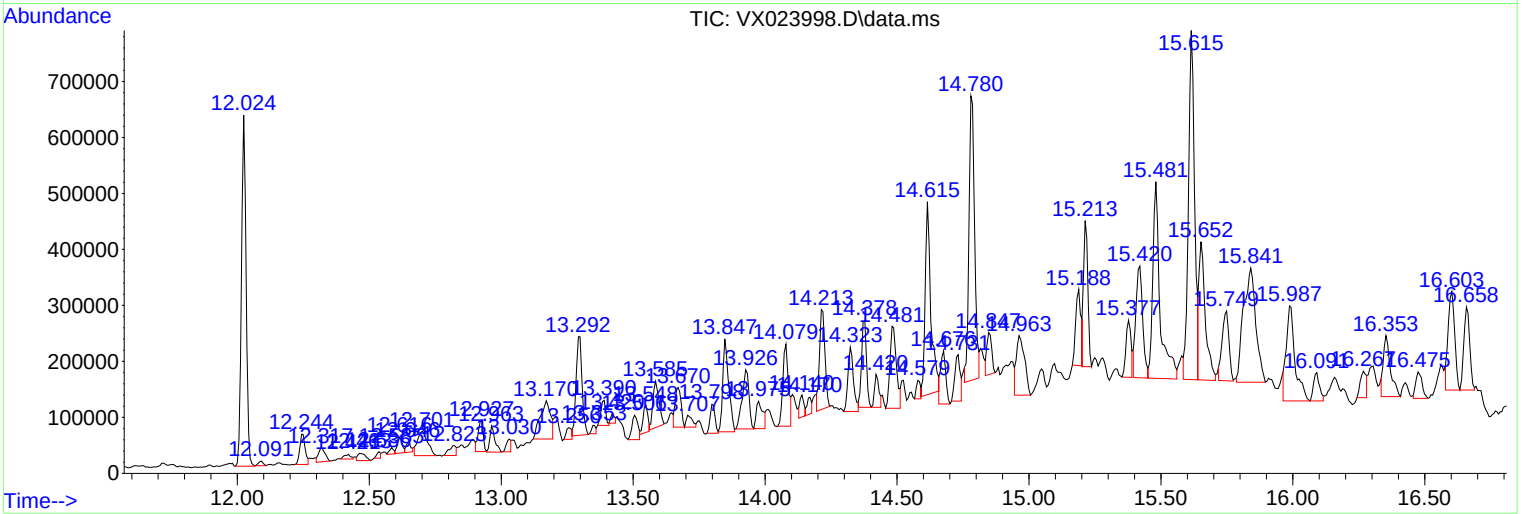
Instrument :
MSVOA_X
ClientSampleId :
VE4-7

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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Data File : VX023998.D
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Operator : JC/MD
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ClientSampleId : VE4-7

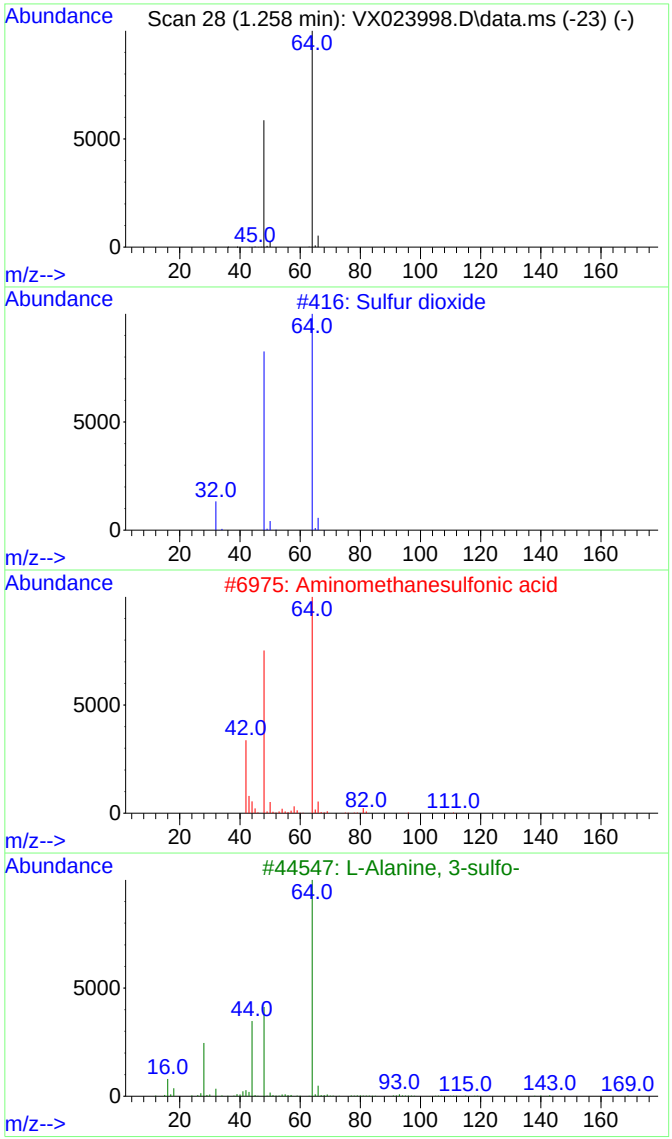
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

