LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110122\
Data File : VX032510.D
Acq On : 01 Nov 2022 14:02
Operator : JC/MD
Sample : N5391-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31845

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\82X102622W.M
Title : SW846 8260

Signal : TIC: VX032510.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.386	206	213	218	rBV	9440	17127	2.75%	0.291%
2	3.111	321	332	343	rBV	17626	40068	6.44%	0.680%
3	3.764	430	439	448	rVB3	4851	12286	1.97%	0.208%
4	5.385	694	705	721	rBV	74644	218420	35.09%	3.705%
5	5.556	721	733	747	rVB	128376	362762	58.28%	6.154%
6	5.958	789	799	813	rBV	81367	215334	34.60%	3.653%
7	6.763	918	931	946	rBV	196835	464437	74.62%	7.878%
8	8.653	1234	1241	1254	rVB	388555	622398	100.00%	10.558%
9	10.055	1465	1471	1480	rBV	400916	534691	85.91%	9.070%
10	11.079	1634	1639	1652	rBV	365678	470944	75.67%	7.989%
11	11.384	1684	1689	1690	rBV	5539	6596	1.06%	0.112%
12	11.451	1695	1700	1703	rBV	5705	6915	1.11%	0.117%
13	11.616	1723	1727	1733	rVB2	8207	11523	1.85%	0.195%
14	11.750	1740	1749	1758	rVB3	6938	12107	1.95%	0.205%
15	11.969	1782	1785	1788	rVB	8246	8787	1.41%	0.149%
16	12.024	1788	1794	1800	rBV	410767	516203	82.94%	8.757%
17	12.085	1800	1804	1808	rBV2	6541	8909	1.43%	0.151%
18	12.268	1825	1834	1838	rBV2	23266	40934	6.58%	0.694%
19	12.317	1838	1842	1852	rVB3	35482	54270	8.72%	0.921%
20	12.408	1852	1857	1859	rBV2	6311	10466	1.68%	0.178%
21	12.463	1862	1866	1871	rVB	17537	22002	3.54%	0.373%
22	12.530	1871	1877	1879	rBV	12076	16018	2.57%	0.272%
23	12.555	1879	1881	1885	rVB	12178	12642	2.03%	0.214%
24	12.616	1886	1891	1894	rBV	28043	33699	5.41%	0.572%
25	12.725	1906	1909	1913	rVB2	14839	22672	3.64%	0.385%
26	12.799	1917	1921	1925	rBV	10173	13451	2.16%	0.228%
27	12.847	1925	1929	1933	rVB2	13667	18451	2.96%	0.313%
28	12.920	1933	1941	1945	rBV	19134	31055	4.99%	0.527%
29	12.963	1945	1948	1954	rVB	24689	31010	4.98%	0.526%
30	13.024	1954	1958	1960	rBV	14510	19883	3.19%	0.337%
31	13.140	1973	1977	1985	rVV5	31309	64327	10.34%	1.091%
32	13.213	1985	1989	1992	rVV2	13942	16576	2.66%	0.281%
33	13.256	1992	1996	1998	rVV4	18356	28982	4.66%	0.492%
34	13.292	1998	2002	2007	rVV3	53455	83835	13.47%	1.422%
35	13.341	2007	2010	2013	rVV2	19636	28717	4.61%	0.487%
36	13.372	2013	2015	2017	rVV	9689	10092	1.62%	0.171%

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ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
31845

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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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Title : SW846 8260

37	13.420	2020	2023	2033	rVB3	27355	43493	6.99%	0.738%
38	13.506	2033	2037	2040	rBV3	11411	17098	2.75%	0.290%
39	13.548	2040	2044	2046	rVV	23863	33015	5.30%	0.560%
40	13.585	2046	2050	2055	rVV2	36949	69399	11.15%	1.177%
41	13.640	2055	2059	2060	rVV	19473	26229	4.21%	0.445%
42	13.664	2060	2063	2069	rVB2	32963	50460	8.11%	0.856%
43	13.750	2075	2077	2081	rVB3	7118	7797	1.25%	0.132%
44	13.792	2081	2084	2088	rBV3	6648	9359	1.50%	0.159%
45	13.853	2088	2094	2099	rVB	46936	68157	10.95%	1.156%
46	13.926	2099	2106	2111	rBV3	51388	80265	12.90%	1.362%
47	13.975	2111	2114	2117	rVV3	14535	17823	2.86%	0.302%
48	14.036	2121	2124	2127	rVB3	12081	13058	2.10%	0.222%
49	14.073	2127	2130	2134	rBV2	29699	36393	5.85%	0.617%
50	14.164	2142	2145	2149	rBV2	5592	9562	1.54%	0.162%
51	14.231	2149	2156	2160	rBV2	87407	160067	25.72%	2.715%
52	14.323	2167	2171	2175	rBV	27575	35014	5.63%	0.594%
53	14.371	2175	2179	2184	rVV	48930	62047	9.97%	1.053%
54	14.420	2184	2187	2192	rVB4	13877	20292	3.26%	0.344%
55	14.481	2192	2197	2202	rBV2	88046	124702	20.04%	2.115%
56	14.615	2215	2219	2225	rBV3	68361	112867	18.13%	1.915%
57	14.670	2225	2228	2233	rVB	45277	62739	10.08%	1.064%
58	14.725	2233	2237	2240	rBV2	16194	24120	3.88%	0.409%
59	14.755	2240	2242	2245	rVB	14613	13203	2.12%	0.224%
60	14.823	2245	2253	2255	rBV4	30212	49105	7.89%	0.833%
61	14.847	2255	2257	2262	rVB3	26685	29906	4.80%	0.507%
62	14.908	2262	2267	2273	rBV2	31495	58961	9.47%	1.000%
63	14.987	2277	2280	2284	rVB5	10003	13596	2.18%	0.231%
64	15.048	2284	2290	2295	rBV2	17455	28764	4.62%	0.488%
65	15.103	2295	2299	2302	rBV6	7130	10473	1.68%	0.178%
66	15.146	2302	2306	2308	rBV4	7782	9602	1.54%	0.163%
67	15.182	2308	2312	2320	rVB	72694	129182	20.76%	2.191%
68	15.249	2320	2323	2325	rBV3	6677	9425	1.51%	0.160%
69	15.329	2331	2336	2339	rBV6	6283	11673	1.88%	0.198%
70	15.377	2339	2344	2351	rVB5	18067	36319	5.84%	0.616%
71	15.487	2352	2362	2365	rBV4	36655	67261	10.81%	1.141%
72	15.524	2365	2368	2373	rVV4	19591	37206	5.98%	0.631%
73	15.572	2373	2376	2378	rVV4	10842	15568	2.50%	0.264%
74	15.615	2378	2383	2387	rVV4	26566	48882	7.85%	0.829%
75	15.652	2387	2389	2396	rVB5	14716	23956	3.85%	0.406%
76	15.847	2417	2421	2424	rBV5	9655	16404	2.64%	0.278%

