Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110420\
Data File : BF122270.D
Acq On : 4 Nov 2020 18:43
Operator : JU/CG
Sample : L4621-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAV-B8-110320-10-20

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_F\METHODS\8270-BF101220.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122270.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.339	550	553	589	rBV	1403983	2211442	18.01%	4.940%
2	6.369	725	728	754	rBV	1438525	2306568	18.79%	5.153%
3	6.710	782	786	797	rVB	558010	555546	4.53%	1.241%
4	7.281	880	883	911	rBV	1273103	1476074	12.02%	3.298%
5	7.992	1001	1004	1012	rBV	691373	652314	5.31%	1.457%
6	9.069	1182	1187	1196	rBV	2235453	2308412	18.80%	5.157%
7	9.186	1203	1207	1215	rVB	203012	226867	1.85%	0.507%
8	9.469	1252	1255	1262	rVB	234675	228651	1.86%	0.511%
9	9.745	1298	1302	1306	rBV	838800	769021	6.26%	1.718%
10	10.545	1434	1438	1451	rBV	1005106	1224486	9.97%	2.736%
11	10.745	1469	1472	1476	rVB	254281	211917	1.73%	0.473%
12	11.233	1552	1555	1557	rBV	786261	648770	5.28%	1.449%
13	11.257	1557	1559	1565	rVB	312277	306312	2.50%	0.684%
14	11.539	1605	1607	1611	rVB	401754	312111	2.54%	0.697%
15	11.621	1616	1621	1624	rBV	4275675	4072637	33.17%	9.098%
16	12.310	1730	1738	1740	rBV	4262036	6595149	53.72%	14.734%
17	12.351	1740	1745	1749	rVV	6697003	12276379	100.00%	27.425%
18	12.410	1752	1755	1759	rVB	2286505	2028435	16.52%	4.532%
19	12.457	1759	1763	1767	rBV	321389	315322	2.57%	0.704%
20	12.686	1798	1802	1809	rVB	264501	368804	3.00%	0.824%
21	12.815	1820	1824	1832	rBV	1969419	1879359	15.31%	4.198%
22	13.051	1860	1864	1872	rVB	458154	541822	4.41%	1.210%
23	13.133	1874	1878	1880	rBV2	264968	243876	1.99%	0.545%
24	13.168	1880	1884	1888	rBV4	137116	251028	2.04%	0.561%
25	13.292	1901	1905	1910	rVV	351374	367304	2.99%	0.821%
26	13.357	1912	1916	1923	rVB7	56246	126672	1.03%	0.283%
27	13.568	1949	1952	1959	rVB2	95062	133915	1.09%	0.299%
28	13.727	1971	1979	1988	rBV6	103760	338986	2.76%	0.757%
29	13.798	1988	1991	1995	rVV	160414	142314	1.16%	0.318%
30	13.880	2001	2005	2009	rVV2	616454	760728	6.20%	1.699%
31	13.910	2009	2010	2017	rVB	134345	128956	1.05%	0.288%
32	14.921	2179	2182	2191	rBV2	91345	195215	1.59%	0.436%
33	15.327	2247	2251	2261	rVV	374693	557363	4.54%	1.245%

