LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040622\
Data File : VX027992.D
Acq On : 06 Apr 2022 12:54
Operator : JC/MD
Sample : N2253-03
Misc : 1.21g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31396

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\82X040522W.M
Title : SW846 8260

Signal : TIC: VX027992.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.105	645	659	675	rVB2	41605	153452	1.52%	0.471%
2	5.391	694	706	712	rBV2	56993	171981	1.71%	0.528%
3	5.495	712	723	736	rVV2	614796	2188965	21.73%	6.723%
4	5.611	736	742	758	rVB	197113	601296	5.97%	1.847%
5	5.812	760	775	790	rBV	771764	2288837	22.72%	7.030%
6	5.958	790	799	810	rBV	63813	177572	1.76%	0.545%
7	6.165	820	833	842	rBV4	80325	333078	3.31%	1.023%
8	6.251	842	847	855	rVV2	49323	129607	1.29%	0.398%
9	6.348	855	863	878	rVB	64154	181260	1.80%	0.557%
10	6.604	893	905	920	rBV	389312	933624	9.27%	2.868%
11	6.763	920	931	943	rBV	162545	392584	3.90%	1.206%
12	7.373	1020	1031	1043	rBV	222068	515136	5.11%	1.582%
13	8.598	1224	1232	1235	rBV	69878	121036	1.20%	0.372%
14	8.653	1235	1241	1246	rVB	313611	513368	5.10%	1.577%
15	8.726	1246	1253	1260	rBV	6320673	10075562	100.00%	30.946%
16	8.909	1278	1283	1289	rBV	92524	135636	1.35%	0.417%
17	9.506	1375	1381	1386	rBV3	68808	132447	1.31%	0.407%
18	9.561	1386	1390	1395	rVB	74242	105225	1.04%	0.323%
19	9.616	1395	1399	1404	rBV	61314	102371	1.02%	0.314%
20	9.829	1427	1434	1439	rBV2	78865	153263	1.52%	0.471%
21	9.903	1441	1446	1451	rVB	86932	139117	1.38%	0.427%
22	10.006	1457	1463	1467	rBV	85783	126660	1.26%	0.389%
23	10.055	1467	1471	1477	rVB	299401	428587	4.25%	1.316%
24	10.195	1487	1494	1499	rBV	623638	877401	8.71%	2.695%
25	10.305	1503	1512	1518	rVV	2190749	3193463	31.70%	9.808%
26	10.360	1518	1521	1532	rVB2	204526	266232	2.64%	0.818%
27	10.646	1562	1568	1576	rVB	602090	821939	8.16%	2.524%
28	11.085	1634	1640	1651	rVB	289149	421948	4.19%	1.296%
29	11.475	1701	1704	1710	rVB	96052	123549	1.23%	0.379%
30	11.756	1746	1750	1759	rVB	77202	111934	1.11%	0.344%
31	12.024	1789	1794	1800	rBV	367481	491214	4.88%	1.509%
32	12.317	1838	1842	1848	rVB5	77362	154402	1.53%	0.474%
33	12.427	1856	1860	1864	rVB	140022	157224	1.56%	0.483%
34	13.170	1975	1982	1986	rBV5	58855	127321	1.26%	0.391%
35	13.292	2000	2002	2007	rVB3	118074	155227	1.54%	0.477%
36	13.426	2018	2024	2029	rBV3	80617	139632	1.39%	0.429%

LSC Area Percent Report

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Operator : JC/MD
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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31396

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\82X040522W.M
Title : SW846 8260

37	13.756	2073	2078	2088	rBV	1375717	1773997	17.61%	5.449%
38	13.853	2091	2094	2100	rVB3	82149	138035	1.37%	0.424%
39	13.926	2100	2106	2112	rBV4	76060	181803	1.80%	0.558%
40	14.231	2149	2156	2162	rBV2	180121	314858	3.12%	0.967%
41	14.481	2193	2197	2205	rVB3	112514	177895	1.77%	0.546%
42	14.615	2216	2219	2222	rBV	142191	211133	2.10%	0.648%
43	14.670	2226	2228	2233	rVB2	76268	101144	1.00%	0.311%
44	15.054	2284	2291	2298	rBV	146528	233622	2.32%	0.718%
45	15.188	2307	2313	2320	rBV3	132325	238514	2.37%	0.733%
46	15.280	2320	2328	2332	rBV7	57605	103628	1.03%	0.318%
47	15.566	2369	2375	2380	rBV	949888	1395236	13.85%	4.285%
48	15.975	2435	2442	2457	rBV	247734	546635	5.43%	1.679%

