LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082120\
Data File : BM027186.D
Acq On : 22 Aug 2020 01:06
Operator : JU/CG
Sample : L3746-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 359

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:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082120.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.199	200	206	213	rBV	84415	109530	3.18%	0.464%
2	4.781	300	305	311	rBV	52083	74653	2.17%	0.317%
3	5.234	376	382	396	rBV	1329384	1789817	51.91%	7.590%
4	6.798	640	648	664	rBV	1287384	1944377	56.40%	8.246%
5	7.228	717	721	731	rBV2	27334	48129	1.40%	0.204%
6	7.610	780	786	795	rVB	472695	731696	21.22%	3.103%
7	8.751	972	980	992	rBV	791889	1291491	37.46%	5.477%
8	10.381	1250	1257	1265	rBV	565768	937738	27.20%	3.977%
9	12.869	1673	1680	1691	rBV	1527932	2217520	64.32%	9.404%
10	13.710	1817	1823	1832	rBV	317744	431178	12.51%	1.829%
11	14.251	1908	1915	1922	rBV	864182	1253507	36.36%	5.316%
12	15.739	2162	2168	2175	rBV	1624742	2215305	64.26%	9.395%
13	16.245	2249	2254	2260	rBV5	23332	61115	1.77%	0.259%
14	16.651	2319	2323	2332	rBV2	80674	120774	3.50%	0.512%
15	16.992	2376	2381	2387	rBV	1044324	1479522	42.91%	6.274%
16	17.915	2533	2538	2545	rBV	252670	362538	10.52%	1.537%
17	18.686	2664	2669	2673	rBV	159777	192817	5.59%	0.818%
18	18.774	2681	2684	2689	rVB	31110	39174	1.14%	0.166%
19	19.056	2728	2732	2734	rBV	27081	34747	1.01%	0.147%
20	19.203	2753	2757	2767	rBV2	132482	201398	5.84%	0.854%
21	19.633	2825	2830	2836	rBV	2958208	3447606	100.00%	14.621%
22	20.345	2948	2951	2956	rVB	51893	58041	1.68%	0.246%
23	20.556	2982	2987	2992	rBV	300282	371615	10.78%	1.576%
24	20.603	2992	2995	2997	rVB2	44663	48949	1.42%	0.208%
25	20.927	3046	3050	3057	rBV	350819	439852	12.76%	1.865%
26	21.186	3089	3094	3100	rBV	1493515	1845183	53.52%	7.825%
27	23.374	3460	3466	3475	rVB	1010807	1832177	53.14%	7.770%

Sum of corrected areas: 23580449

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082120\
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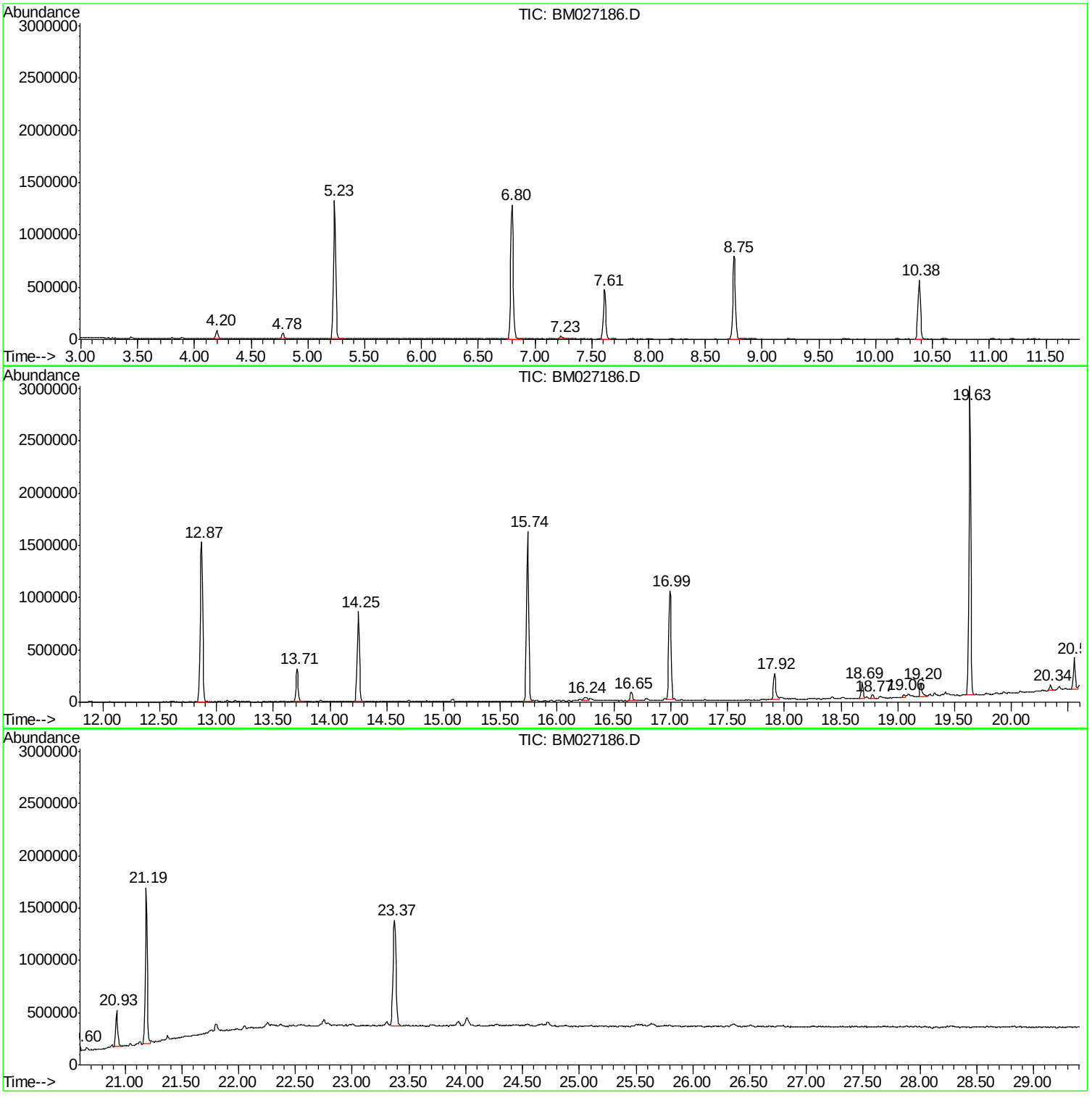
Acq On : 22 Aug 2020 01:06
Operator : JU/CG
Sample : L3746-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 359