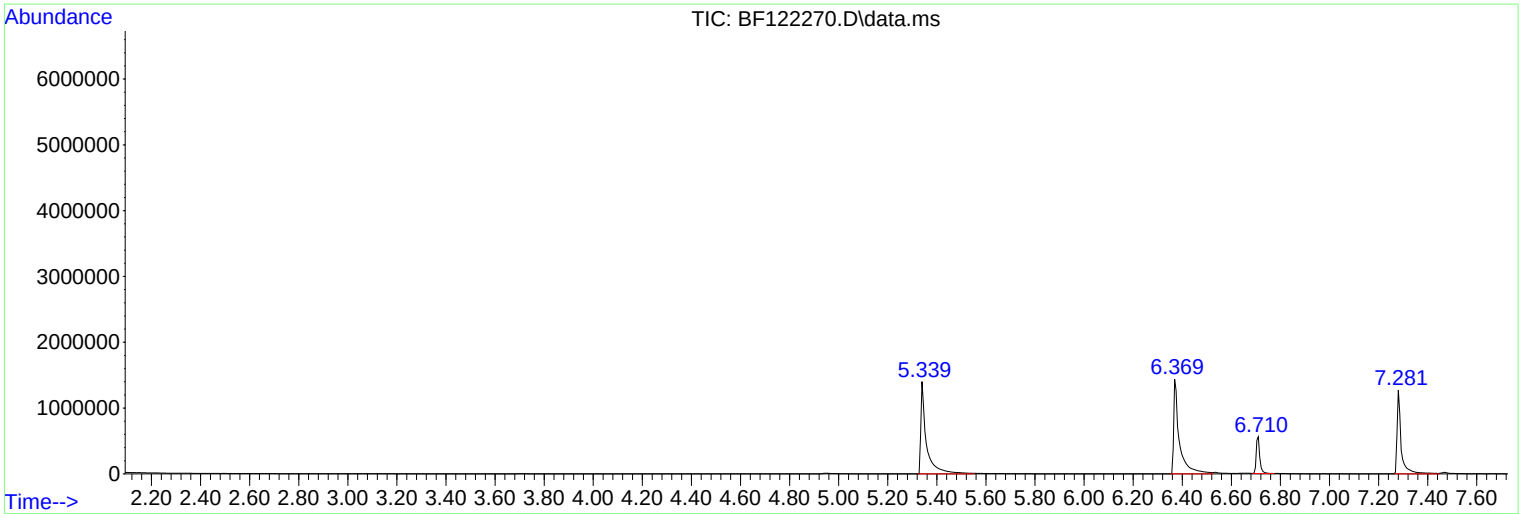
Sum of corrected areas: 44762755

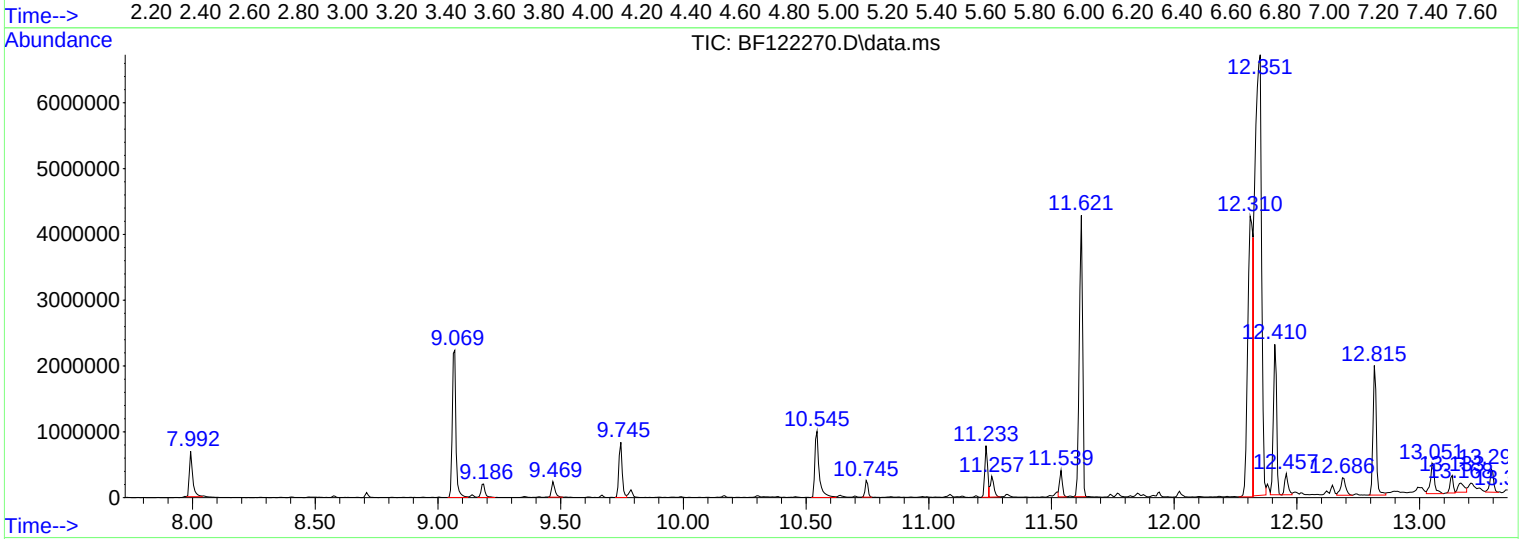
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110420\
Data File : BF122270.D
Acq On : 4 Nov 2020 18:43
Operator : JU/CG
Sample : L4621-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

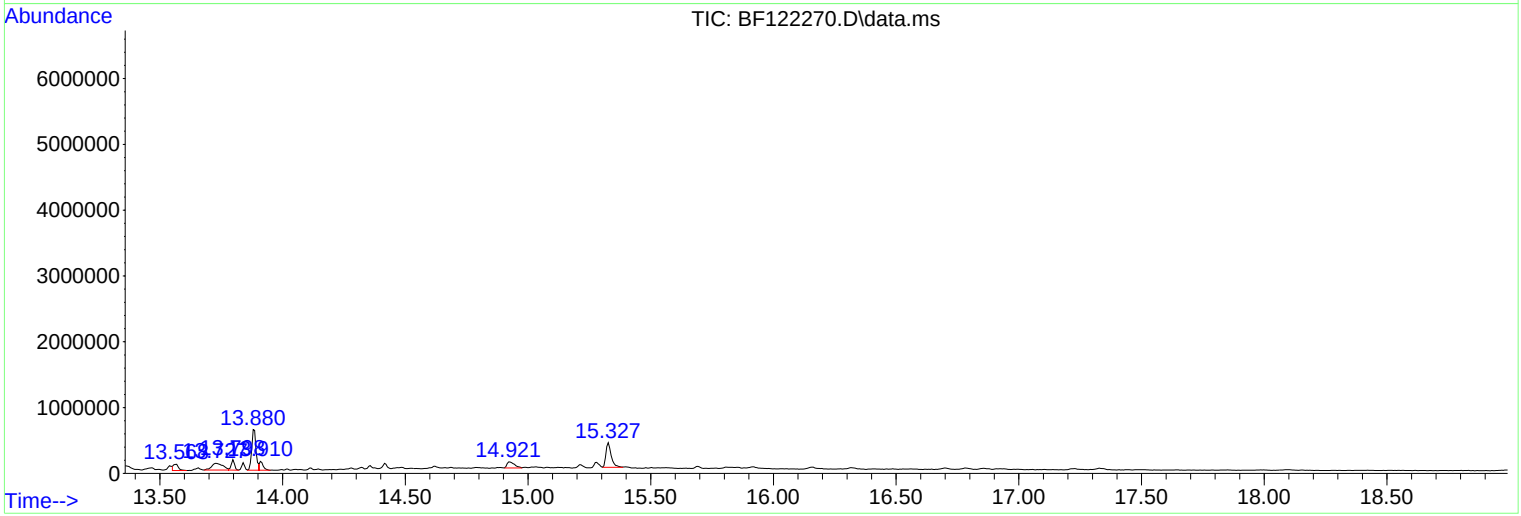
Instrument :
BNA_F
ClientSampleId :
PAV-B8-110320-10-20

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110420\
Data File : BF122270.D
Acq On : 4 Nov 2020 18:43
Operator : JU/CG
Sample : L4621-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAV-B8-110320-10-20

