LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM022717\
Data File : BM009037.D
Acq On : 27 Feb 2017 19:57
Operator : SJ/MA
Sample : I1943-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DABS1

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM022317.M
Title : SVOA CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.328	37	41	45	rBV2	244218	348759	3.12%	0.531%
2	4.452	228	232	237	rBV	97394	132010	1.18%	0.201%
3	4.616	253	260	275	rBV	7879260	11169209	100.00%	17.016%
4	5.946	481	486	495	rBV2	171423	267518	2.40%	0.408%
5	7.046	668	673	685	rVB2	164274	302547	2.71%	0.461%
6	7.228	698	704	714	rBV	587071	924317	8.28%	1.408%
7	7.422	731	737	745	rVB	624038	991360	8.88%	1.510%
8	7.898	811	818	823	rBV	691837	1134341	10.16%	1.728%
9	8.457	905	913	922	rBV2	146675	294687	2.64%	0.449%
10	8.592	929	936	945	rBV2	445572	742997	6.65%	1.132%
11	9.063	1009	1016	1023	rBV	769515	1294136	11.59%	1.972%
12	9.781	1131	1138	1147	rBV	635193	1029901	9.22%	1.569%
13	10.310	1221	1228	1237	rBV	929865	1505177	13.48%	2.293%
14	10.698	1287	1294	1302	rBV	887275	1476665	13.22%	2.250%
15	11.575	1434	1443	1450	rBV	947879	1450891	12.99%	2.210%
16	12.910	1662	1670	1678	rBV2	165668	251268	2.25%	0.383%
17	13.939	1838	1845	1850	rBV	1805781	2489393	22.29%	3.792%
18	13.986	1850	1853	1859	rVB	120722	161174	1.44%	0.246%
19	14.227	1889	1894	1902	rVB	1770196	2561240	22.93%	3.902%
20	14.533	1940	1946	1957	rBV2	1202156	1922867	17.22%	2.929%
21	14.722	1972	1978	1985	rBV2	152492	250616	2.24%	0.382%
22	14.998	2021	2025	2035	rBV2	127348	200967	1.80%	0.306%
23	15.527	2108	2115	2122	rBV	2395949	3455854	30.94%	5.265%
24	15.639	2126	2134	2144	rBV	897122	1255953	11.24%	1.913%
25	15.910	2176	2180	2186	rBV	170533	224780	2.01%	0.342%
26	16.221	2229	2233	2241	rBV2	103488	157986	1.41%	0.241%
27	17.280	2405	2413	2419	rBV	1653850	2370456	21.22%	3.611%
28	17.380	2422	2430	2440	rBV	2748826	3973603	35.58%	6.054%
29	17.980	2527	2532	2538	rBV	188359	276533	2.48%	0.421%
30	18.151	2556	2561	2572	rBV2	258150	359346	3.22%	0.547%
31	19.427	2773	2778	2783	rBV2	176670	237725	2.13%	0.362%
32	19.668	2813	2819	2826	rBV	3699322	4891513	43.79%	7.452%
33	20.386	2935	2941	2959	rBV	4078831	5610811	50.23%	8.548%
34	21.139	3066	3069	3075	rVB4	153957	181946	1.63%	0.277%

LSC Area Percent Report

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Data File : BM009037.D
Acq On : 27 Feb 2017 19:57
Operator : SJ/MA
Sample : I1943-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DABS1

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM022317.M
Title : SVOA CALIBRATION

35	21.450	3117	3122	3128	rBV	2592234	3246428	29.07%	4.946%
36	23.644	3488	3495	3504	rVB2	2759933	5331584	47.73%	8.122%
37	23.791	3514	3520	3530	rVB	1571258	3163431	28.32%	4.819%

Sum of corrected areas: 65639989

LSC Report - Integrated Chromatogram

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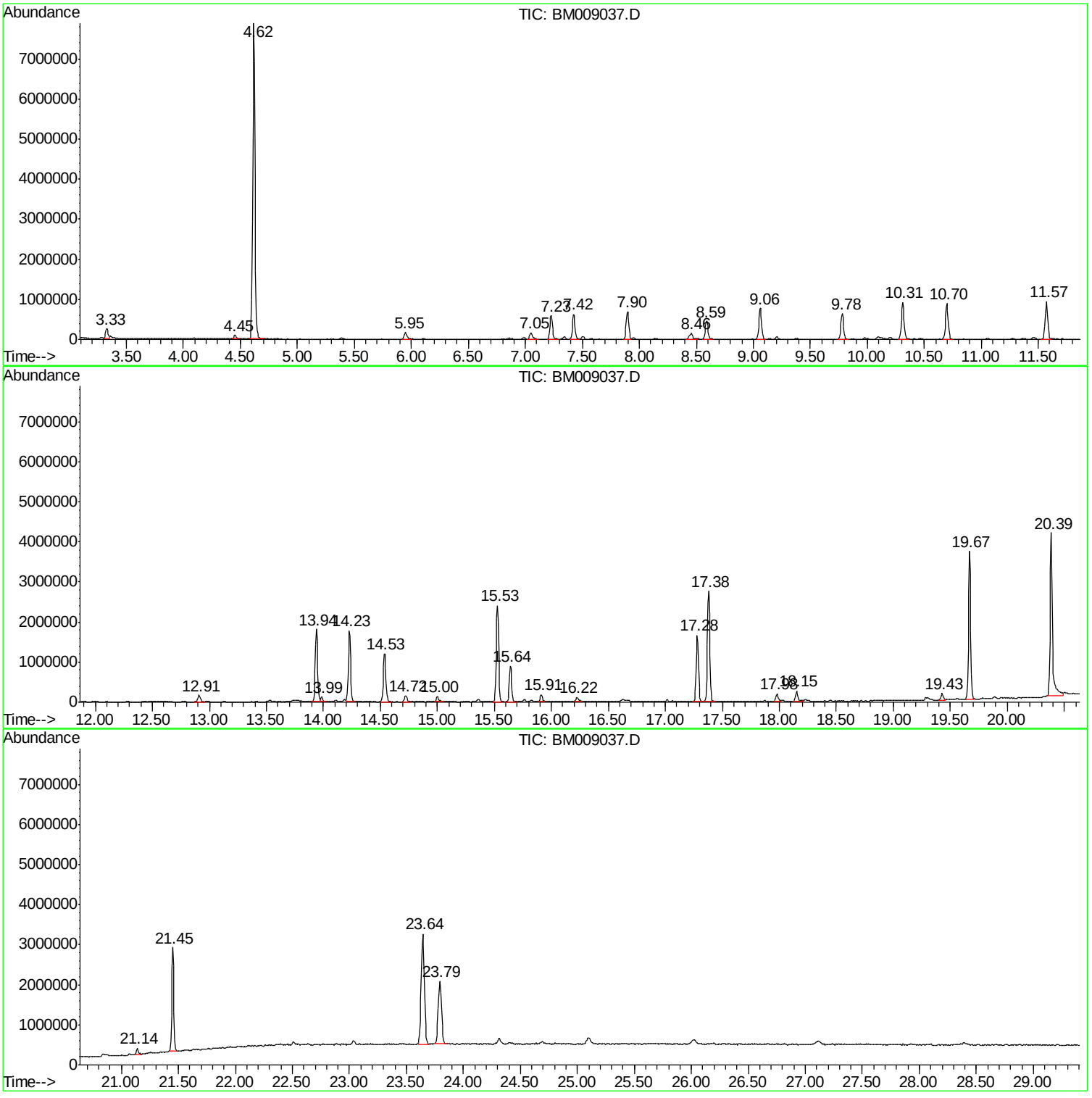
Data File : BM009037.D
Acq On : 27 Feb 2017 19:57
Operator : SJ/MA
Sample : I1943-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DABS1

