LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101922\
Data File : VX032215.D
Acq On : 19 Oct 2022 18:09
Operator : JC/MD
Sample : N5114-04 10X
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-0095

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\82X101922W.M
Title : SW846 8260

Signal : TIC: VX032215.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.946	296	305	317	rBV	8481	20197	1.37%	0.222%
2	5.385	694	705	715	rBV2	95847	278612	18.89%	3.062%
3	5.550	715	732	741	rBV2	164023	617654	41.88%	6.787%
4	5.824	763	777	789	rBV	83545	240061	16.28%	2.638%
5	5.958	789	799	819	rVV	109735	288335	19.55%	3.168%
6	6.184	823	836	843	rVV7	9011	34696	2.35%	0.381%
7	6.354	855	864	876	rVB5	6401	18074	1.23%	0.199%
8	6.610	896	906	917	rVB	42056	99097	6.72%	1.089%
9	6.763	921	931	946	rBV	236068	559340	37.93%	6.146%
10	7.379	1023	1032	1041	rVB2	19152	43006	2.92%	0.473%
11	8.647	1234	1240	1246	rBV	511973	798848	54.17%	8.778%
12	8.720	1246	1252	1265	rVB	988125	1474838	100.00%	16.206%
13	10.055	1466	1471	1478	rVB	487544	646354	43.83%	7.102%
14	10.195	1488	1494	1499	rBV	14313	20345	1.38%	0.224%
15	10.305	1499	1512	1517	rVV2	16981	38238	2.59%	0.420%
16	10.360	1517	1521	1530	rVB	26857	35779	2.43%	0.393%
17	10.780	1582	1590	1594	rBV3	14260	22626	1.53%	0.249%
18	10.860	1594	1603	1606	rBV5	9340	17174	1.16%	0.189%
19	11.079	1634	1639	1650	rVB	453063	581368	39.42%	6.388%
20	11.384	1685	1689	1694	rBV	11643	21222	1.44%	0.233%
21	11.475	1701	1704	1709	rVB	32148	39701	2.69%	0.436%
22	11.573	1715	1720	1724	rBV	192188	239880	16.26%	2.636%
23	11.616	1724	1727	1733	rVB2	9608	17257	1.17%	0.190%
24	11.756	1746	1750	1753	rBV	17530	24457	1.66%	0.269%
25	11.829	1757	1762	1766	rBV	62901	81143	5.50%	0.892%
26	11.890	1769	1772	1777	rVB3	17797	23676	1.61%	0.260%
27	11.969	1782	1785	1789	rVV	21466	26849	1.82%	0.295%
28	12.024	1789	1794	1800	rVV	508141	648881	44.00%	7.130%
29	12.103	1800	1807	1812	rVB5	13504	27368	1.86%	0.301%
30	12.244	1825	1830	1833	rBV2	16095	23262	1.58%	0.256%
31	12.317	1837	1842	1848	rBV5	12524	25957	1.76%	0.285%
32	12.420	1856	1859	1863	rBV	22898	28097	1.91%	0.309%
33	12.463	1863	1866	1872	rVB4	10305	17729	1.20%	0.195%
34	12.524	1872	1876	1880	rBV	63503	84186	5.71%	0.925%
35	12.683	1899	1902	1905	rBV	11090	15585	1.06%	0.171%
36	12.719	1905	1908	1913	rVB4	26251	36309	2.46%	0.399%

LSC Area Percent Report

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Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-0095

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\82X101922W.M
Title : SW846 8260

37	12.817	1921	1924	1931	rVB3	42367	56154	3.81%	0.617%
38	12.890	1931	1936	1943	rBV4	40831	87851	5.96%	0.965%
39	12.987	1947	1952	1957	rVB3	148564	221665	15.03%	2.436%
40	13.042	1957	1961	1965	rVB2	32944	36459	2.47%	0.401%
41	13.091	1965	1969	1976	rVB6	11786	19428	1.32%	0.213%
42	13.176	1977	1983	1986	rBV6	14366	27104	1.84%	0.298%
43	13.237	1986	1993	1995	rBV5	22005	38438	2.61%	0.422%
44	13.292	1999	2002	2008	rVB3	72167	108747	7.37%	1.195%
45	13.347	2008	2011	2014	rBV2	23962	29829	2.02%	0.328%
46	13.384	2014	2017	2019	rBV	44833	50199	3.40%	0.552%
47	13.414	2019	2022	2026	rBV5	36456	42495	2.88%	0.467%
48	13.499	2033	2036	2041	rVB6	19768	29673	2.01%	0.326%
49	13.591	2048	2051	2056	rBV6	14383	25911	1.76%	0.285%
50	13.682	2061	2066	2067	rBV5	27049	39316	2.67%	0.432%
51	13.737	2072	2075	2078	rVV2	53059	72769	4.93%	0.800%
52	13.768	2078	2080	2083	rVV3	34366	38626	2.62%	0.424%
53	13.798	2083	2085	2088	rVV2	35391	45661	3.10%	0.502%
54	13.841	2088	2092	2096	rVV3	53852	85464	5.79%	0.939%
55	13.908	2100	2103	2111	rVB6	29533	61067	4.14%	0.671%
56	14.103	2132	2135	2138	rVV	21393	24986	1.69%	0.275%
57	14.219	2152	2154	2159	rVB5	17654	26183	1.78%	0.288%
58	14.438	2183	2190	2194	rBV	201611	251924	17.08%	2.768%
59	14.499	2198	2200	2207	rVB2	18026	29003	1.97%	0.319%
60	14.566	2207	2211	2215	rVB4	10008	17728	1.20%	0.195%
61	14.615	2215	2219	2221	rBV2	27379	35156	2.38%	0.386%
62	14.792	2244	2248	2252	rVB5	12013	17307	1.17%	0.190%
63	15.188	2308	2313	2321	rBV5	26032	57811	3.92%	0.635%
64	15.493	2358	2363	2368	rBV4	15648	28721	1.95%	0.316%
65	15.560	2369	2374	2380	rBV	167375	245994	16.68%	2.703%
66	16.103	2457	2463	2467	rBV8	6762	14822	1.00%	0.163%
67	16.377	2503	2508	2513	rVB4	10612	17807	1.21%	0.196%