Sum of corrected areas: 32558650

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MSVOA_X
ClientSampleId :
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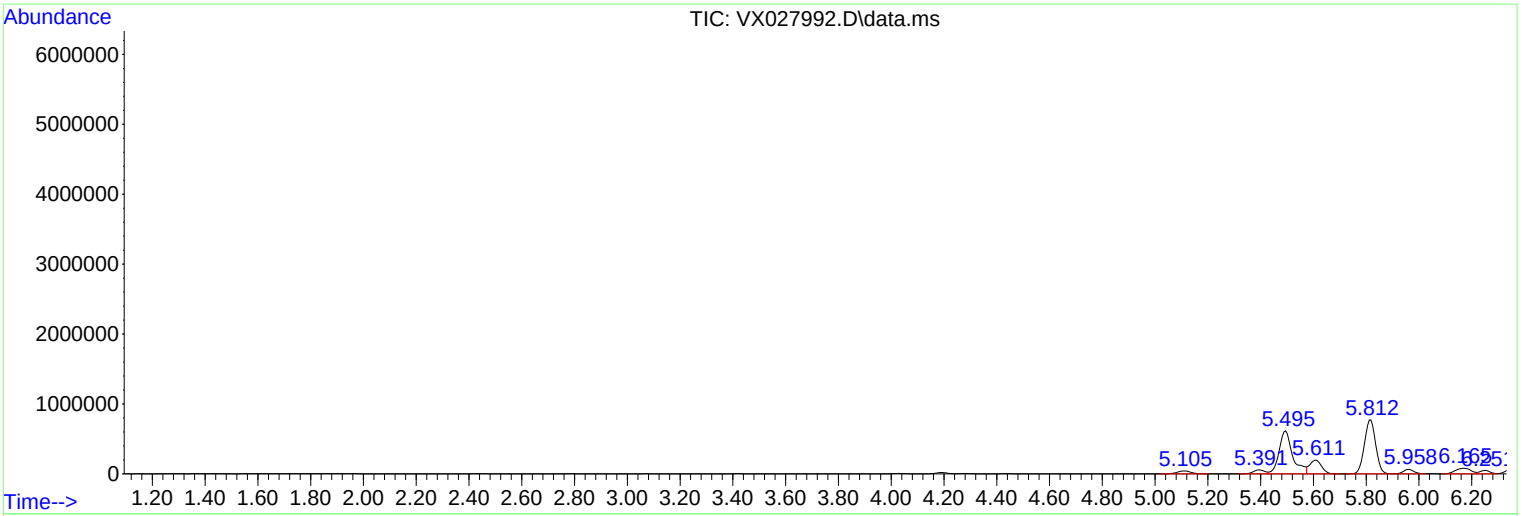
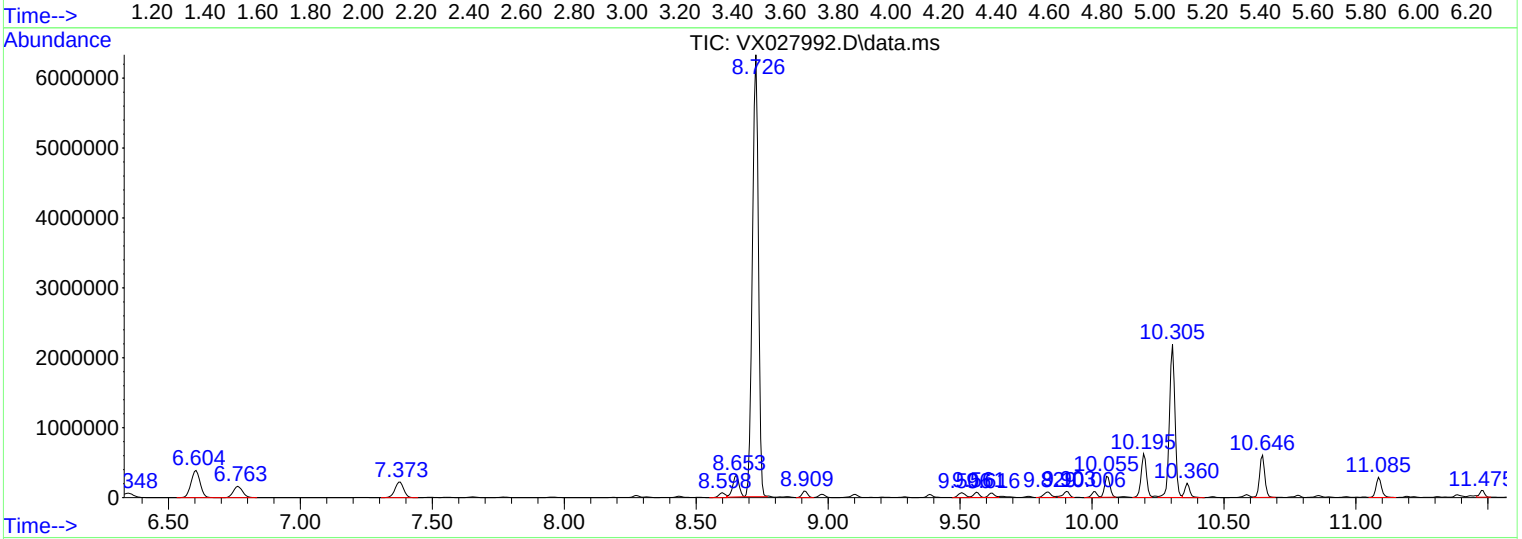
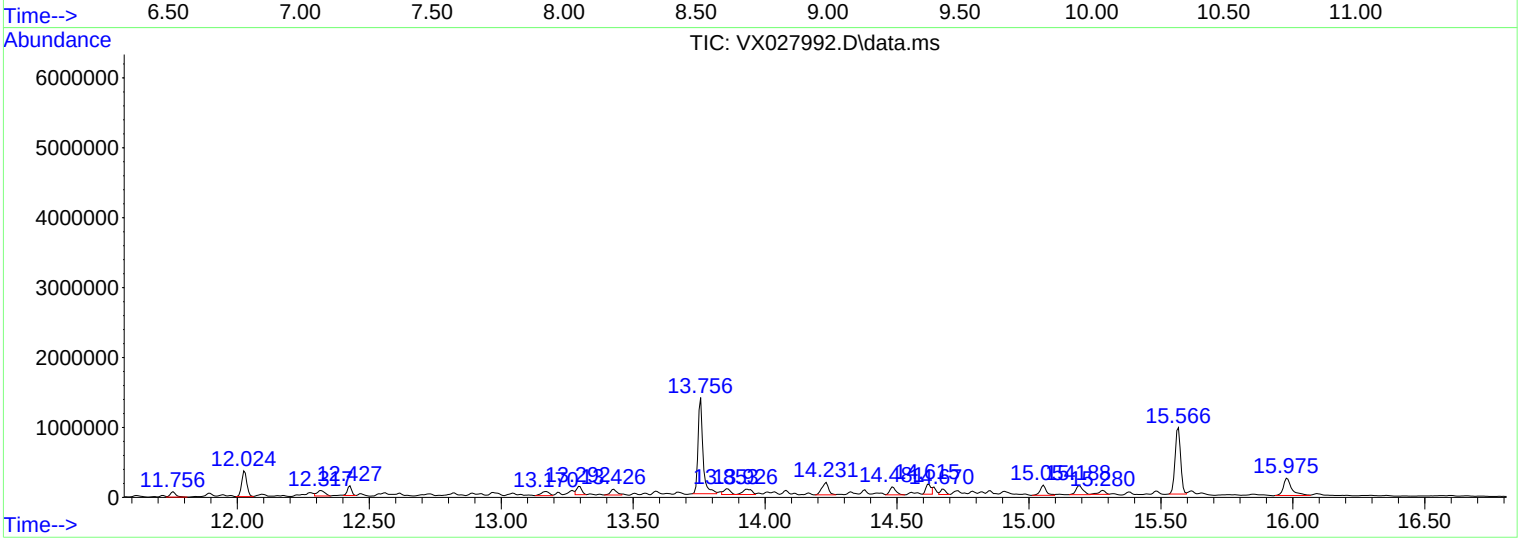
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040522W.M
Quant Title : SW846 8260