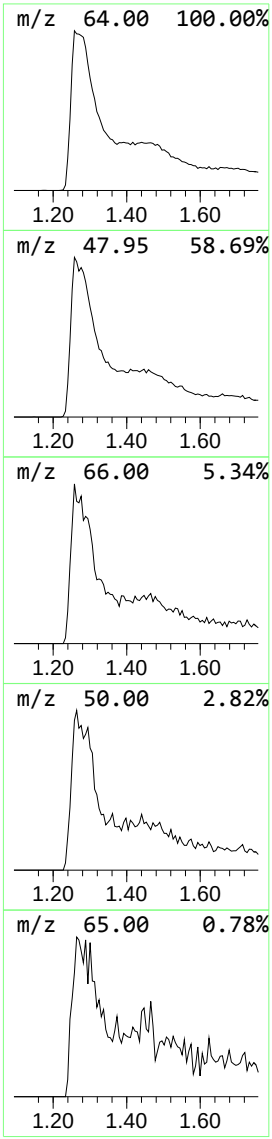
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.258	104.29 ug/l	999176	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3





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Data File : VX023998.D
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Sample : M3561-15
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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VE4-7

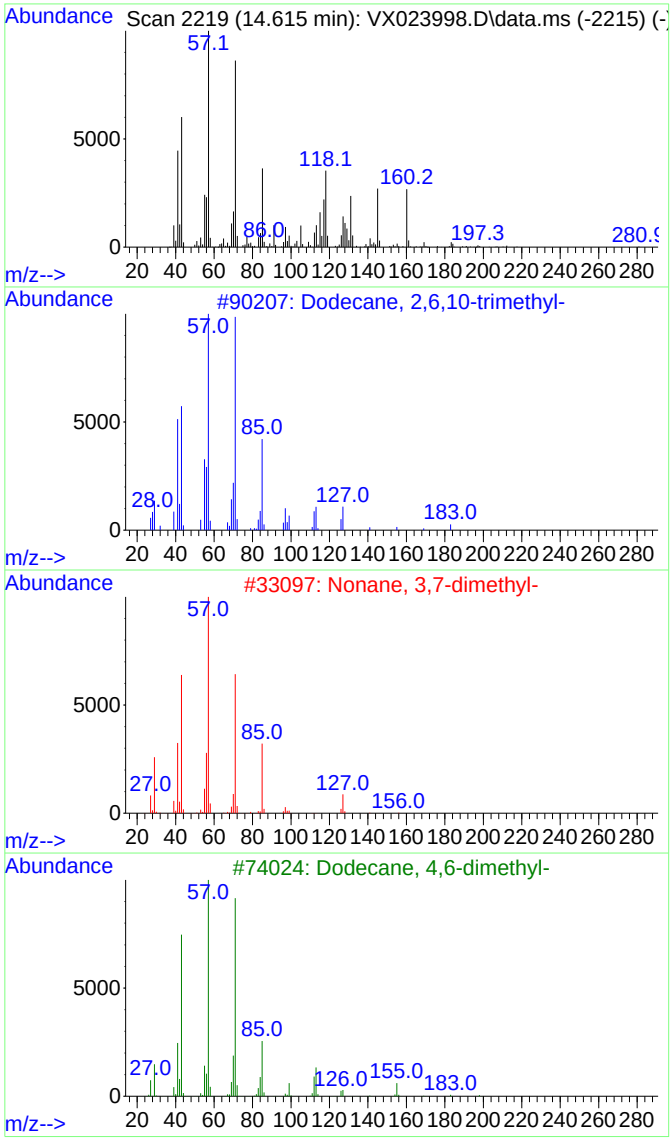
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

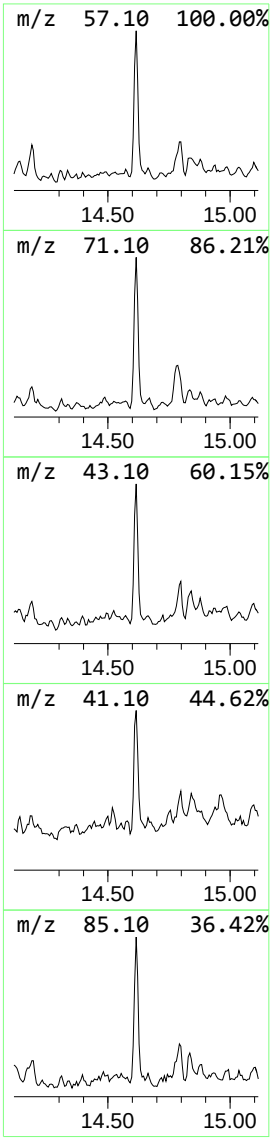
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Dodecane, 2,6,10-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.615	33.39 ug/l	511880	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	50
2	Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	46
3	Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	46
4	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	43
5	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082721\
Data File : VX023998.D
Acq On : 27 Aug 2021 17:31
Operator : JC/MD
Sample : M3561-15
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VE4-7