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ClientSampleId :
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Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
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Title : SW846 8260

77	15.883	2424	2427	2434	rVB6	8967	18095	2.91%	0.307%
78	16.024	2447	2450	2456	rVB7	8077	13881	2.23%	0.235%
79	16.091	2456	2461	2463	rBV4	8563	13879	2.23%	0.235%
80	16.298	2492	2495	2500	rVB7	5111	7617	1.22%	0.129%
81	16.371	2500	2507	2519	rVB2	15492	34955	5.62%	0.593%
82	16.597	2542	2544	2549	rVB4	5728	6819	1.10%	0.116%
83	16.658	2549	2554	2559	rVV3	5000	10851	1.74%	0.184%
84	16.719	2561	2564	2569	rVB6	4289	6873	1.10%	0.117%

Sum of corrected areas: 5895001

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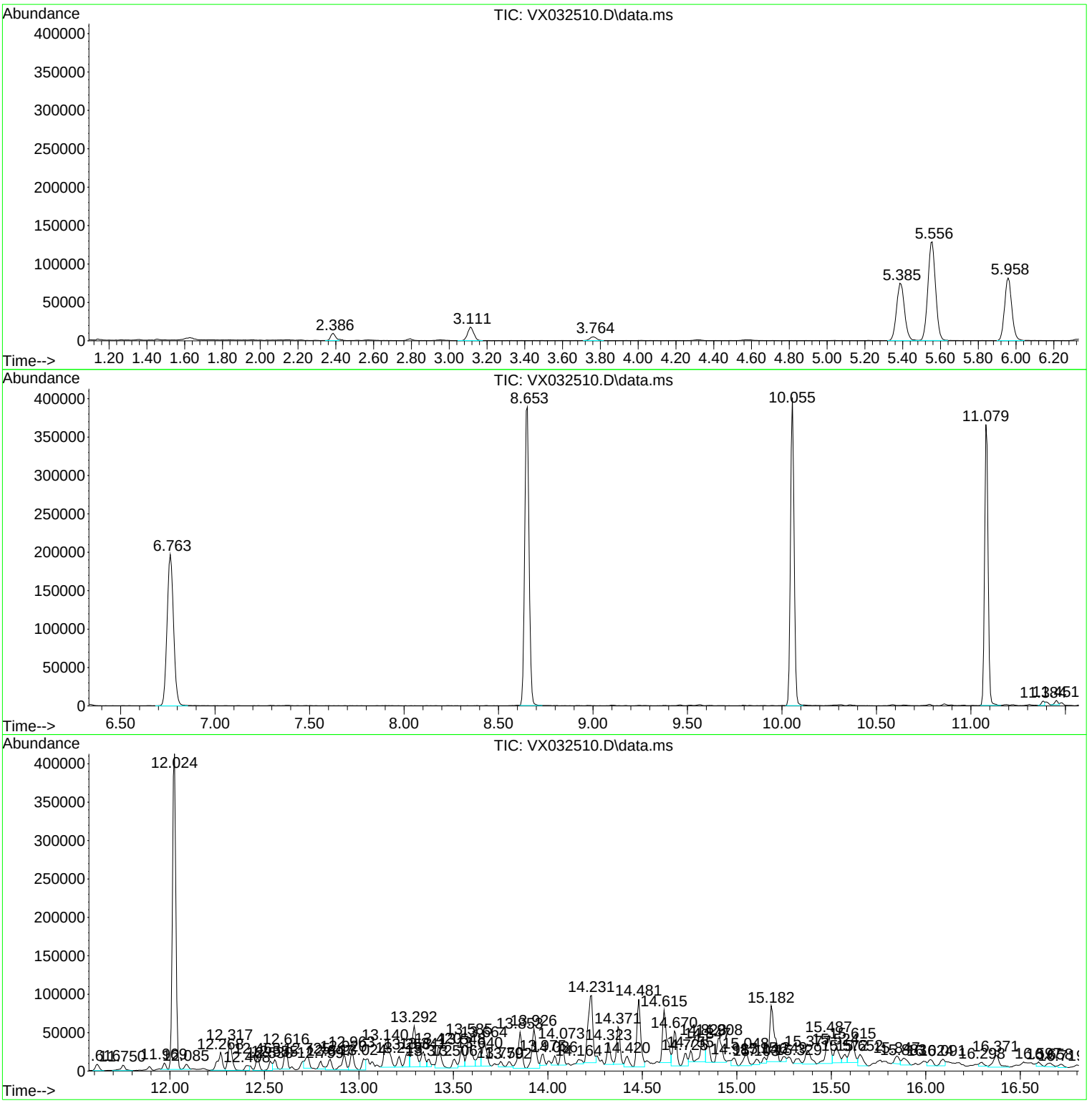
Instrument :
MSVOA_X
ClientSampleId :
31845

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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



