LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031021\
Data File : BM029081.D
Acq On : 10 Mar 2021 22:02
Operator : CG/JU
Sample : M1607-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : NB-07-030921

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-BM022321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029081.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.234	377	382	403	rBB	141305	222326	28.72%	5.341%
2	6.863	653	659	671	rBV	146640	235416	30.41%	5.656%
3	6.969	671	677	684	rVB	8253	12683	1.64%	0.305%
4	7.663	790	795	802	rBB	40199	57818	7.47%	1.389%
5	8.839	989	995	1004	rBV	84056	133388	17.23%	3.204%
6	10.457	1264	1270	1279	rVB	49713	80031	10.34%	1.923%
7	12.945	1687	1693	1703	rBV	228760	317505	41.01%	7.628%
8	14.333	1924	1929	1935	rVB2	71705	101416	13.10%	2.436%
9	15.833	2179	2184	2192	rBV	137586	193011	24.93%	4.637%
10	16.045	2215	2220	2228	rBV4	3893	8415	1.09%	0.202%
11	17.080	2389	2396	2401	rBV	87218	116703	15.07%	2.804%
12	17.745	2504	2509	2514	rBV	159720	185881	24.01%	4.466%
13	17.974	2545	2548	2553	rBV2	12499	19949	2.58%	0.479%
14	18.715	2670	2674	2679	rVB	13790	18358	2.37%	0.441%
15	18.892	2699	2704	2707	rBV	648235	774246	100.00%	18.600%
16	18.927	2707	2710	2721	rVB2	535769	689700	89.08%	16.569%
17	19.056	2728	2732	2737	rVB	111281	120922	15.62%	2.905%
18	19.262	2764	2767	2772	rBV5	9849	15893	2.05%	0.382%
19	19.709	2837	2843	2848	rBV	384478	488483	63.09%	11.735%
20	20.974	3055	3058	3065	rVB	50805	76663	9.90%	1.842%
21	21.256	3102	3106	3114	rVB	114093	150990	19.50%	3.627%
22	23.409	3468	3472	3479	rVB2	79518	142737	18.44%	3.429%

Sum of corrected areas: 4162534

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031021\
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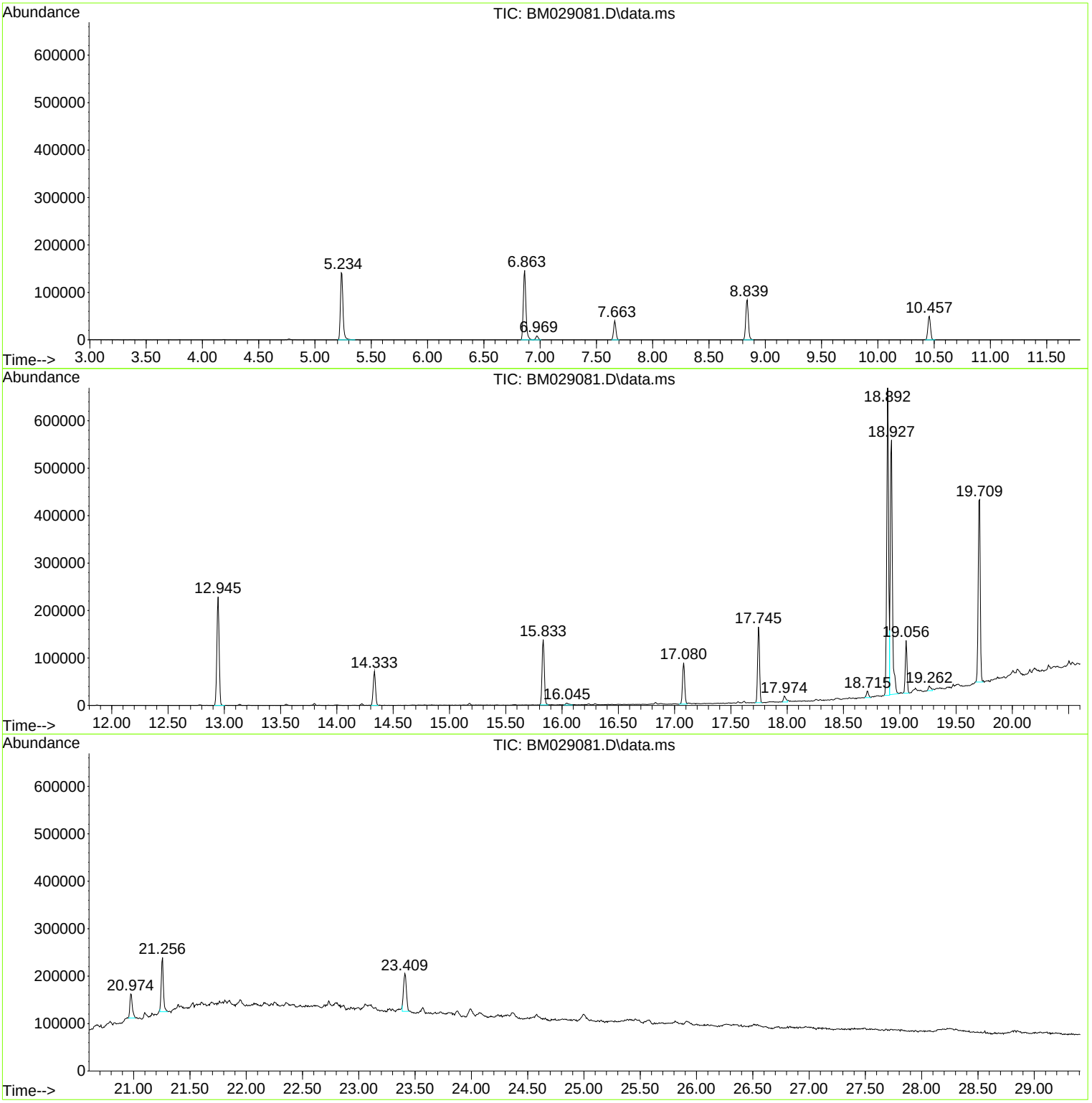
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-07-030921