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM022317.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM022717\
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Acq On : 27 Feb 2017 19:57
Operator : SJ/MA
Sample : I1943-12
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ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DABS1

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM022317.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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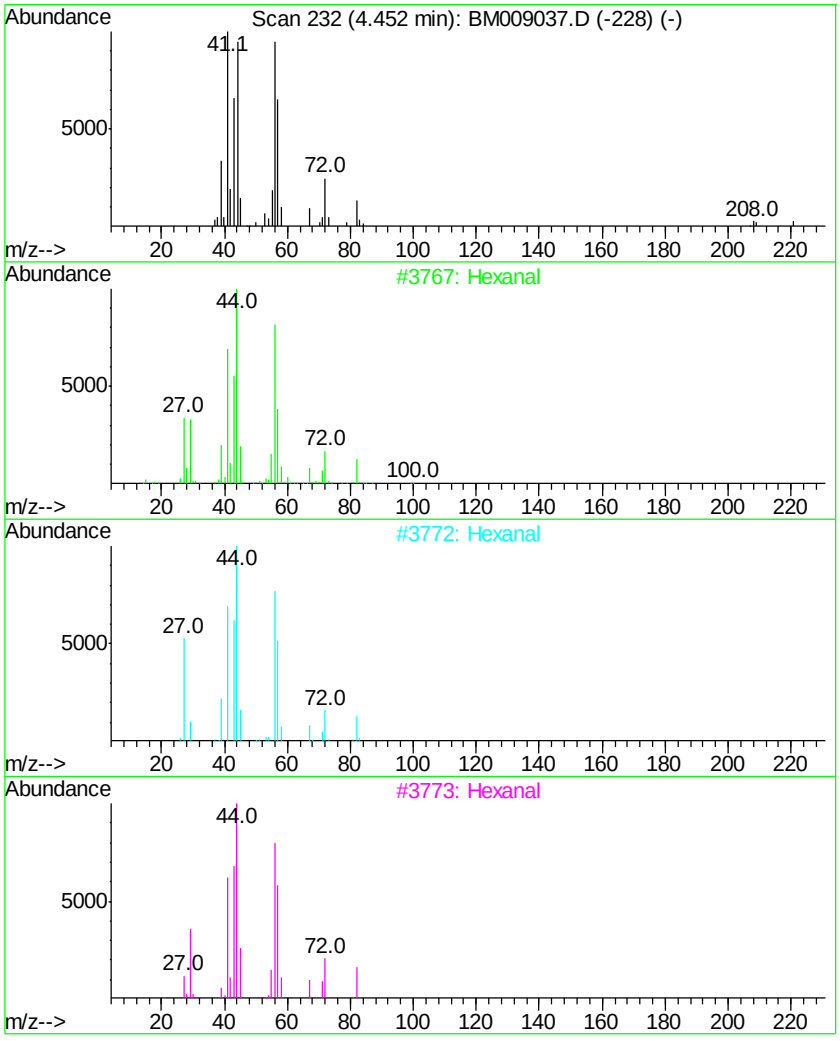
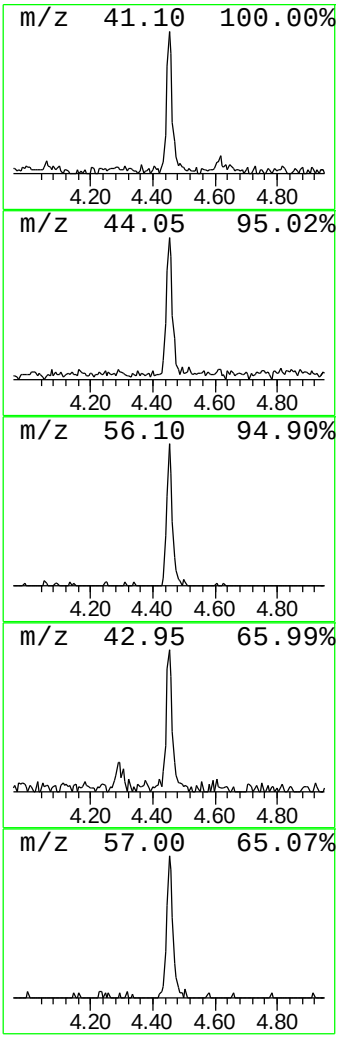
Peak Number 1 Hexanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.45	2.33 ng/ul	132010	1,4-Dichlorobenzene-d4	7.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal	100	C6H12O	000066-25-1	78
2	Hexanal	100	C6H12O	000066-25-1	72
3	Hexanal	100	C6H12O	000066-25-1	64
4	Hexanal	100	C6H12O	000066-25-1	43
5	Glutaraldehyde	100	C5H8O2	000111-30-8	38





Library Search Compound Report

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Data File : BM009037.D
Acq On : 27 Feb 2017 19:57
Operator : SJ/MA
Sample : I1943-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DABS1