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ClientSampleId :
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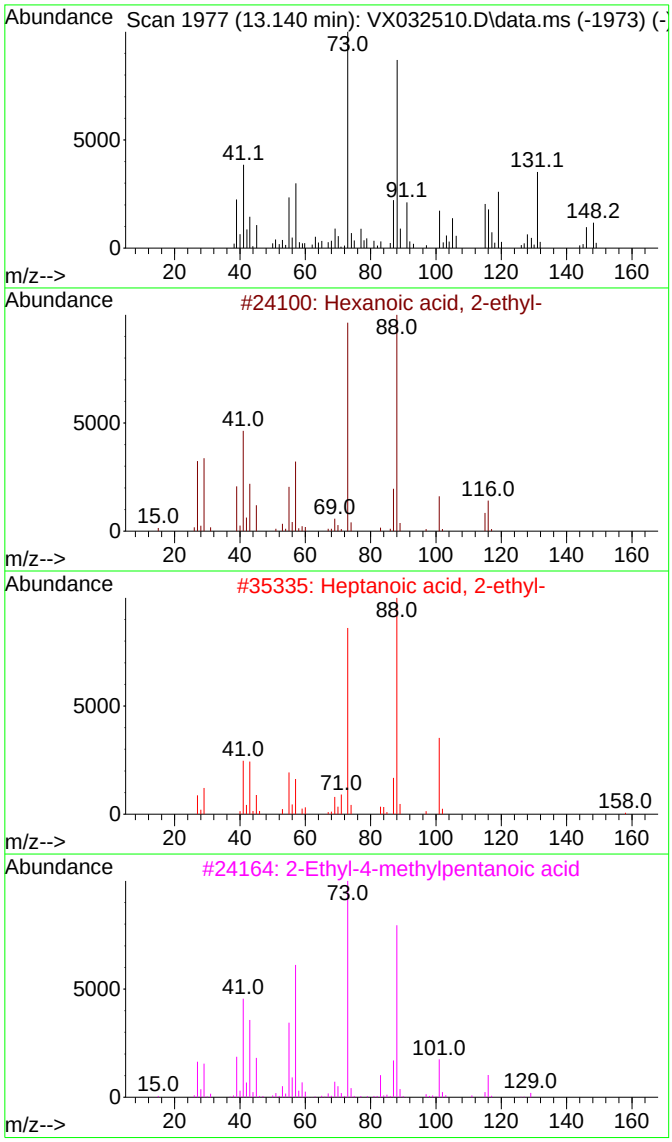
Quant Title : SW846 8260

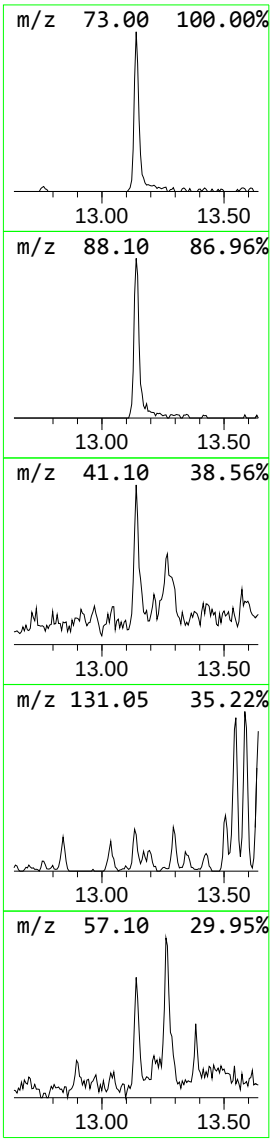
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Hexanoic acid, 2-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.140	6.23 ug/l	64327	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	52
2	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	43
3	2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	38
4	Methyl 2-methylhexanoate	144	C8H16O2	002177-81-3	35
5	Hexanoic acid, ethyl ester	144	C8H16O2	000123-66-0	35





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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

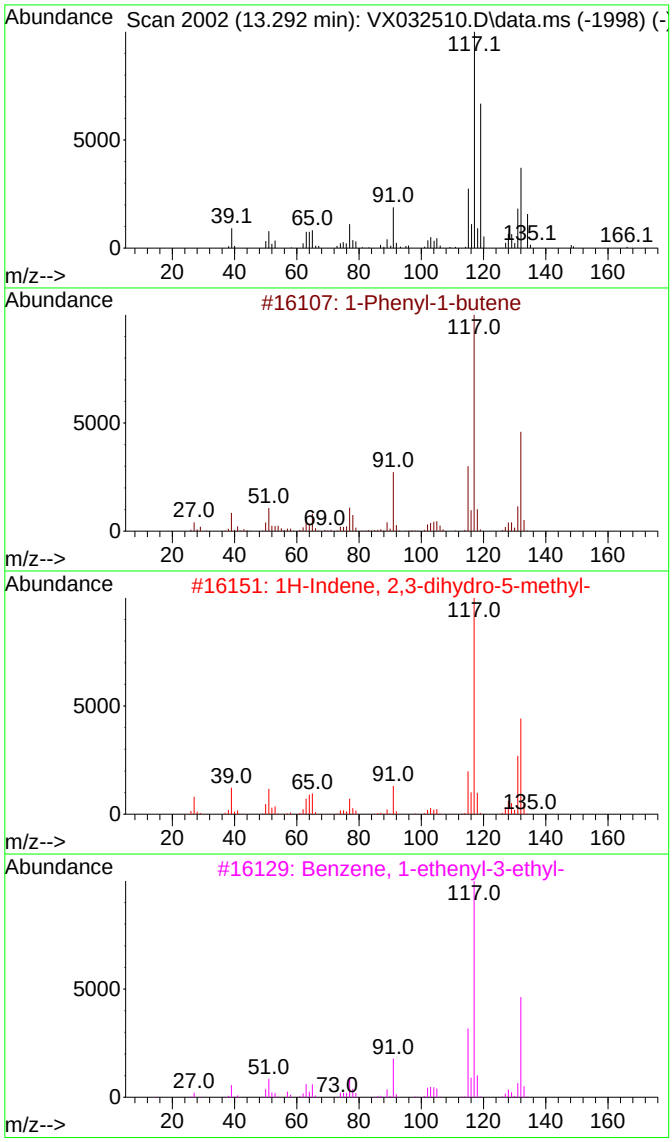
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

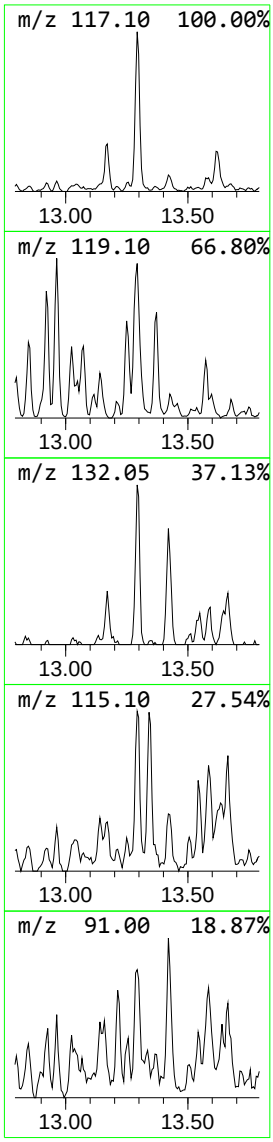
****

Peak Number 2 1-Phenyl-1-butene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	8.12 ug/l	83835	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenyl-1-butene	132	C10H12	000824-90-8	95
2	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	92
3	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	92
4	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	91
5	2,4-Dimethylstyrene	132	C10H12	002234-20-0	91