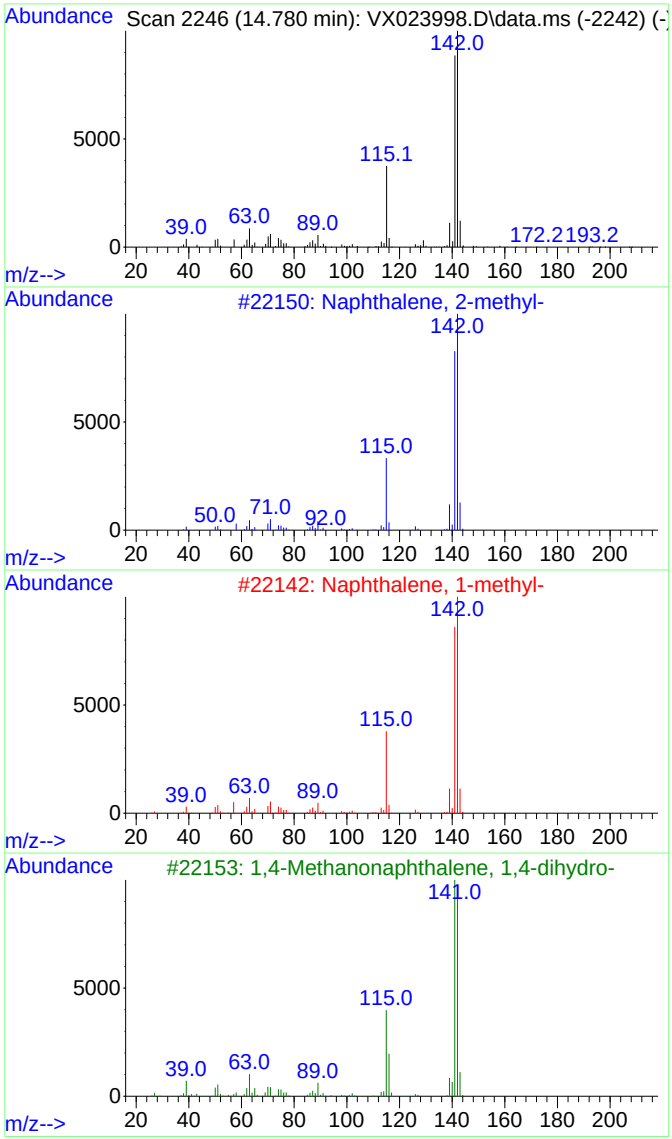
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

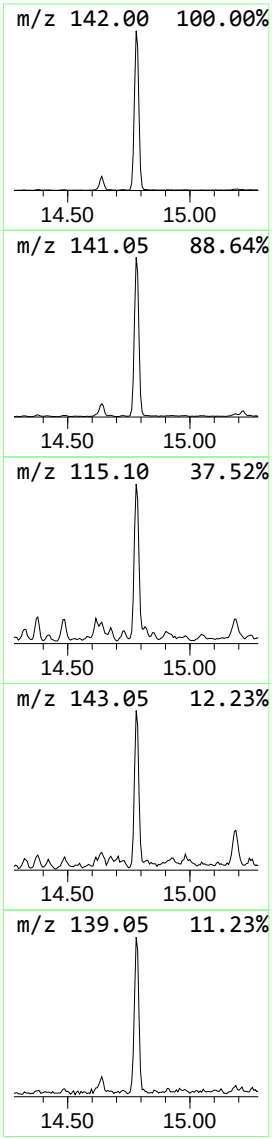
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	49.27 ug/l	755322	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	94
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64





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ALS Vial : 22 Sample Multiplier: 1

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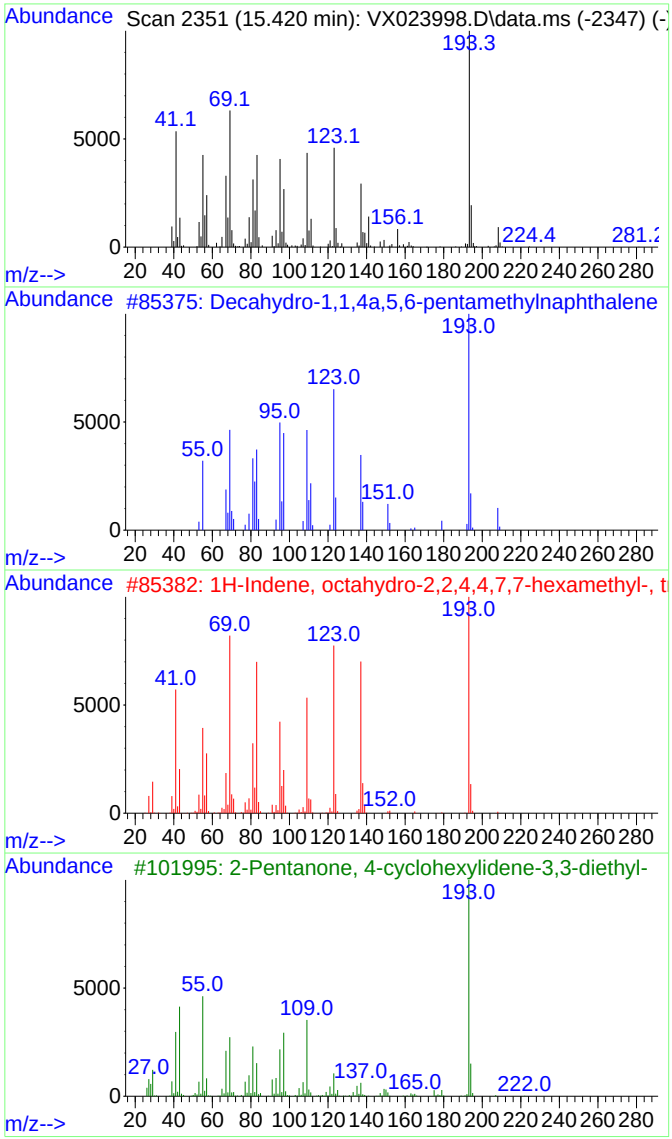
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

