LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111120\
Data File : BP003936.D
Acq On : 11 Nov 2020 23:55
Operator : CG/JU
Sample : L4622-05 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : PAV-B12-10-17

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_P\METHODS\8270-BP110320.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP003936.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.928	3	7	27	rVB	1340541	2134525	3.22%	1.476%
2	5.811	489	497	510	rBV	912920	1419033	2.14%	0.981%
3	7.452	768	776	790	rBV	896543	1459326	2.20%	1.009%
4	8.281	910	917	924	rVB	635015	1028344	1.55%	0.711%
5	9.446	1102	1115	1125	rBV	575579	993773	1.50%	0.687%
6	11.116	1389	1399	1405	rBV	850798	1511773	2.28%	1.046%
7	13.528	1802	1809	1817	rBV	1336794	1924578	2.91%	1.331%
8	14.904	2037	2043	2050	rVB	1185869	1737310	2.62%	1.202%
9	16.387	2290	2295	2300	rBV	889282	1224057	1.85%	0.847%
10	17.639	2502	2508	2512	rBV	1367279	1900016	2.87%	1.314%
11	18.133	2589	2592	2598	rVB	991116	1100965	1.66%	0.761%
12	18.263	2608	2614	2619	rBV	13062442	16120768	24.34%	11.150%
13	19.345	2792	2798	2801	rBV	18832535	28270713	42.69%	19.554%
14	19.392	2801	2806	2813	rVB2	33945910	66222448	100.00%	45.803%
15	19.498	2819	2824	2829	rVB	6601053	7933089	11.98%	5.487%
16	19.833	2878	2881	2886	rVB	647041	766234	1.16%	0.530%
17	20.139	2929	2933	2938	rVB	2063254	2445596	3.69%	1.692%
18	20.345	2964	2968	2969	rBV	638116	770874	1.16%	0.533%
19	20.433	2979	2983	2987	rVB	1790979	1938681	2.93%	1.341%
20	20.539	2997	3001	3004	rBV	1046900	1177833	1.78%	0.815%
21	20.575	3004	3007	3013	rVV4	424187	762929	1.15%	0.528%
22	21.674	3190	3194	3198	rVB	1328202	1737176	2.62%	1.202%

Sum of corrected areas: 144580041

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111120\
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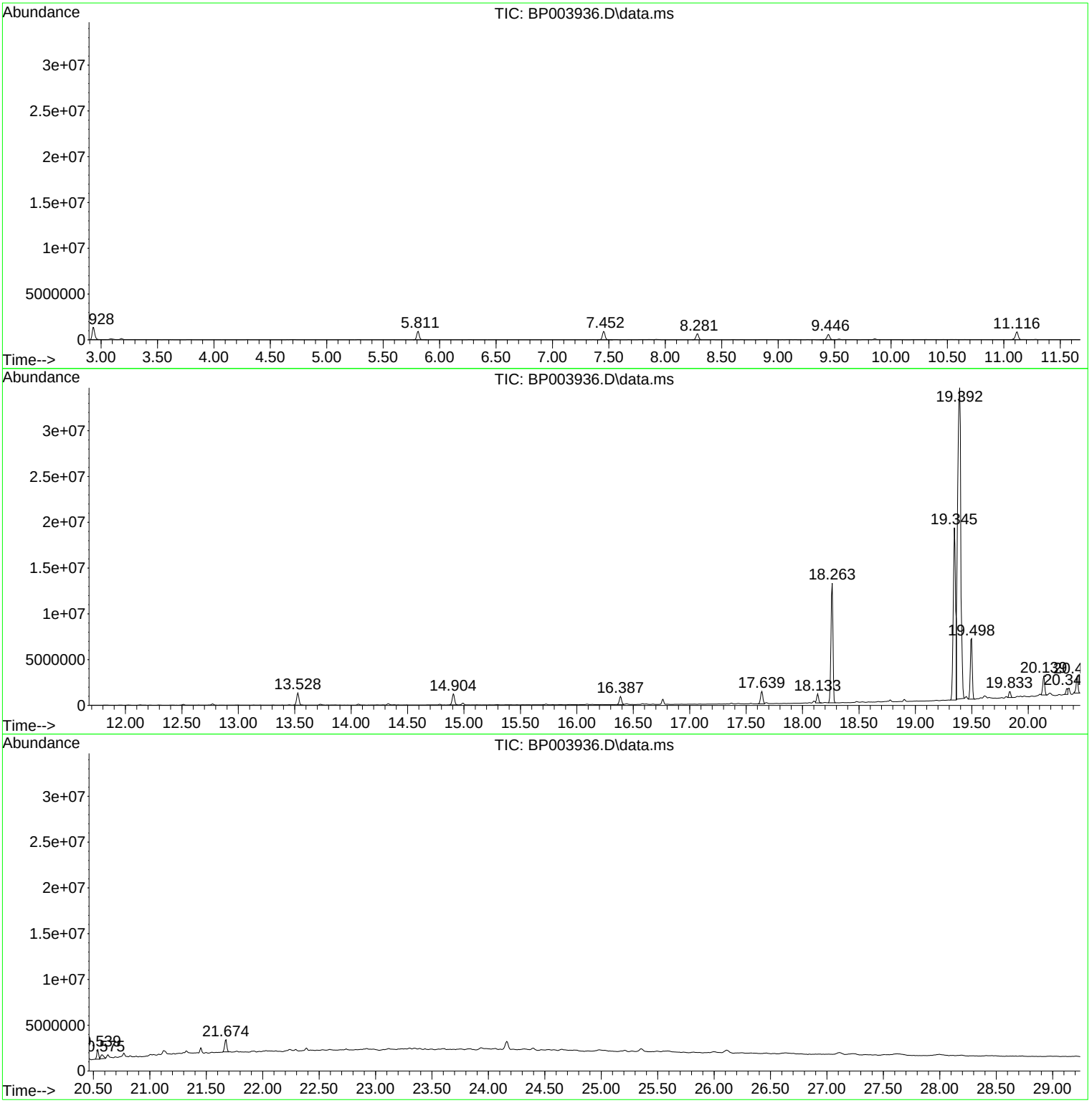
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PAV-B12-10-17

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.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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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