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Instrument :
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ClientSampleId :
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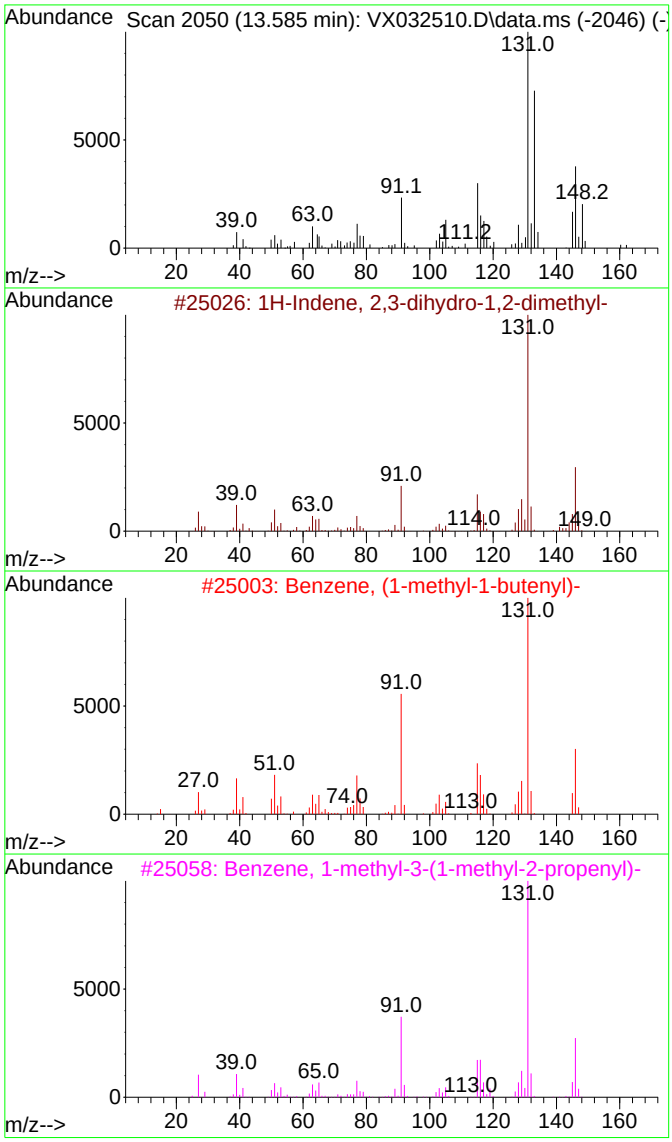
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

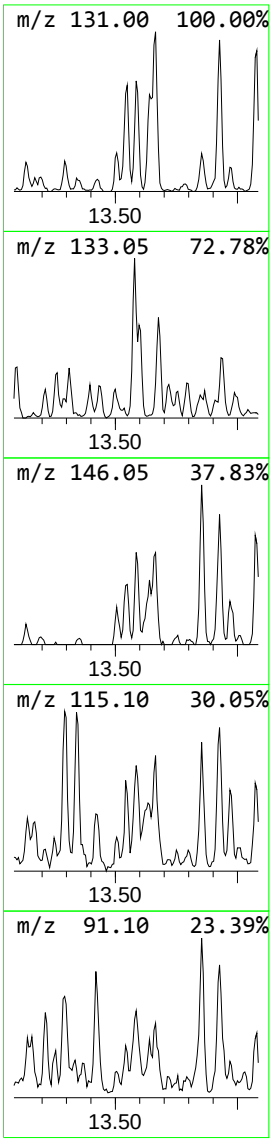
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.585	6.72 ug/l	69399	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	70
2	Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	70
3	Benzene, 1-methyl-3-(1-methyl-2-...	146	C11H14	052161-57-6	70
4	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	64
5	Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	64





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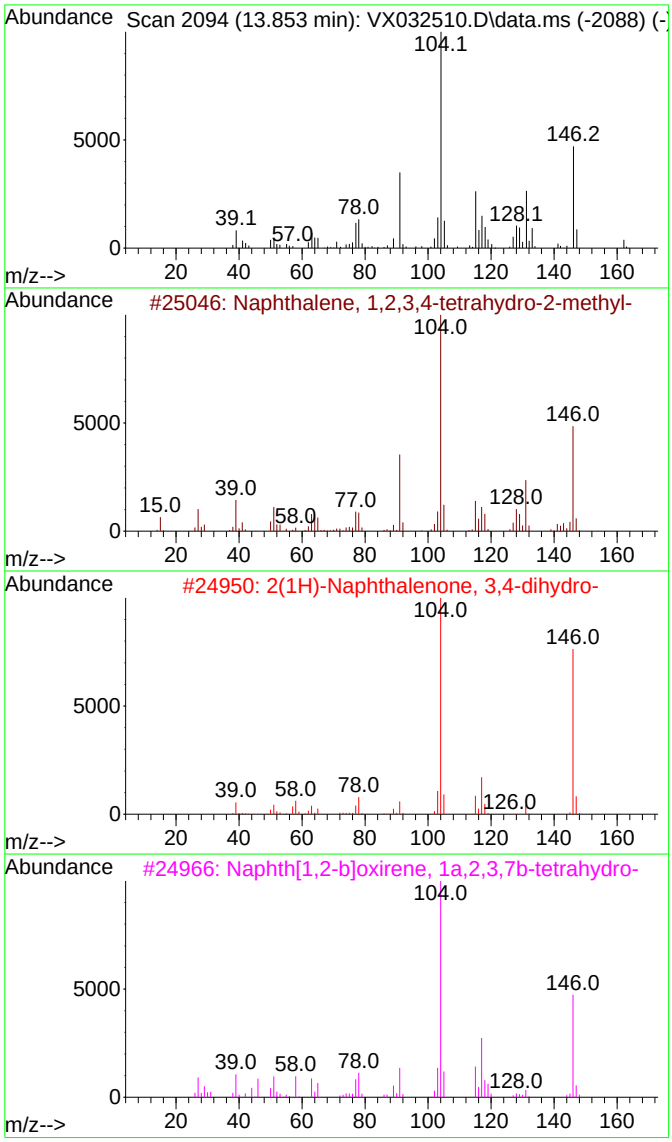
Quant Title : SW846 8260