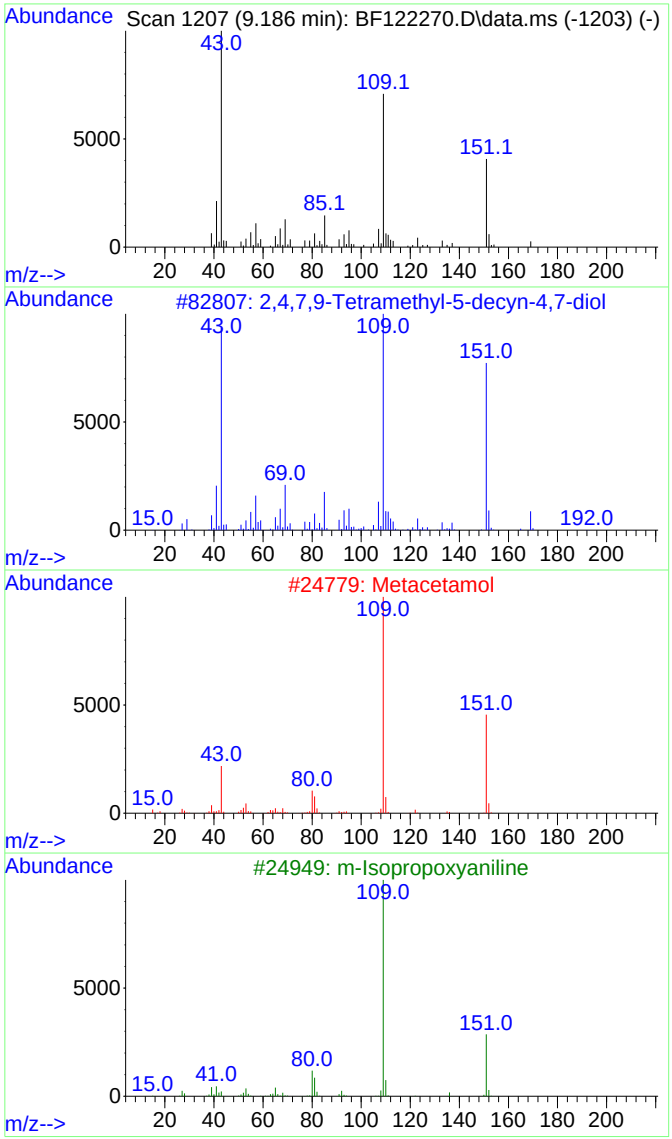
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

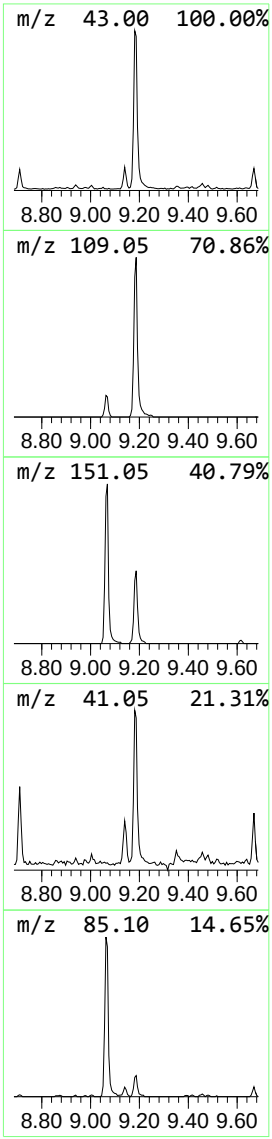
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.186	5.90 ng	226867	Acenaphthene-d10	9.745

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	Metacetamol	151	C8H9NO2	000621-42-1	58
3	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	53
4	Cyclohexanol, 3,3,5-trimethyl-	142	C9H18O	000116-02-9	35
5	Ethanone, 1-(1,4-dimethyl-3-cycl...	152	C10H16O	043219-68-7	32





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Data File : BF122270.D
Acq On : 4 Nov 2020 18:43
Operator : JU/CG
Sample : L4621-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAV-B8-110320-10-20

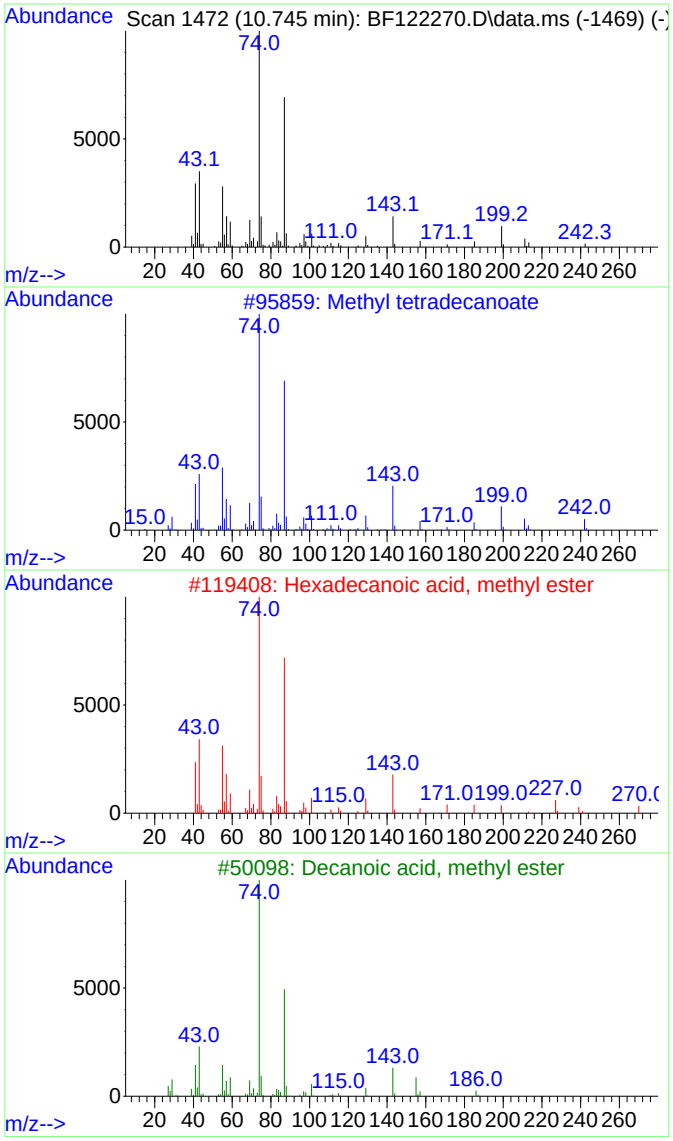
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

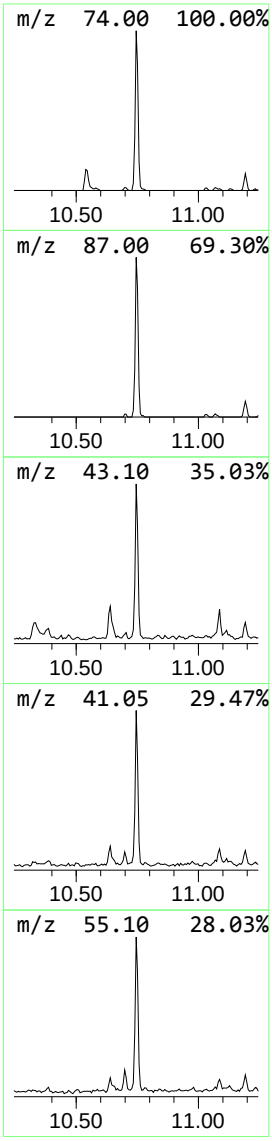
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Methyl tetradecanoate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.745	6.53 ng	211917	Phenanthrene-d10	11.233