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082120\
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Instrument : BNA_M
ClientSampleId : 359

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

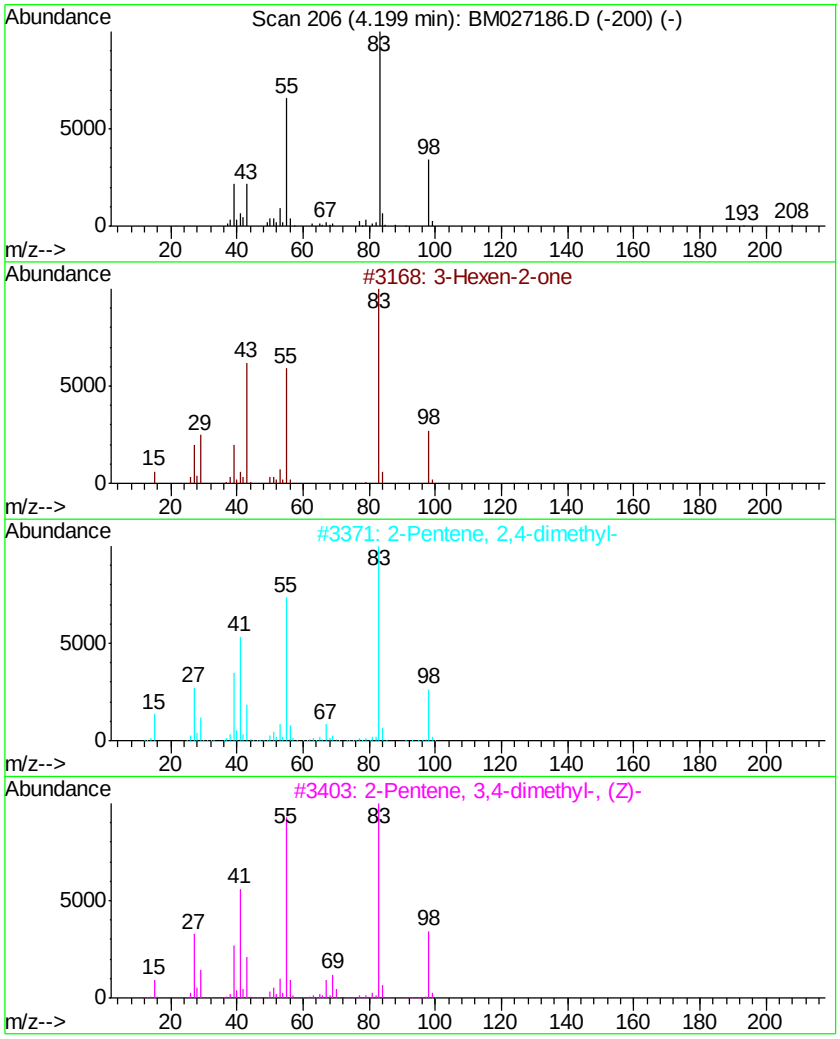
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