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.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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Data File : BM029081.D
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Instrument :
BNA_M
ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

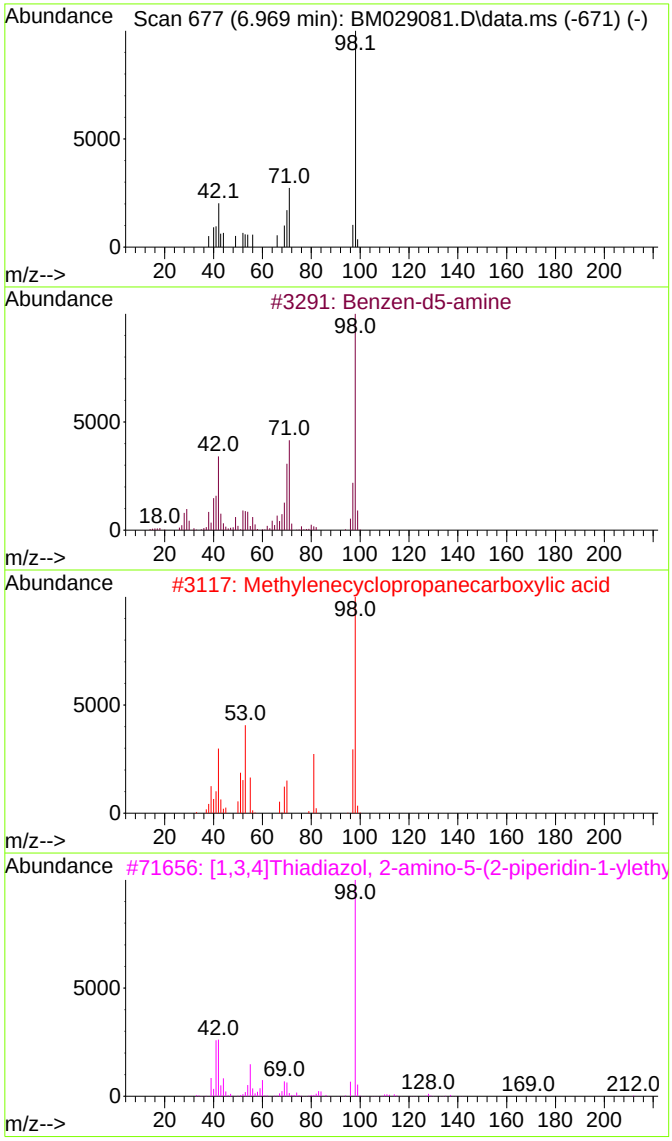
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

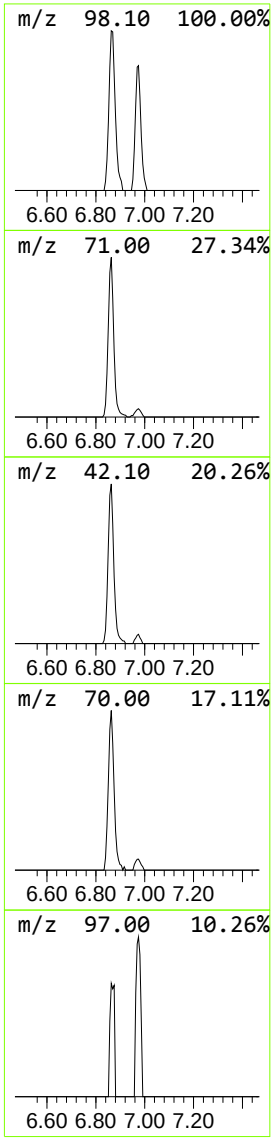
****

Peak Number 1 Benzen-d5-amine Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.969	4.39 ng	12683	1,4-Dichlorobenzene-d4	7.663

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzen-d5-amine	98	C6H2D5N	004165-61-1	50
2	Methylenecyclopropanecarboxylic ...	98	C5H6O2	062266-36-8	42
3	[1,3,4]Thiadiazol, 2-amino-5-(2-...	212	C9H16N4S	1000303-12-6	36
4	1,2-Cyclopentanedione	98	C5H6O2	003008-40-0	36
5	Piperidine, 1,1'-methylenebis-	182	C11H22N2	000880-09-1	36





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Data File : BM029081.D
Acq On : 10 Mar 2021 22:02
Operator : CG/JU
Sample : M1607-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : NB-07-030921