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl tetradecanoate	242	C15H30O2	000124-10-7	93
2	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	87
3	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	86
4	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	86
5	Undecanoic acid, 10-methyl-, met...	214	C13H26O2	005129-56-6	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110420\
Data File : BF122270.D
Acq On : 4 Nov 2020 18:43
Operator : JU/CG
Sample : L4621-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAV-B8-110320-10-20

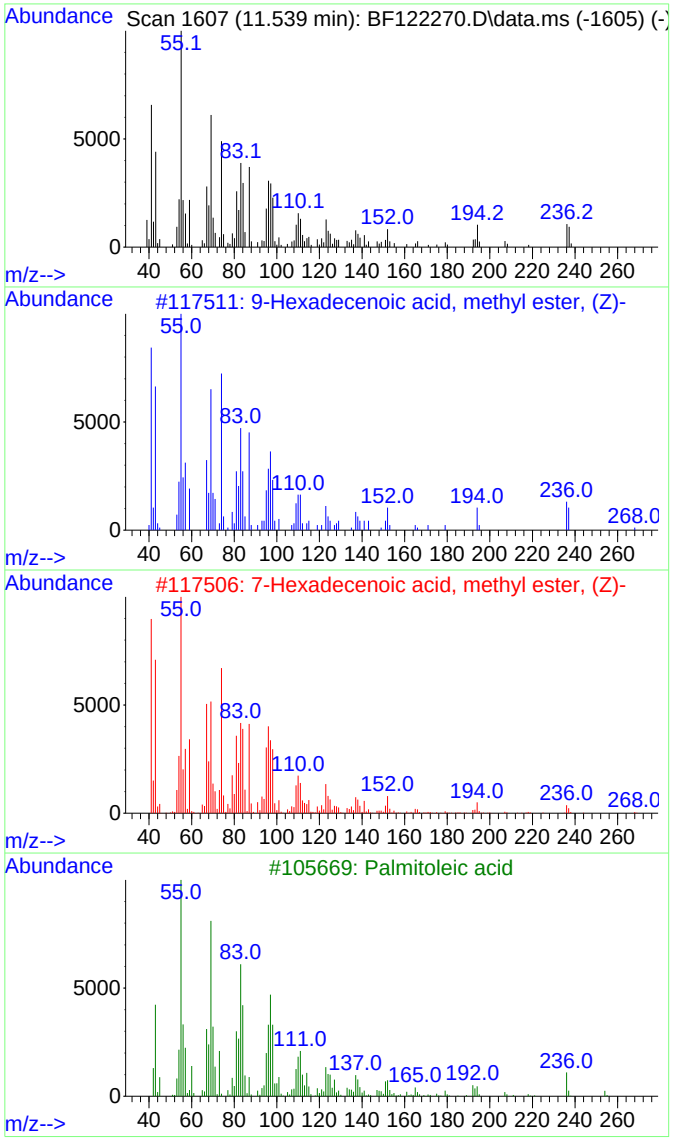
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

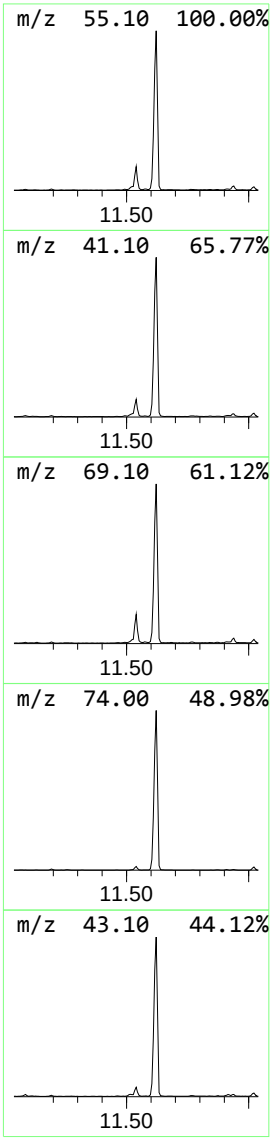
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 9-Hexadecenoic acid, methyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.539	9.62 ng	312111	Phenanthrene-d10	11.233

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	91
2	7-Hexadecenoic acid, methyl este...	268	C17H32O2	056875-67-3	62
3	Palmitoleic acid	254	C16H30O2	000373-49-9	53
4	Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	52
5	Chloromethyl 7-chlorododecanoate	282	C13H24Cl2O2	080419-03-0	49





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Data File : BF122270.D
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Operator : JU/CG
Sample : L4621-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAV-B8-110320-10-20