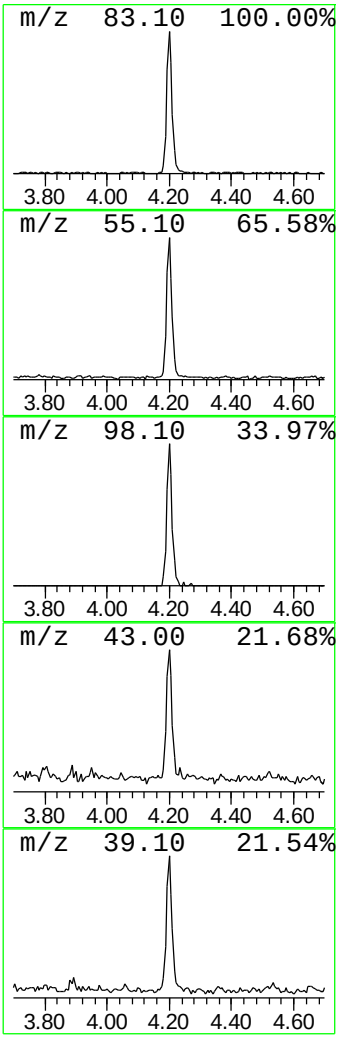
****

Peak Number 1 3-Hexen-2-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.20	2.99 ng	109530	1,4-Dichlorobenzene-d4	7.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	91
2	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
3	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4	Furan, 2-methoxy-	98	C5H6O2	025414-22-6	86
5	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082120\
Data File : BM027186.D
Acq On : 22 Aug 2020 01:06
Operator : JU/CG
Sample : L3746-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 359

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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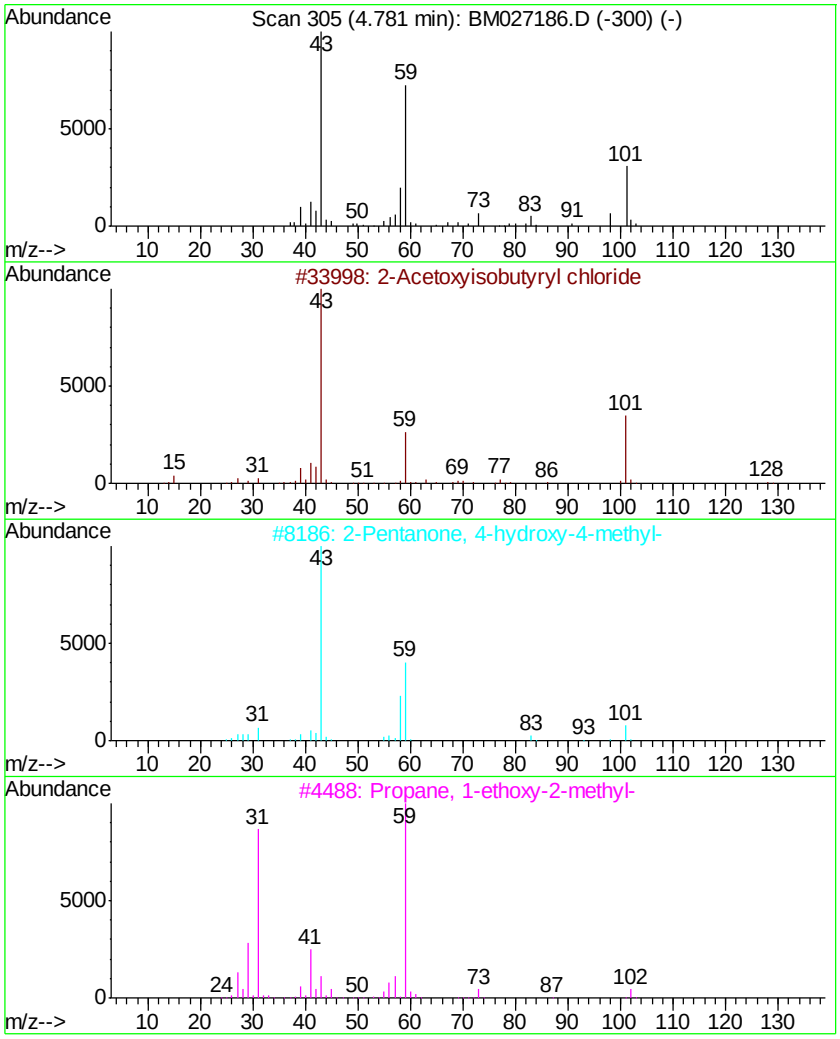
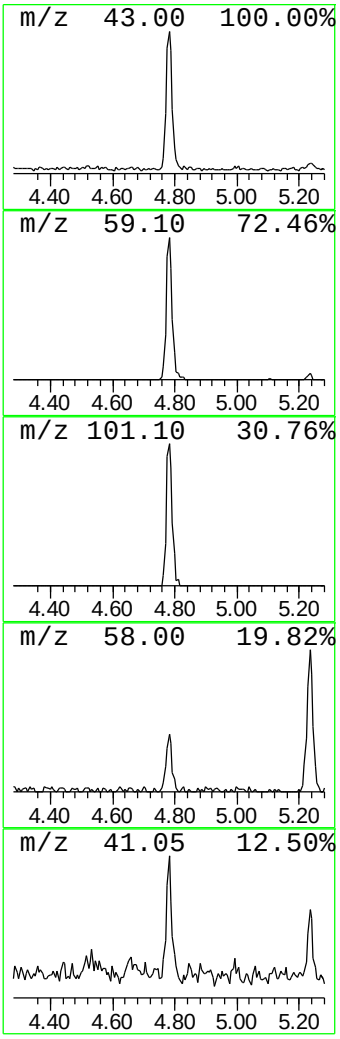
Peak Number 2 unknown4.78 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.78	2.04 ng	74653	1,4-Dichlorobenzene-d4	7.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Acetoxyisobutyryl chloride	164	C6H9ClO3	040635-66-3	42
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25
4	2-Butanol, 1-methoxy-	104	C5H12O2	053778-73-7	23
5	Hexaethylene glycol dimethyl ether	310	C14H30O7	001072-40-8	23