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







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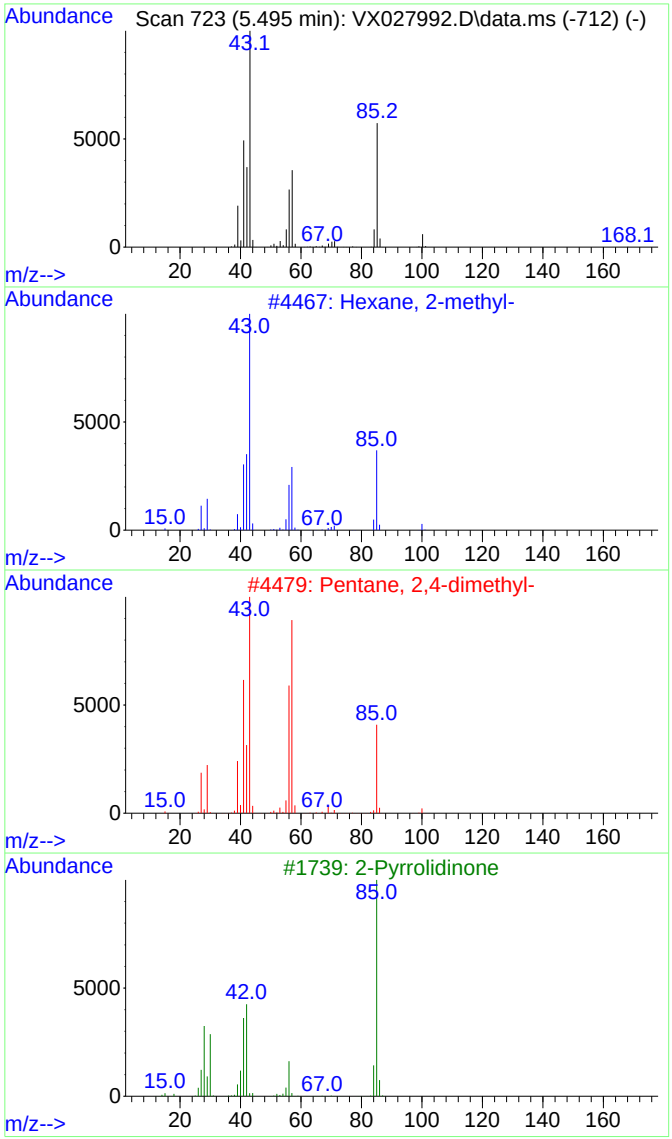
Quant Title : SW846 8260

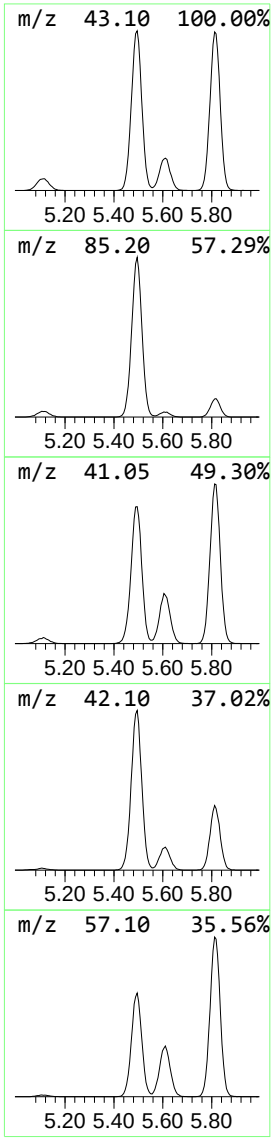
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Hexane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.495	50.00 ug/l	2188970	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2-methyl-	100	C7H16	000591-76-4	90
2	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	72
3	2-Pyrrolidinone	85	C4H7NO	000616-45-5	59
4	Pentane, 3-ethyl-2,4-dimethyl-	128	C9H20	001068-87-7	50
5	2-Pentanone, 3-ethyl-3-methyl-	128	C8H16O	019780-65-5	50





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Operator : JC/MD
Sample : N2253-03
Misc : 1.21g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31396

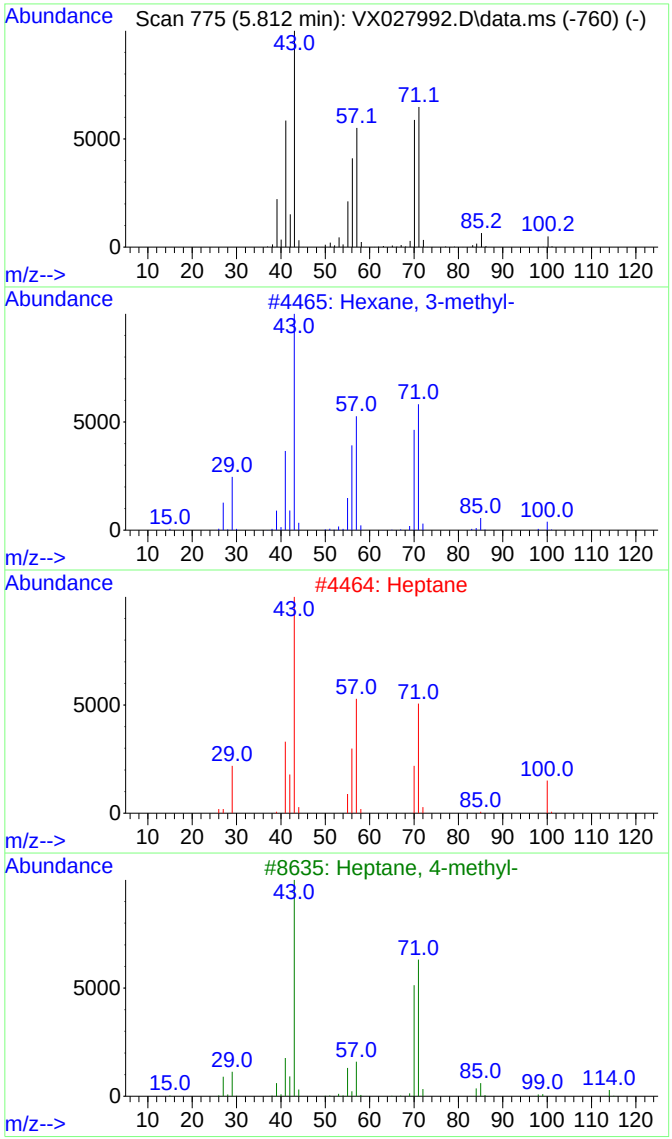
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040522W.M
Quant Title : SW846 8260