Sum of corrected areas: 9100499

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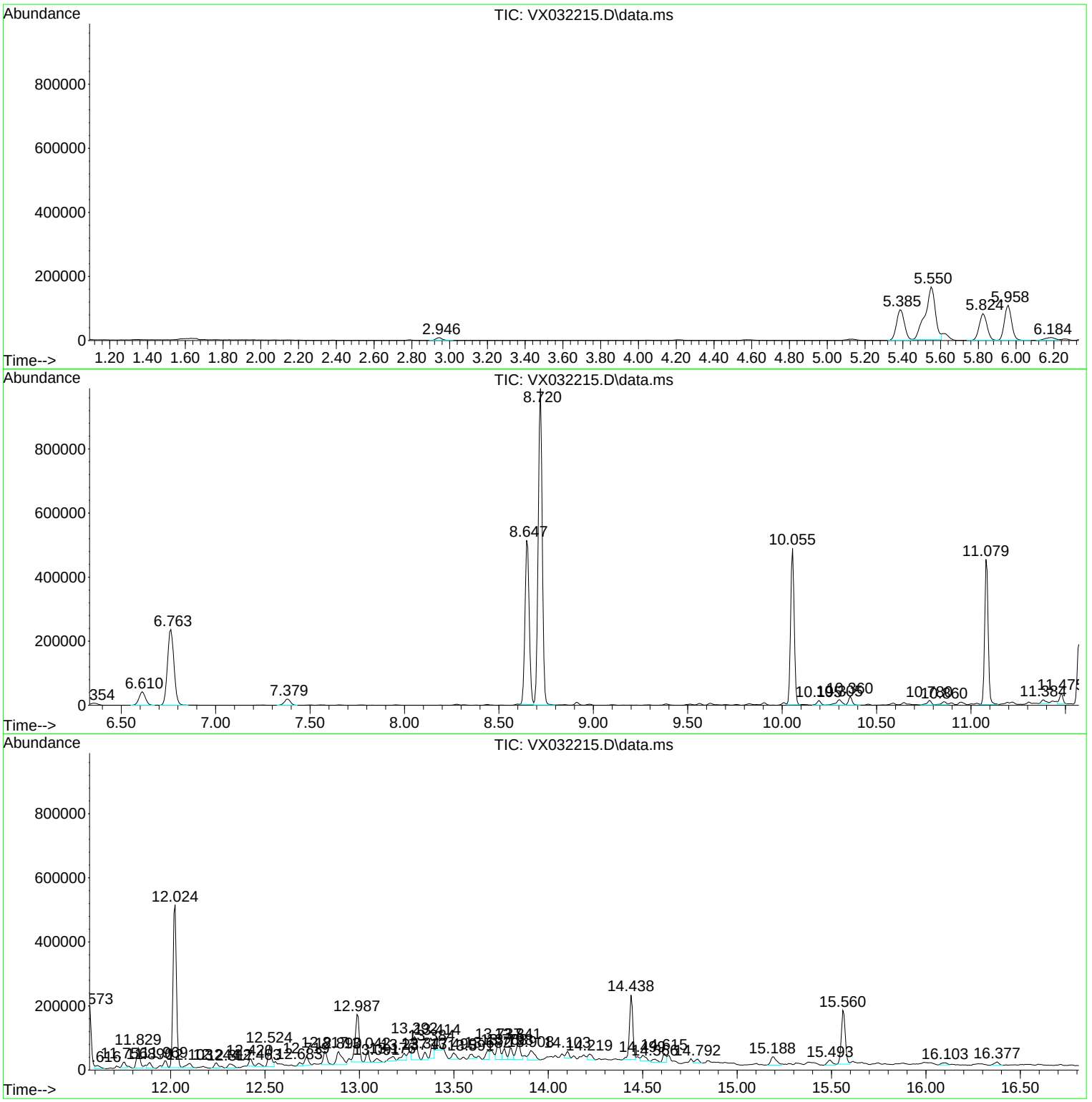
Instrument :
MSVOA_X
ClientSampleId :
FMC-0095

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101922\
Data File : VX032215.D
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

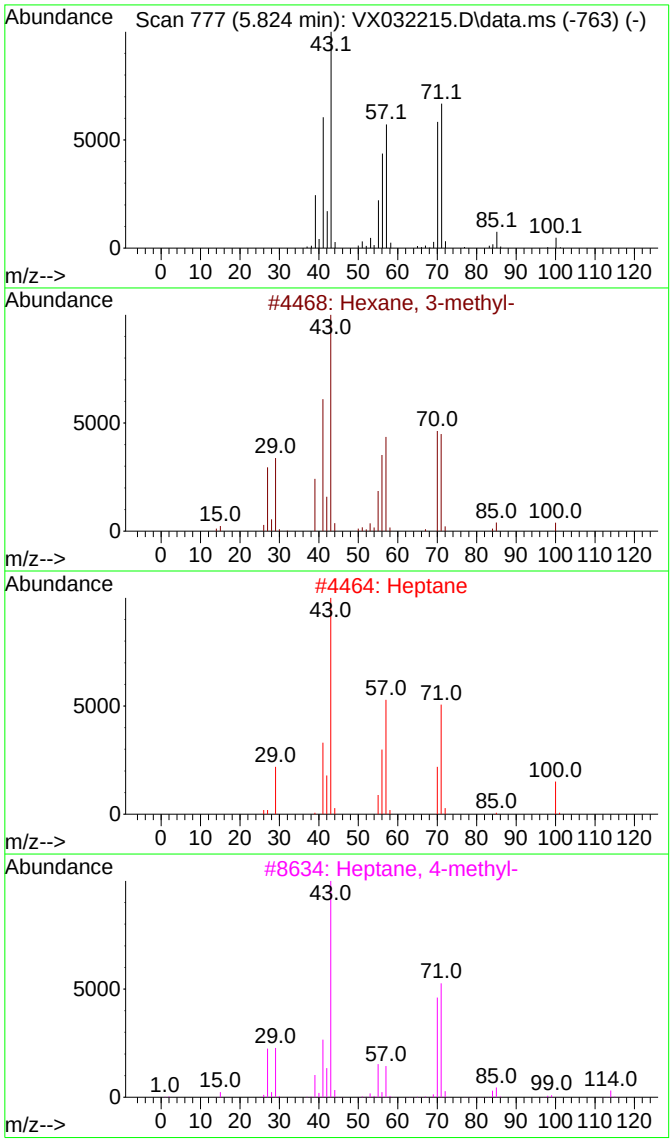
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