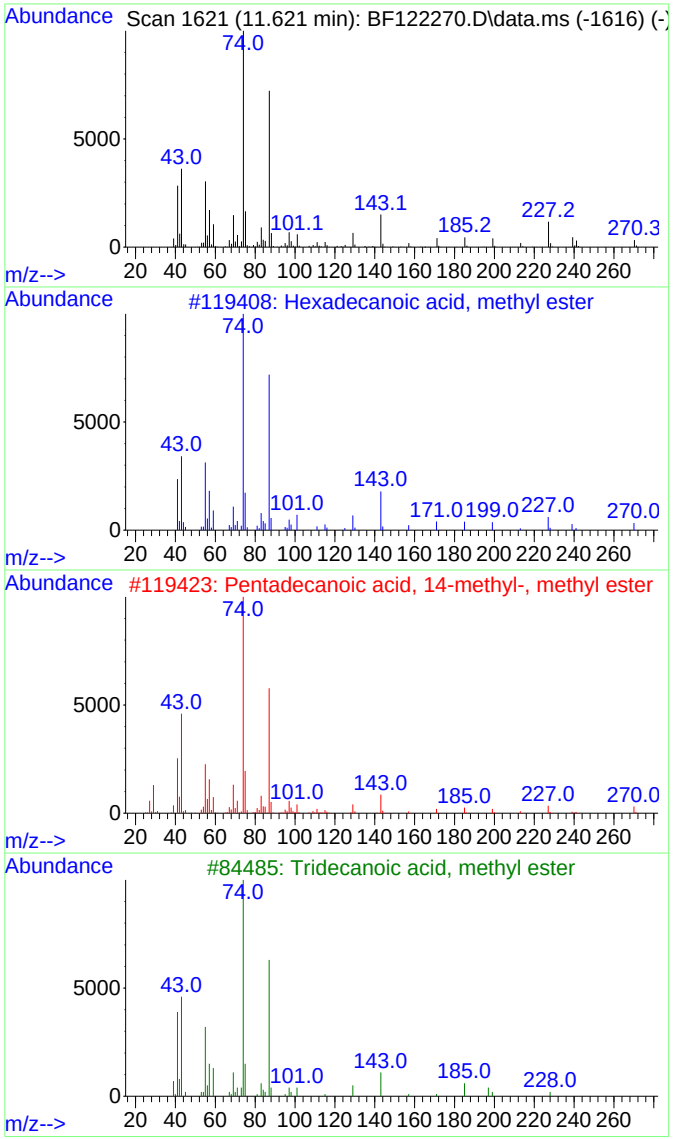
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

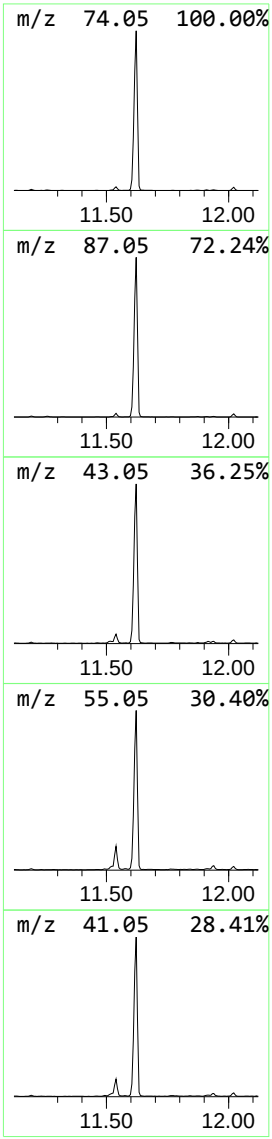
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.621	125.55 ng	4072640	Phenanthrene-d10	11.233

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	90
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110420\
Data File : BF122270.D
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Operator : JU/CG
Sample : L4621-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAV-B8-110320-10-20

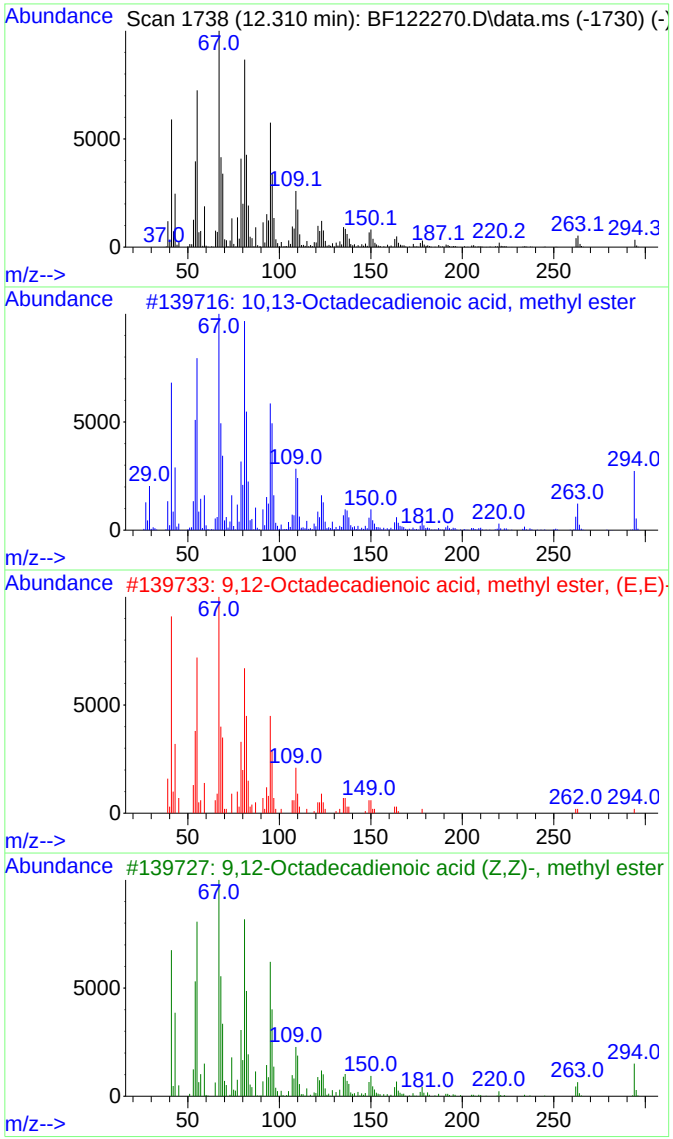
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

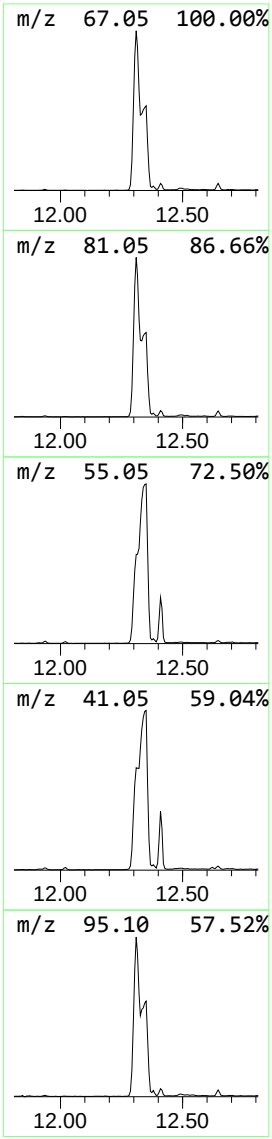
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 10,13-Octadecadienoic acid,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.310	203.31 ng	6595150	Phenanthrene-d10	11.233

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
3	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
4	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
5	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	99