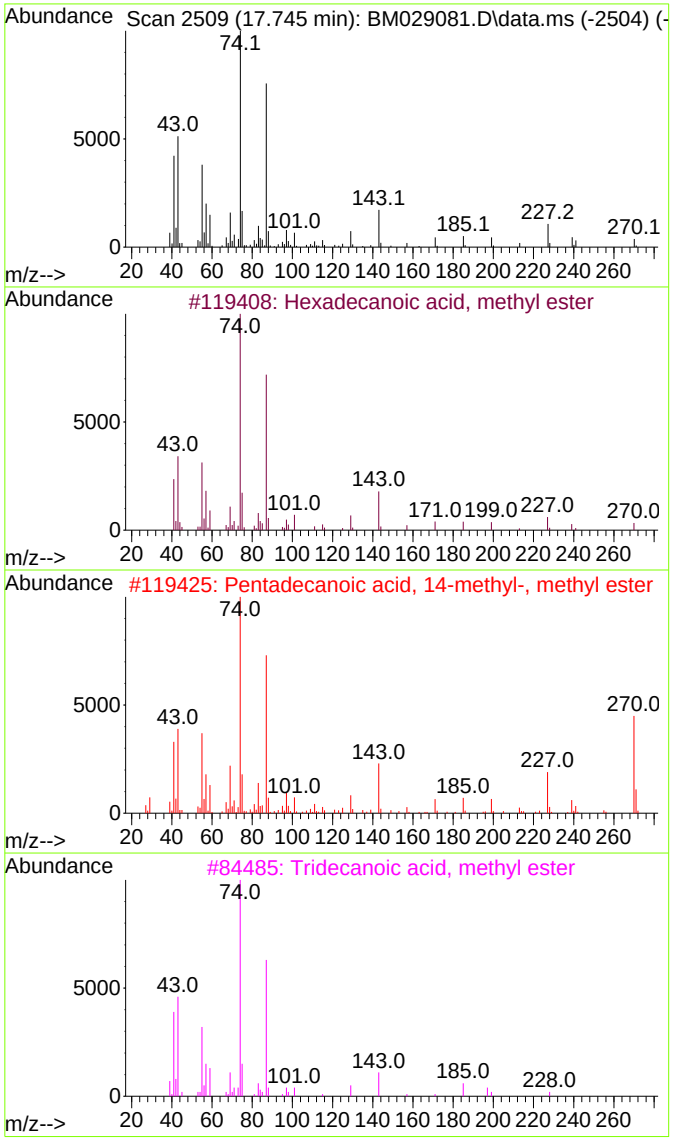
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

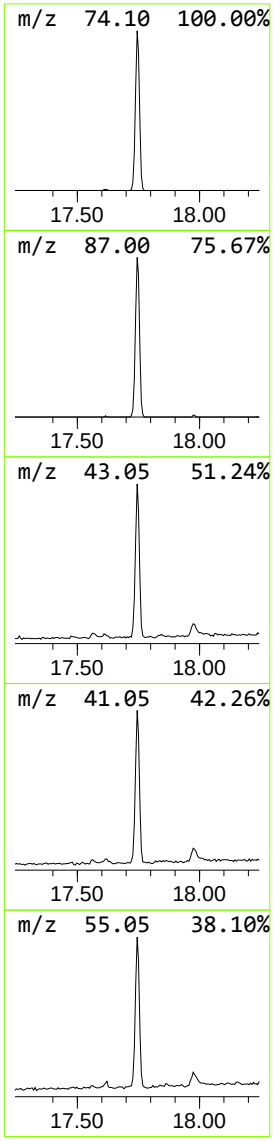
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.745	31.86 ng	185881	Phenanthrene-d10	17.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	95
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	93
4	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	87
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86





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Data File : BM029081.D
Acq On : 10 Mar 2021 22:02
Operator : CG/JU
Sample : M1607-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : NB-07-030921