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM022317.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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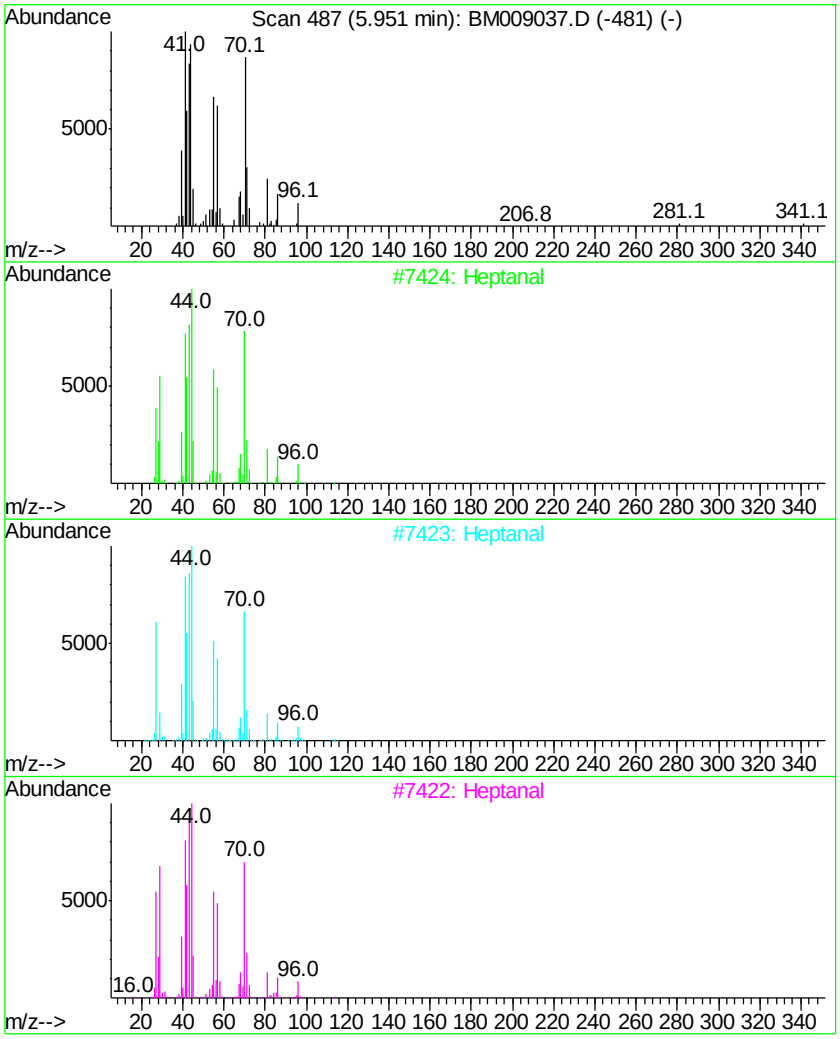
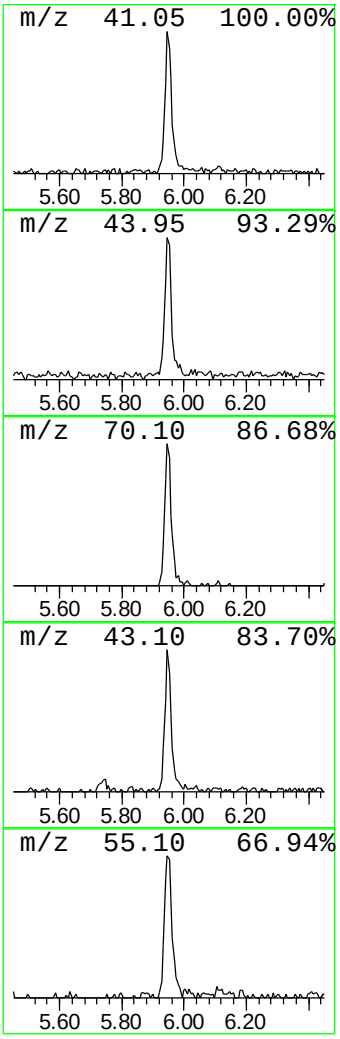
Peak Number 3 Heptanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.95	4.72 ng/ul	267518	1,4-Dichlorobenzene-d4	7.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanal	114	C7H14O	000111-71-7	72
2	Heptanal	114	C7H14O	000111-71-7	64
3	Heptanal	114	C7H14O	000111-71-7	50
4	2-Butene, 2-methyl-	70	C5H10	000513-35-9	43
5	Heptanal	114	C7H14O	000111-71-7	42





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM022717\
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Acq On : 27 Feb 2017 19:57
Operator : SJ/MA
Sample : I1943-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DABS1