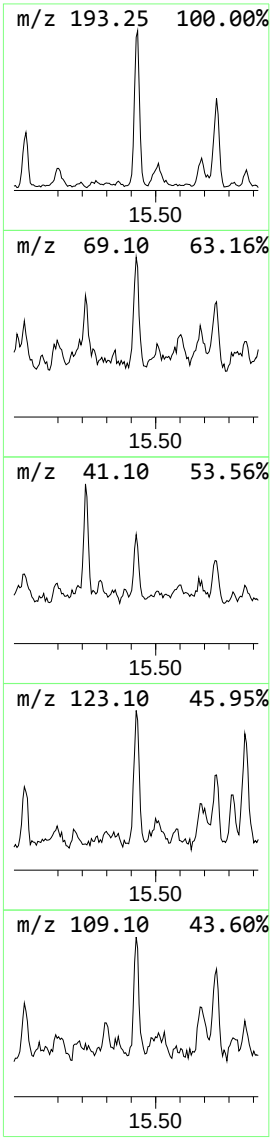
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.420	22.84 ug/l	350091	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	55
2	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	43
3	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	40
4	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	38
5	2-Dodecen-1-yl(-)succinic anhydride	266	C16H26O3	019780-11-1	32





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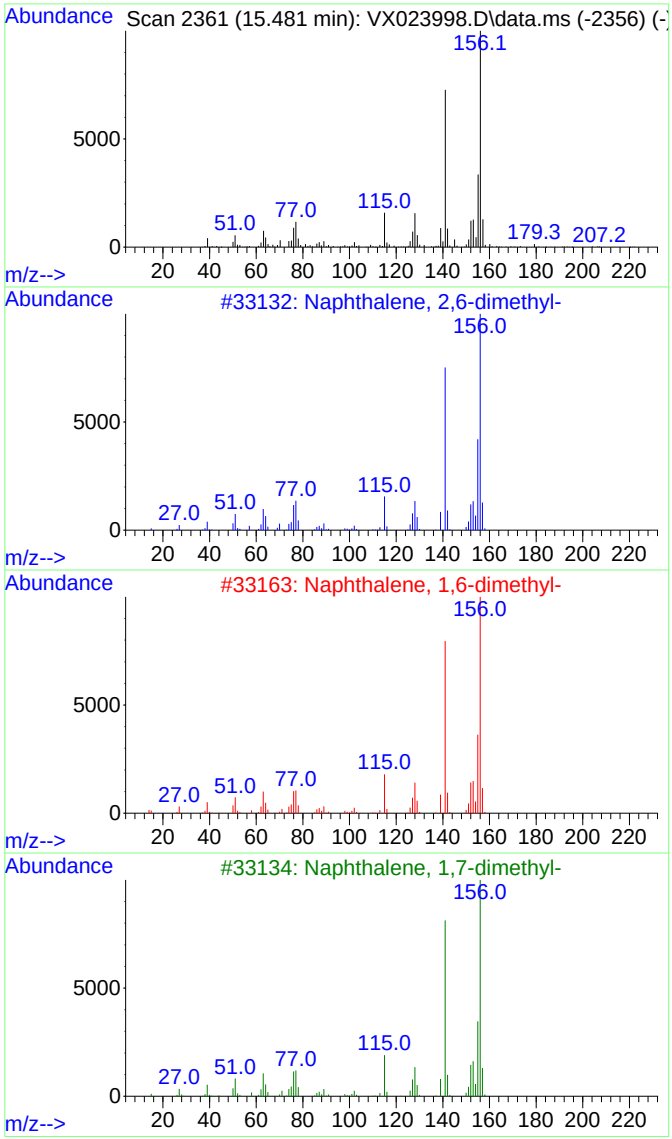
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

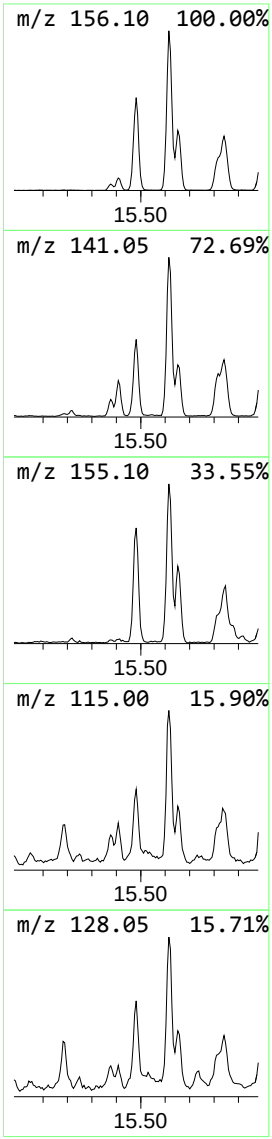
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Naphthalene, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.481	44.04 ug/l	675167	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, 1,6-dimethyl-	156	C12H12	000575-43-9	97
3	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96
4	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	96
5	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082721\
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Operator : JC/MD
Sample : M3561-15
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VE4-7