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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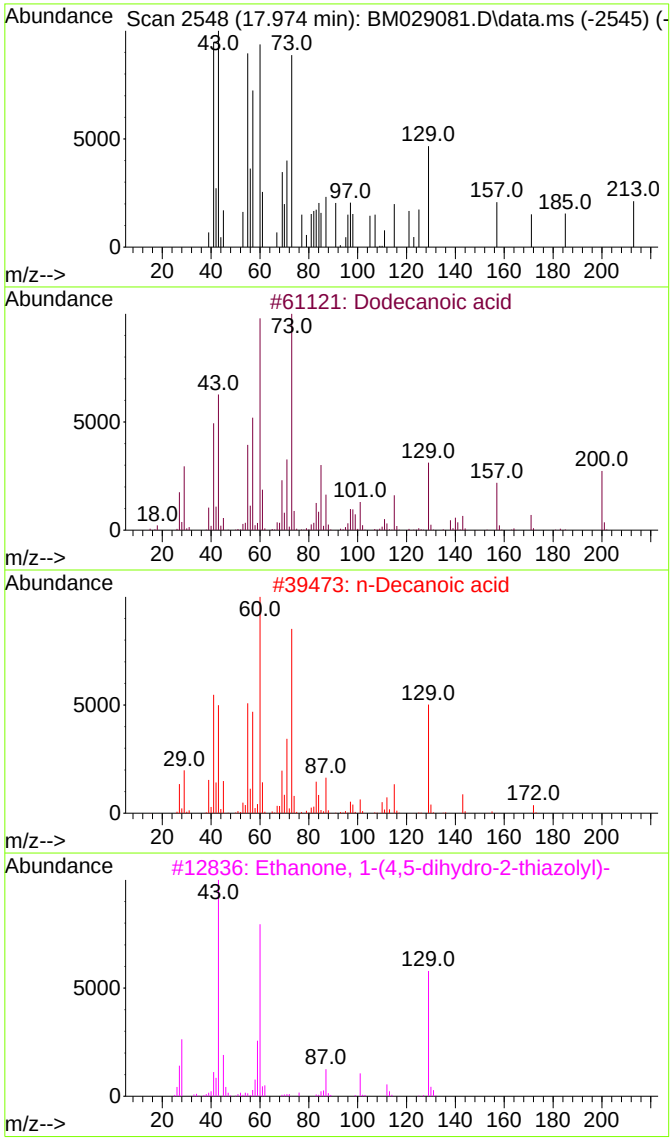
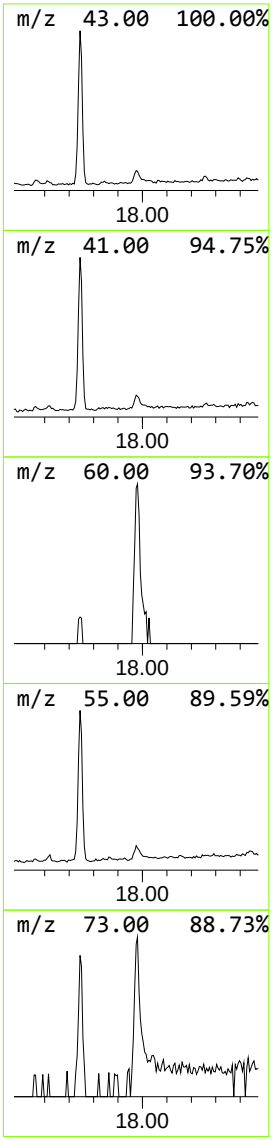
****

Peak Number 3 Dodecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.974	3.42 ng	19949	Phenanthrene-d10	17.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	59
2	n-Decanoic acid	172	C10H20O2	000334-48-5	59
3	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	38
4	Nonanoic acid	158	C9H18O2	000112-05-0	27
5	.alpha.-D-Glucopyranoside, O-.al...	504	C18H32O16	000597-12-6	27





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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-07-030921

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

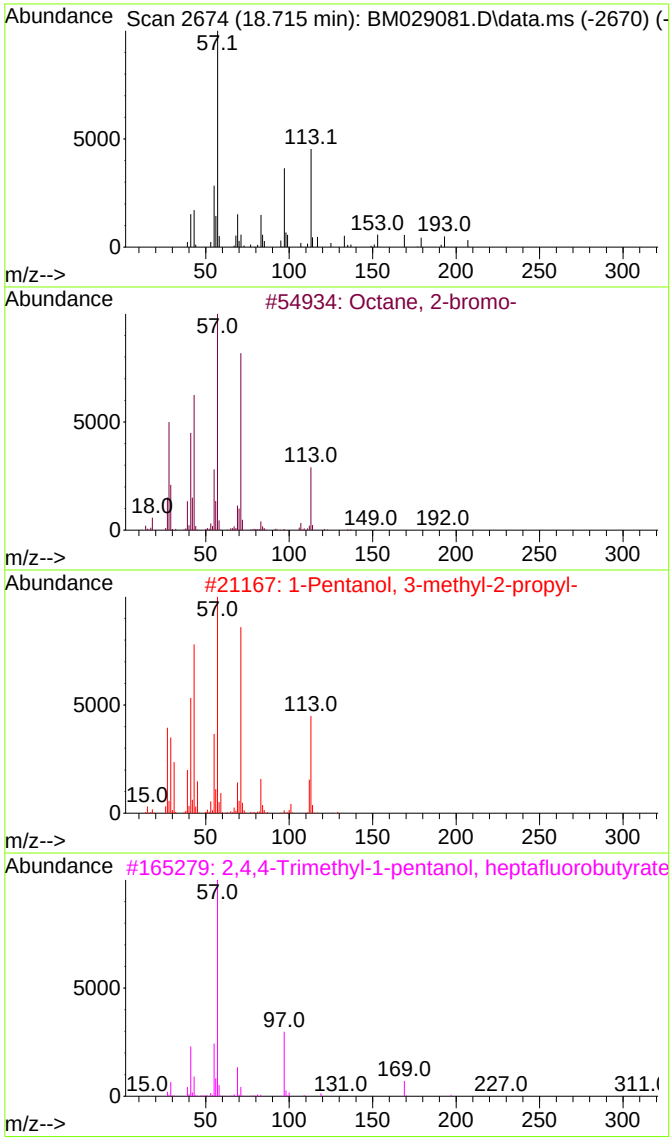
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