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM022317.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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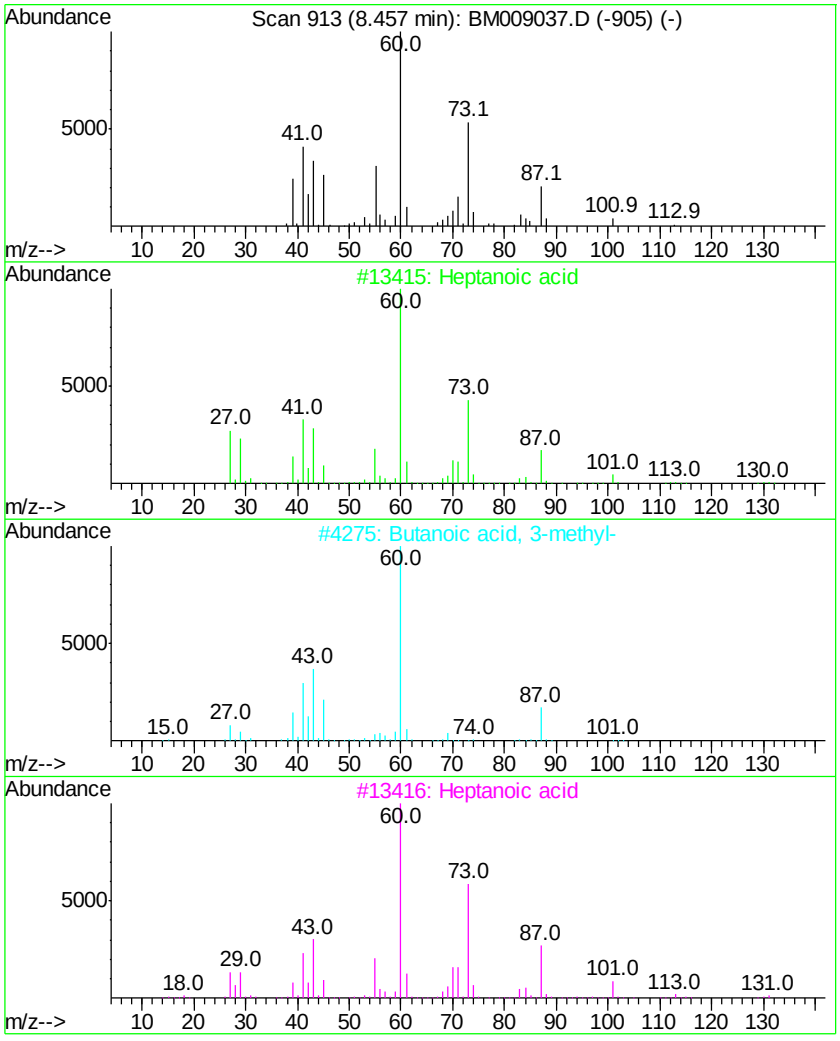
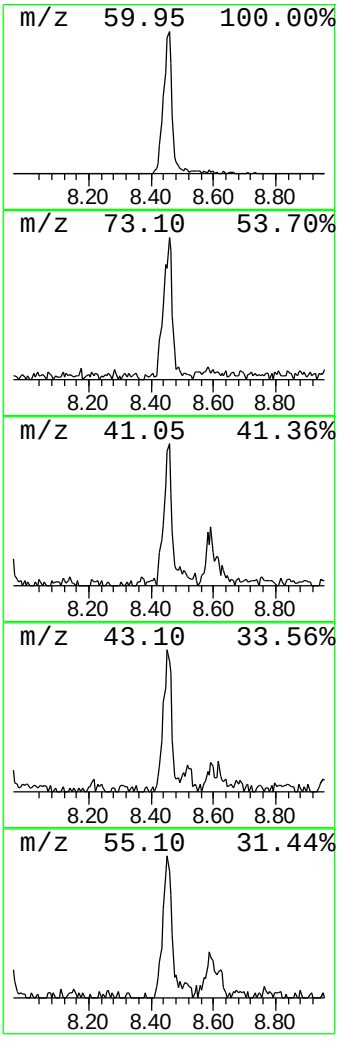
Peak Number 4 Heptanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.46	5.20 ng/ul	294687	1,4-Dichlorobenzene-d4	7.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanoic acid	130	C7H14O2	000111-14-8	72
2	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	64
3	Heptanoic acid	130	C7H14O2	000111-14-8	56
4	Hexanoic acid	116	C6H12O2	000142-62-1	53
5	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	50





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Sample : I1943-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DABS1

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM022317.M
Quant Title : SVOA CALIBRATION

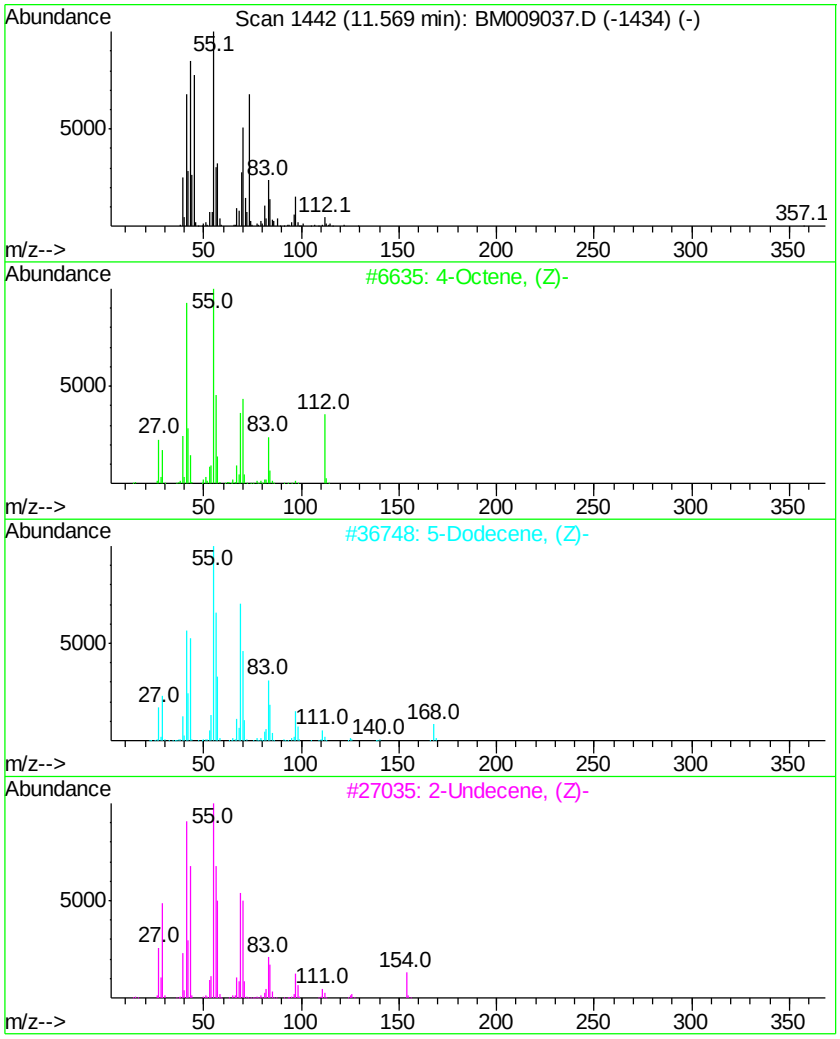
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