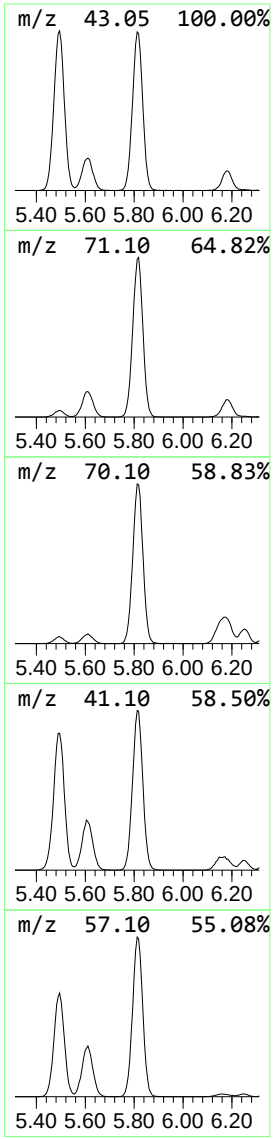
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Hexane, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.812	52.28 ug/l	2288840	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-	100	C7H16	000589-34-4	91
2	Heptane	100	C7H16	000142-82-5	80
3	Heptane, 4-methyl-	114	C8H18	000589-53-7	59
4	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53
5	Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	50





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Operator : JC/MD
Sample : N2253-03
Misc : 1.21g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31396

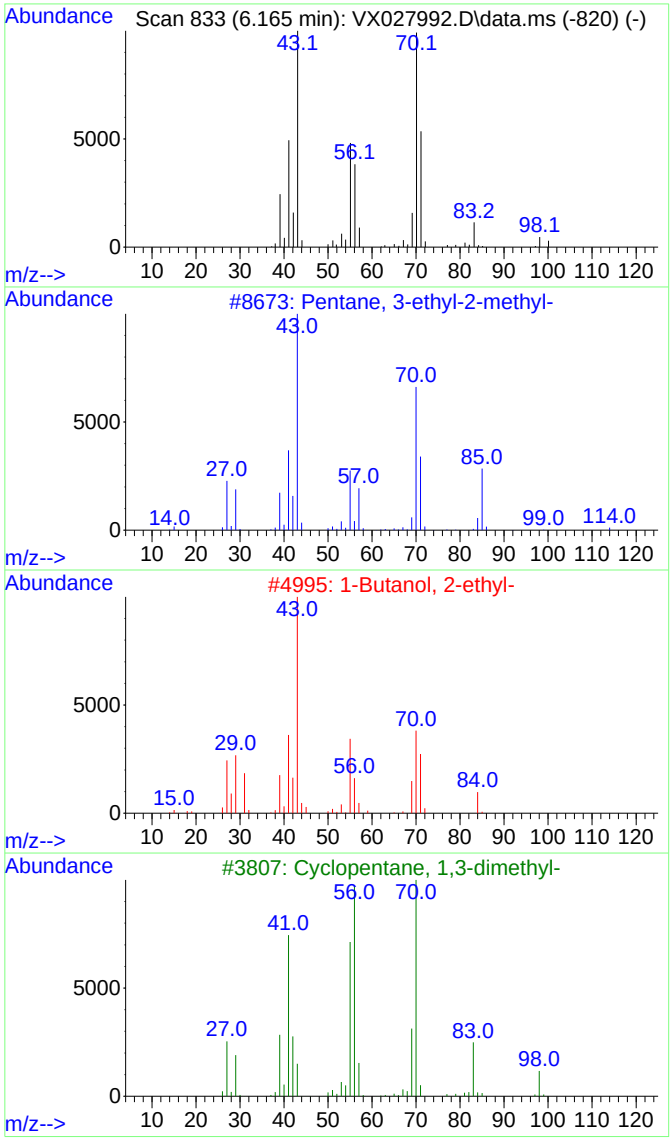
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040522W.M
Quant Title : SW846 8260

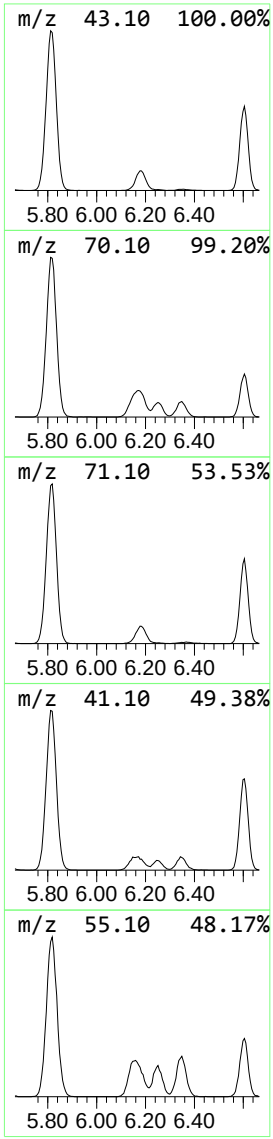
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Pentane, 3-ethyl-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.165	42.42 ug/l	333078	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-ethyl-2-methyl-	114	C8H18	000609-26-7	59
2	1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	50
3	Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	46
4	Hexane, 3-methyl-	100	C7H16	000589-34-4	43
5	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	38





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Operator : JC/MD
Sample : N2253-03
Misc : 1.21g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31396

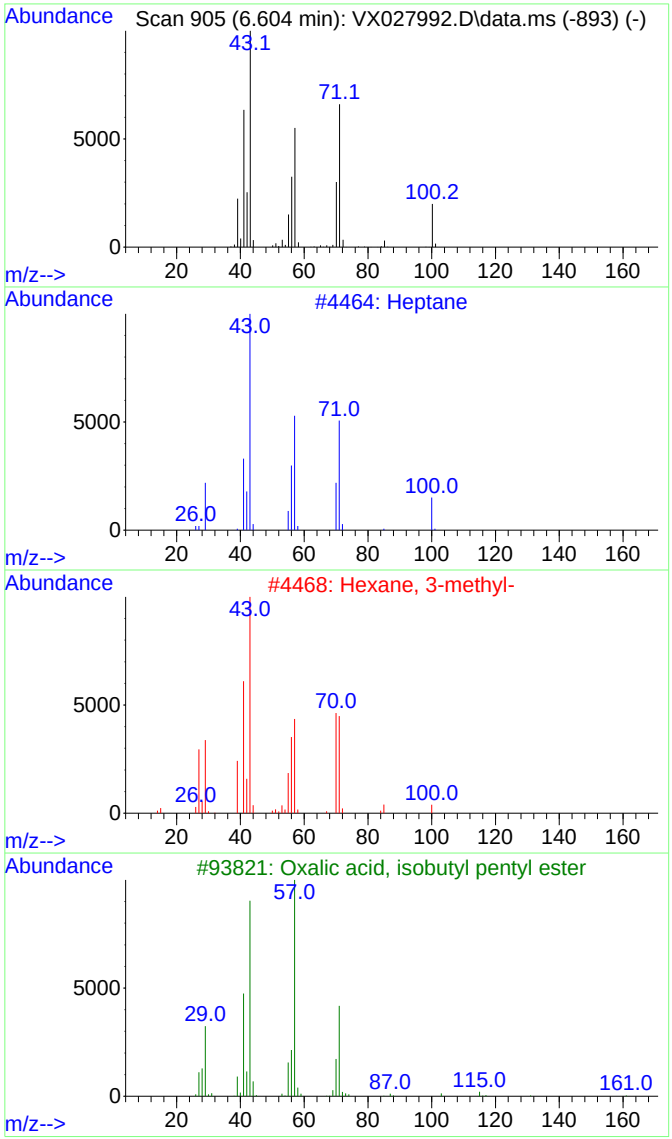
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040522W.M
Quant Title : SW846 8260