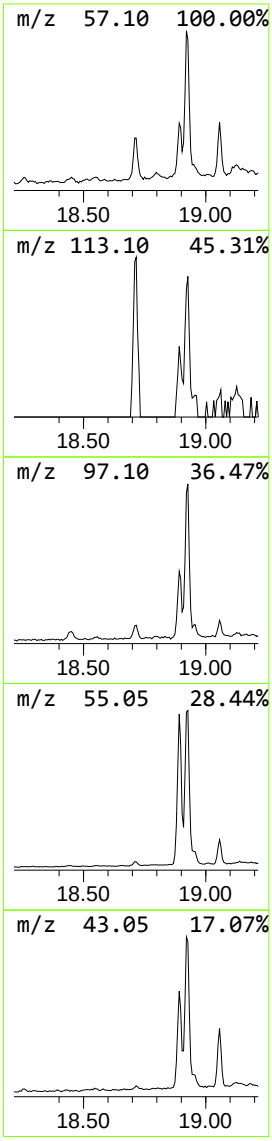
****

Peak Number 4 unknown18.715 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.715	3.15 ng	18358	Phenanthrene-d10	17.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2-bromo-	192	C8H17Br	000557-35-7	43
2	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	37
3	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	27
4	Heptane, 4-(bromomethyl)-	192	C8H17Br	101654-29-9	25
5	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	25





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Operator : CG/JU
Sample : M1607-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-07-030921

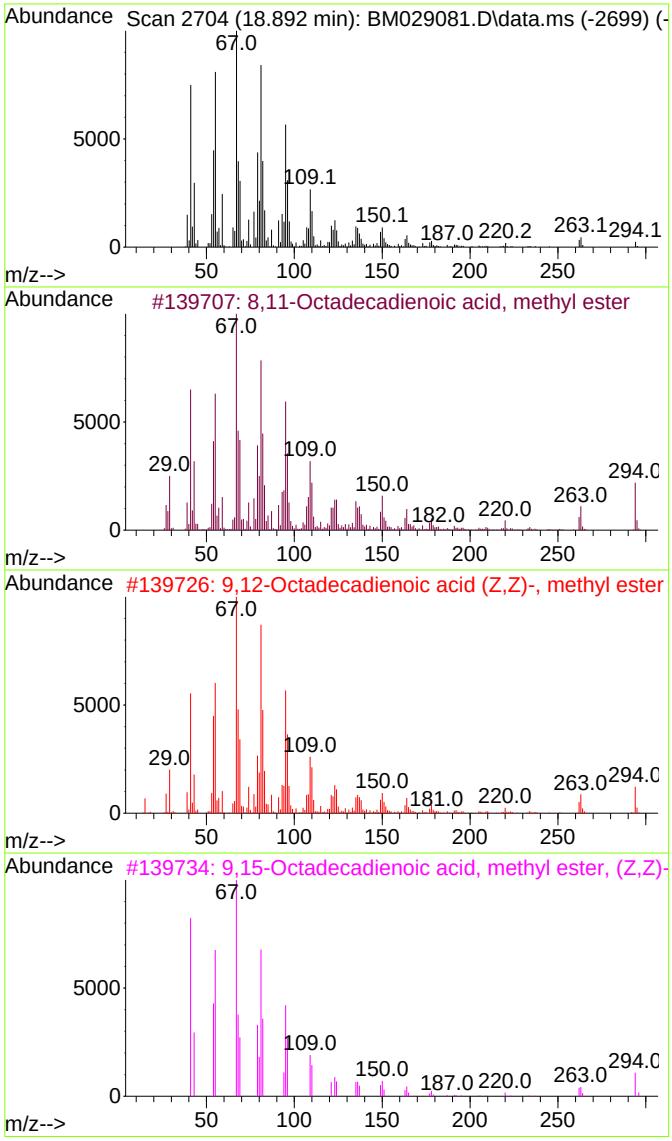
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

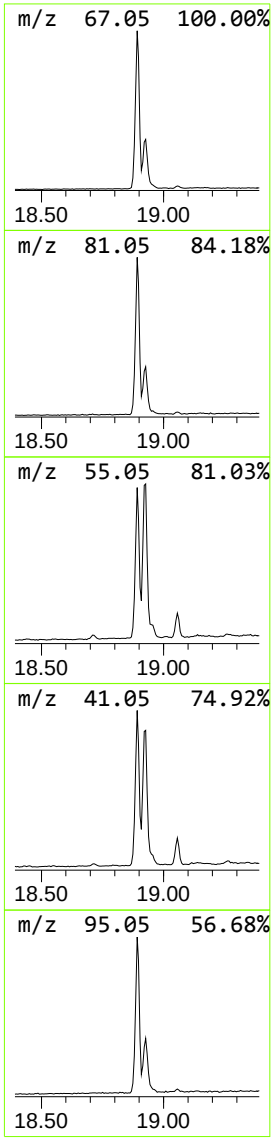
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 8,11-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.892	132.69 ng	774246	Phenanthrene-d10	17.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	99
2	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
3	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
5	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	99





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Data File : BM029081.D
Acq On : 10 Mar 2021 22:02
Operator : CG/JU
Sample : M1607-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-07-030921