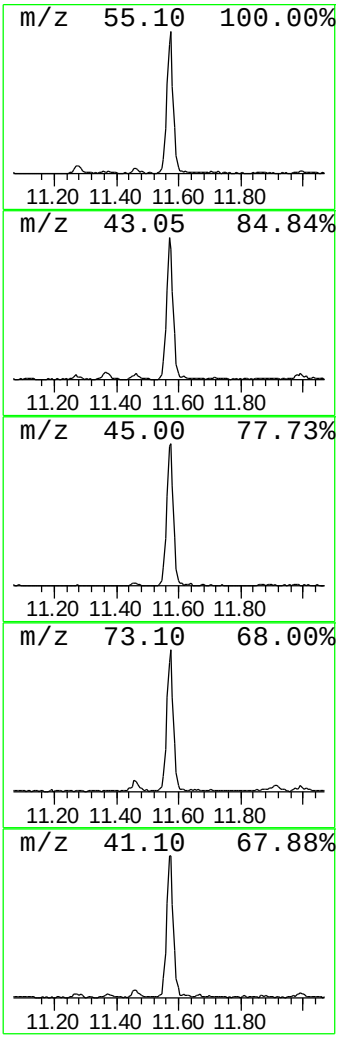
****

Peak Number 5 (DEL) Alkane: Cyclic11.57 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.57	19.65 ng/ul	1450890	Naphthalene-d8	10.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Octene, (Z)-	112	C8H16	007642-15-1	46
2	5-Dodecene, (Z)-	168	C12H24	007206-28-2	43
3	2-Undecene, (Z)-	154	C11H22	000821-96-5	43
4	n-Nonane, 1-[1-cycloazapropyl]-	169	C11H23N	014924-95-9	43
5	4-Octene, 2,6-dimethyl-, [S-(Z)]-	140	C10H20	062960-77-4	38





Library Search Compound Report

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ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DABS1

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM022317.M
Quant Title : SVOA CALIBRATION

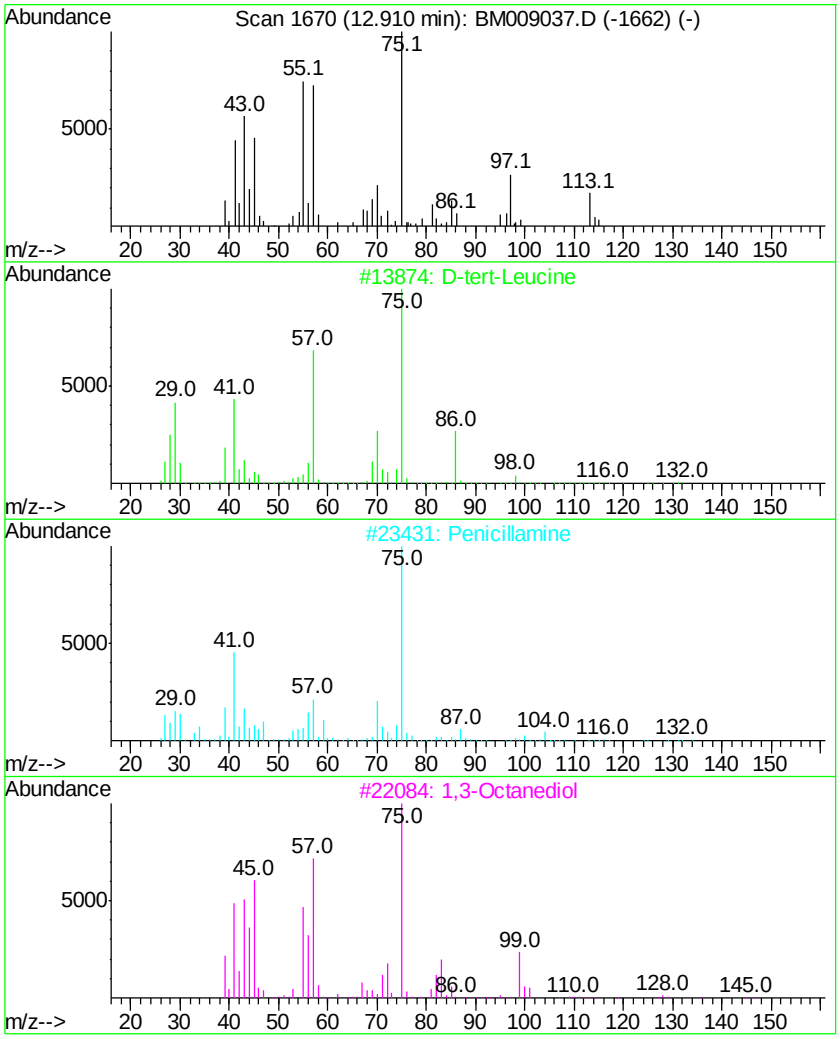
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

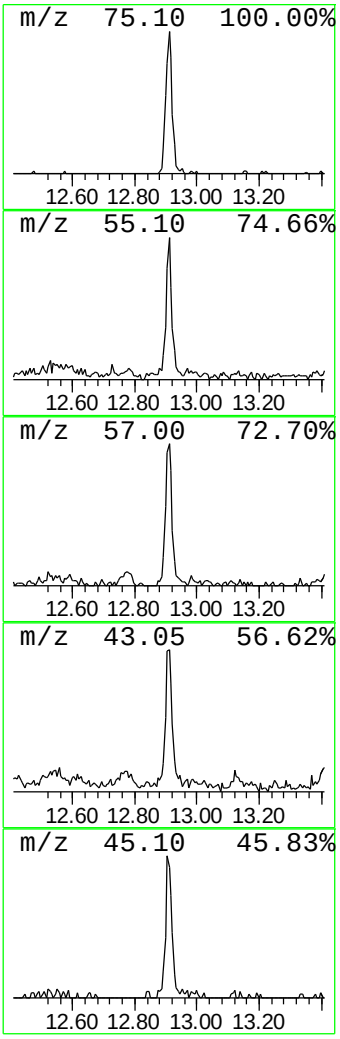
****

Peak Number 6 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.91	2.61 ng/ul	251268	Acenaphthene-d10	14.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D-tert-Leucine	131	C6H13NO2	026782-71-8	35
2	Penicillamine	149	C5H11NO2S	000052-67-5	32
3	1,3-Octanediol	146	C8H18O2	023433-05-8	23
4	E-10-Dodecen-1-ol propionate	240	C15H28O2	1000130-97-6	16
5	Ethanethioamide	75	C2H5NS	000062-55-5	12





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ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DABS1