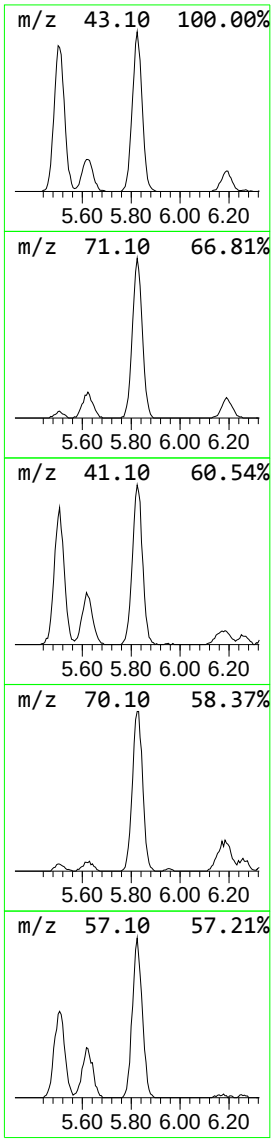
****

Peak Number 1 Hexane, 3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.824	19.43 ug/l	240061	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-	100	C7H16	000589-34-4	94
2	Heptane	100	C7H16	000142-82-5	80
3	Heptane, 4-methyl-	114	C8H18	000589-53-7	59
4	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	53
5	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101922\
Data File : VX032215.D
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Operator : JC/MD
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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-0095

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

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

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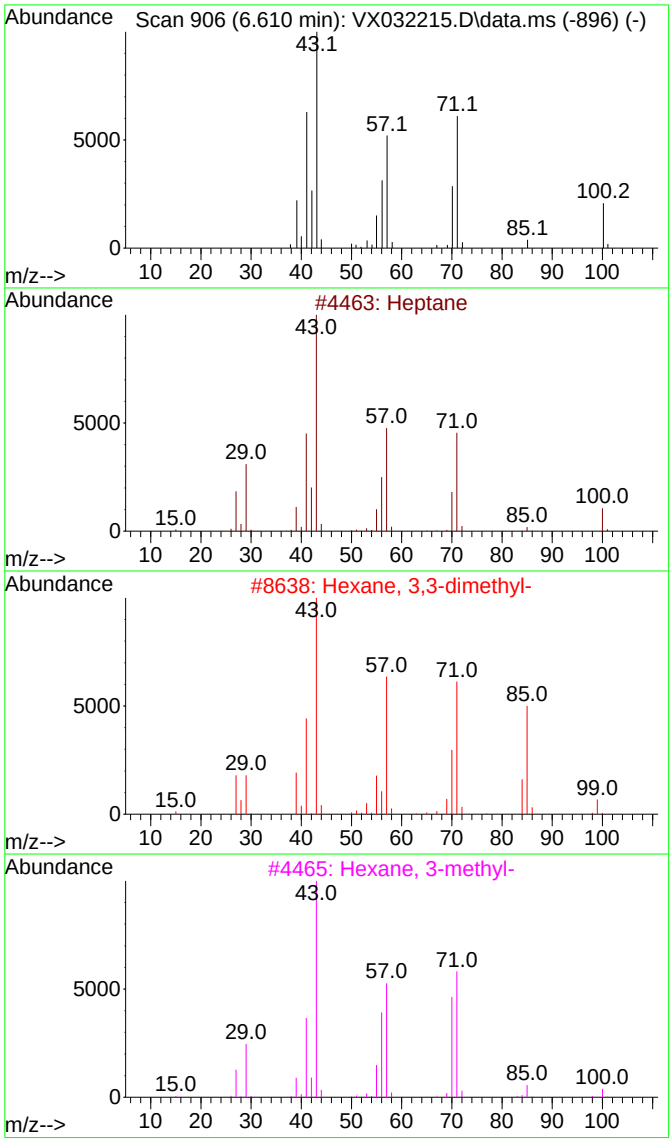
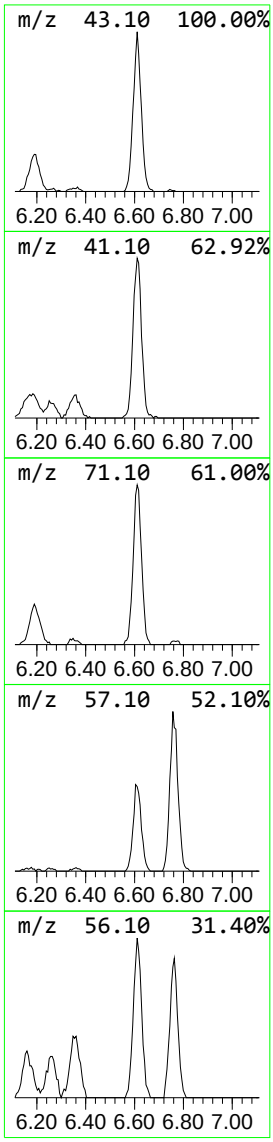
Peak Number 2 Heptane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.610	8.86 ug/l	99097	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	87
2	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	47
3	Hexane, 3-methyl-	100	C7H16	000589-34-4	40
4	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	38
5	3-Hexanone	100	C6H12O	000589-38-8	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101922\
Data File : VX032215.D
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Operator : JC/MD
Sample : N5114-04 10X
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-0095

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

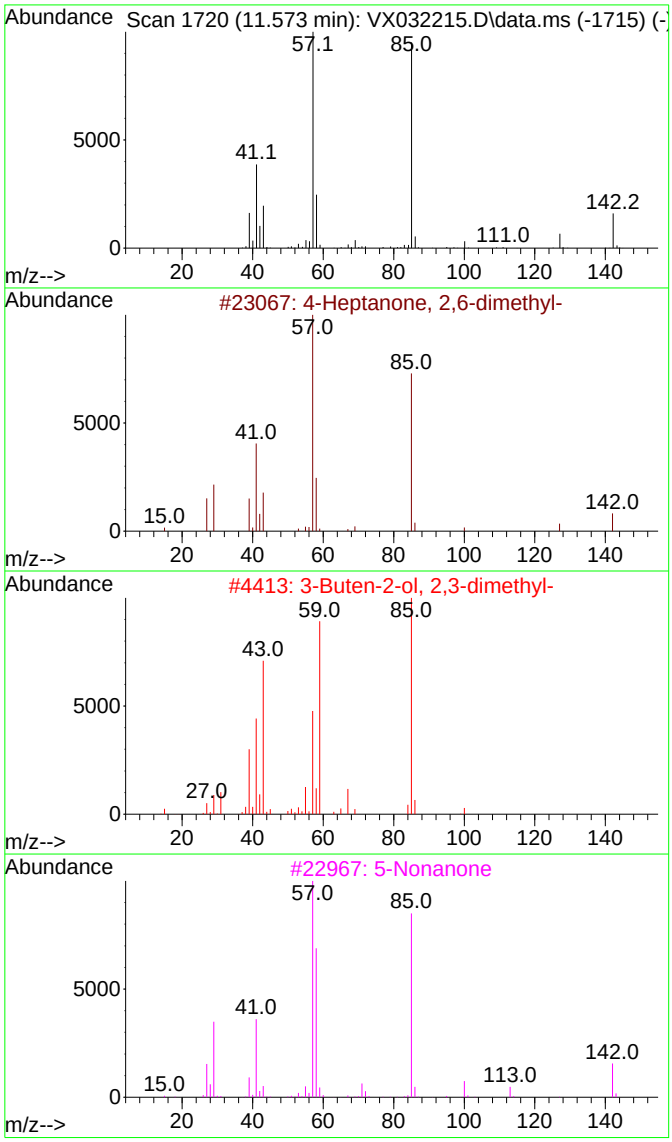
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