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Sample : L4621-05
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ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
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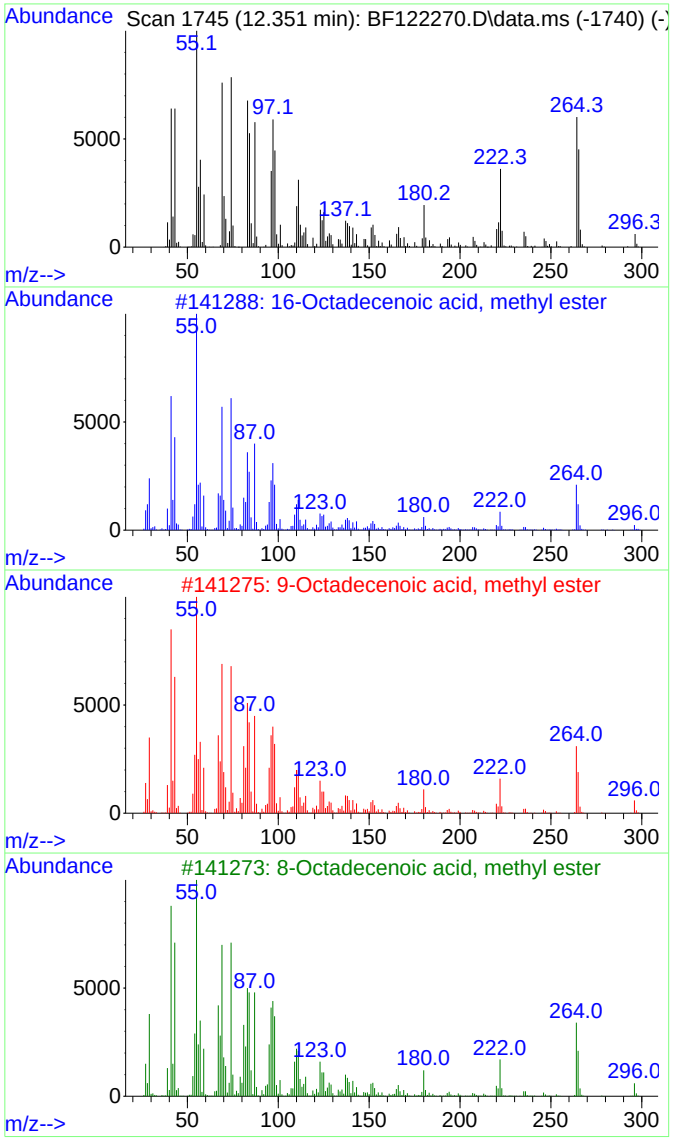
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

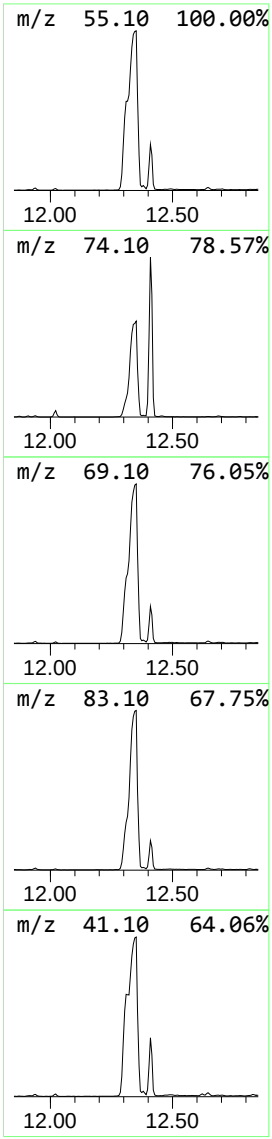
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 16-Octadecenoic acid, methy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.351	378.45 ng	12276400	Phenanthrene-d10	11.233

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	98
2	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	96
3	8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	92
4	7-Octadecenoic acid, methyl ester	296	C19H36O2	057396-98-2	91
5	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	90





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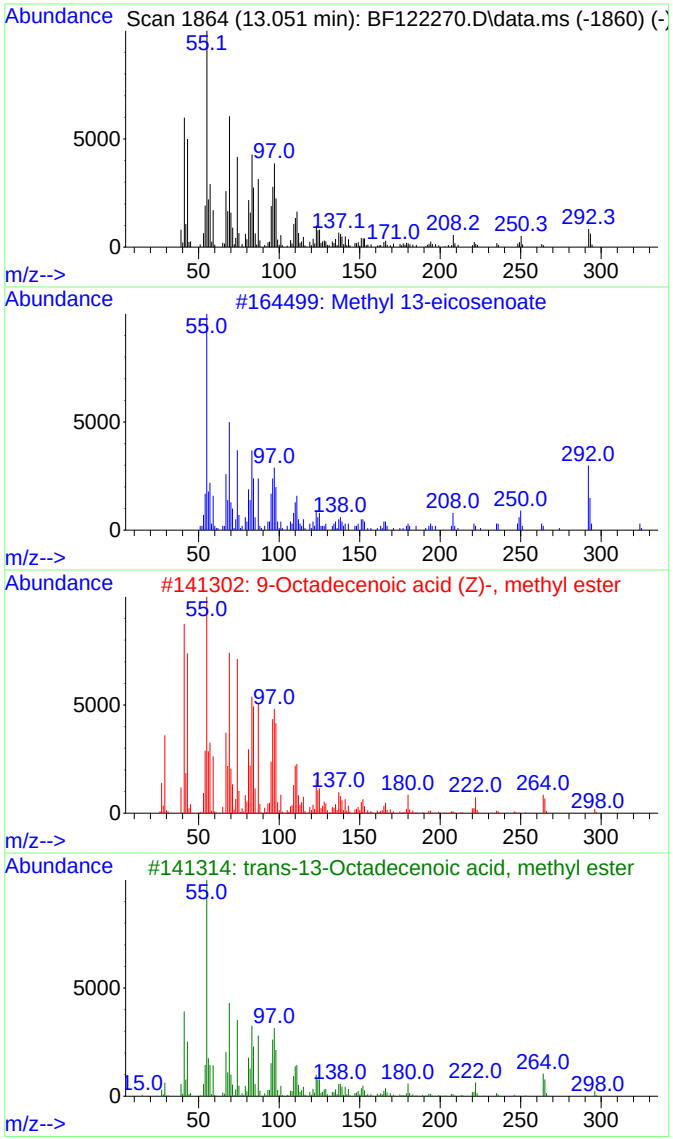
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