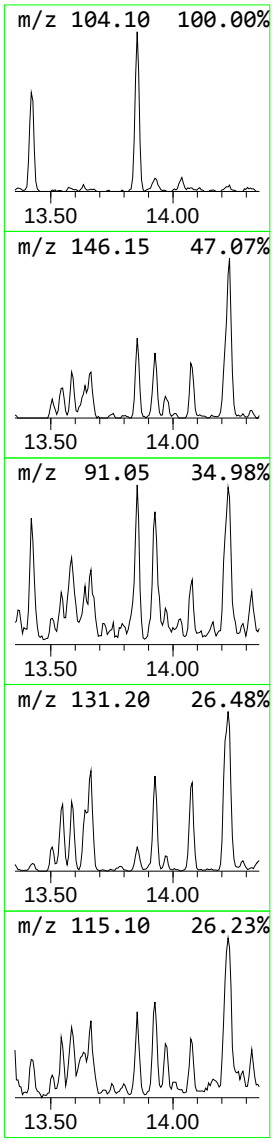
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.853	6.60 ug/l	68157	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	003877-19-8	94
2	2(1H)-Naphthalenone, 3,4-dihydro-	146	C10H10O	000530-93-8	58
3	Naphth[1,2-b]oxirene, 1a,2,3,7b-...	146	C10H10O	002461-34-9	58
4	Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	47
5	2-Azetidinone, 4-phenyl-	147	C9H9NO	005661-55-2	38





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ALS Vial : 11 Sample Multiplier: 1

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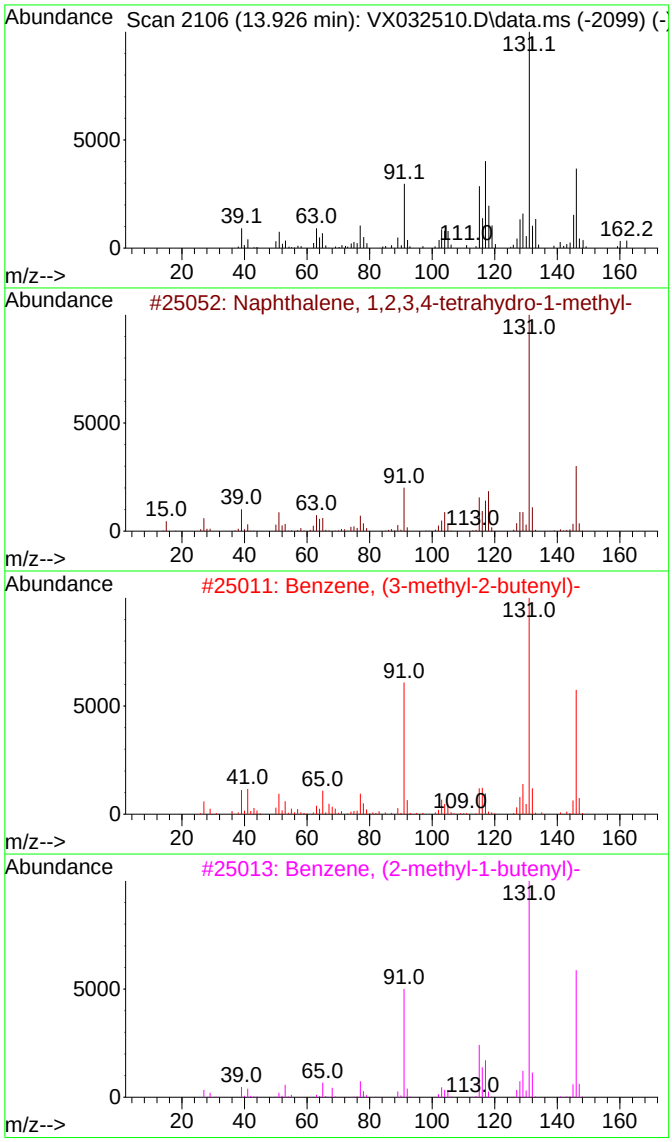
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

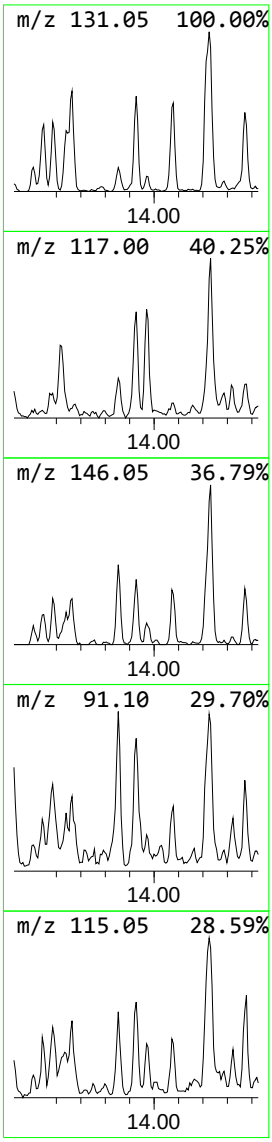
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.926	7.77 ug/l	80265	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	92
2	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	92
3	Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	91
4	Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	83
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	160	C12H16	078920-29-3	76