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082120\
Data File : BM027186.D
Acq On : 22 Aug 2020 01:06
Operator : JU/CG
Sample : L3746-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 359

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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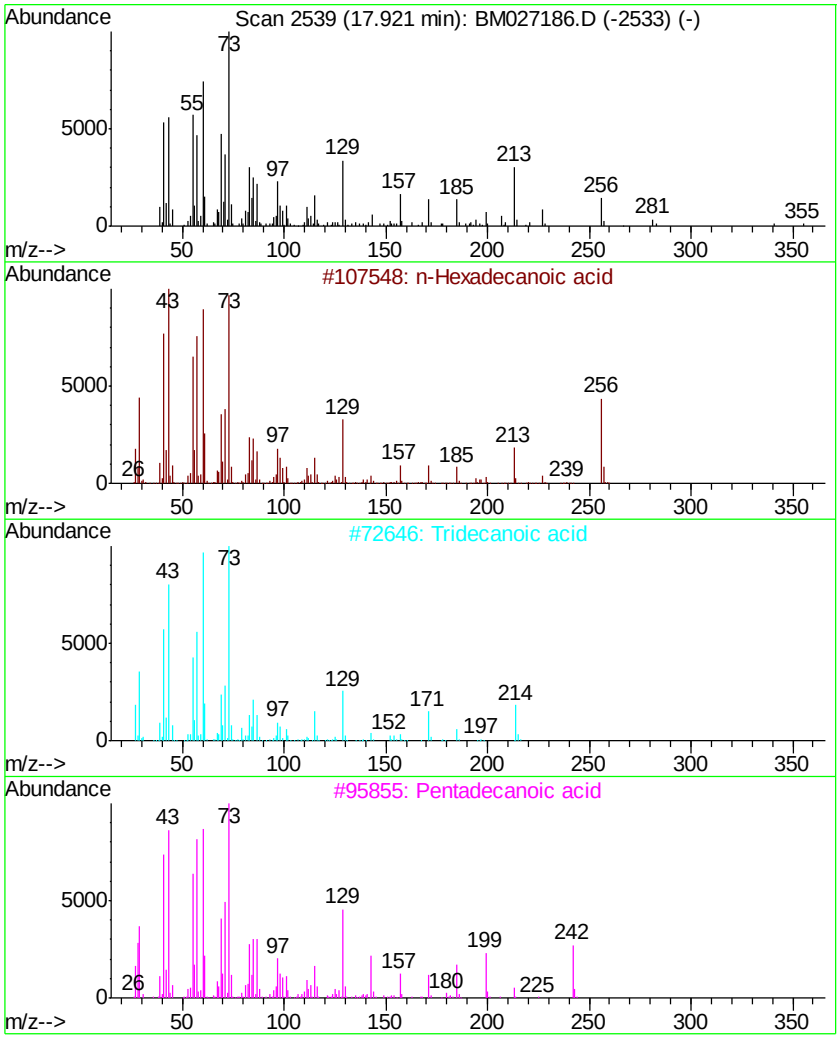
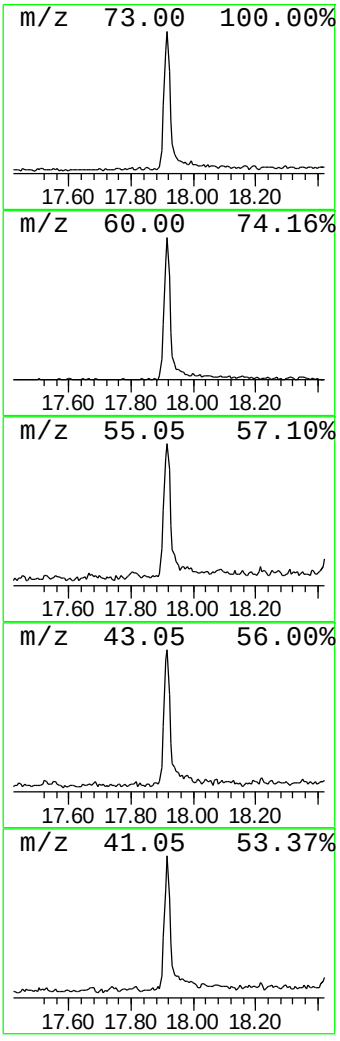
Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.92	4.90 ng	362538	Phenanthrene-d10	16.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	62
5	Dodecanoic acid	200	C12H24O2	000143-07-7	49