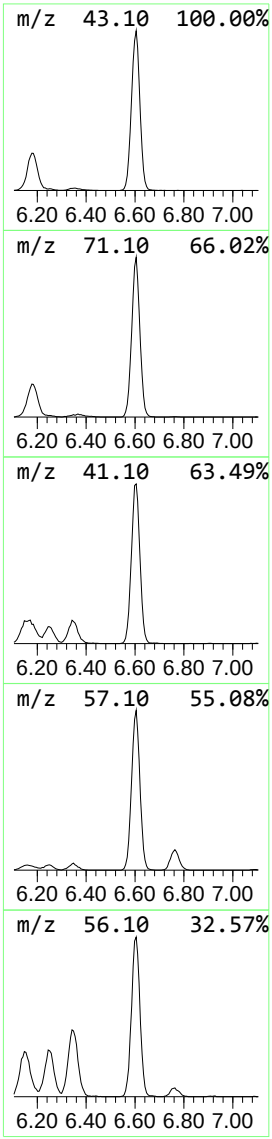
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Heptane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.604	118.91 ug/l	933624	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	91
2	Hexane, 3-methyl-	100	C7H16	000589-34-4	47
3	Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	40
4	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	38
5	Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	38





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Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040522W.M
Quant Title : SW846 8260

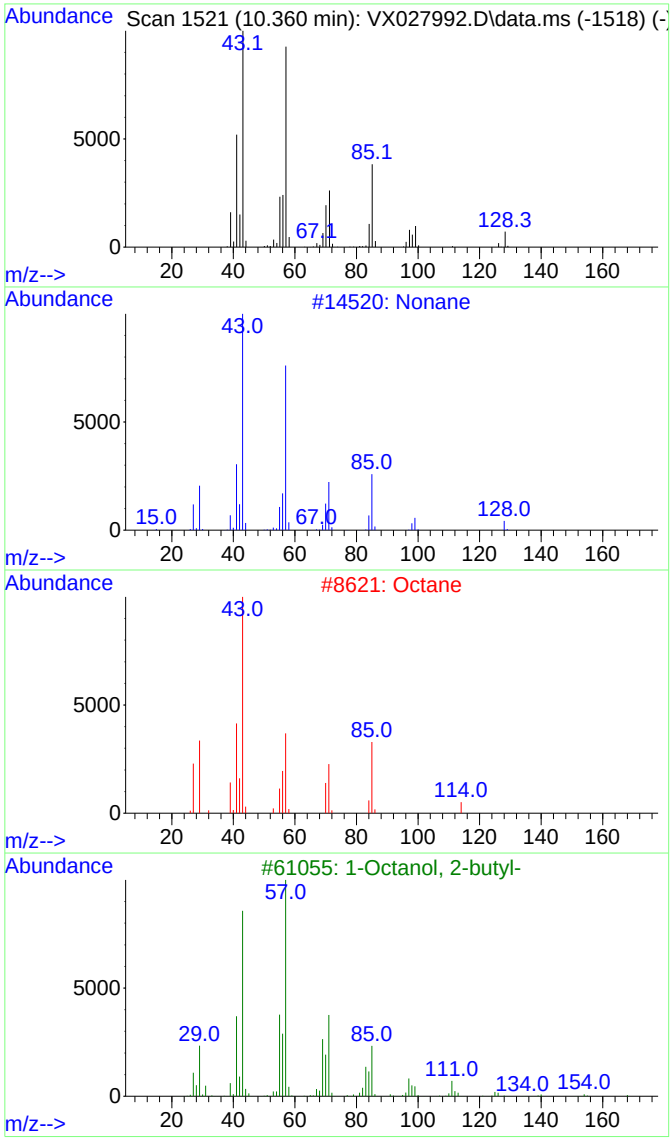
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

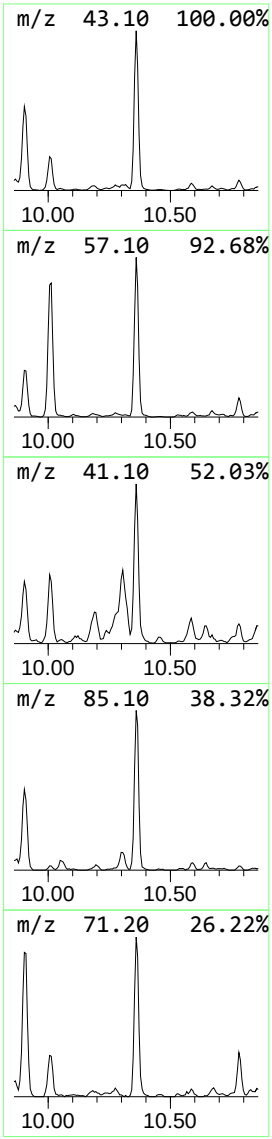
****

Peak Number 5 Nonane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.360	31.06 ug/l	266232	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane	128	C9H20	000111-84-2	93
2	Octane	114	C8H18	000111-65-9	64
3	1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	64
4	4,4-Dimethyl octane	142	C10H22	015869-95-1	53
5	Isobutyl nonyl carbonate	244	C14H28O3	959311-27-4	50