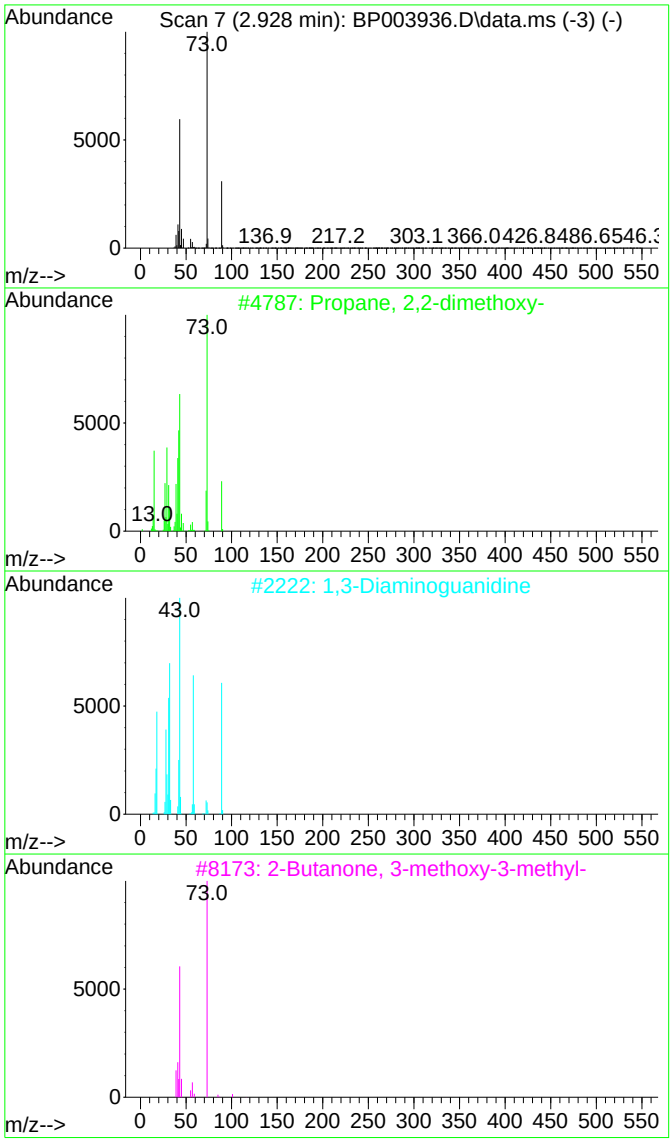
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

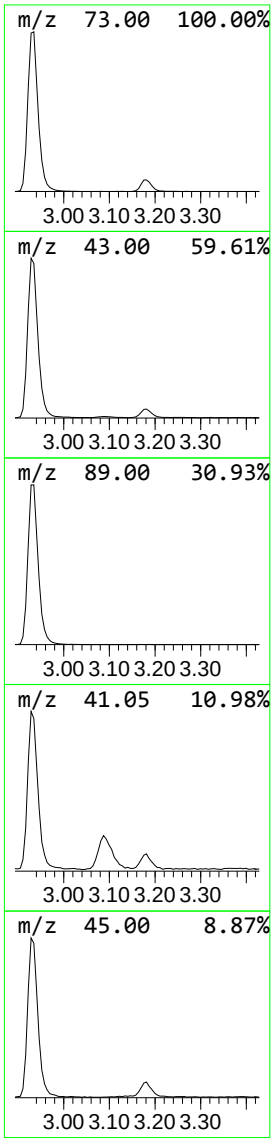
****

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.928	41.51 ng	2134530	1,4-Dichlorobenzene-d4	8.281

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	50
2	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
3	2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	9
4	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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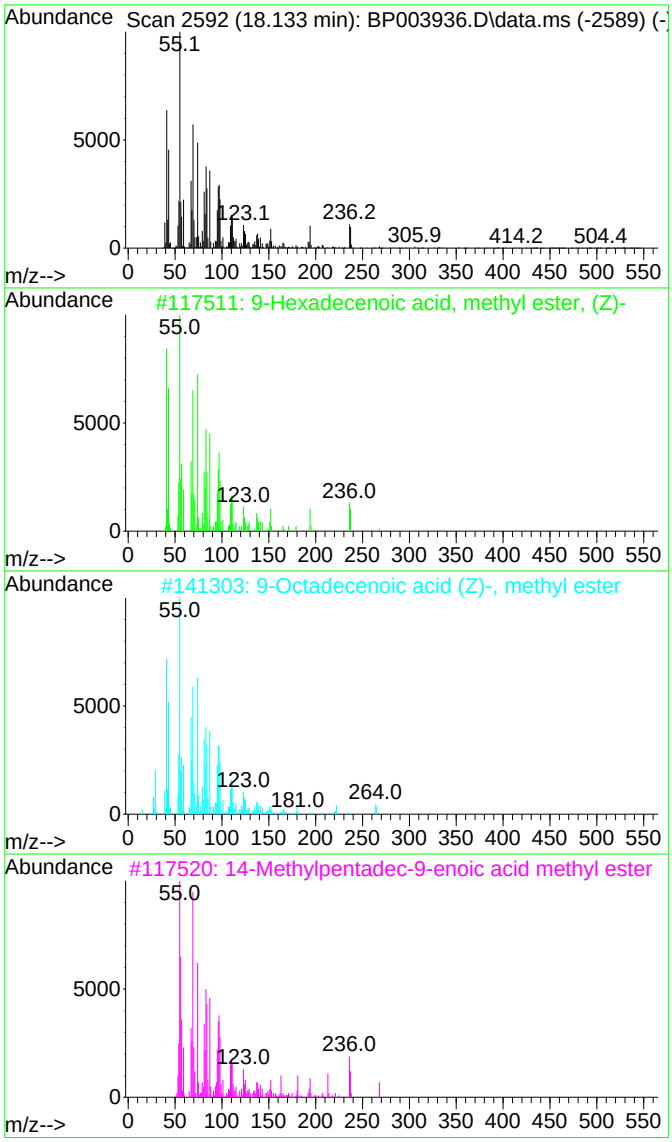
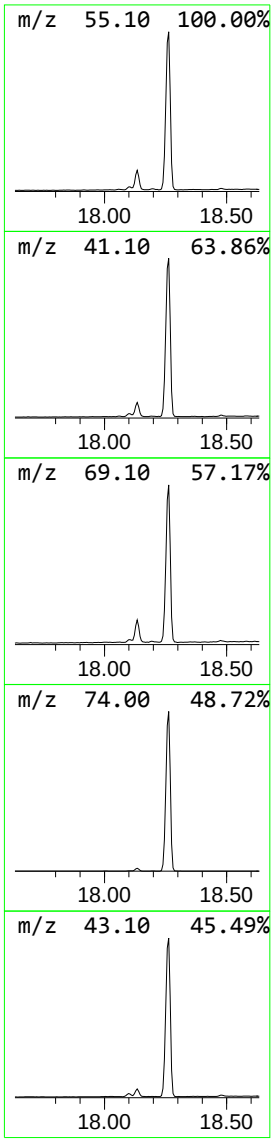
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 9-Hexadecenoic acid, methyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.134	11.59 ng	1100970	Phenanthrene-d10	17.639