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Data File : BM027186.D
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Operator : JU/CG
Sample : L3746-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 359

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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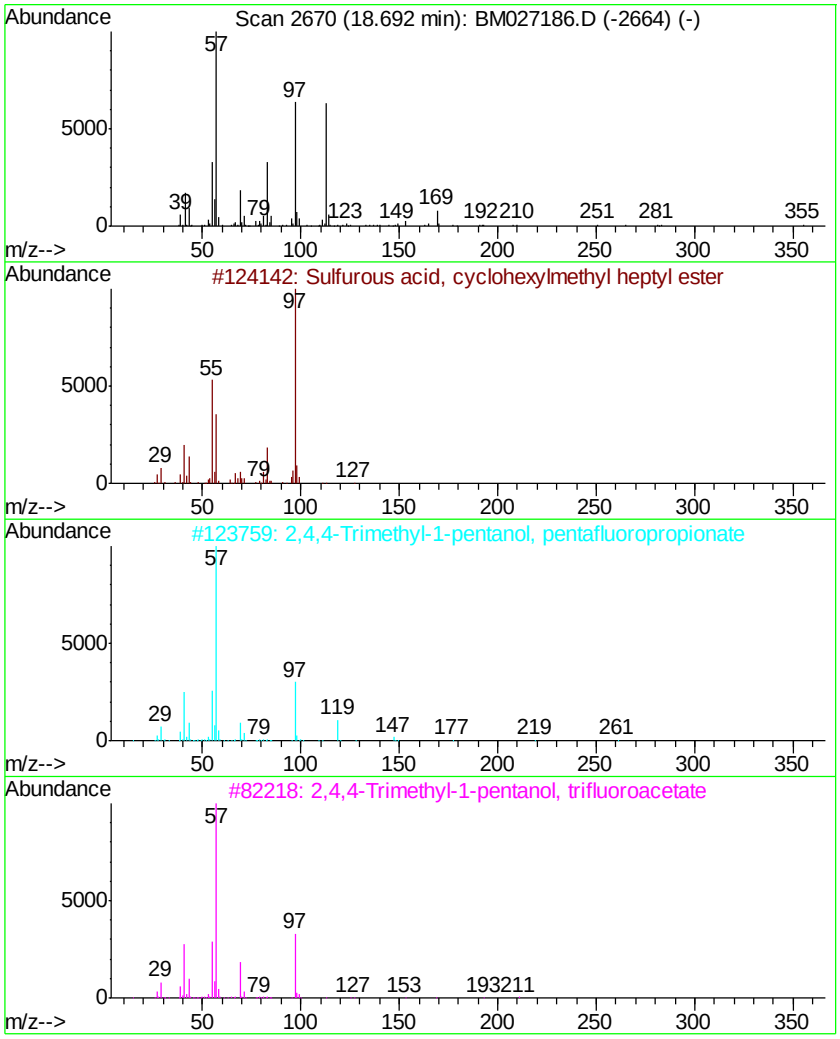
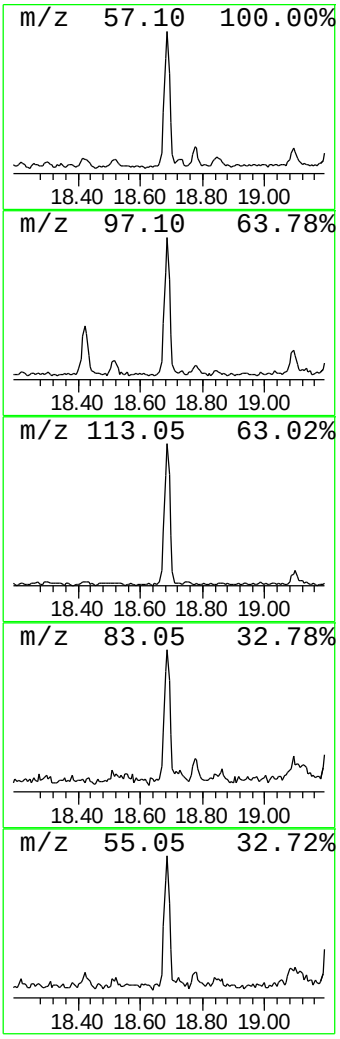
Peak Number 4 unknown18.69 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.69	2.61 ng	192817	Phenanthrene-d10	16.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, cyclohexylmethyl...	276	C14H28O3S	1000309-21-7	37
2	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	35
3	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	25
4	Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1000309-21-6	25
5	Pentyl ethylphosphonofluoridate	182	C7H16FO2P	162085-84-9	22