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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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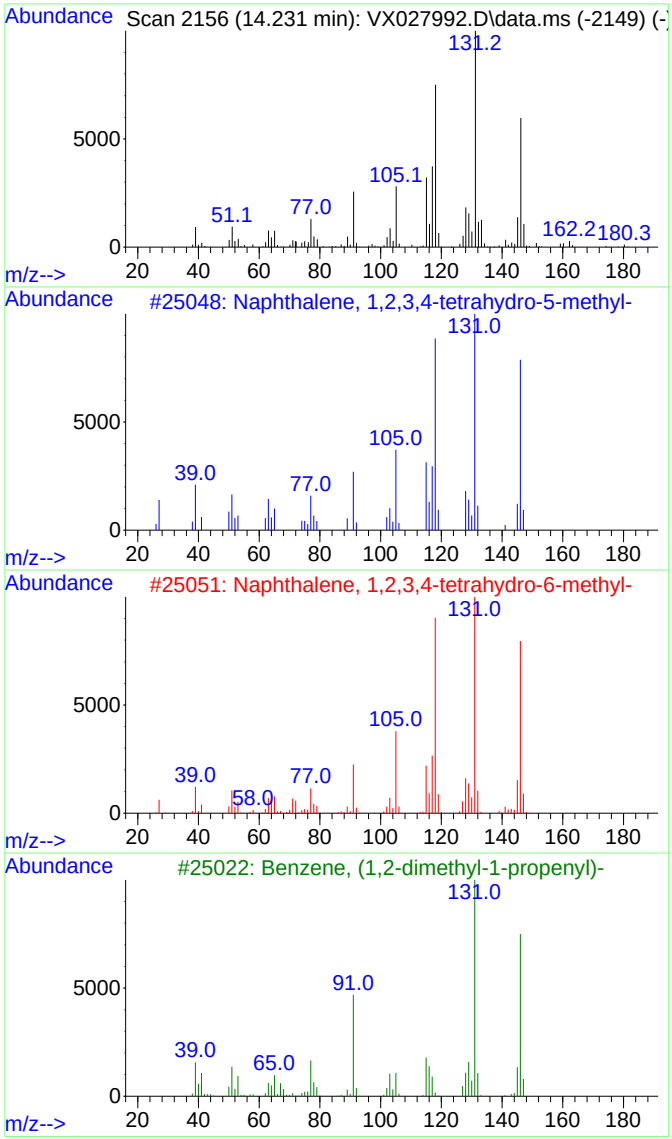
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040522W.M
Quant Title : SW846 8260

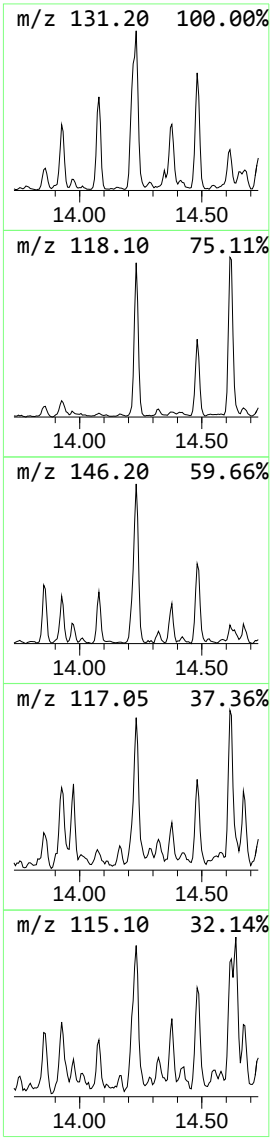
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.231	32.05 ug/l	314858	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	97
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	95
3	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	90
4	1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	60
5	Benzene, (2-methyl-1-methylenepr...	146	C11H14	017498-71-4	60





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Instrument :
MSVOA_X
ClientSampleId :
31396

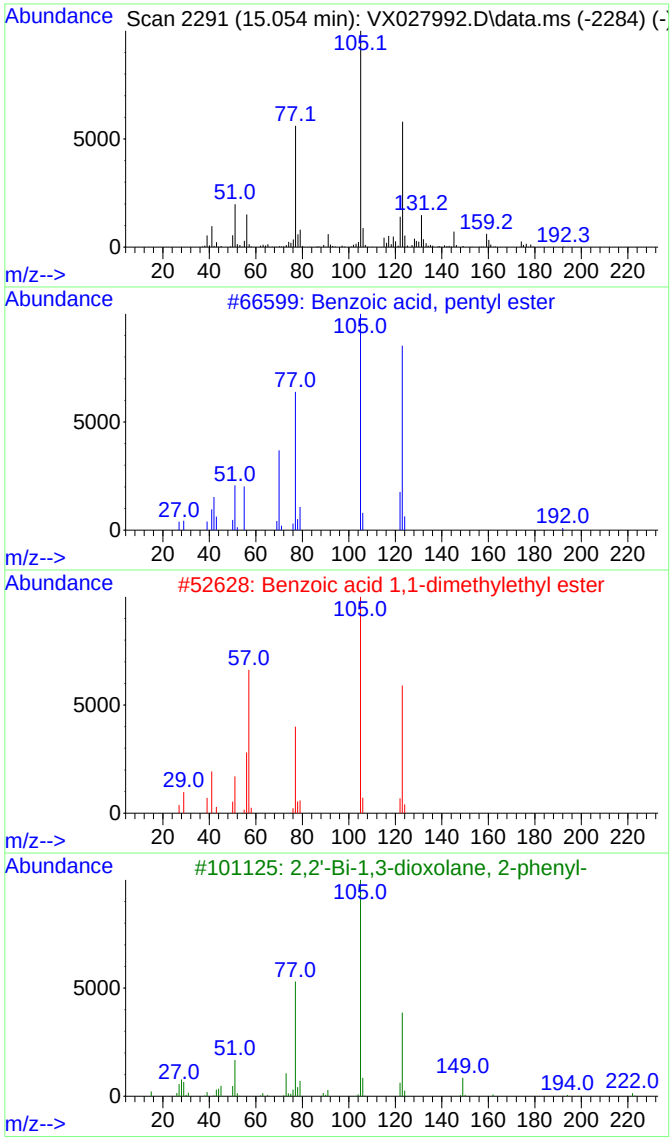
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040522W.M
Quant Title : SW846 8260

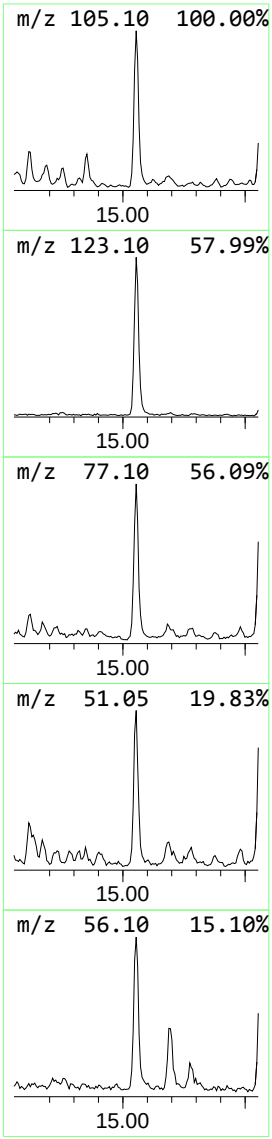
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzoic acid, pentyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.054	23.78 ug/l	233622	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, pentyl ester	192	C12H16O2	002049-96-9	72
2	Benzoic acid 1,1-dimethylethyl e...	178	C11H14O2	000774-65-2	64
3	2,2'-Bi-1,3-dioxolane, 2-phenyl-	222	C12H14O4	021504-04-1	59
4	Butyl benzoate	178	C11H14O2	000136-60-7	53
5	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	45