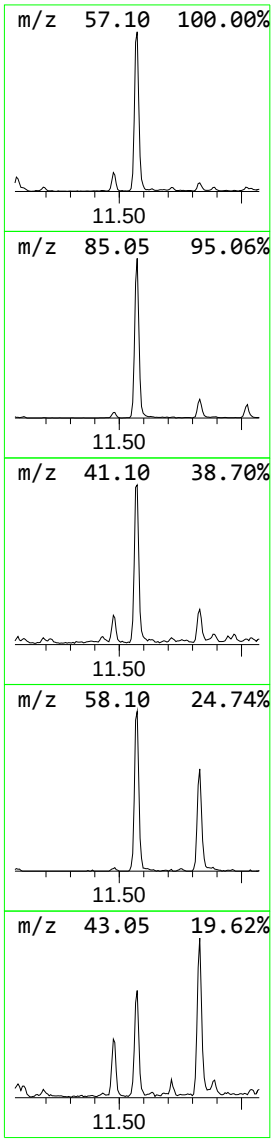
****

Peak Number 3 4-Heptanone, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.573	18.48 ug/l	239880	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	94
2	3-Buten-2-ol, 2,3-dimethyl-	100	C6H12O	010473-13-9	59
3	5-Nonanone	142	C9H18O	000502-56-7	53
4	2(3H)-Furanone, dihydro-5-propyl-	128	C7H12O2	000105-21-5	47
5	4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	42





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101922\
Data File : VX032215.D
Acq On : 19 Oct 2022 18:09
Operator : JC/MD
Sample : N5114-04 10X
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-0095

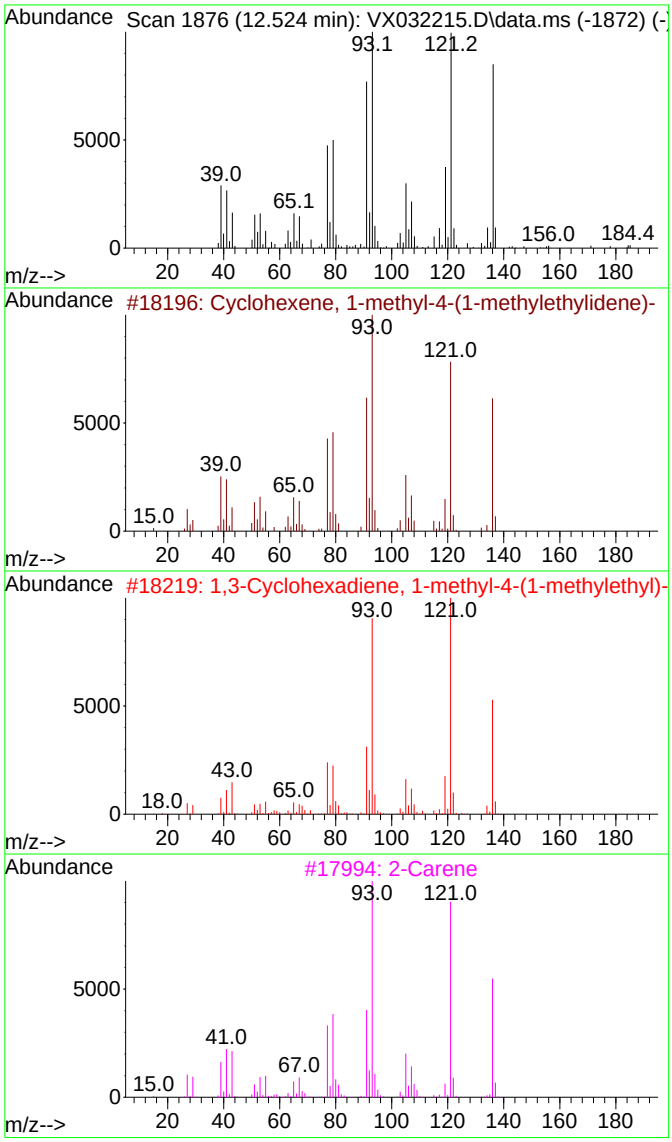
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

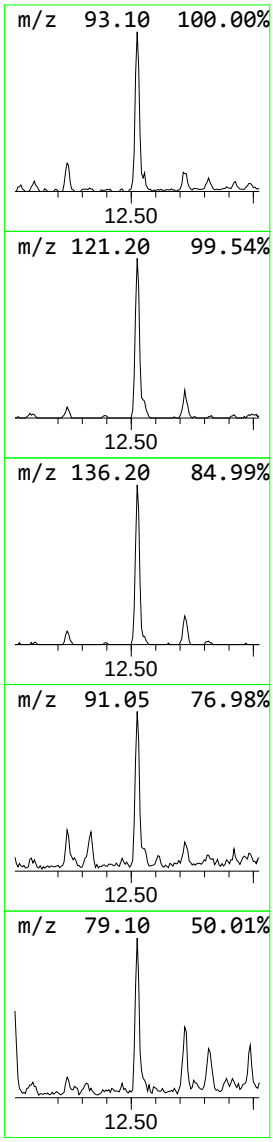
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclohexene, 1-methyl-4-(1-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.524	6.49 ug/l	84186	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	000586-62-9	98
2	1,3-Cyclohexadiene, 1-methyl-4-(...	136	C10H16	000099-86-5	95
3	2-Carene	136	C10H16	000554-61-0	95
4	Cyclohexene, 3-methyl-6-(1-methy...	136	C10H16	000586-63-0	94
5	Bicyclo[2.2.1]hept-2-ene, 1,7,7-...	136	C10H16	000464-17-5	90