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082120\
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Acq On : 22 Aug 2020 01:06
Operator : JU/CG
Sample : L3746-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 359

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

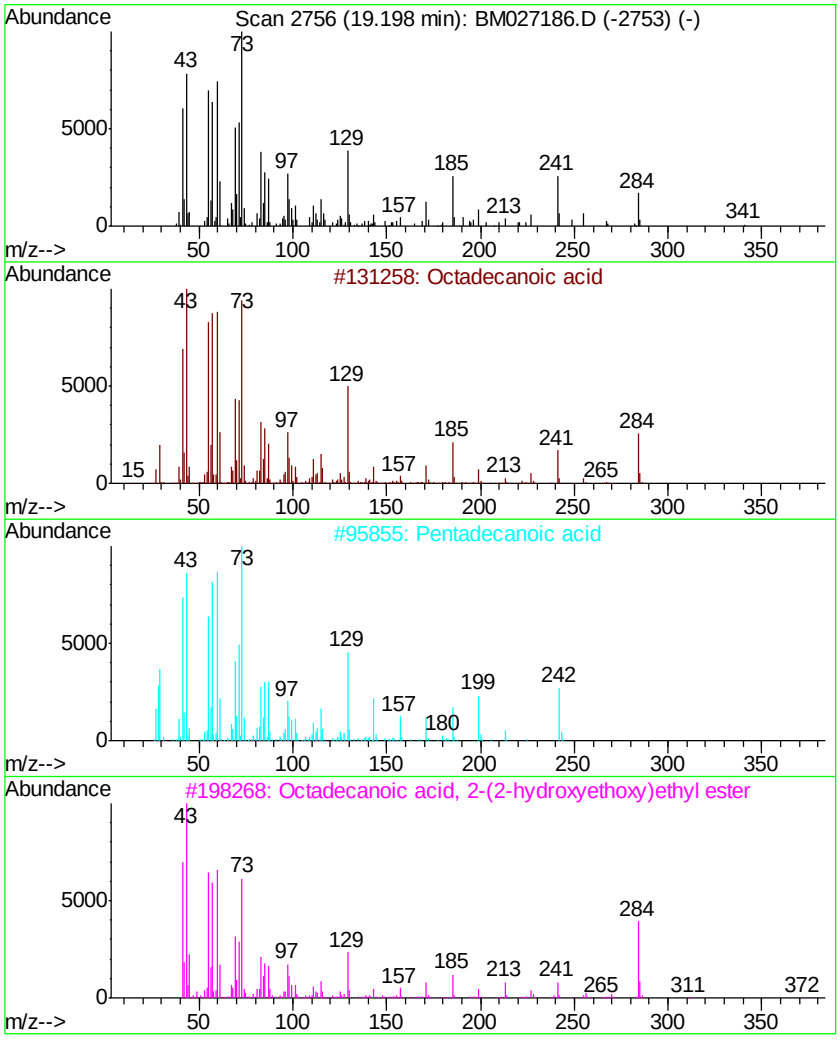
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

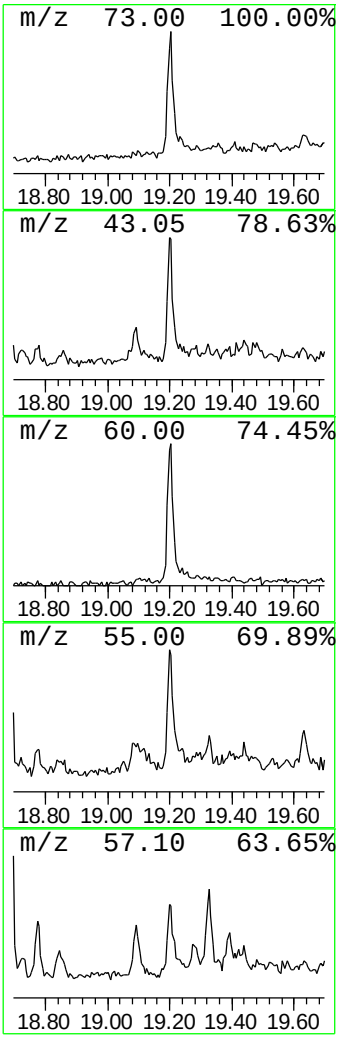
****

Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.20	2.18 ng	201398	Chrysene-d12	21.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64
4	.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	30
5	n-Decanoic acid	172	C10H20O2	000334-48-5	22