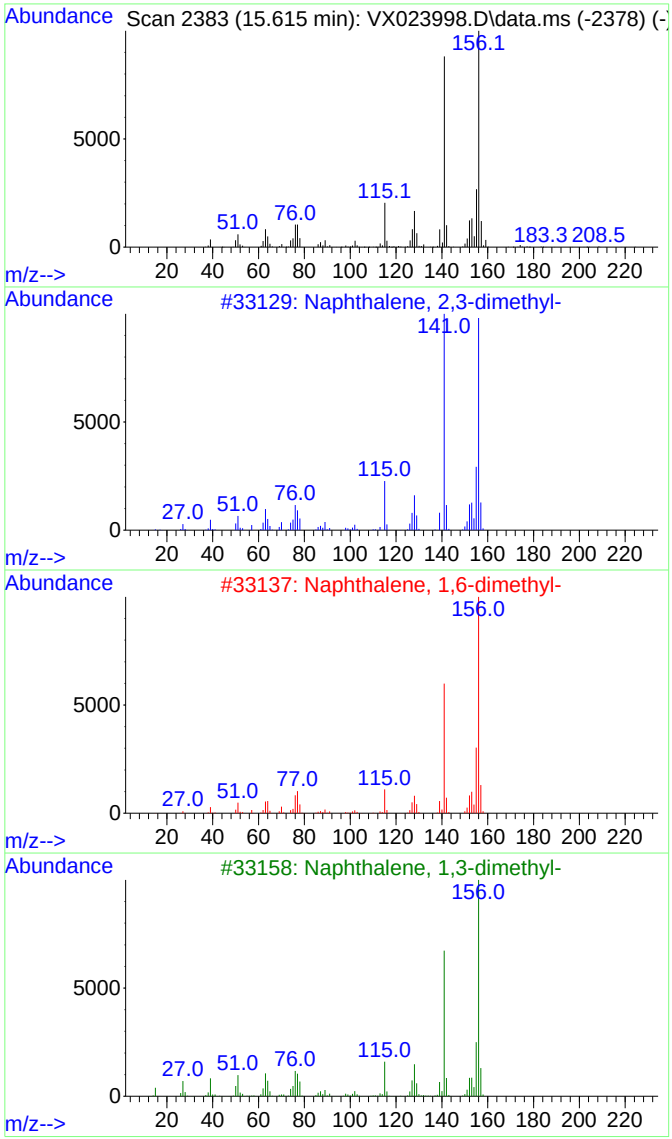
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

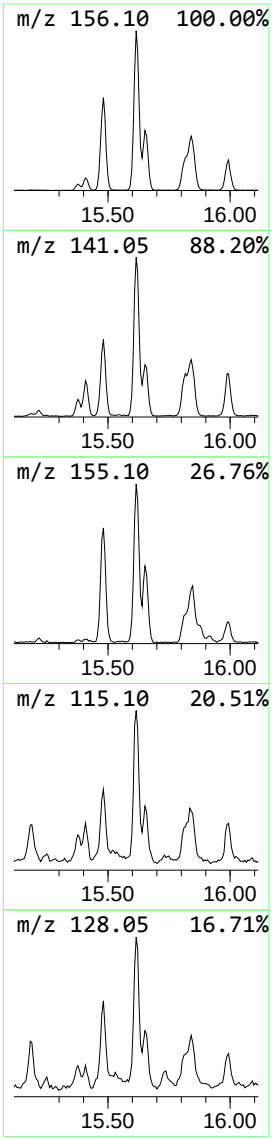
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Naphthalene, 2,3-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	66.56 ug/l	1020270	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, 1,6-dimethyl-	156	C12H12	000575-43-9	97
3	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
4	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
5	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082721\
Data File : VX023998.D
Acq On : 27 Aug 2021 17:31
Operator : JC/MD
Sample : M3561-15
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VE4-7