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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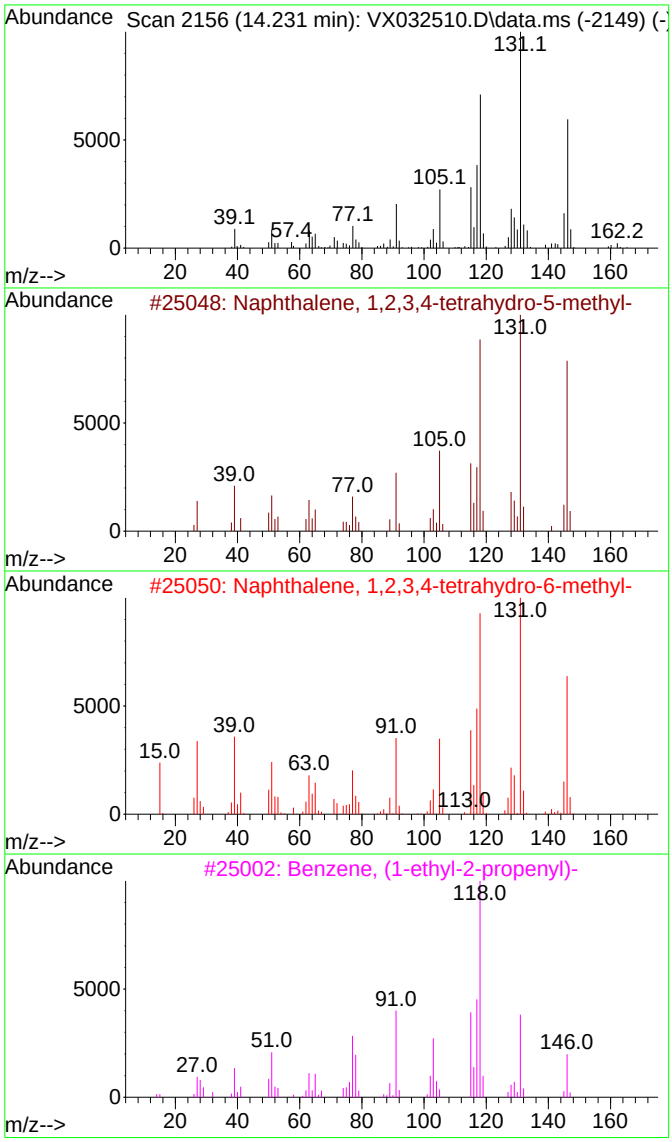
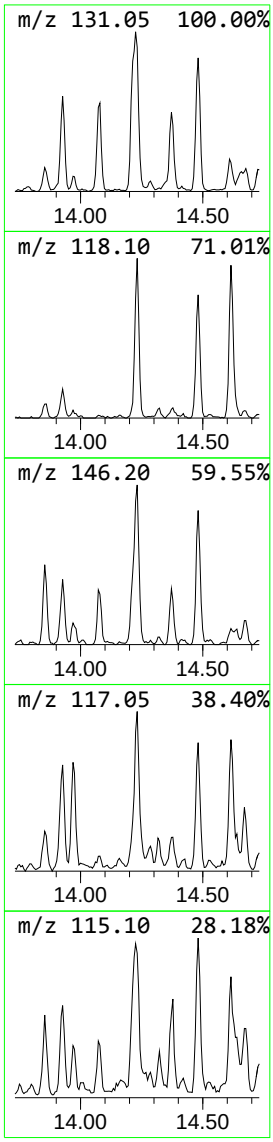
****
Peak Number 6 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.231	15.50 ug/l	160067	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	98
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	97
3	Benzene, (1-ethyl-2-propenyl)-	146	C11H14	019947-22-9	81
4	1H-Inden-1-one, 2,3-dihydro-2-me...	146	C10H10O	017496-14-9	81
5	Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	70





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110122\
Data File : VX032510.D
Acq On : 01 Nov 2022 14:02
Operator : JC/MD
Sample : N5391-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31845

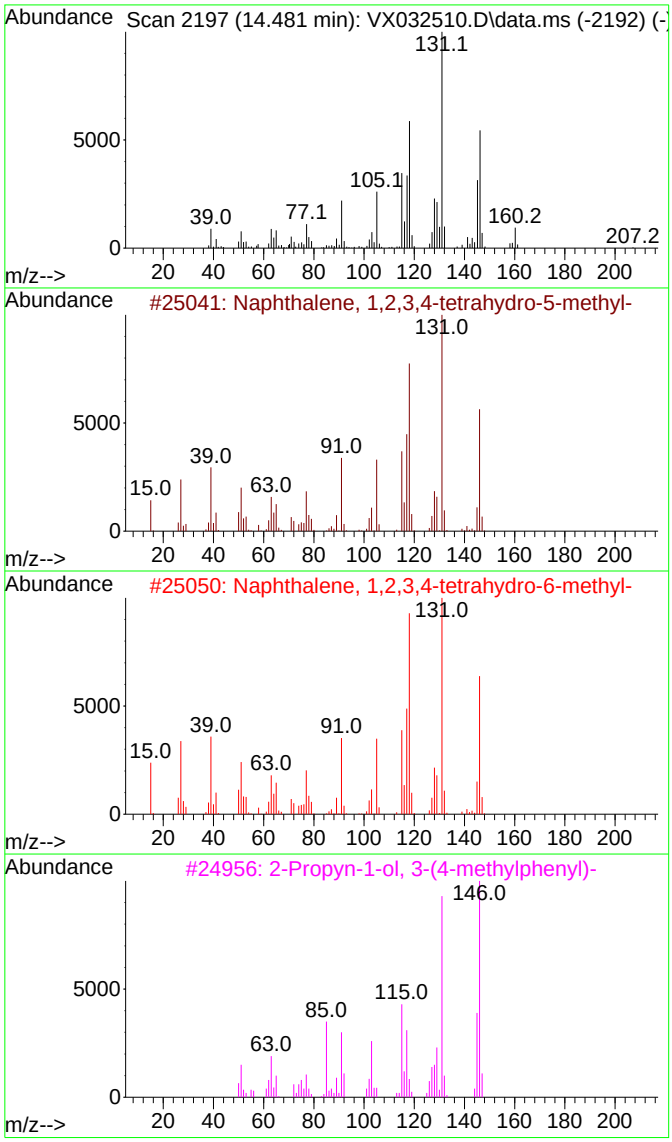
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

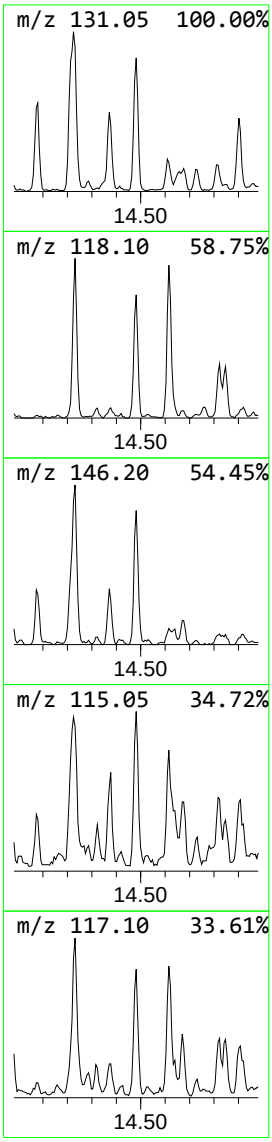
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.481	12.08 ug/l	124702	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	90
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	89
3	2-Propyn-1-ol, 3-(4-methylphenyl)-	146	C10H10O	016017-24-6	68
4	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	58
5	2-Propenal, 3-(4-methylphenyl)-	146	C10H10O	001504-75-2	58





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110122\
Data File : VX032510.D
Acq On : 01 Nov 2022 14:02
Operator : JC/MD
Sample : N5391-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31845