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM022317.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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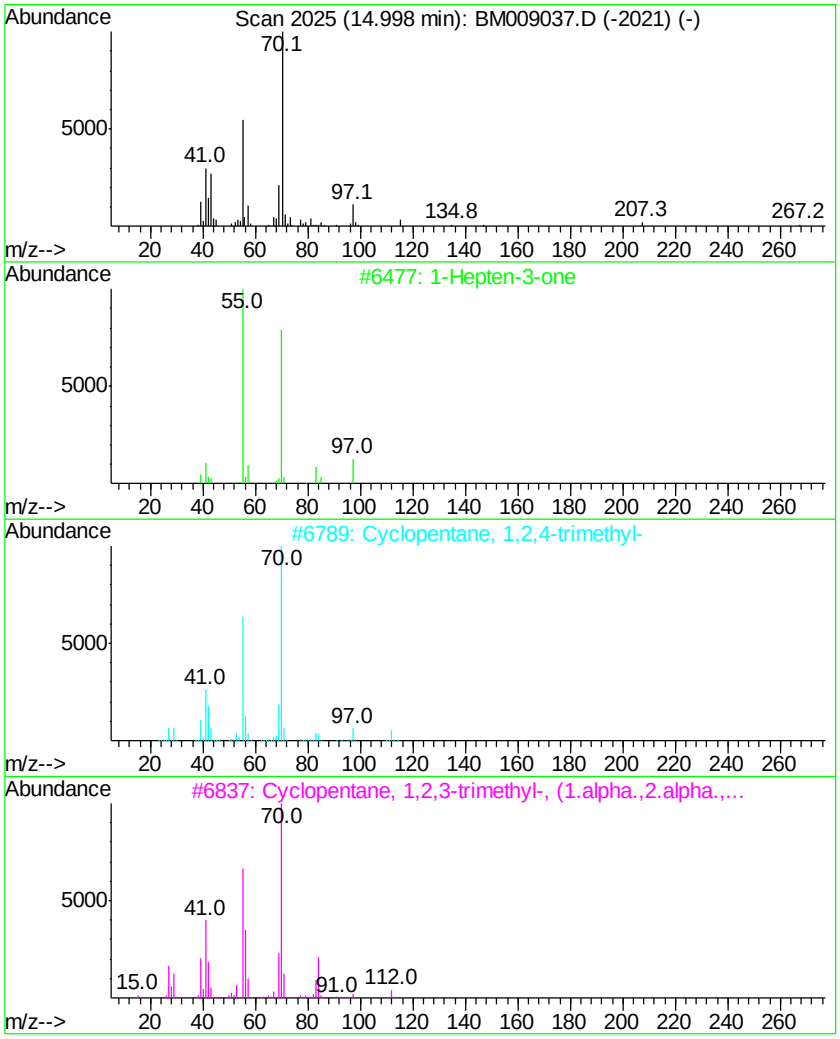
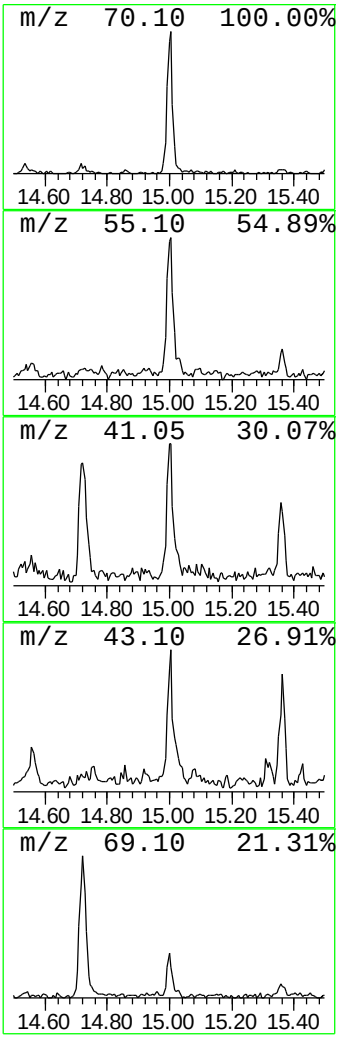
Peak Number 7 1-Hepten-3-one Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.00	2.09 ng/ul	200967	Acenaphthene-d10	14.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hepten-3-one	112	C7H12O	002918-13-0	50
2	Cyclopentane, 1,2,4-trimethyl-	112	C8H16	002815-58-9	50
3	Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	002613-69-6	50
4	Tridecane, 3-methylene-	196	C14H28	019780-34-8	50
5	Cyclopentane, 1,2,3-trimethyl-	112	C8H16	002815-57-8	45