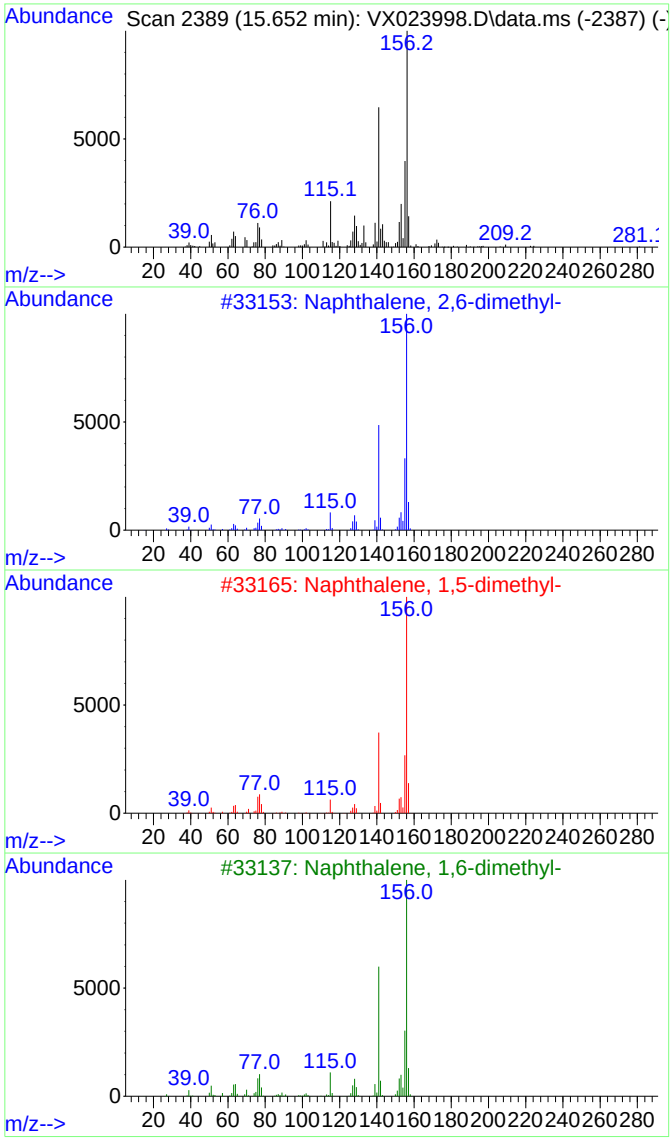
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

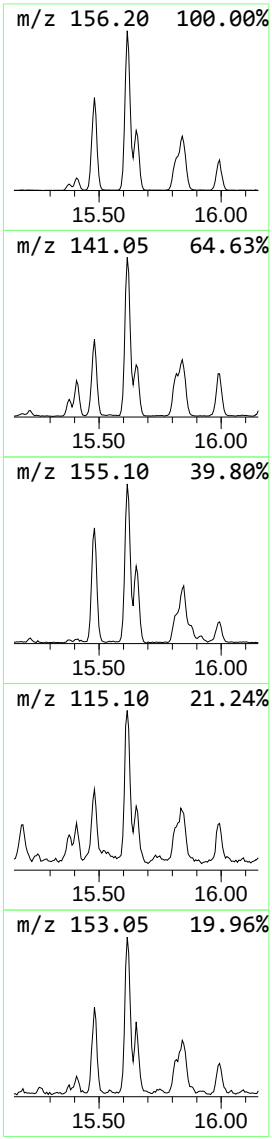
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Naphthalene, 1,5-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.652	26.50 ug/l	406255	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	94
2	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	93
3	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	93
4	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	90
5	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	86





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082721\
Data File : VX023998.D
Acq On : 27 Aug 2021 17:31
Operator : JC/MD
Sample : M3561-15
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VE4-7

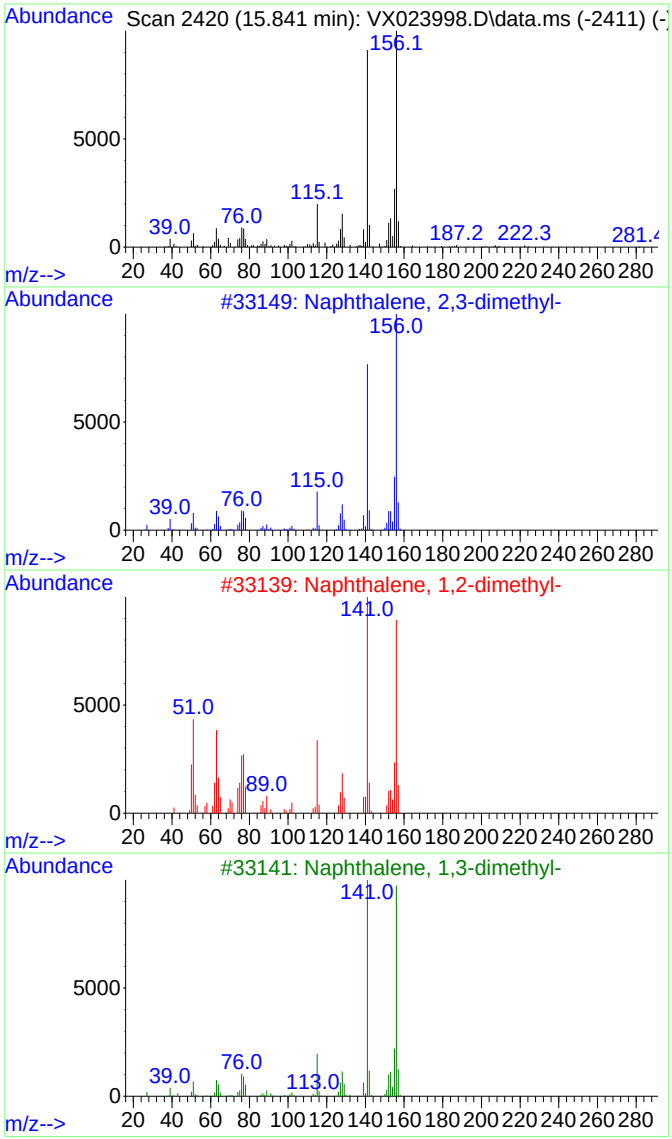
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