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Operator : JC/MD
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Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

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

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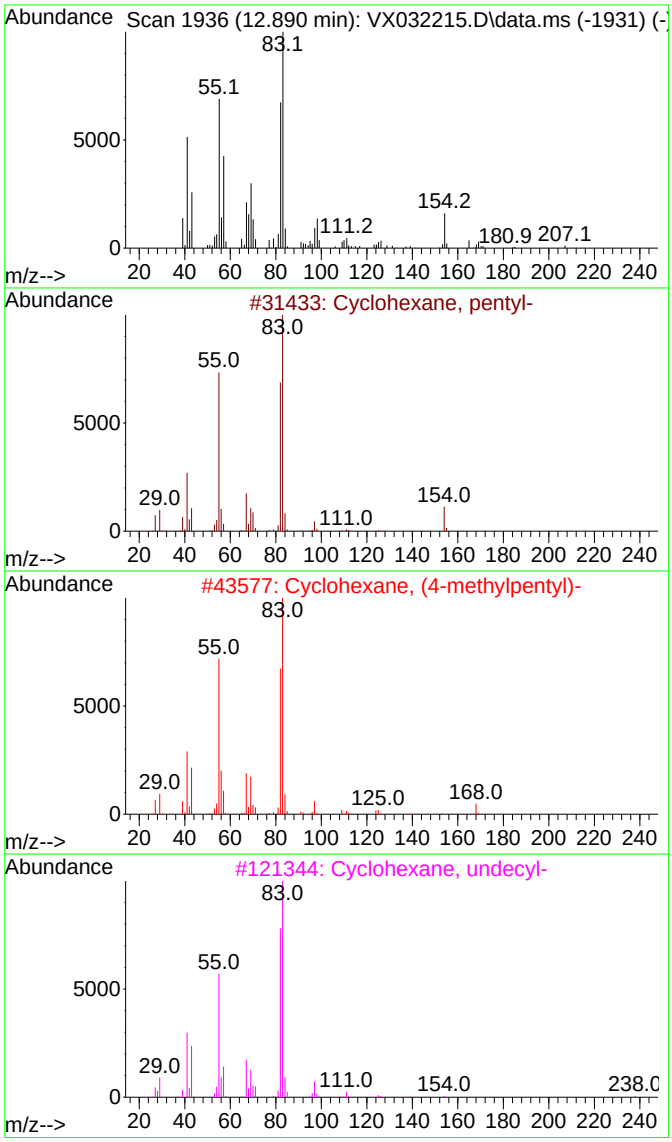
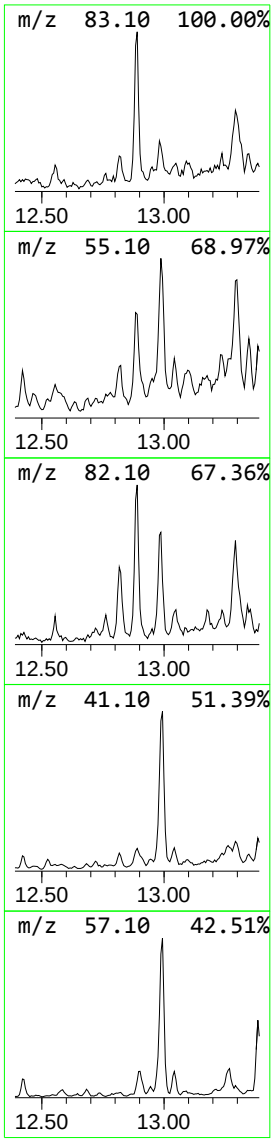
Peak Number 5 Cyclohexane, pentyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.890	6.77 ug/l	87851	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, pentyl-	154	C11H22	004292-92-6	87
2	Cyclohexane, (4-methylpentyl)-	168	C12H24	061142-20-9	72
3	Cyclohexane, undecyl-	238	C17H34	054105-66-7	72
4	Cyclohexane, propyl-	126	C9H18	001678-92-8	72
5	Cyclohexane, butyl-	140	C10H20	001678-93-9	64





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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-0095

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

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

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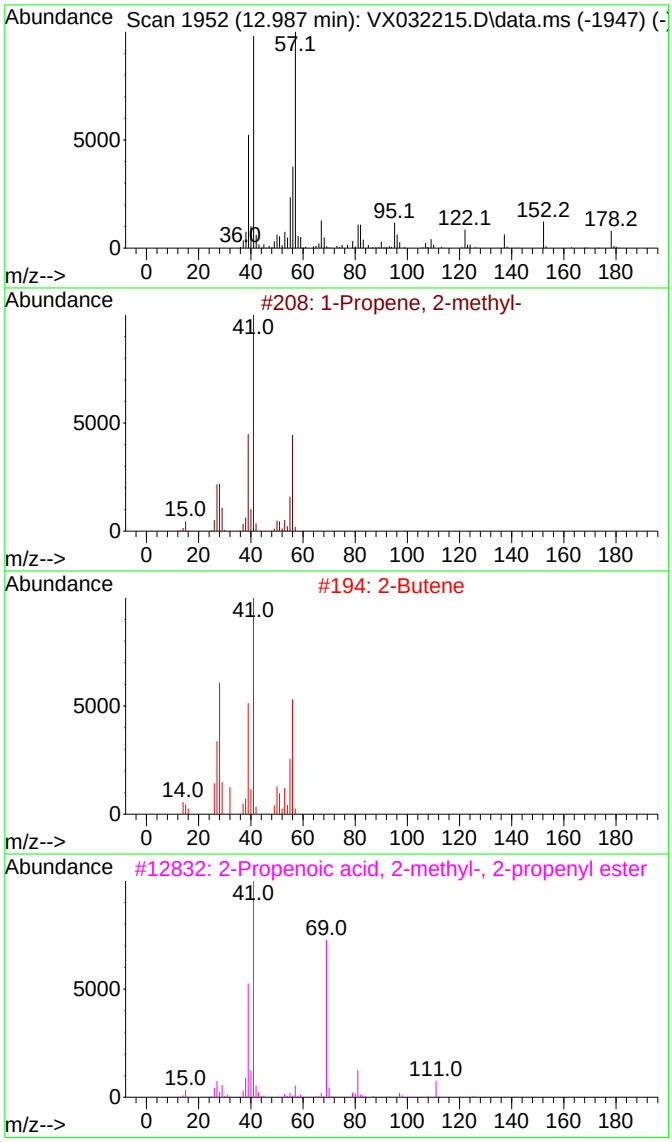
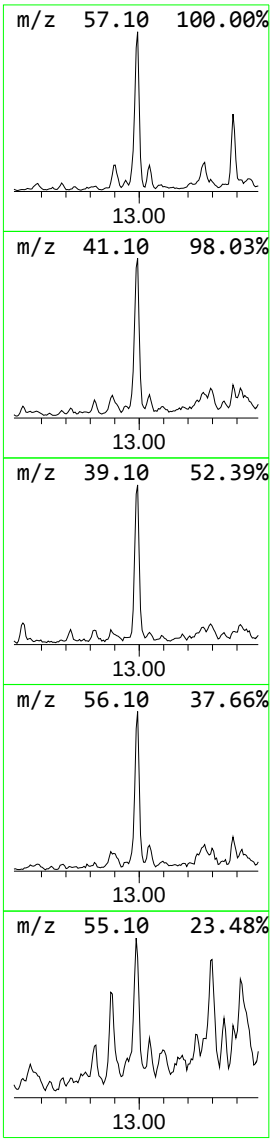
Peak Number 6 unknown12.987 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.987	17.08 ug/l	221665	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 2-methyl-	56	C4H8	000115-11-7	43
2	2-Butene	56	C4H8	000107-01-7	43
3	2-Propenoic acid, 2-methyl-, 2-p...	126	C7H10O2	000096-05-9	25
4	Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	20
5	1-Methyldecahydronaphthalene	152	C11H20	002958-75-0	20