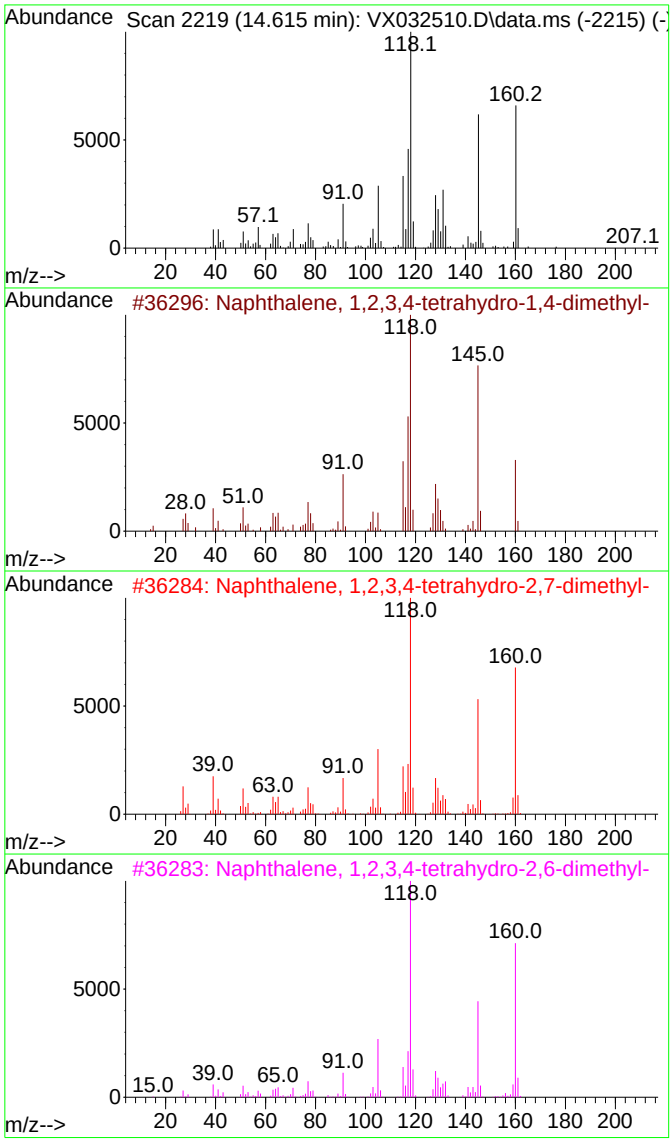
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

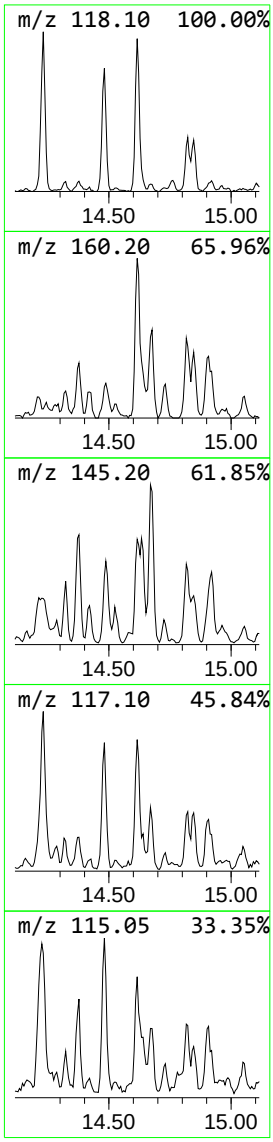
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.615	10.93 ug/l	112867	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	87
2	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	76
3	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	74
4	Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	70
5	Benzene, (3-methyl-1-methylenebu...	160	C12H16	038212-14-5	62





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110122\
Data File : VX032510.D
Acq On : 01 Nov 2022 14:02
Operator : JC/MD
Sample : N5391-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31845

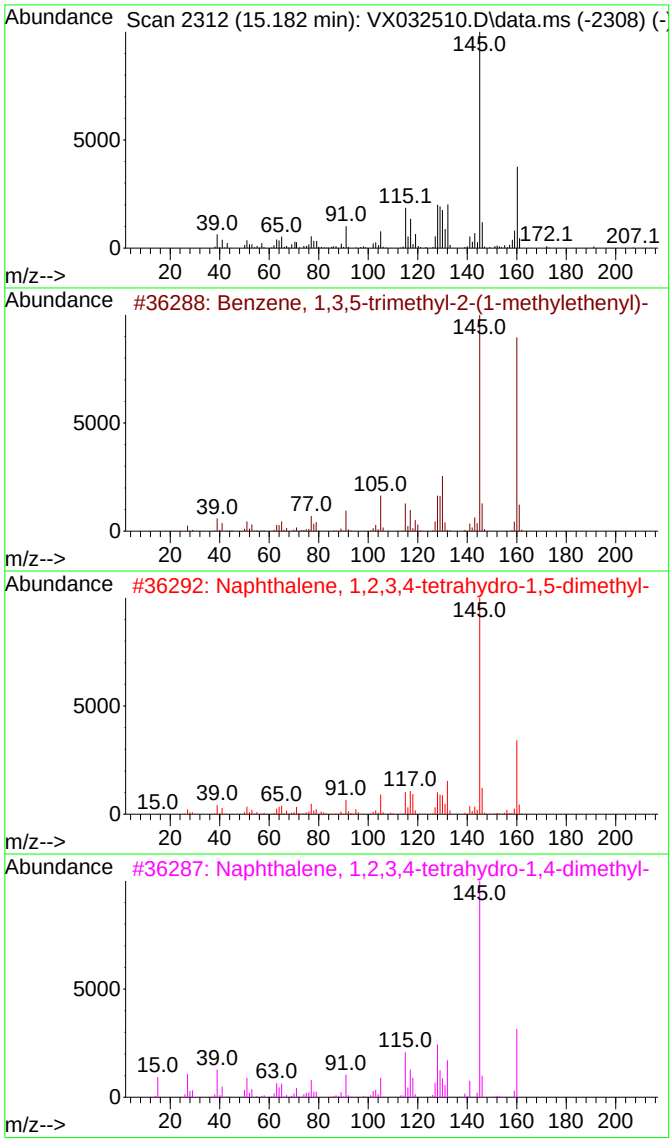
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