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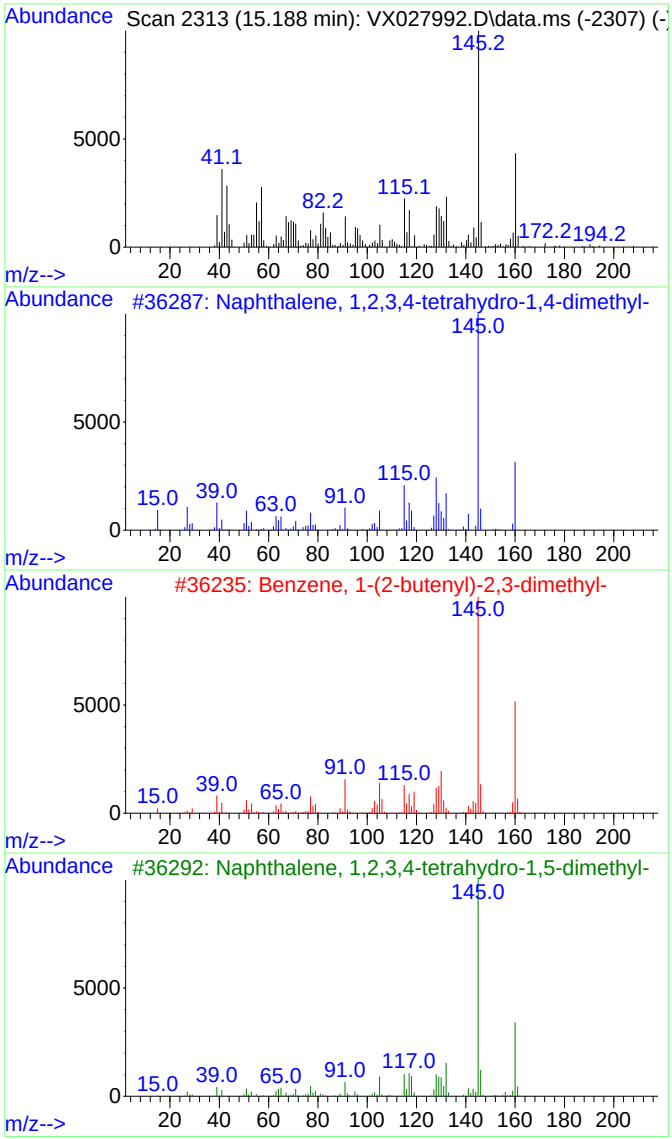
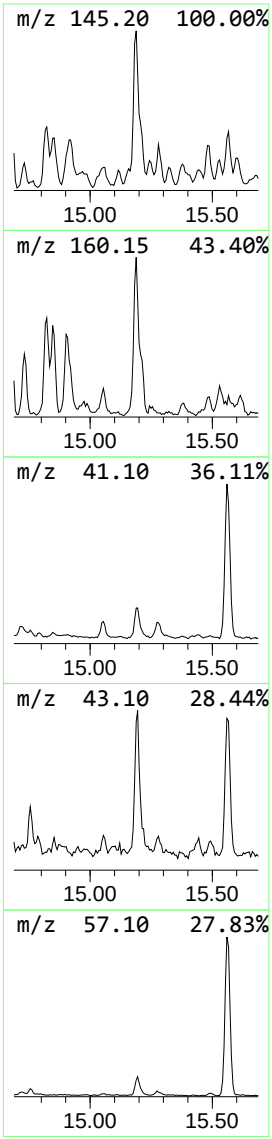
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.188	24.28 ug/l	238514	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	93
2	Benzene, 1-(2-butenyl)-2,3-dimet...	160	C12H16	054340-85-1	91
3	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021564-91-0	91
4	Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	90
5	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	020027-77-4	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040622\
Data File : VX027992.D
Acq On : 06 Apr 2022 12:54
Operator : JC/MD
Sample : N2253-03
Misc : 1.21g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31396

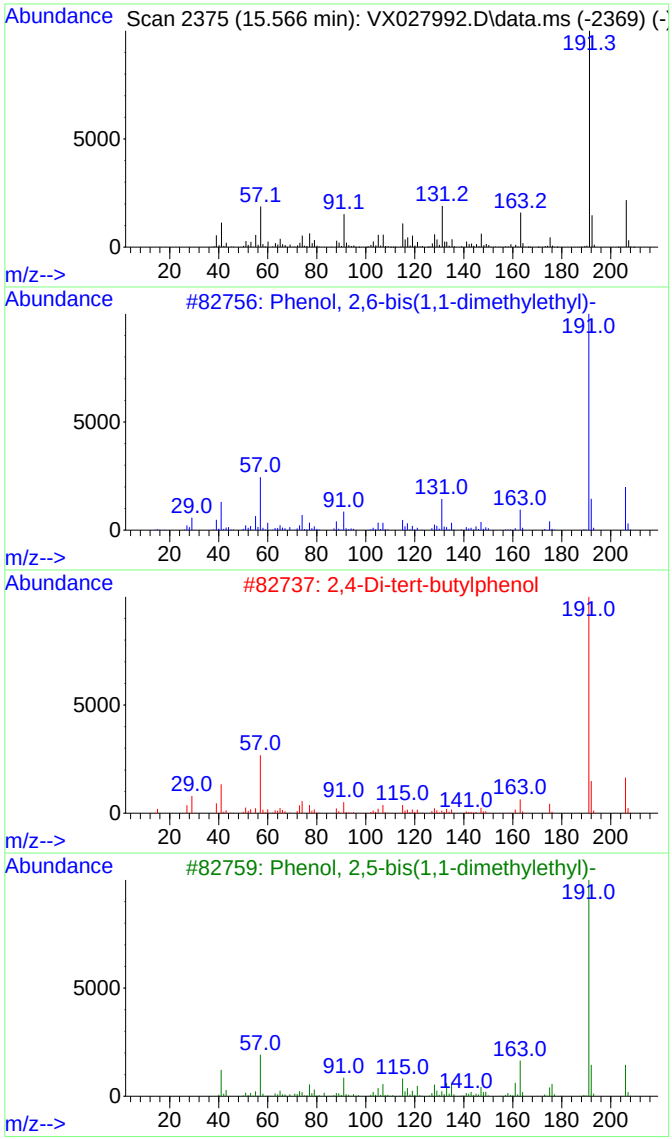
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040522W.M
Quant Title : SW846 8260