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101922\
Data File : VX032215.D
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Operator : JC/MD
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Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-0095

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

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

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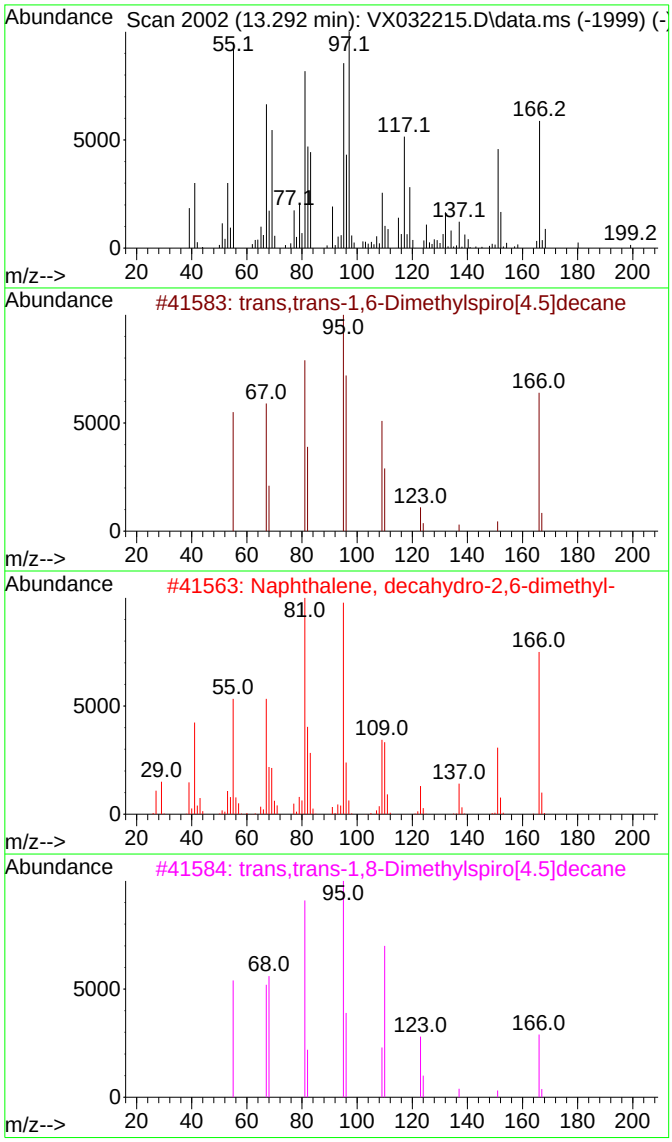
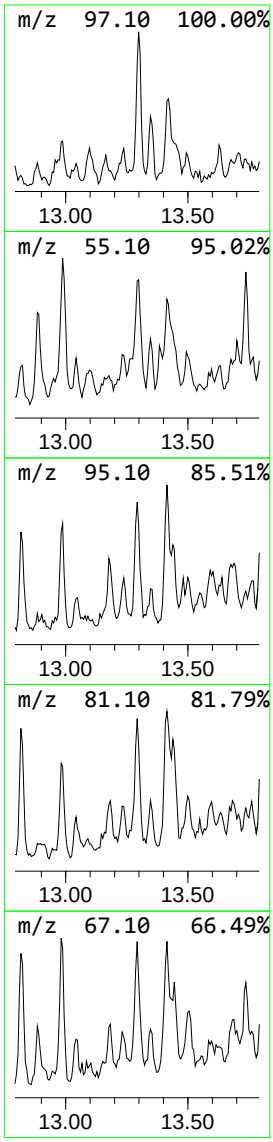
Peak Number 7 unknown13.292 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	8.38 ug/l	108747	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans,trans-1,6-Dimethylspiro[4....	166	C12H22	1000111-72-1	46
2	Naphthalene, decahydro-2,6-dimet...	166	C12H22	001618-22-0	46
3	trans,trans-1,8-Dimethylspiro[4....	166	C12H22	1000111-72-8	46
4	trans, cis-3-Ethylbicyclo[4.4.0]...	166	C12H22	066660-43-3	43
5	Naphthalene, decahydro-1,2-dimet...	166	C12H22	003604-14-6	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101922\
Data File : VX032215.D
Acq On : 19 Oct 2022 18:09
Operator : JC/MD
Sample : N5114-04 10X
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-0095