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	99
2	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	98
3	14-Methylpentadec-9-enoic acid m...	268	C17H32O2	1000365-89-7	91
4	Methyl 11-hexadecenoate	268	C17H32O2	1000336-35-5	91
5	Methyl hexadec-9-enoate	268	C17H32O2	010030-74-7	90





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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
PAV-B12-10-17

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
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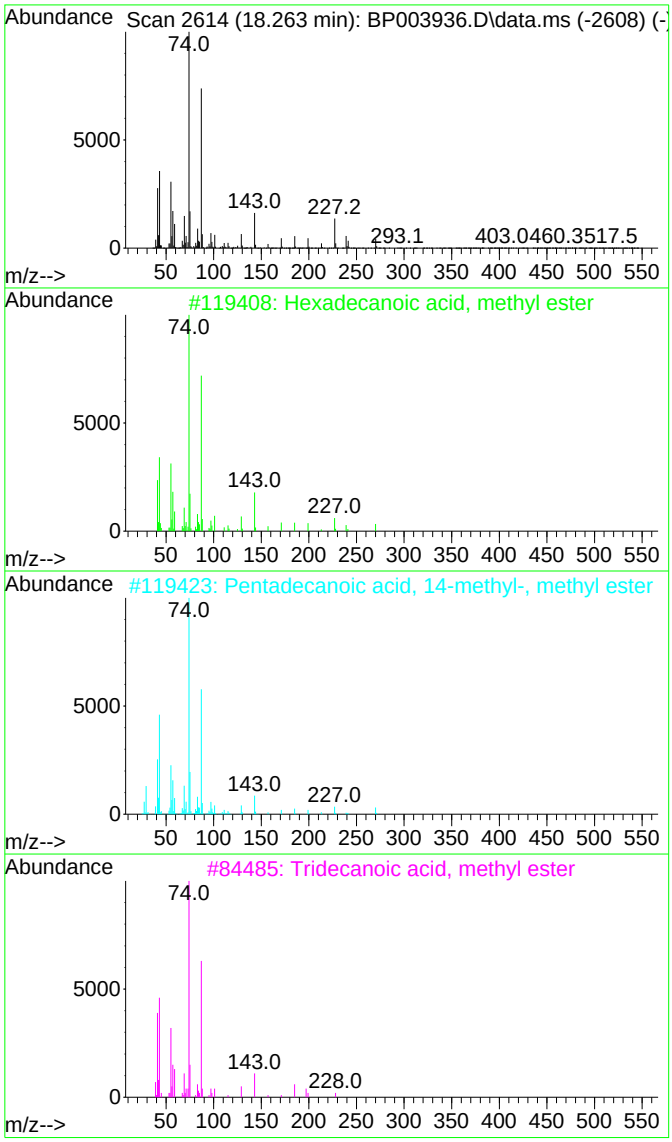
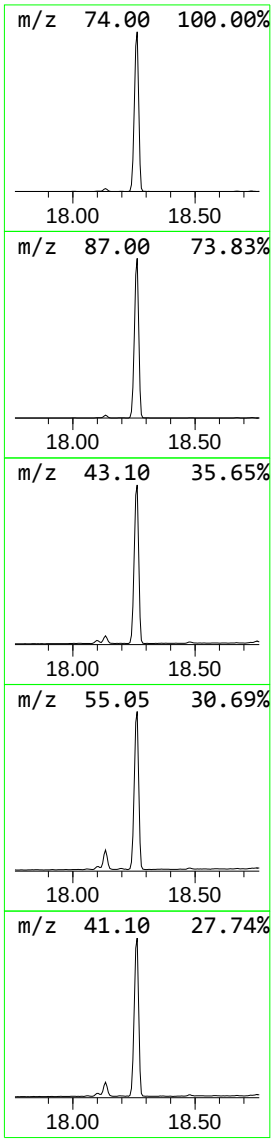
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.263	169.69 ng	16120800	Phenanthrene-d10	17.639

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	96
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
4	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	87
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	87





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Sample : L4622-05 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PAV-B12-10-17

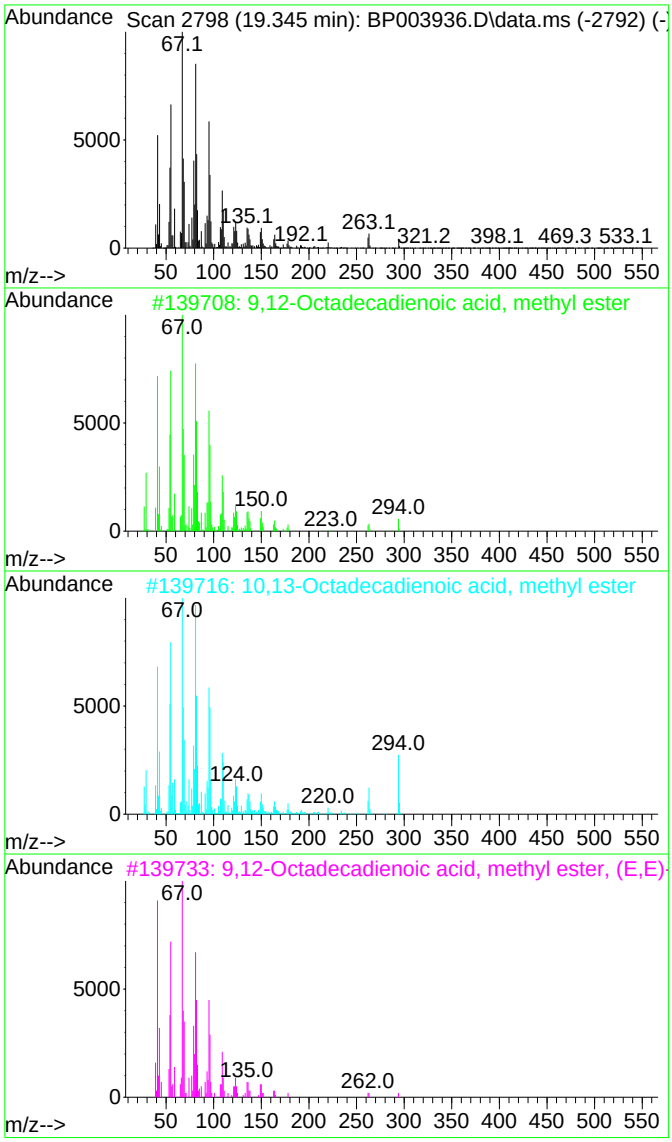
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