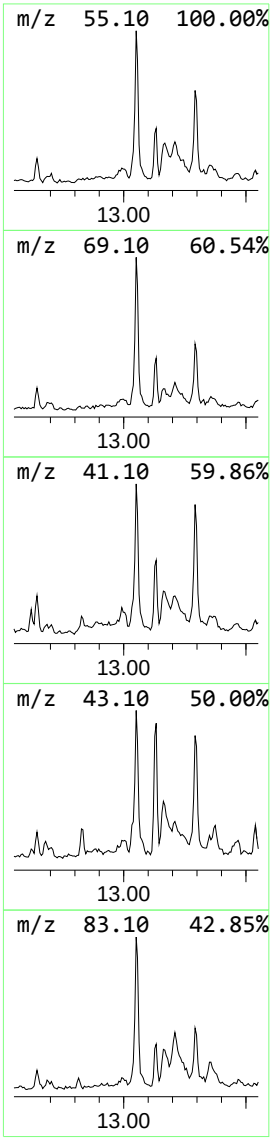
****

Peak Number 7 Methyl 13-eicosenoate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.051	14.24 ng	541822	Chrysene-d12	13.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 13-eicosenoate	324	C21H40O2	1000336-48-4	91
2	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	90
3	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	90
4	Methyl 9-heptadecenoate or 9-17:1	282	C18H34O2	1000336-38-0	83
5	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110420\
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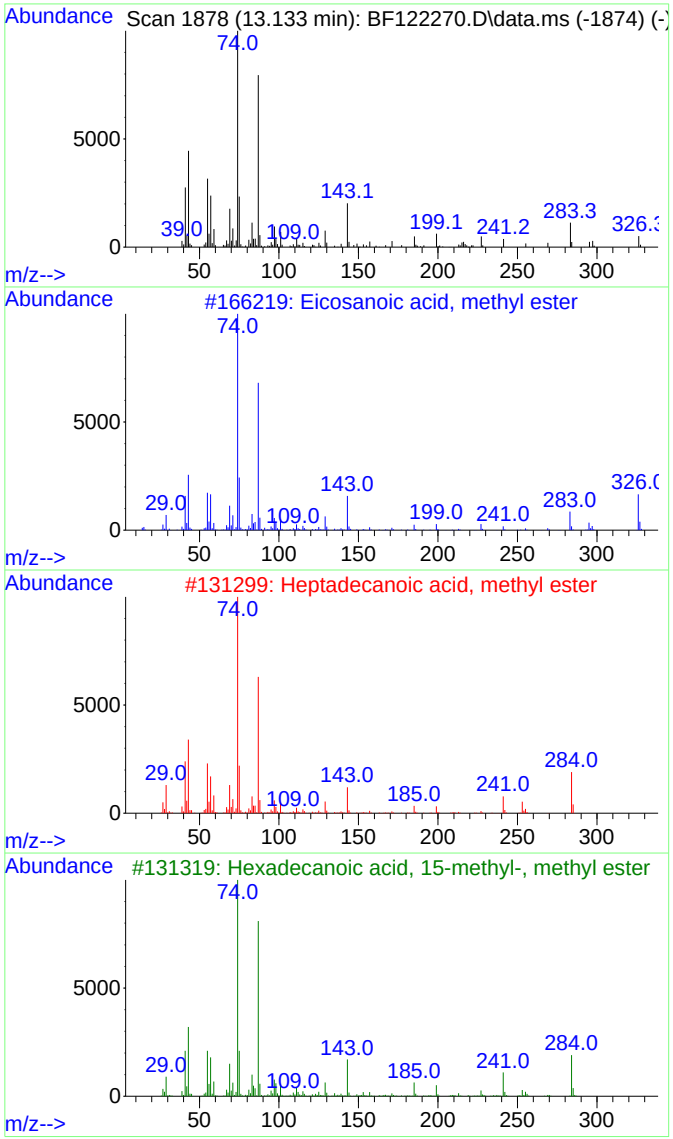
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

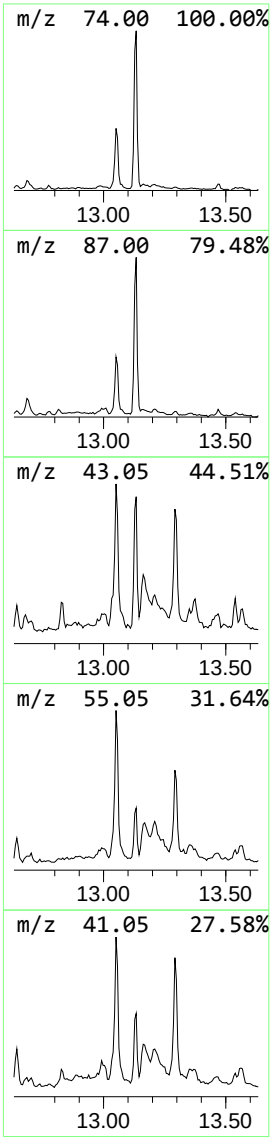
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Eicosanoic acid, methyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.133	6.41 ng	243876	Chrysene-d12	13.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	96
2	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	93
3	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	93
4	Methyl stearate	298	C19H38O2	000112-61-8	90
5	Hexadecanoic acid, 14-methyl-, m...	284	C18H36O2	002490-49-5	87





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Data File : BF122270.D
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Operator : JU/CG
Sample : L4621-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAV-B8-110320-10-20