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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM022317.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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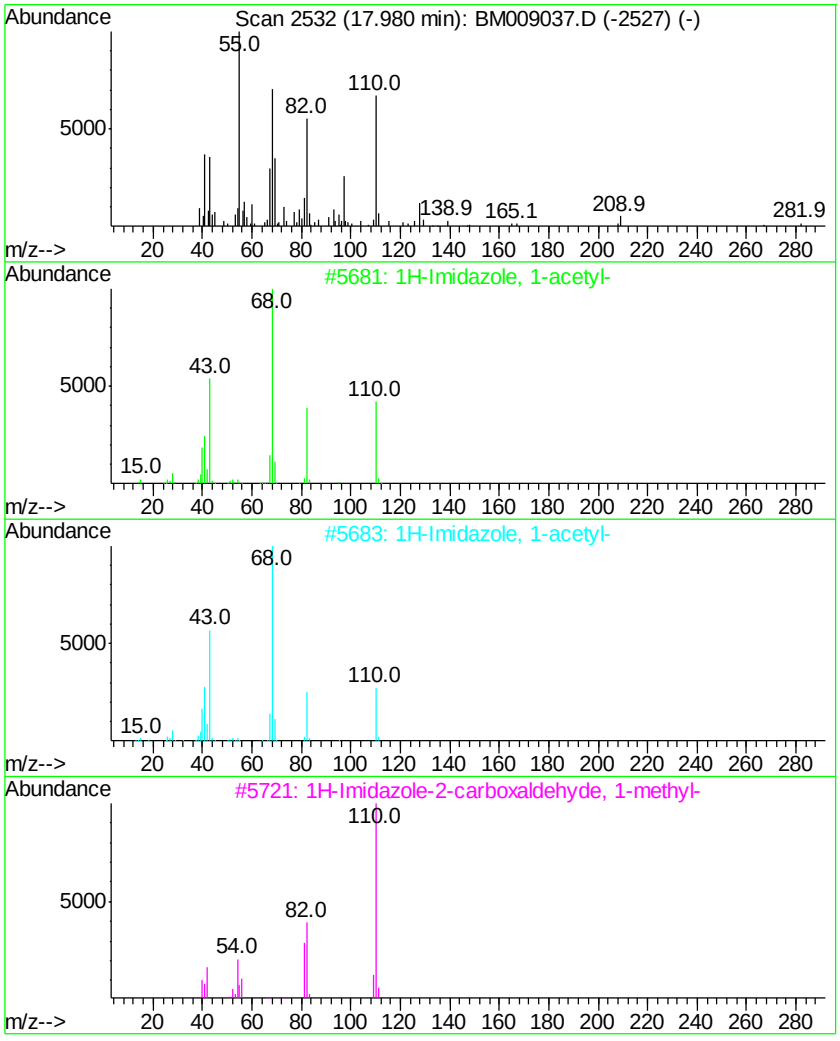
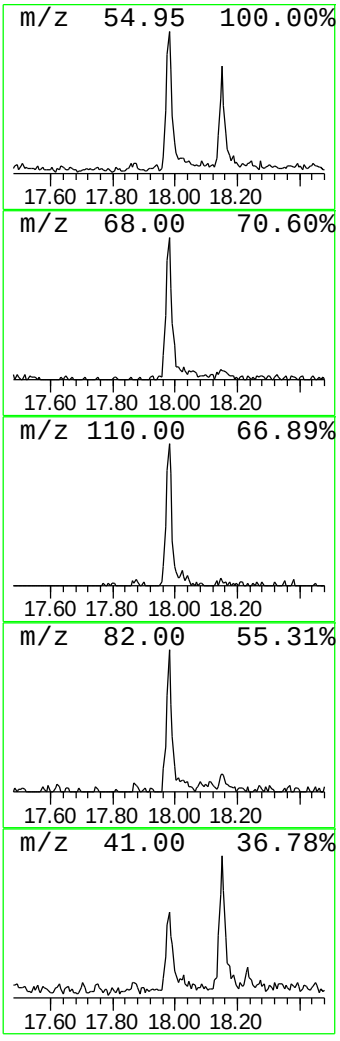
Peak Number 8 unknown-02 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.98	2.33 ng/ul	276533	Phenanthrene-d10	17.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Imidazole, 1-acetyl-	110	C5H6N2O	002466-76-4	35
2	1H-Imidazole, 1-acetyl-	110	C5H6N2O	002466-76-4	35
3	1H-Imidazole-2-carboxaldehyde, 1...	110	C5H6N2O	013750-81-7	27
4	1-(Dimethylamino)pyrrole	110	C6H10N2	078307-76-3	22
5	4-Amino-2(1H)-pyridinone	110	C5H6N2O	038767-72-5	14





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ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM022317.M
Quant Title : SVOA CALIBRATION

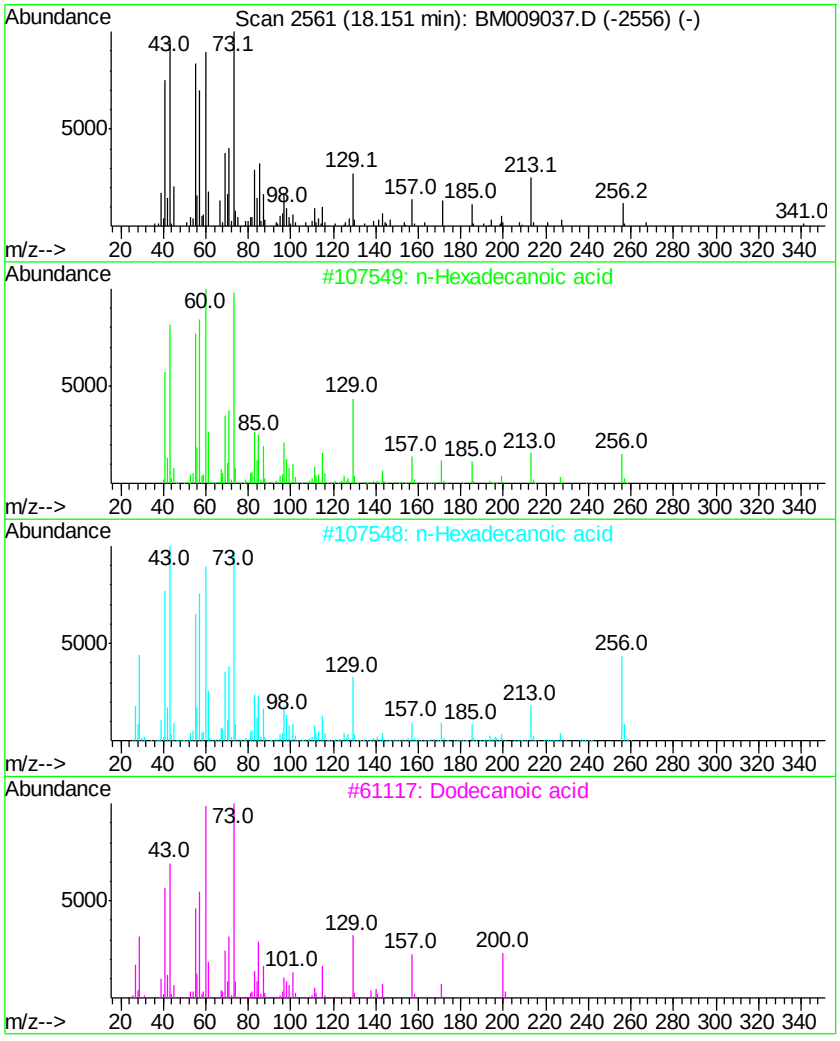
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

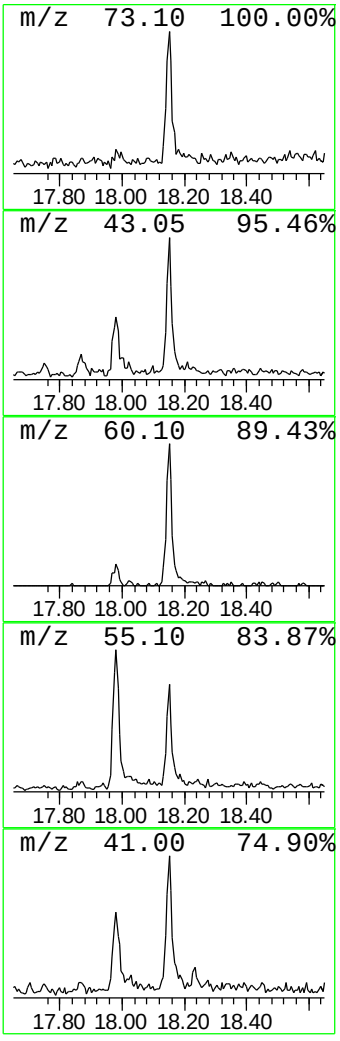
****

Peak Number 9 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.15	3.03 ng/ul	359346	Phenanthrene-d10	17.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
3	Dodecanoic acid	200	C12H24O2	000143-07-7	76
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76
5	Dodecanoic acid	200	C12H24O2	000143-07-7	76