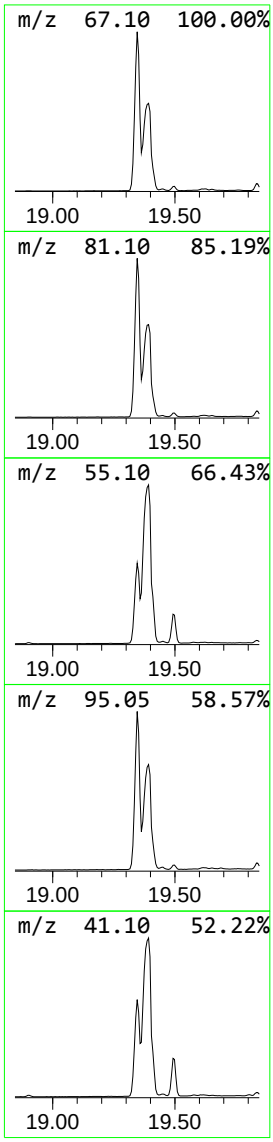
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 9,12-Octadecadienoic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.345	297.58 ng	28270700	Phenanthrene-d10	17.639

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
2	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
3	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
4	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
5	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99





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Operator : CG/JU
Sample : L4622-05 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PAV-B12-10-17

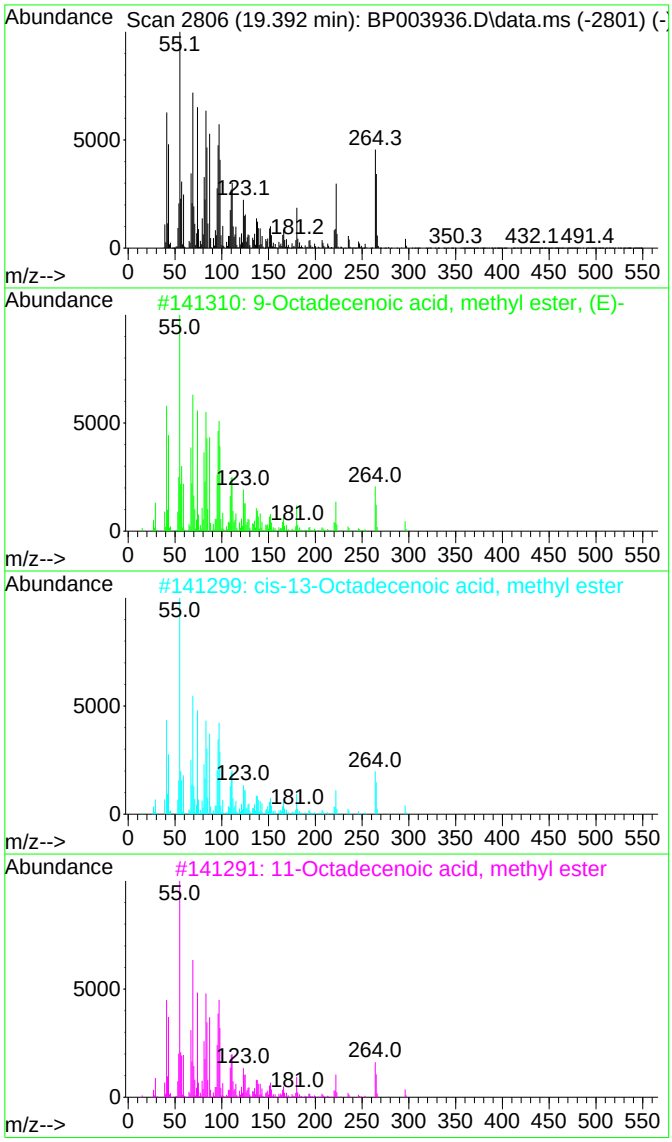
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

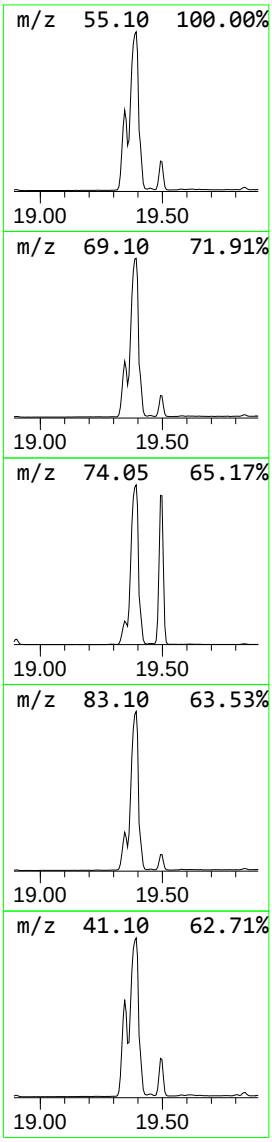
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 9-Octadecenoic acid, methyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.392	697.07 ng	66222400	Phenanthrene-d10	17.639

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99
2	cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1000333-58-3	99
3	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	99
4	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
5	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	98





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ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : PAV-B12-10-17