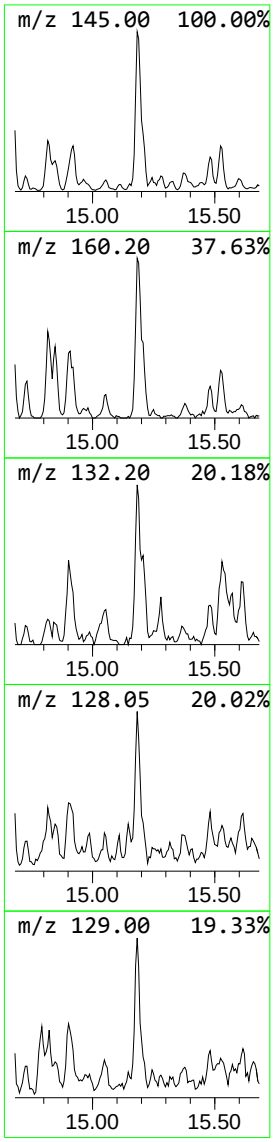
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1,3,5-trimethyl-2-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.182	12.51 ug/l	129182	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	90
2	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021564-91-0	87
3	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	87
4	Benzene, 1-(2-butenyl)-2,3-dimet...	160	C12H16	054340-85-1	81
5	Benzene, 4-(2-butenyl)-1,2-dimet...	160	C12H16	054340-86-2	70





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110122\
Data File : VX032510.D
Acq On : 01 Nov 2022 14:02
Operator : JC/MD
Sample : N5391-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31845

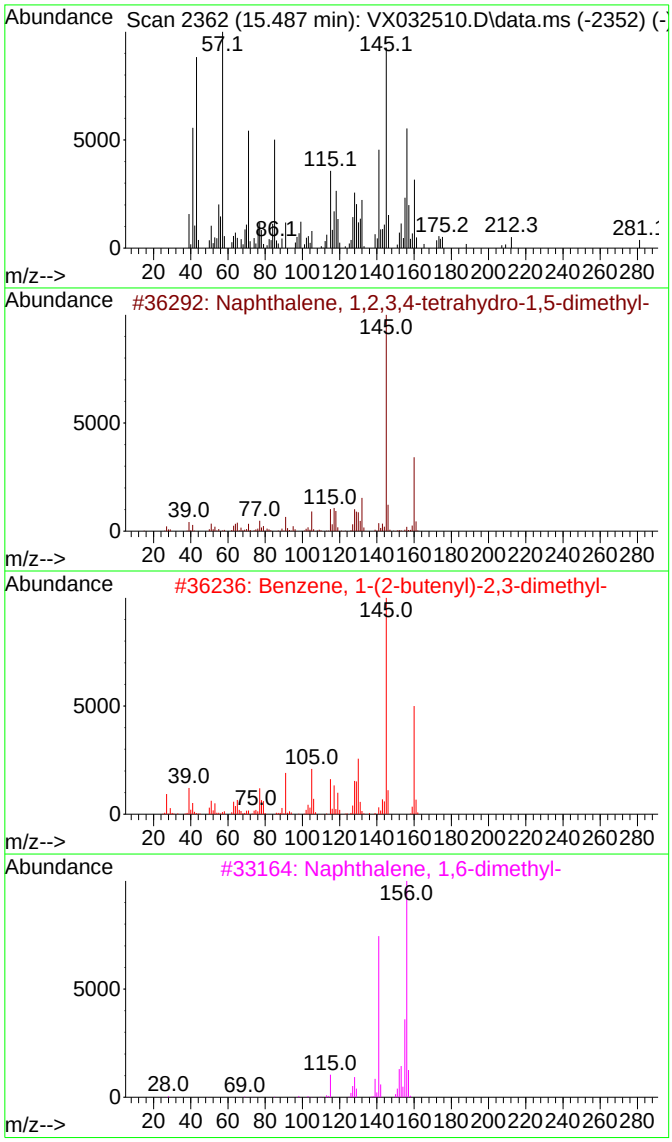
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

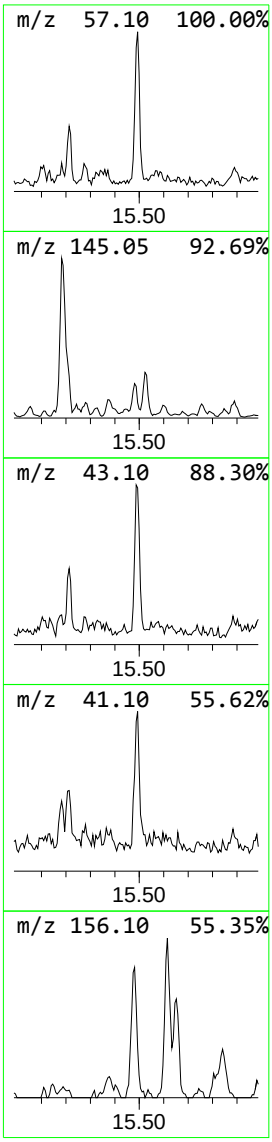
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 unknown15.487 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.487	6.51 ug/l	67261	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021564-91-0	45
2	Benzene, 1-(2-butenyl)-2,3-dimet...	160	C12H16	054340-85-1	42
3	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	42
4	1H-Indene, 2,3-dihydro-1,1,3-tri...	160	C12H16	002613-76-5	42
5	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	41





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110122\
Data File : VX032510.D
Acq On : 01 Nov 2022 14:02
Operator : JC/MD
Sample : N5391-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31845

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.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
Hexanoic acid, ...	13.140	6.2	ug/l	64327	4	12.024	516203	50.0
1-Phenyl-1-butene	13.292	8.1	ug/l	83835	4	12.024	516203	50.0
1H-Indene, 2,3-...	13.585	6.7	ug/l	69399	4	12.024	516203	50.0
Naphthalene, 1,...	13.853	6.6	ug/l	68157	4	12.024	516203	50.0
Naphthalene, 1,...	13.926	7.8	ug/l	80265	4	12.024	516203	50.0
Naphthalene, 1,...	14.231	15.5	ug/l	160067	4	12.024	516203	50.0
Naphthalene, 1,...	14.481	12.1	ug/l	124702	4	12.024	516203	50.0
Naphthalene, 1,...	14.615	10.9	ug/l	112867	4	12.024	516203	50.0
Benzene, 1,3,5-...	15.182	12.5	ug/l	129182	4	12.024	516203	50.0
unknown15.487	15.487	6.5	ug/l	67261	4	12.024	516203	50.0