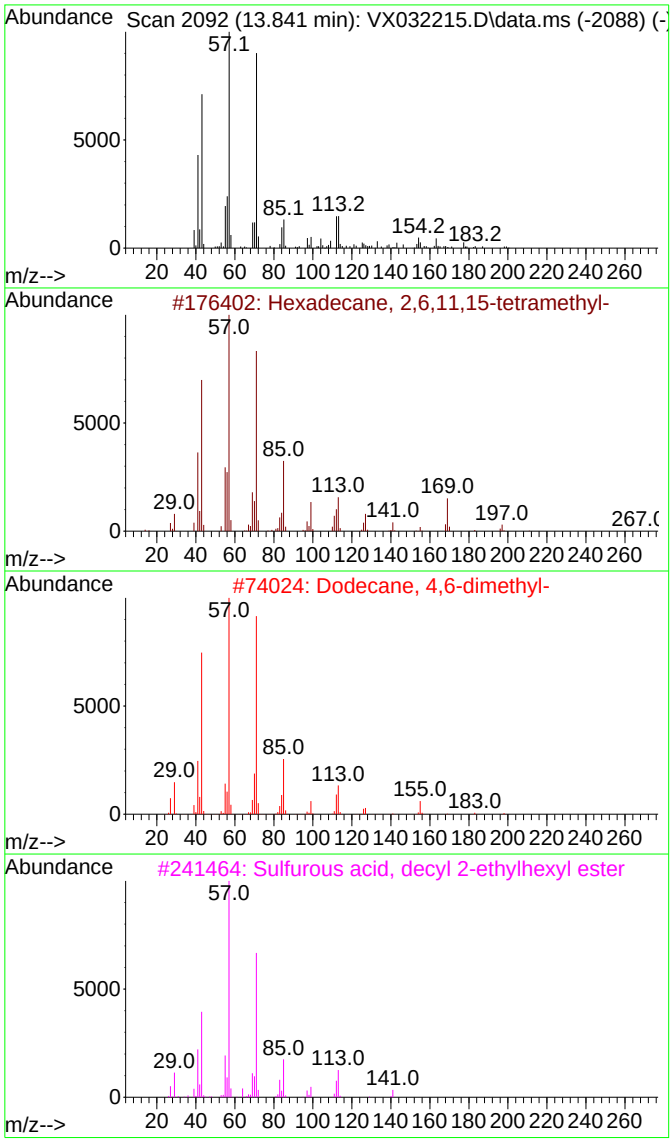
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

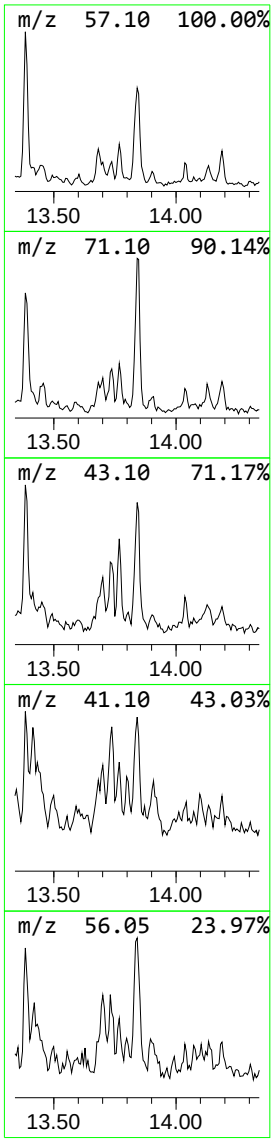
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Hexadecane, 2,6,11,15-tetra... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.841	6.59 ug/l	85464	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,11,15-tetramethyl-	282	C20H42	000504-44-9	72
2	Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	64
3	Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	64
4	Tridecane, 7-methyl-	198	C14H30	026730-14-3	64
5	Octane, 3-ethyl-	142	C10H22	005881-17-4	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101922\
Data File : VX032215.D
Acq On : 19 Oct 2022 18:09
Operator : JC/MD
Sample : N5114-04 10X
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-0095

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

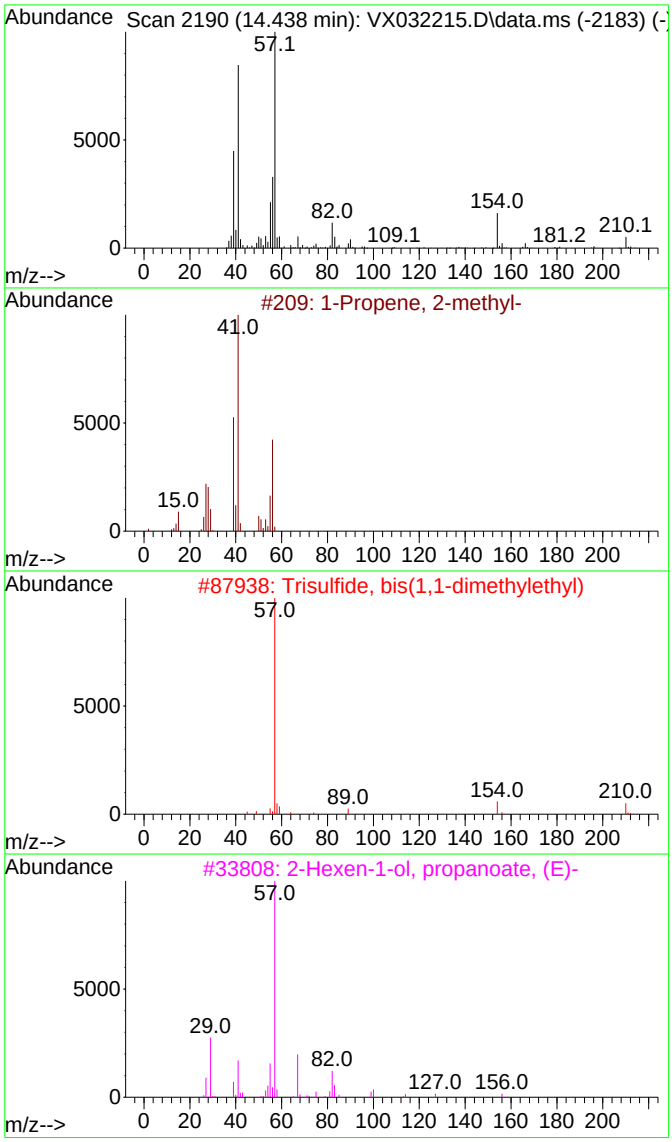
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