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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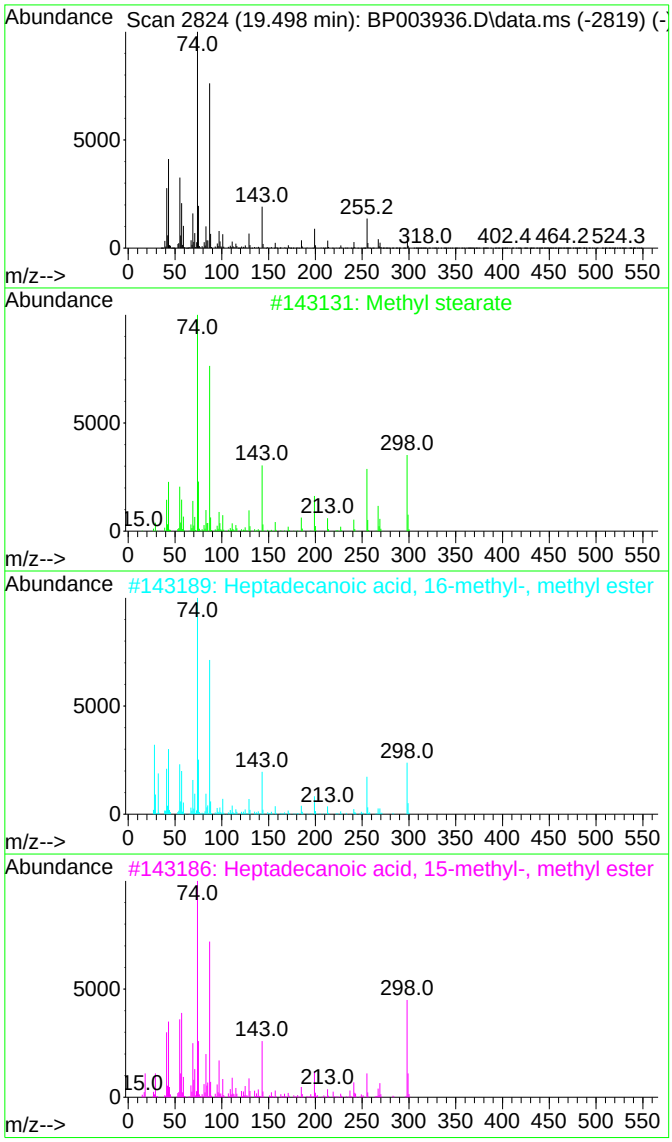
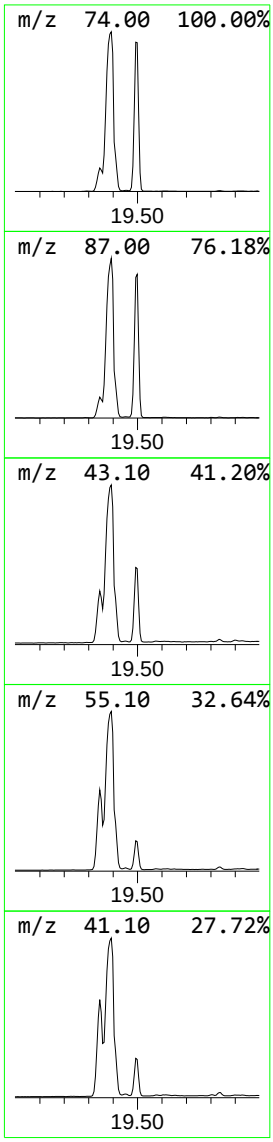
****

Peak Number 6 Methyl stearate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.498	83.51 ng	7933090	Phenanthrene-d10	17.639

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	92
3	Heptadecanoic acid, 15-methyl-, ...	298	C19H38O2	054833-55-5	90
4	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	87
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	87





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Instrument :
BNA_P
ClientSampleId :
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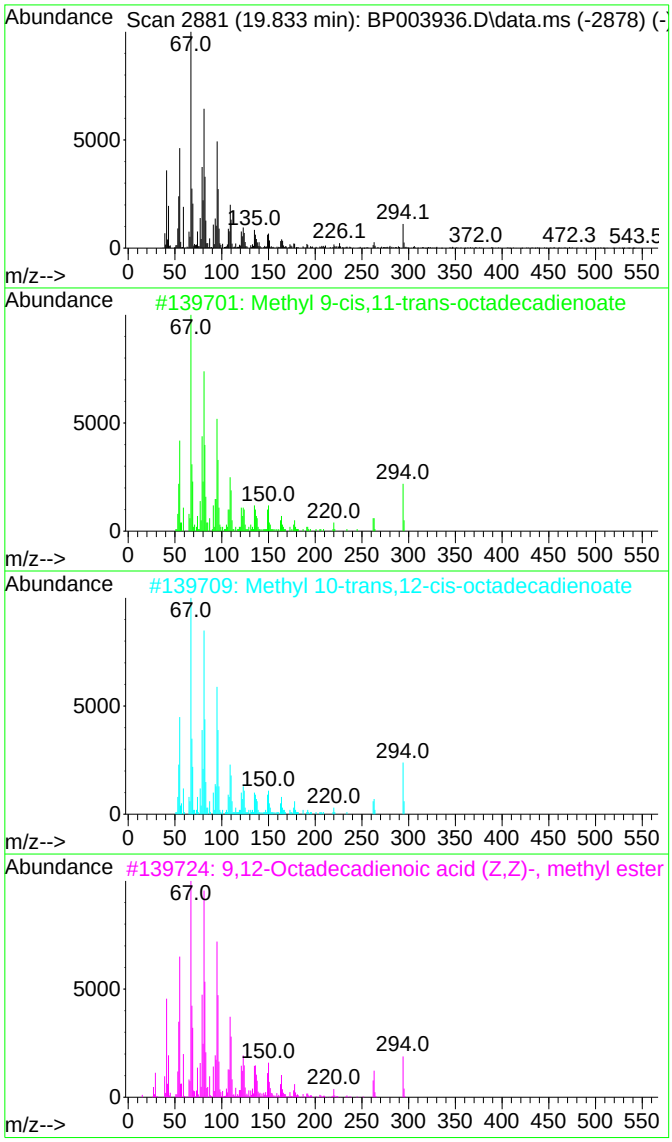
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