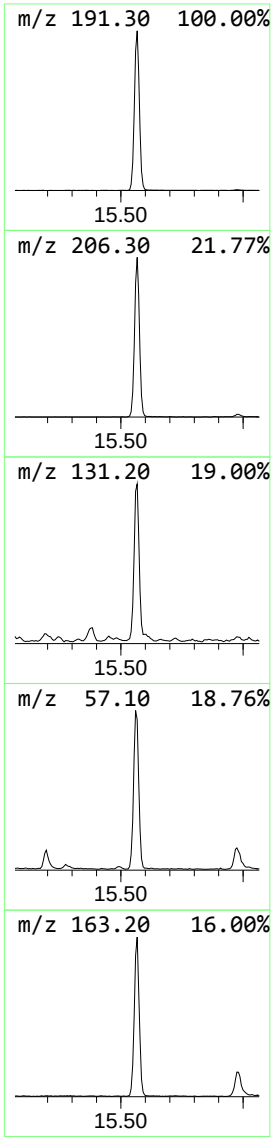
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.566	142.02 ug/l	1395240	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	94
2	2,4-Di-tert-butylphenol	206	C14H22O	000096-76-4	83
3	Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	83
4	Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	74
5	3-(4-(tert-Butyl)phenyl)-2-methy...	206	C14H22O	056107-04-1	74





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040622\
Data File : VX027992.D
Acq On : 06 Apr 2022 12:54
Operator : JC/MD
Sample : N2253-03
Misc : 1.21g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31396

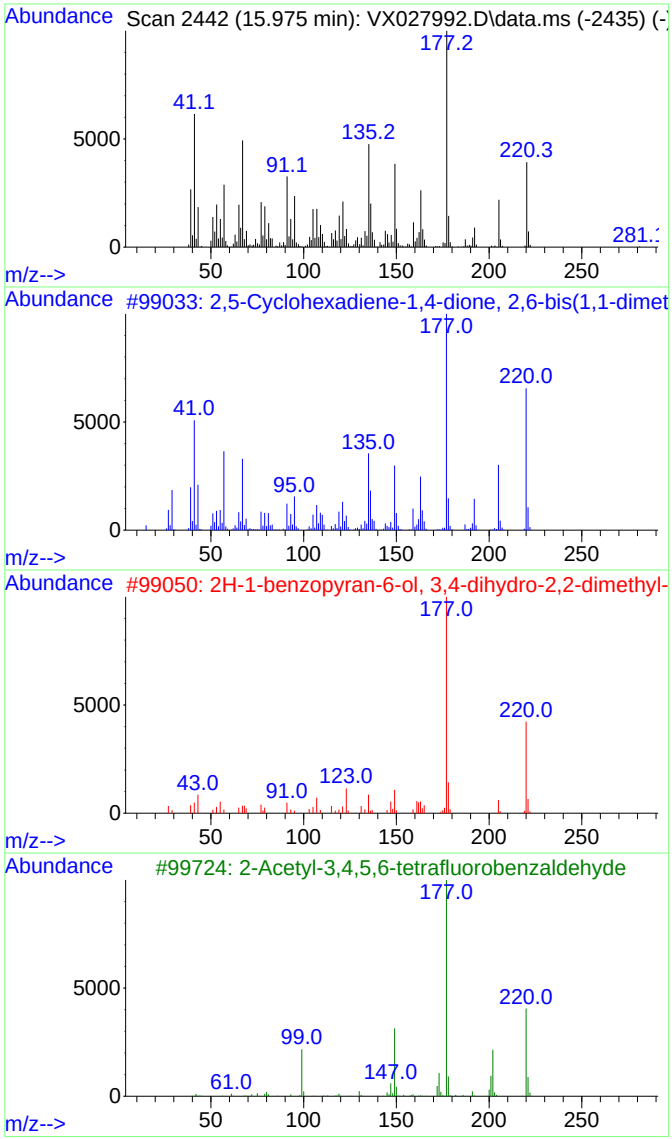
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040522W.M
Quant Title : SW846 8260

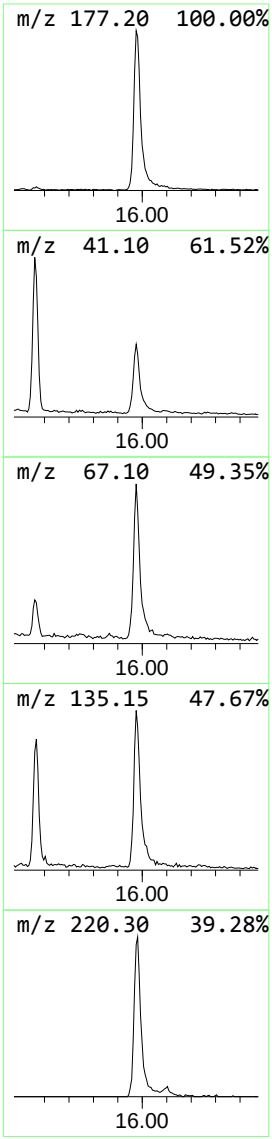
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.975	55.64 ug/l	546635	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	99
2	2H-1-benzopyran-6-ol, 3,4-dihydr...	220	C14H20O2	1000396-25-4	80
3	2-Acetyl-3,4,5,6-tetrafluorobenz...	220	C9H4F4O2	1000461-12-2	43
4	4-Propylbenzaldehyde diethyl acetal	222	C14H22O2	089557-35-7	38
5	1,3,5,7-Tetramethyl-adamantane	192	C14H24	001687-36-1	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040622\
Data File : VX027992.D
Acq On : 06 Apr 2022 12:54
Operator : JC/MD
Sample : N2253-03
Misc : 1.21g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31396

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040522W.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, 2-methyl-	5.495	50.0	ug/l	2188970	1	5.550	2188970	50.0
Hexane, 3-methyl-	5.812	52.3	ug/l	2288840	1	5.550	2188970	50.0
Pentane, 3-ethy...	6.165	42.4	ug/l	333078	2	6.763	392584	50.0
Heptane	6.604	118.9	ug/l	933624	2	6.763	392584	50.0
Nonane	10.360	31.1	ug/l	266232	3	10.055	428587	50.0
Naphthalene, 1,...	14.231	32.0	ug/l	314858	4	12.024	491214	50.0
Benzoic acid, p...	15.054	23.8	ug/l	233622	4	12.024	491214	50.0
Naphthalene, 1,...	15.188	24.3	ug/l	238514	4	12.024	491214	50.0
Phenol, 2,6-bis...	15.566	142.0	ug/l	1395240	4	12.024	491214	50.0
2,5-Cyclohexadi...	15.975	55.6	ug/l	546635	4	12.024	491214	50.0