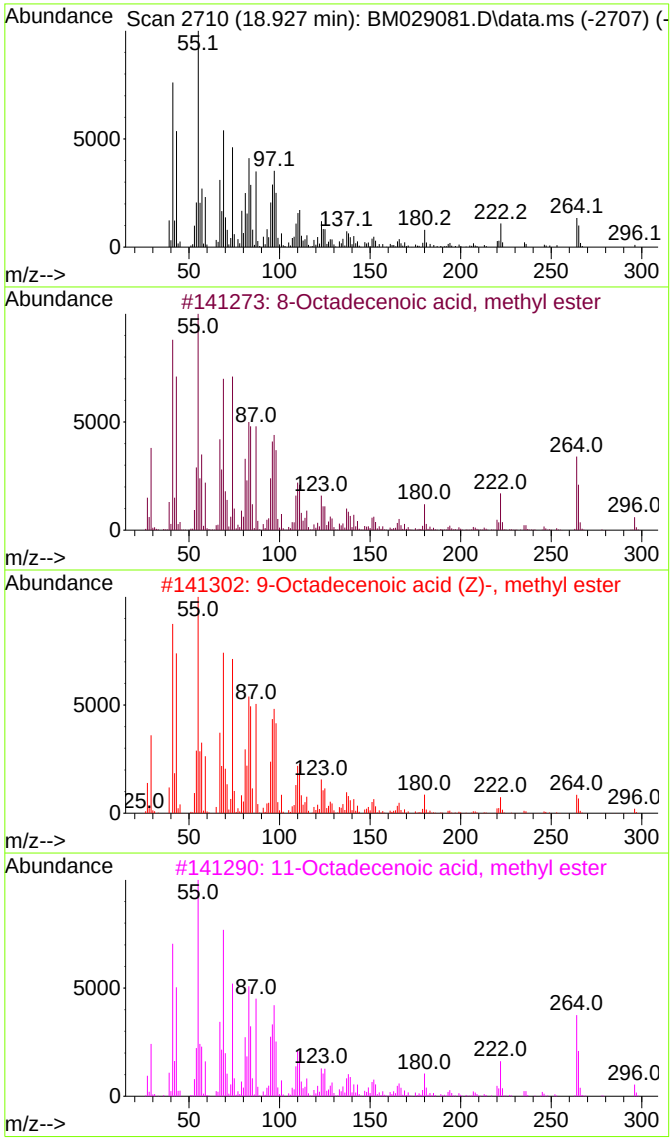
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

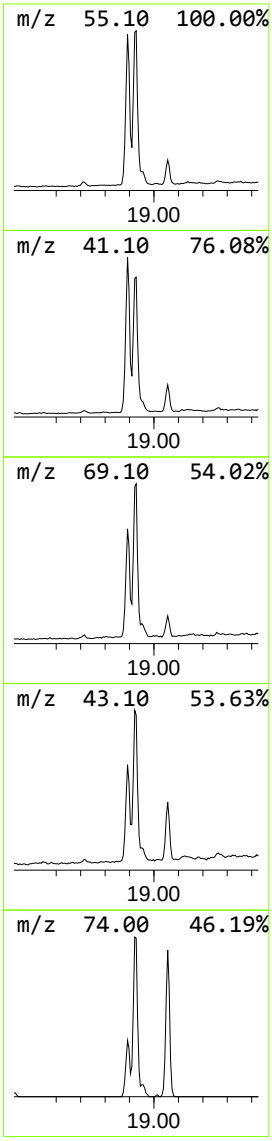
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 8-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.927	118.20 ng	689700	Phenanthrene-d10	17.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	99
2	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
3	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	99
4	7-Octadecenoic acid, methyl ester	296	C19H36O2	057396-98-2	97
5	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	96





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Data File : BM029081.D
Acq On : 10 Mar 2021 22:02
Operator : CG/JU
Sample : M1607-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : NB-07-030921

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

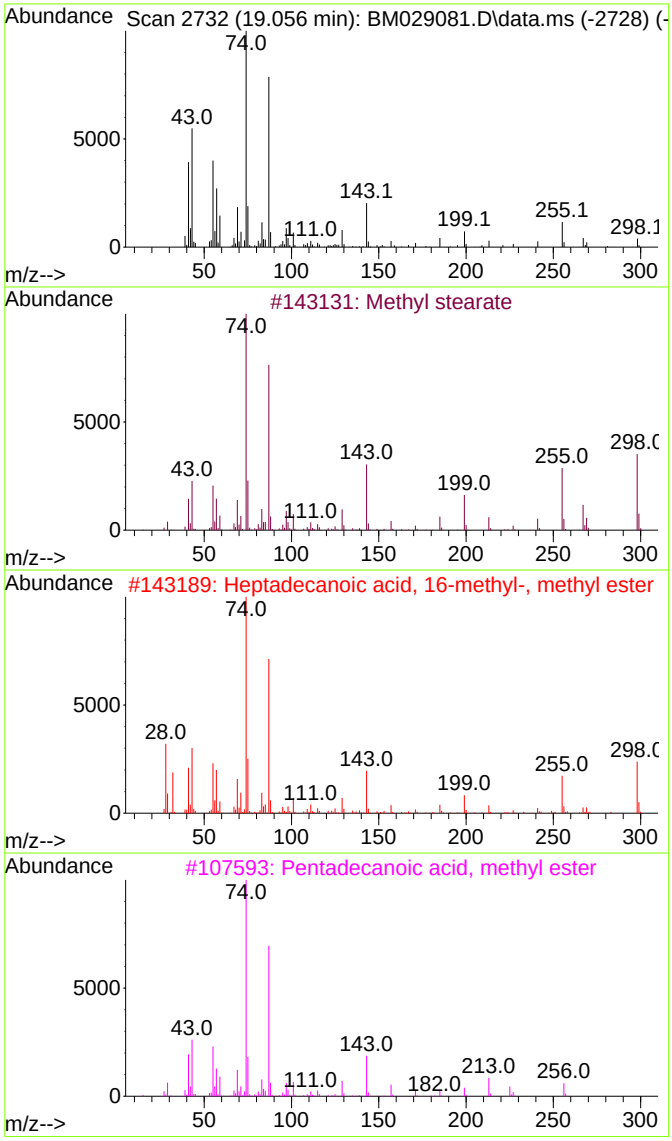
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