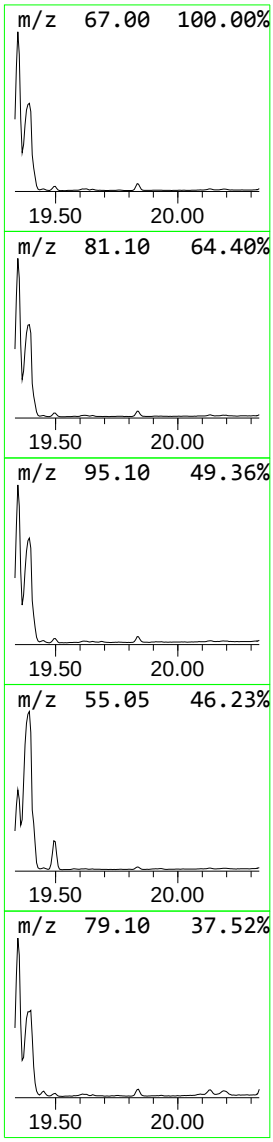
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Methyl 9-cis,11-trans-octad... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.833	8.82 ng	766234	Chrysene-d12	21.674

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	95
2	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	95
3	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	94
4	9,11-Octadecadienoic acid, methy...	294	C19H34O2	013038-47-6	93
5	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	90





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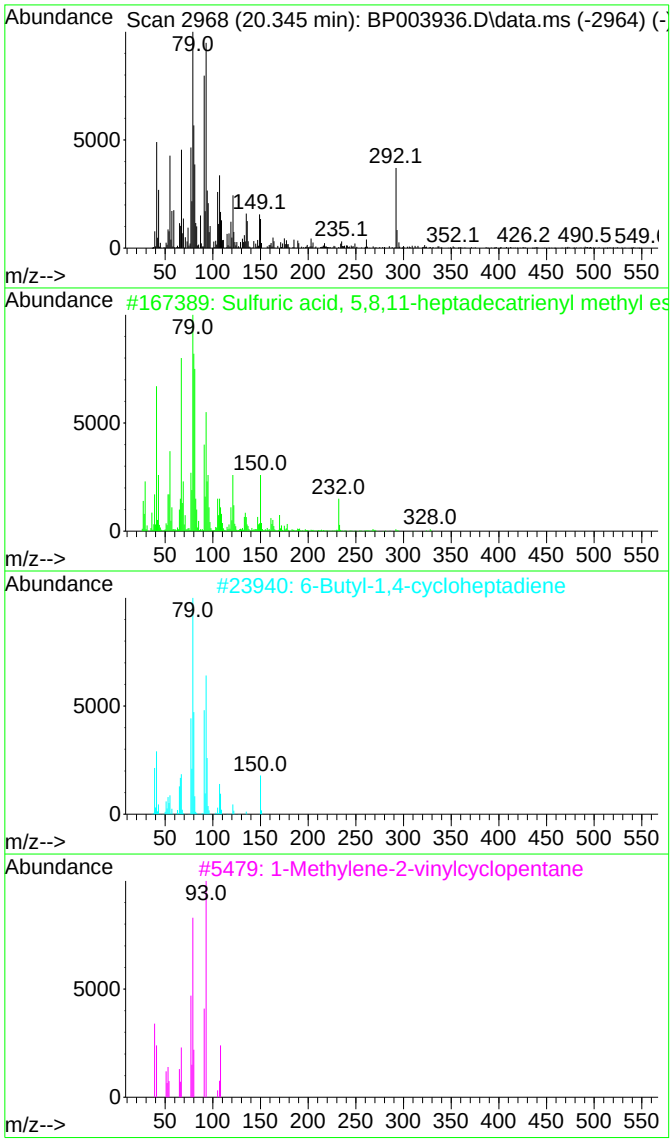
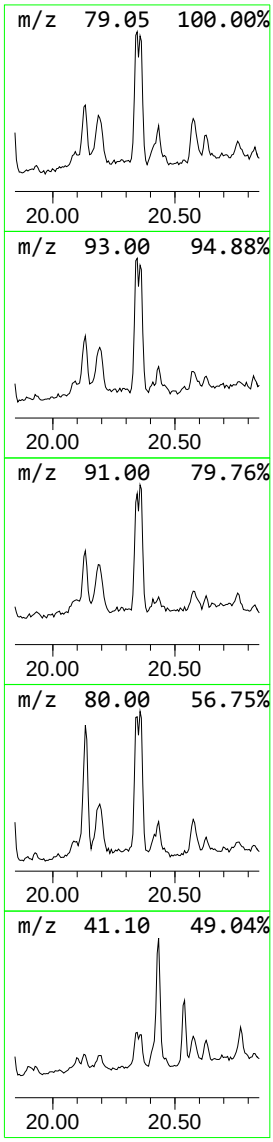
****
Peak Number 8 Sulfuric acid, 5,8,11-hepta... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.345	8.88 ng	770874	Chrysene-d12	21.674

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfuric acid, 5,8,11-heptadecat...	328	C18H32O3S	056554-67-7	86
2	6-Butyl-1,4-cycloheptadiene	150	C11H18	022735-58-6	68
3	1-Methylene-2-vinylcyclopentane	108	C8H12	006196-78-7	64
4	Bicyclo[4.1.0]heptane, 7-methylene-	108	C8H12	054211-14-2	64
5	Camphene	136	C10H16	000079-92-5	58