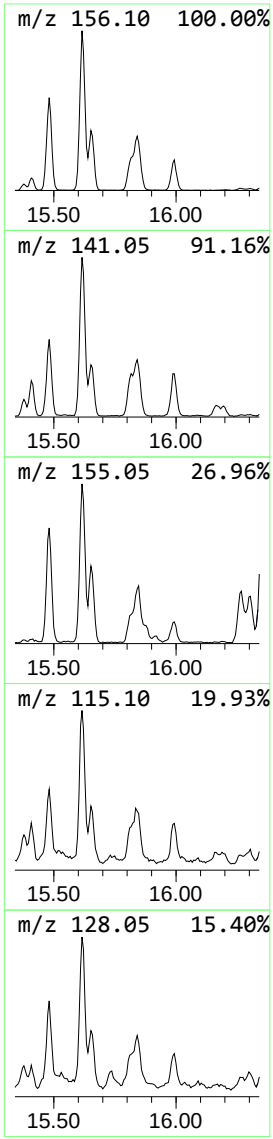
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Naphthalene, 1,2-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.841	42.82 ug/l	656415	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	97
2	Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	97
3	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96
4	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
5	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	95





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082721\
Data File : VX023998.D
Acq On : 27 Aug 2021 17:31
Operator : JC/MD
Sample : M3561-15
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VE4-7

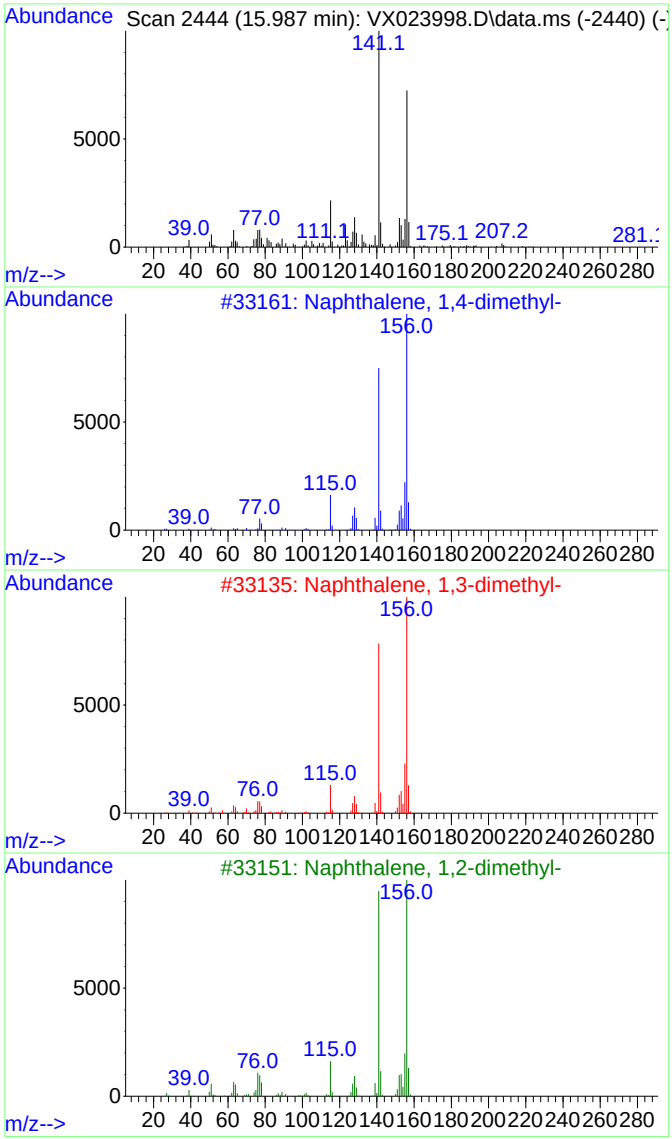
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

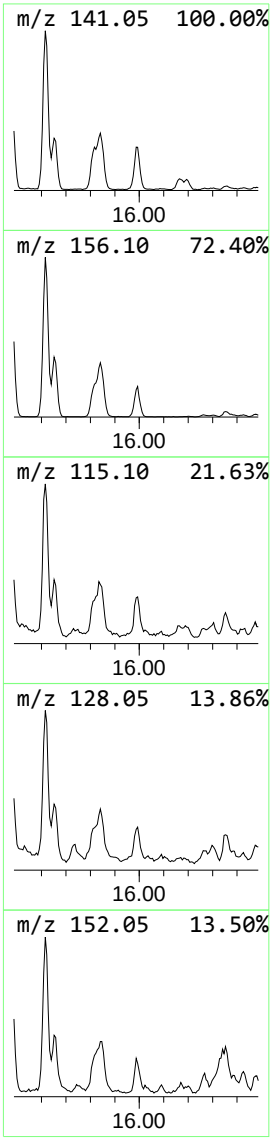
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Naphthalene, 1,4-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.987	25.52 ug/l	391198	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	95
2	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	95
3	Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	95
4	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	94
5	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	87





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082721\
Data File : VX023998.D
Acq On : 27 Aug 2021 17:31
Operator : JC/MD
Sample : M3561-15
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VE4-7