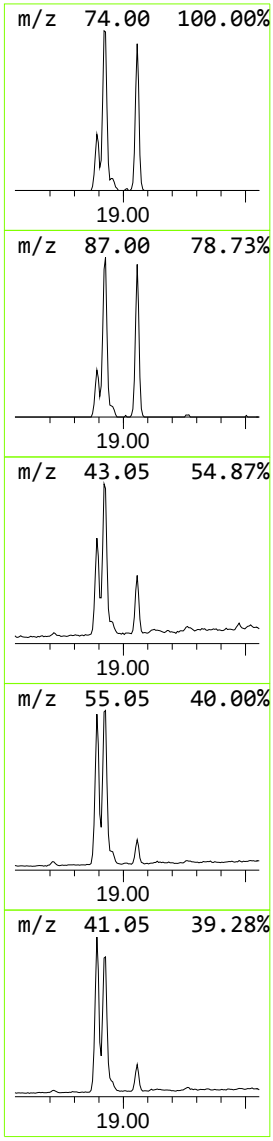
****

Peak Number 7 Methyl stearate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.056	20.72 ng	120922	Phenanthrene-d10	17.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	98
2	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	95
3	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	87
4	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	86
5	Undecanoic acid, 10-methyl-, met...	214	C13H26O2	005129-56-6	80





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Data File : BM029081.D
Acq On : 10 Mar 2021 22:02
Operator : CG/JU
Sample : M1607-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : NB-07-030921

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

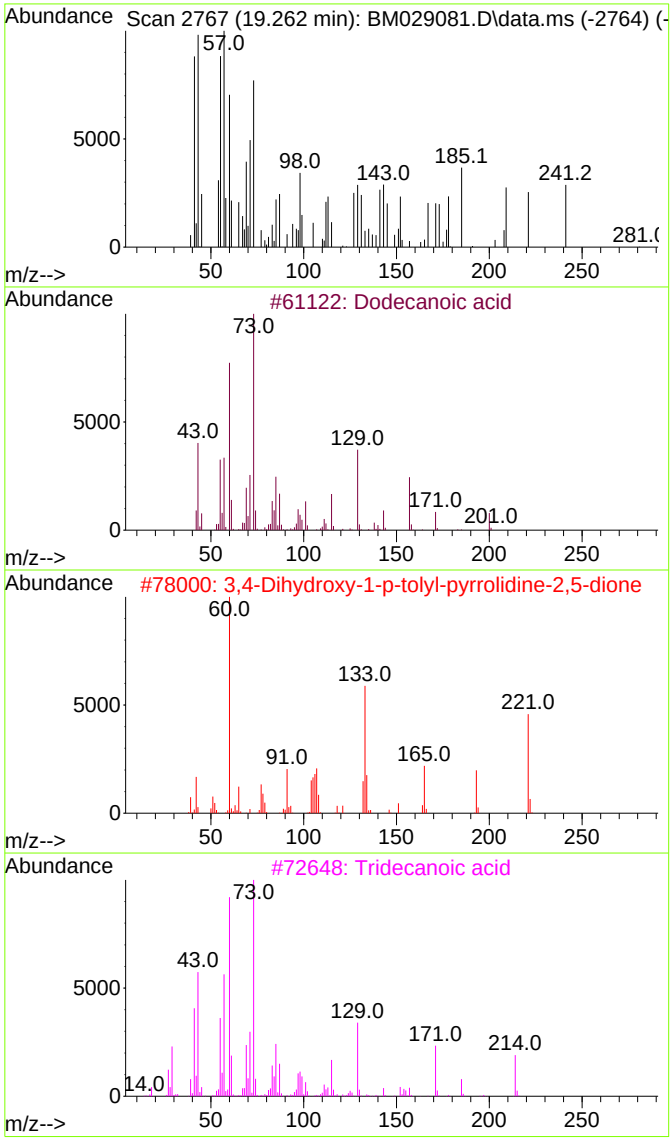
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

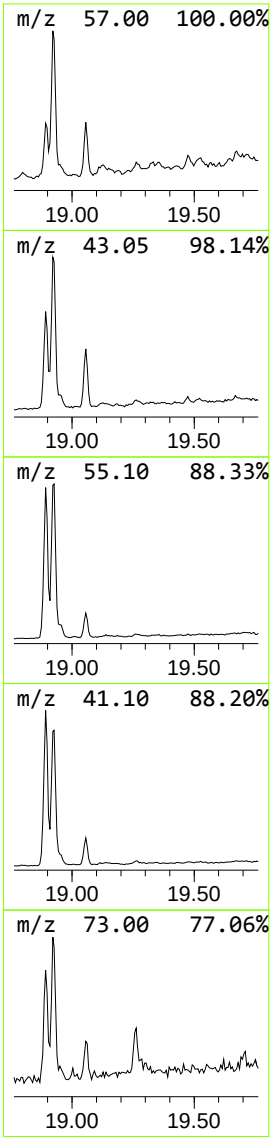
****

Peak Number 8 unknown19.262 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.262	2.11 ng	15893	Chrysene-d12	21.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	10
2	3,4-Dihydroxy-1-p-tolyl-pyrrolid...	221	C11H11NO4	1000317-72-5	10
3	Tridecanoic acid	214	C13H26O2	000638-53-9	10
4	4-Bromobutanoic acid, butyl ester	222	C8H15BrO2	003540-75-8	9
5	Methyl isopropylidene-.beta.-d-a...	204	C9H16O5	1000129-88-1	9