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Sample : L3746-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 359

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

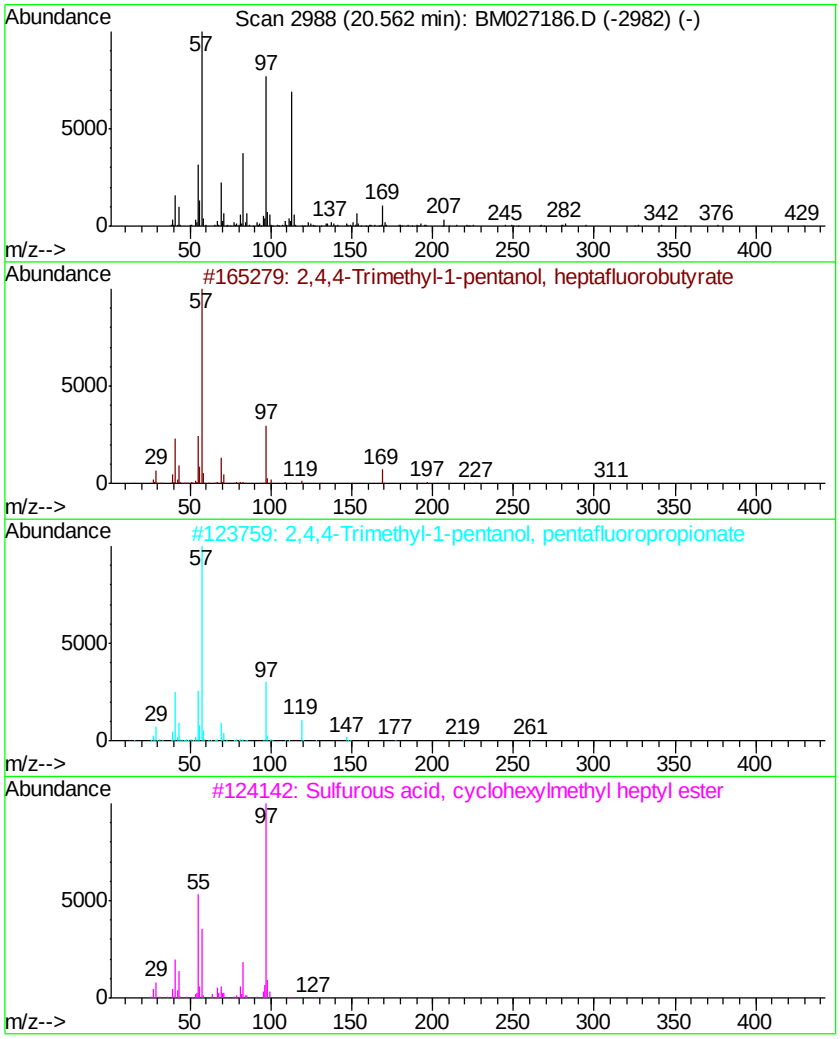
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

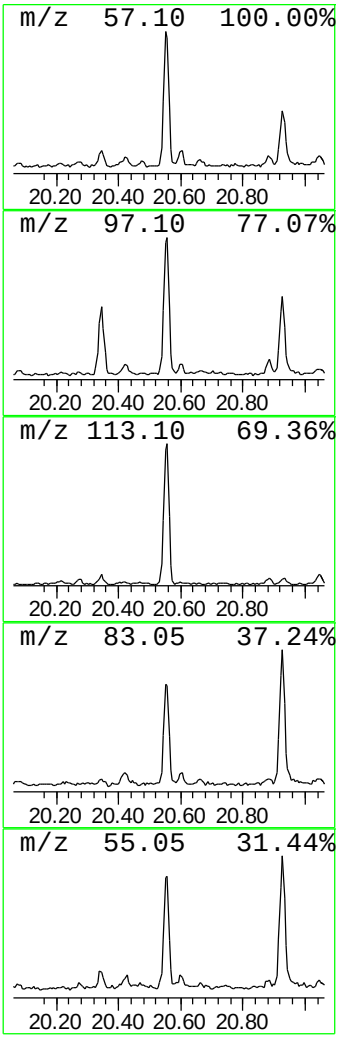
****

Peak Number 6 unknown20.56 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.56	4.03 ng	371615	Chrysene-d12	21.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	38
2	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	38
3	Sulfurous acid, cyclohexylmethyl...	276	C14H28O3S	1000309-21-7	38
4	Cyclohexane, 1-methyl-2-pentyl-	168	C12H24	054411-01-7	35
5	Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	35