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Instrument : BNA_M
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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM022317.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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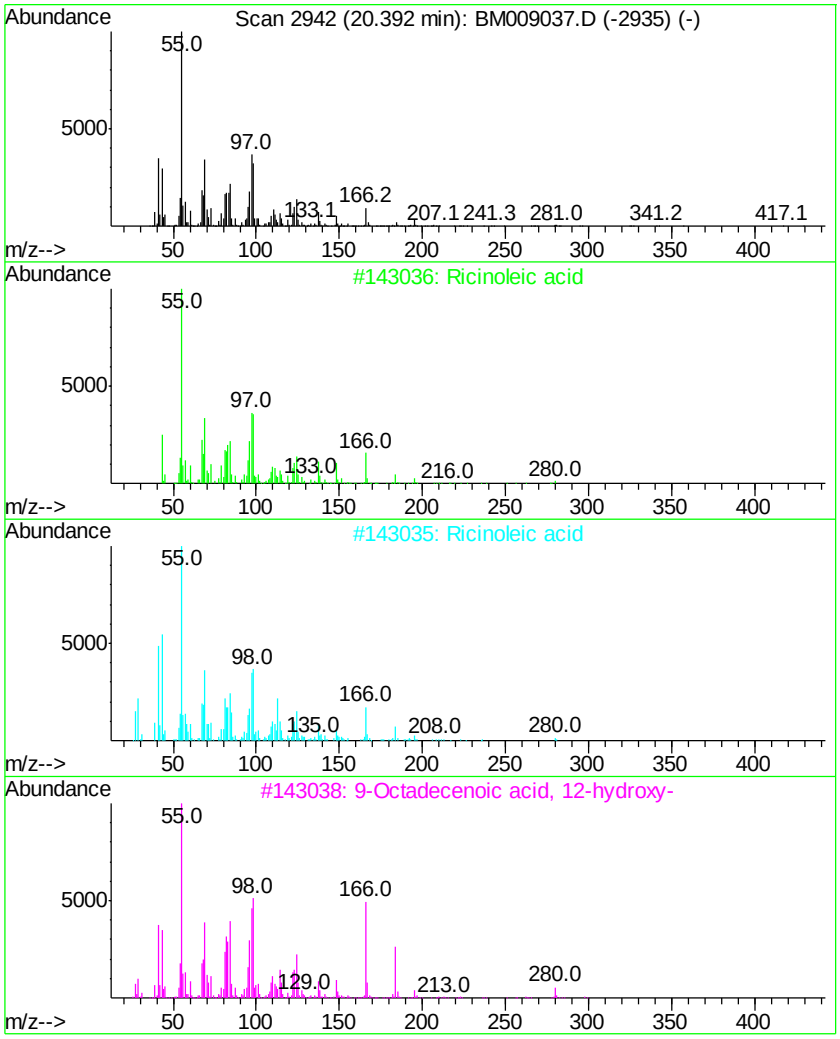
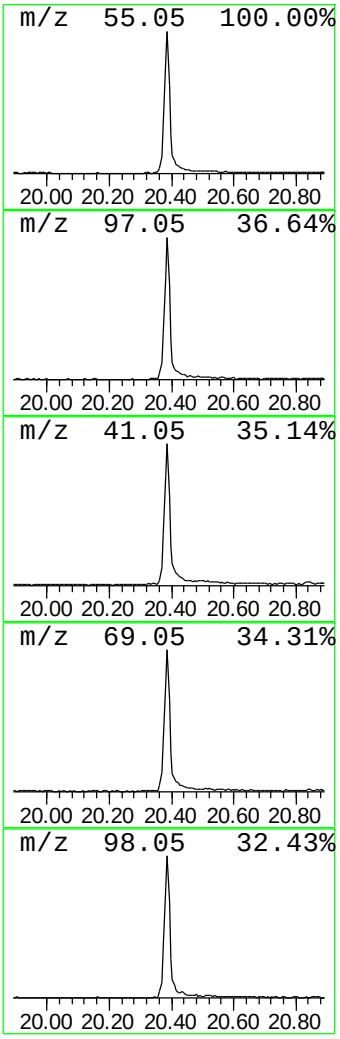
Peak Number 10 Ricinoleic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.39	34.57 ng/ul	5610810	Chrysene-d12	21.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ricinoleic acid	298	C18H34O3	000141-22-0	87
2	Ricinoleic acid	298	C18H34O3	000141-22-0	86
3	9-Octadecenoic acid, 12-hydroxy-	298	C18H34O3	007431-95-0	80
4	Ricinoleic acid	298	C18H34O3	000141-22-0	49
5	Z-7-Tetradecenoic acid	226	C14H26O2	1000130-98-4	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM022717\
Data File : BM009037.D
Acq On : 27 Feb 2017 19:57
Operator : SJ/MA
Sample : I1943-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DABS1

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM022317.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Hexanal	4.45	2.3	ng/ul	132010	1	7.90	1134340	20.0
Heptanal	5.95	4.7	ng/ul	267518	1	7.90	1134340	20.0
Heptanoic acid	8.46	5.2	ng/ul	294687	1	7.90	1134340	20.0
(DEL) Alkane: Cyc...	11.57	19.6	ng/ul	1450890	2	10.70	1476670	20.0
unknown-01	12.91	2.6	ng/ul	251268	3	14.53	1922870	20.0
1-Hepten-3-one	15.00	2.1	ng/ul	200967	3	14.53	1922870	20.0
unknown-02	17.98	2.3	ng/ul	276533	4	17.28	2370460	20.0
n-Hexadecanoic acid	18.15	3.0	ng/ul	359346	4	17.28	2370460	20.0
Ricinoleic acid	20.39	34.6	ng/ul	5610810	5	21.45	3246430	20.0