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ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : NB-07-030921

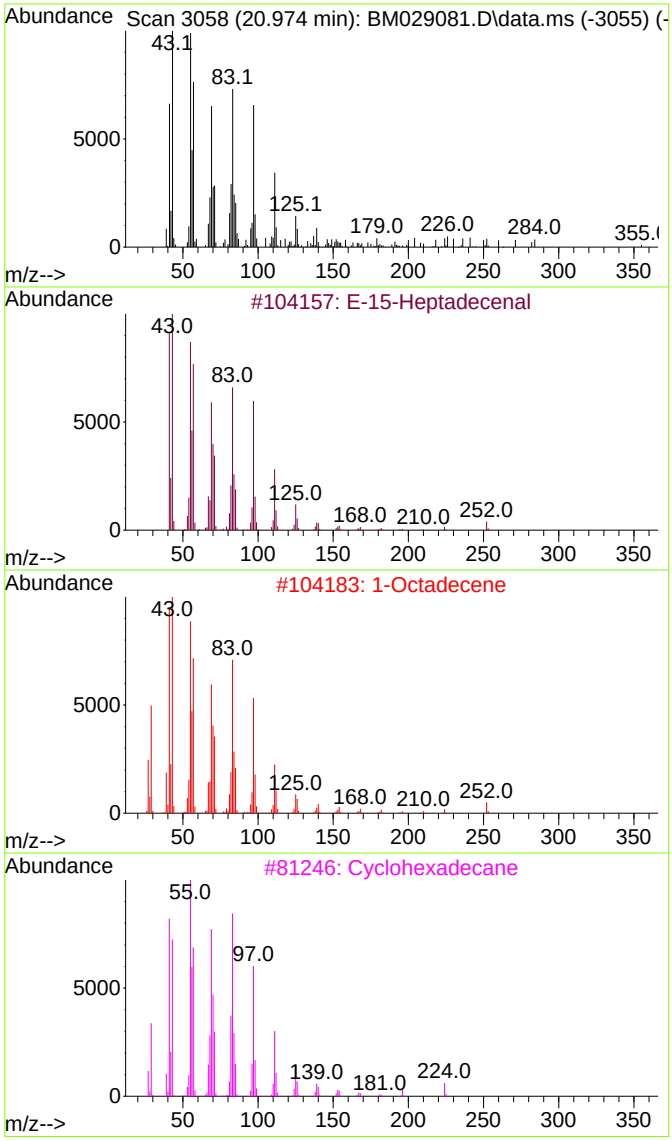
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

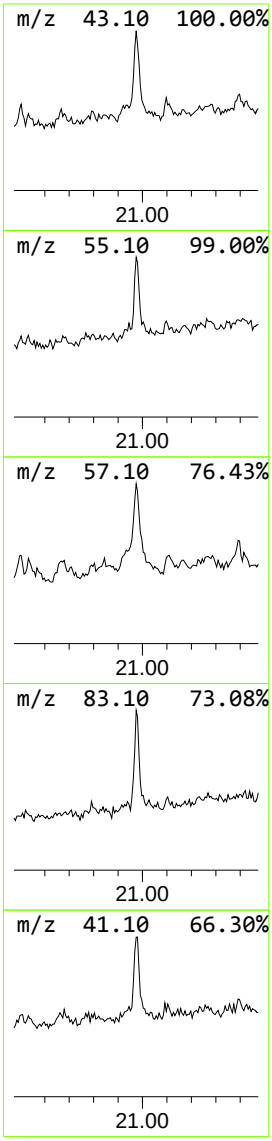
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 E-15-Heptadecenal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.974	10.15 ng	76663	Chrysene-d12	21.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal	252	C17H32O	1000130-97-9	95
2	1-Octadecene	252	C18H36	000112-88-9	93
3	Cyclohexadecane	224	C16H32	000295-65-8	91
4	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	90
5	Cycloeicosane	280	C20H40	000296-56-0	90





Tentatively Identified Compound (LSC) summary

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Data File : BM029081.D
Acq On : 10 Mar 2021 22:02
Operator : CG/JU
Sample : M1607-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : NB-07-030921

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
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
Benzen-d5-amine	6.969	4.4	ng	12683	1	7.663	57818	20.0
Hexadecanoic ac...	17.745	31.9	ng	185881	4	17.080	116703	20.0
Dodecanoic acid	17.974	3.4	ng	19949	4	17.080	116703	20.0
unknown18.715	18.715	3.1	ng	18358	4	17.080	116703	20.0
8,11-Octadecadi...	18.892	132.7	ng	774246	4	17.080	116703	20.0
8-Octadecenoic ...	18.927	118.2	ng	689700	4	17.080	116703	20.0
Methyl stearate	19.056	20.7	ng	120922	4	17.080	116703	20.0
unknown19.262	19.262	2.1	ng	15893	5	21.256	150990	20.0
E-15-Heptadecenal	20.974	10.2	ng	76663	5	21.256	150990	20.0