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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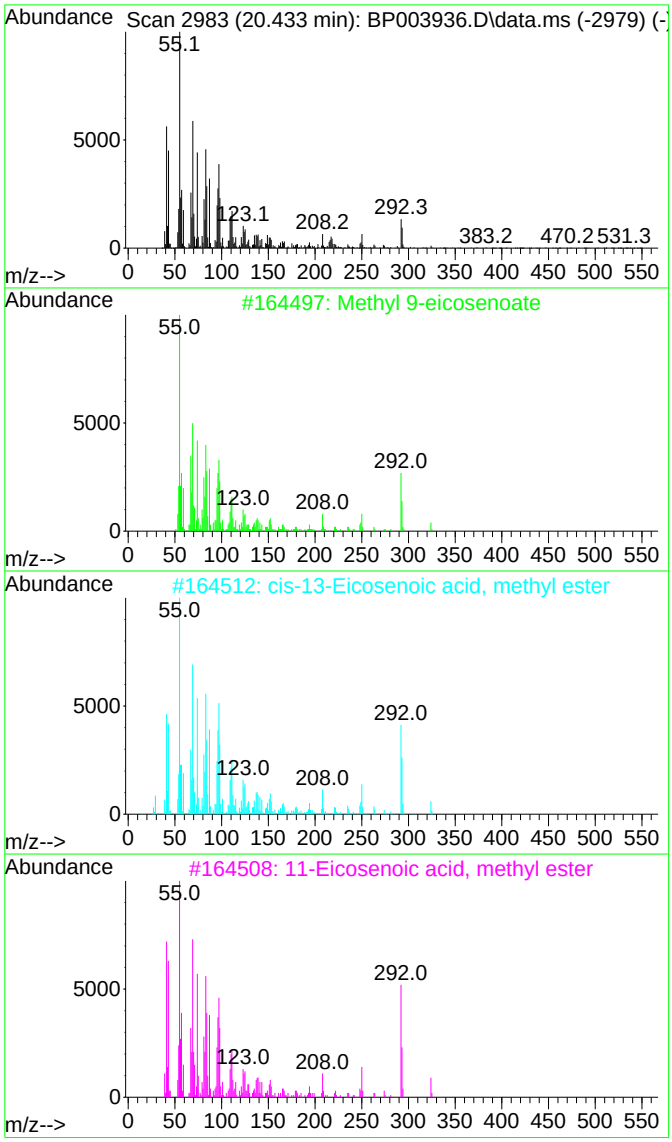
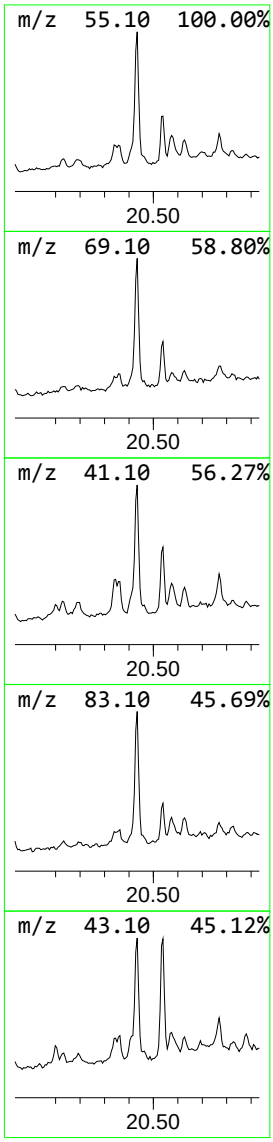
Peak Number 9 Methyl 9-eicosenoate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.433	22.32 ng	1938680	Chrysene-d12	21.674

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 9-eicosenoate	324	C21H40O2	1000336-50-5	99
2	cis-13-Eicosenoic acid, methyl e...	324	C21H40O2	1000333-52-1	91
3	11-Eicosenoic acid, methyl ester	324	C21H40O2	003946-08-5	91
4	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	90
5	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	90





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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
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TIC Integration Parameters: LSCINT.P

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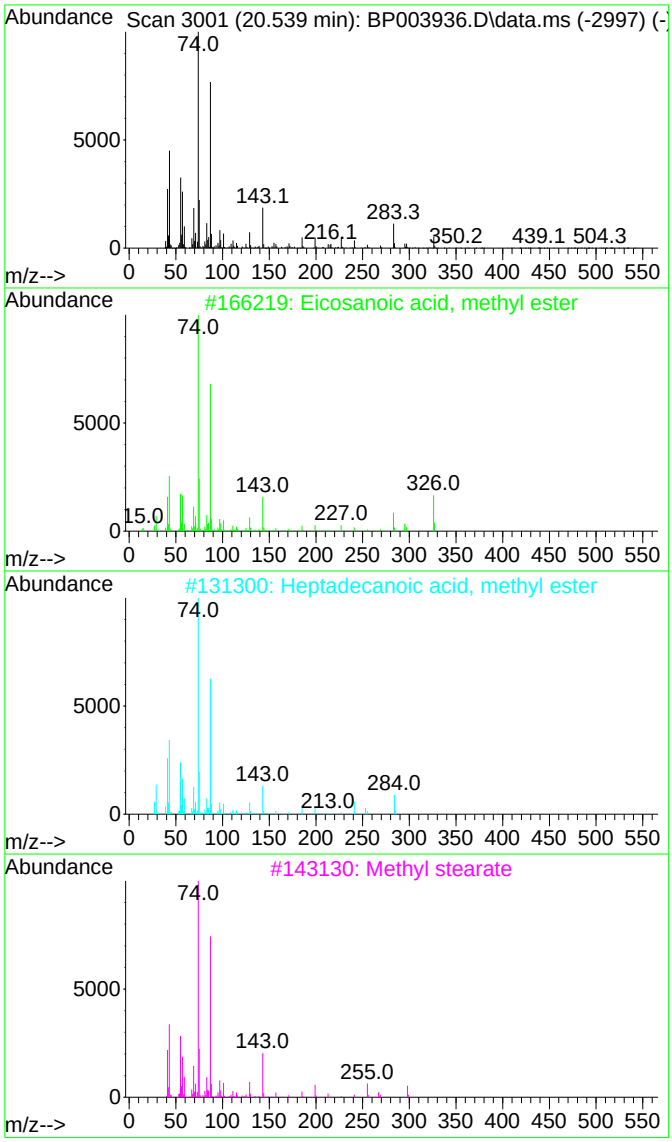
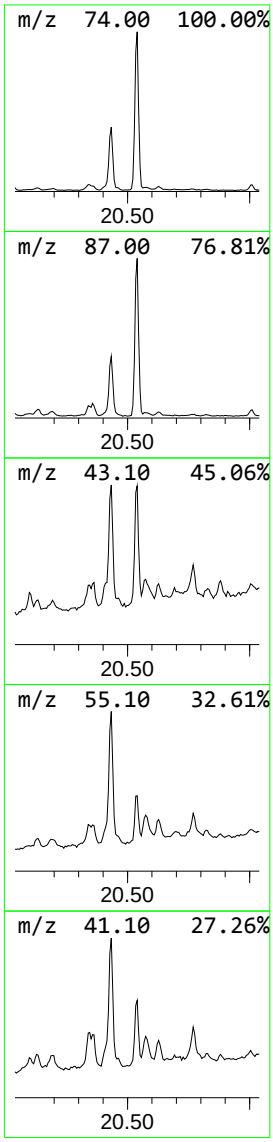
Peak Number 10 Eicosanoic acid, methyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.539	13.56 ng	1177830	Chrysene-d12	21.674