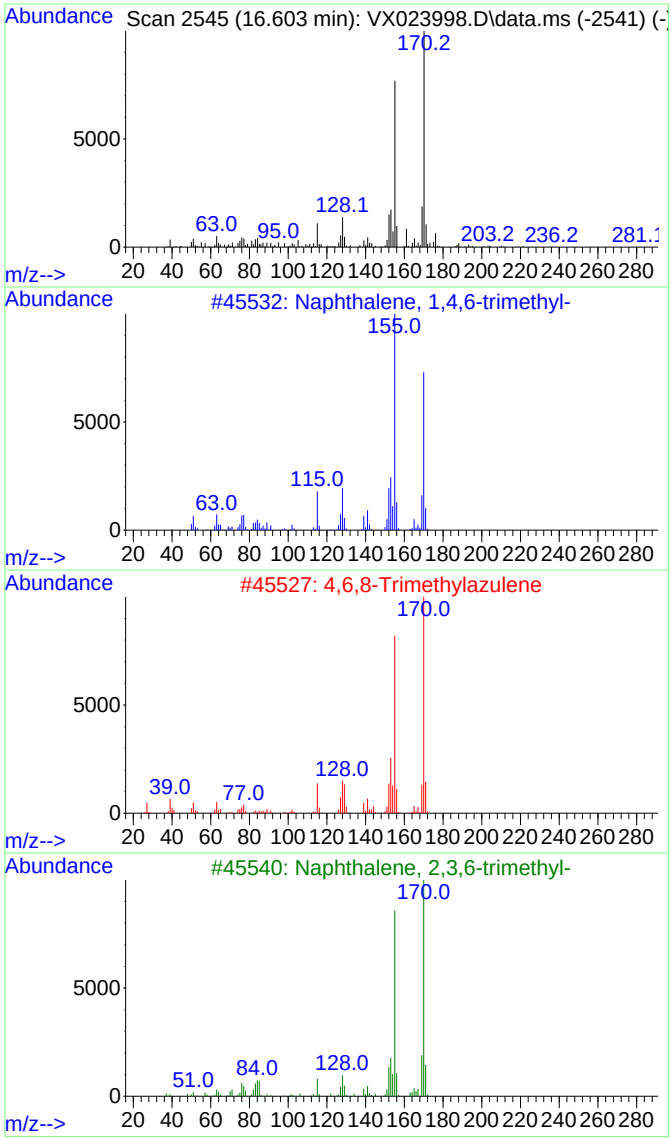
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081721W.M
Quant Title : SW846 8260

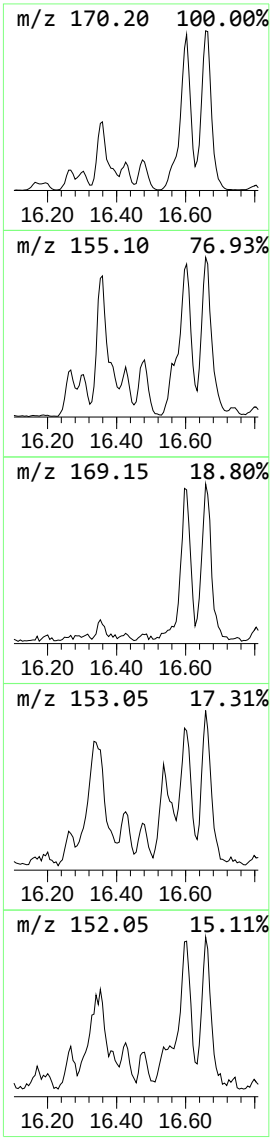
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, 1,4,6-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.603	19.38 ug/l	297152	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,4,6-trimethyl-	170	C13H14	002131-42-2	96
2	4,6,8-Trimethylazulene	170	C13H14	000941-81-1	94
3	Naphthalene, 2,3,6-trimethyl-	170	C13H14	000829-26-5	94
4	Naphthalene, 1,6,7-trimethyl-	170	C13H14	002245-38-7	94
5	Naphthalene, 1,4,5-trimethyl-	170	C13H14	002131-41-1	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082721\
Data File : VX023998.D
Acq On : 27 Aug 2021 17:31
Operator : JC/MD
Sample : M3561-15
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : VE4-7

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
Sulfur dioxide	1.258	104.3	ug/l	999176	1	5.562	479022	50.0
Dodecane, 2,6,1...	14.615	33.4	ug/l	511880	4	12.024	766465	50.0
Naphthalene, 1-...	14.780	49.3	ug/l	755322	4	12.024	766465	50.0
Decahydro-1,1,4...	15.420	22.8	ug/l	350091	4	12.024	766465	50.0
Naphthalene, 2,...	15.481	44.0	ug/l	675167	4	12.024	766465	50.0
Naphthalene, 2,...	15.615	66.6	ug/l	1020270	4	12.024	766465	50.0
Naphthalene, 1,...	15.652	26.5	ug/l	406255	4	12.024	766465	50.0
Naphthalene, 1,...	15.841	42.8	ug/l	656415	4	12.024	766465	50.0
Naphthalene, 1,...	15.987	25.5	ug/l	391198	4	12.024	766465	50.0
Naphthalene, 1,...	16.603	19.4	ug/l	297152	4	12.024	766465	50.0