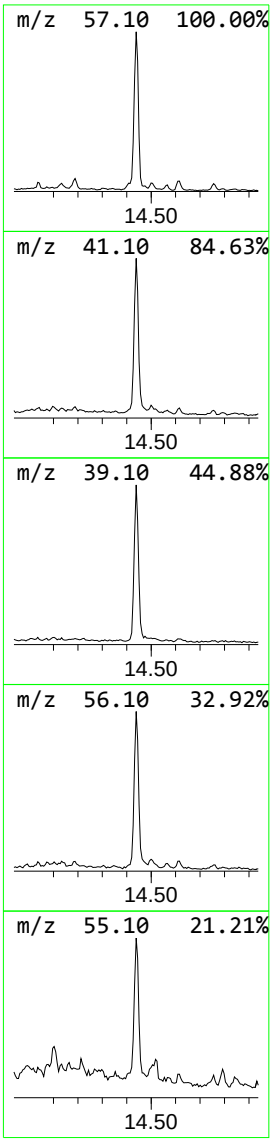
****

Peak Number 9 unknown14.438 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.438	19.41 ug/l	251924	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 2-methyl-	56	C4H8	000115-11-7	43
2	Trisulfide, bis(1,1-dimethylethyl)	210	C8H18S3	004253-90-1	43
3	2-Hexen-1-ol, propanoate, (E)-	156	C9H16O2	053398-80-4	14
4	1-Hexene, 4-methyl-	98	C7H14	003769-23-1	12
5	2-Butene, (Z)-	56	C4H8	000590-18-1	11





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101922\
Data File : VX032215.D
Acq On : 19 Oct 2022 18:09
Operator : JC/MD
Sample : N5114-04 10X
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-0095

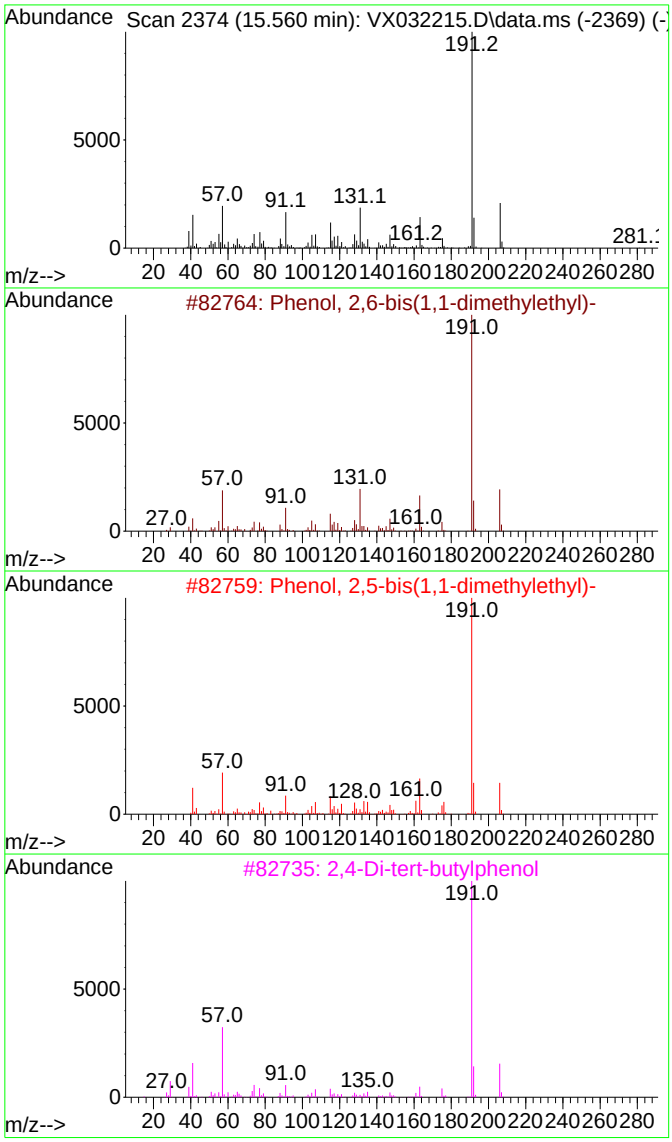
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

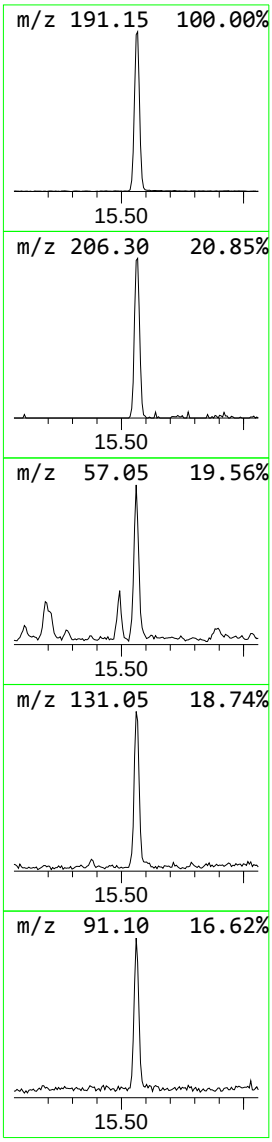
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.560	18.96 ug/l	245994	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	98
2	Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	83
3	2,4-Di-tert-butylphenol	206	C14H22O	000096-76-4	83
4	Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	81
5	3-(4-(tert-Butyl)phenyl)-2-methy...	206	C14H22O	056107-04-1	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101922\
Data File : VX032215.D
Acq On : 19 Oct 2022 18:09
Operator : JC/MD
Sample : N5114-04 10X
Misc : 1.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FMC-0095

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.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
Hexane, 3-methyl-	5.824	19.4	ug/l	240061	1	5.550	617654	50.0
Heptane	6.610	8.9	ug/l	99097	2	6.763	559340	50.0
4-Heptanone, 2,...	11.573	18.5	ug/l	239880	4	12.024	648881	50.0
Cyclohexene, 1-...	12.524	6.5	ug/l	84186	4	12.024	648881	50.0
Cyclohexane, pe...	12.890	6.8	ug/l	87851	4	12.024	648881	50.0
unknown12.987	12.987	17.1	ug/l	221665	4	12.024	648881	50.0
unknown13.292	13.292	8.4	ug/l	108747	4	12.024	648881	50.0
Hexadecane, 2,6...	13.841	6.6	ug/l	85464	4	12.024	648881	50.0
unknown14.438	14.438	19.4	ug/l	251924	4	12.024	648881	50.0
Phenol, 2,6-bis...	15.560	19.0	ug/l	245994	4	12.024	648881	50.0