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	98
2	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	94
3	Methyl stearate	298	C19H38O2	000112-61-8	93
4	Methyl 18-methylnonadecanoate	326	C21H42O2	1000352-20-6	90
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111120\
Data File : BP003936.D
Acq On : 11 Nov 2020 23:55
Operator : CG/JU
Sample : L4622-05 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PAV-B12-10-17

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

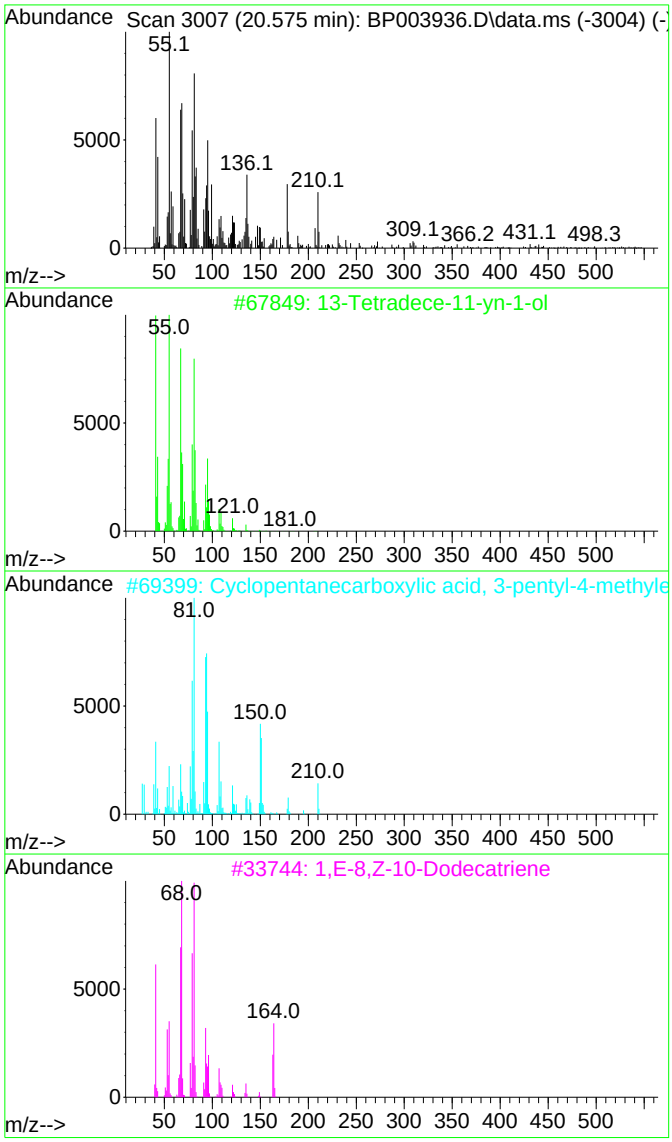
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

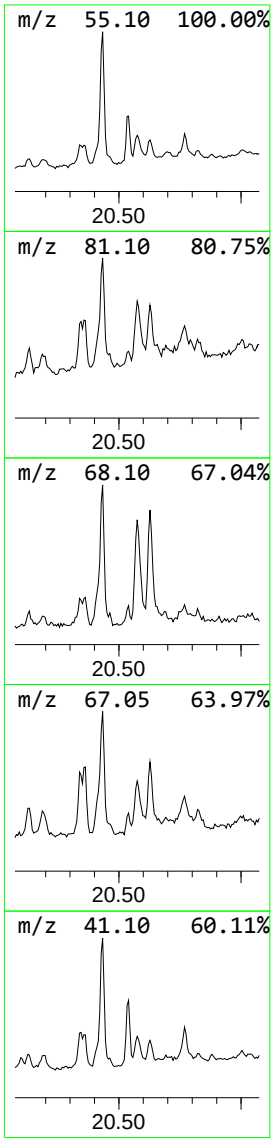
****

Peak Number 11 13-Tetradece-11-yn-1-ol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.575	8.78 ng	762929	Chrysene-d12	21.674

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Tetradece-11-yn-1-ol	208	C14H24O	1000131-00-4	70
2	Cyclopentanecarboxylic acid, 3-p...	210	C13H22O2	1000154-24-9	60
3	1,E-8,Z-10-Dodecatriene	164	C12H20	1000098-05-5	60
4	Z,Z-3,13-Octadecadien-1-ol	266	C18H34O	1000131-10-9	55
5	Methyl 7,8-octadecadienoate	294	C19H34O2	1000336-44-6	51





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111120\
Data File : BP003936.D
Acq On : 11 Nov 2020 23:55
Operator : CG/JU
Sample : L4622-05 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : PAV-B12-10-17

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.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
Propane, 2,2-di...	2.928	41.5	ng	2134530	1	8.281	1028340	20.0
9-Hexadecenoic ...	18.134	11.6	ng	1100970	4	17.639	1900020	20.0
Hexadecanoic ac...	18.263	169.7	ng	16120800	4	17.639	1900020	20.0
9,12-Octadecadi...	19.345	297.6	ng	28270700	4	17.639	1900020	20.0
9-Octadecenoic ...	19.392	697.1	ng	66222400	4	17.639	1900020	20.0
Methyl stearate	19.498	83.5	ng	7933090	4	17.639	1900020	20.0
Methyl 9-cis,11...	19.833	8.8	ng	766234	5	21.674	1737180	20.0
Sulfuric acid, ...	20.345	8.9	ng	770874	5	21.674	1737180	20.0
Methyl 9-eicose...	20.433	22.3	ng	1938680	5	21.674	1737180	20.0
Eicosanoic acid...	20.539	13.6	ng	1177830	5	21.674	1737180	20.0
13-Tetradece-11...	20.575	8.8	ng	762929	5	21.674	1737180	20.0