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

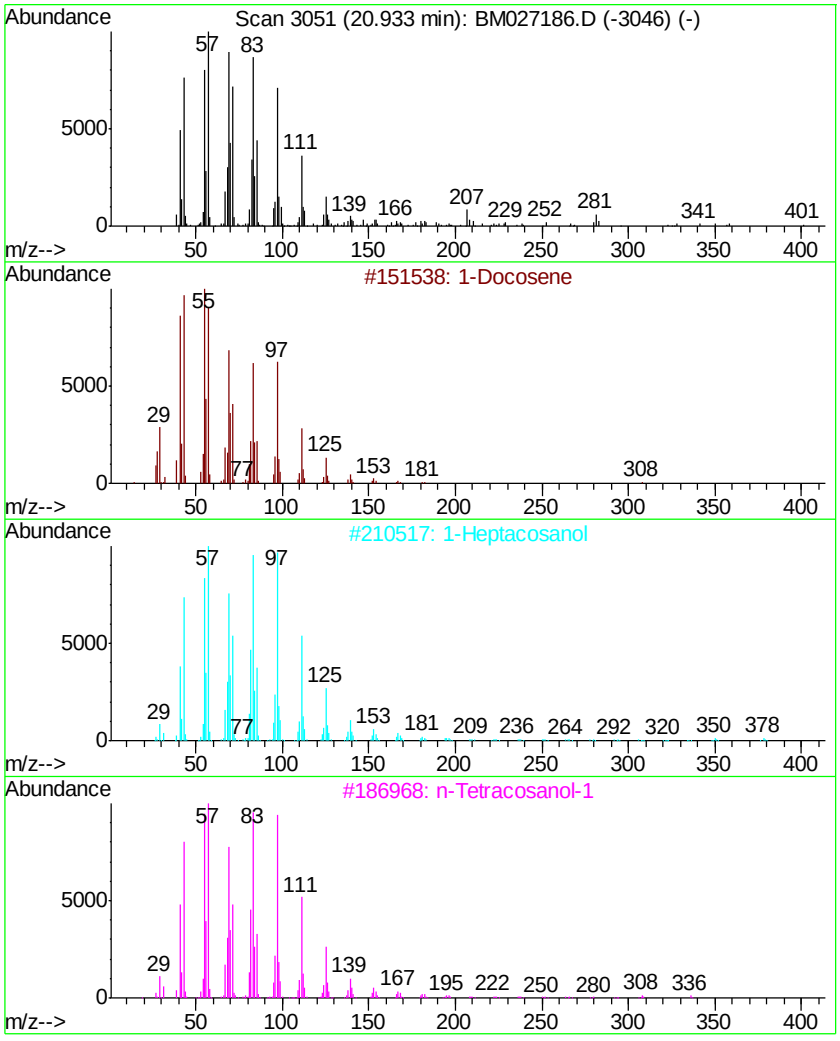
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

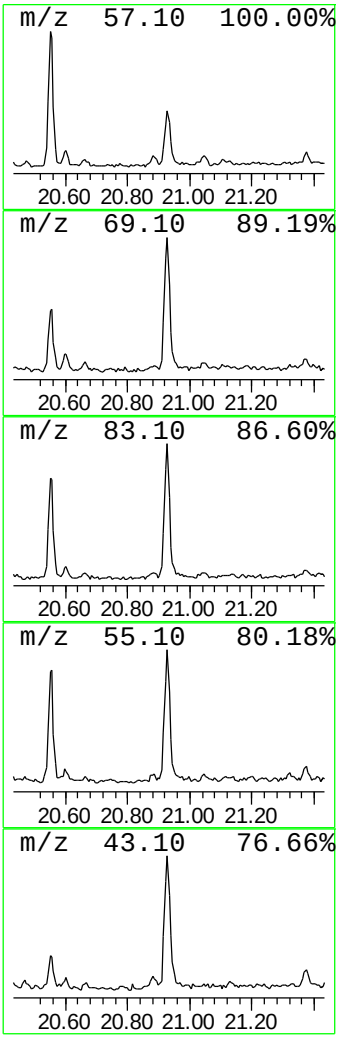
****

Peak Number 7 1-Docosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.93	4.77 ng	439852	Chrysene-d12	21.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	81
2	1-Heptacosanol	396	C27H56O	002004-39-9	76
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	70
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	64
5	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM082120\
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Quant Title : ASP BNA STANDARDS FOR 5 POINT 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
3-Hexen-2-one	4.20	3.0	ng	109530	1	7.61	731696	20.0
unknown4.78	4.78	2.0	ng	74653	1	7.61	731696	20.0
n-Hexadecanoic acid	17.92	4.9	ng	362538	4	16.99	1479520	20.0
unknown18.69	18.69	2.6	ng	192817	4	16.99	1479520	20.0
Octadecanoic acid	19.20	2.2	ng	201398	5	21.19	1845180	20.0
unknown20.56	20.56	4.0	ng	371615	5	21.19	1845180	20.0
1-Docosene	20.93	4.8	ng	439852	5	21.19	1845180	20.0