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

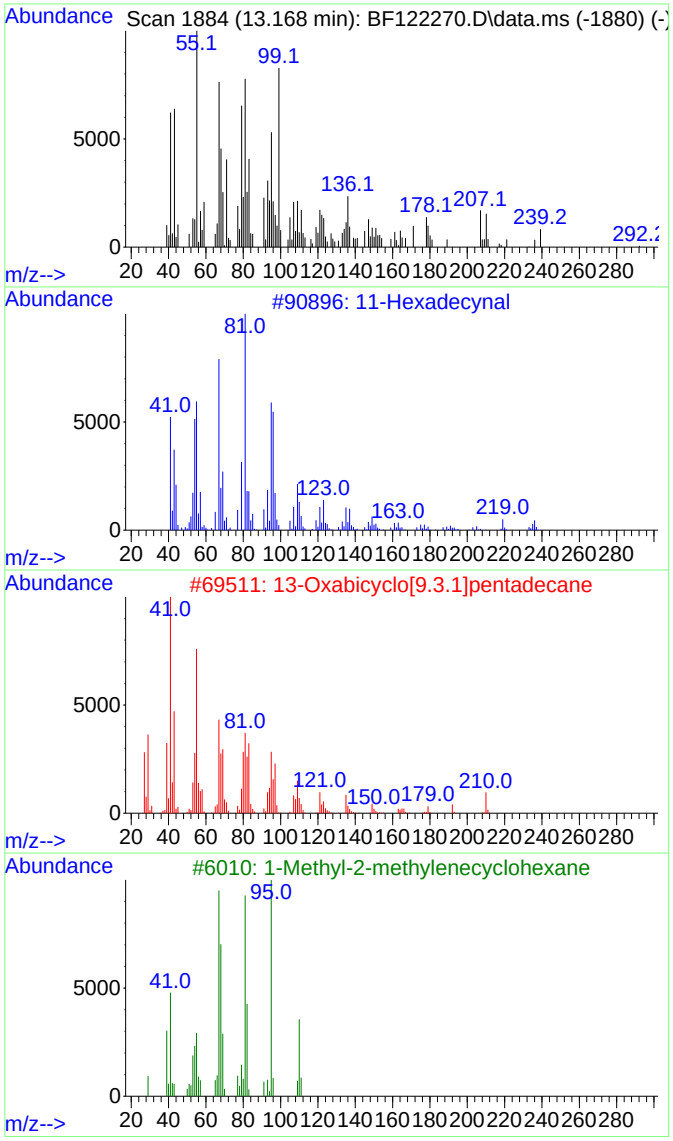
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

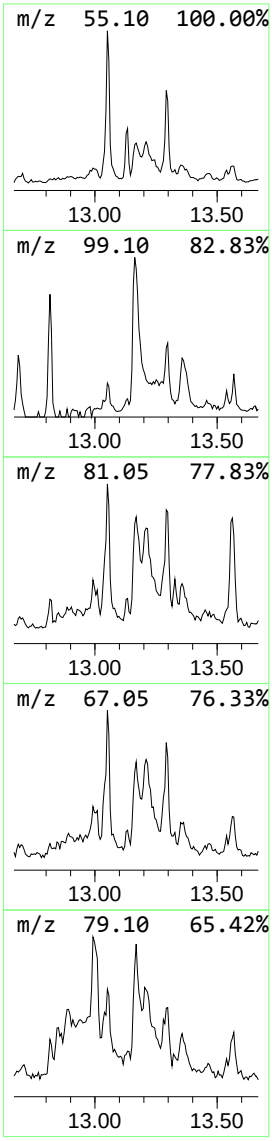
****

Peak Number 9 11-Hexadecynal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.168	6.60 ng	251028	Chrysene-d12	13.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Hexadecynal	236	C16H28O	086426-73-5	70
2	13-Oxabicyclo[9.3.1]pentadecane	210	C14H26O	051547-45-6	62
3	1-Methyl-2-methylenecyclohexane	110	C8H14	002808-75-5	50
4	9,12-Octadecadien-1-ol, (Z,Z)-	266	C18H34O	000506-43-4	49
5	Z-1,6-Tridecadiene	180	C13H24	1000130-98-3	46





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Data File : BF122270.D
Acq On : 4 Nov 2020 18:43
Operator : JU/CG
Sample : L4621-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAV-B8-110320-10-20

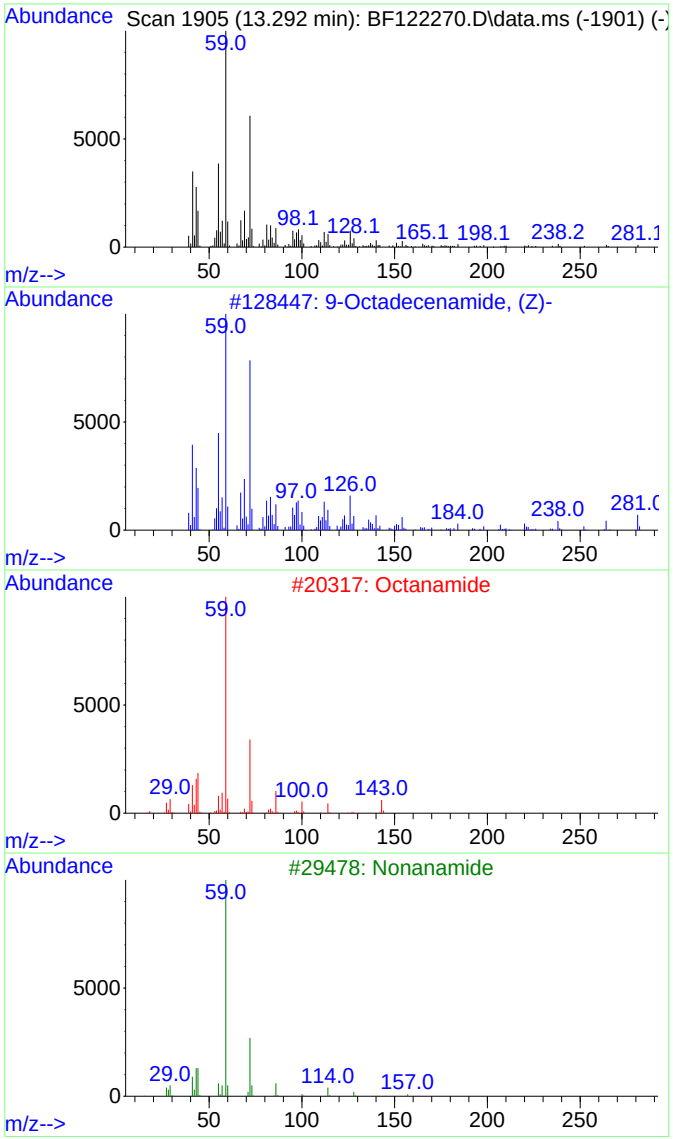
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

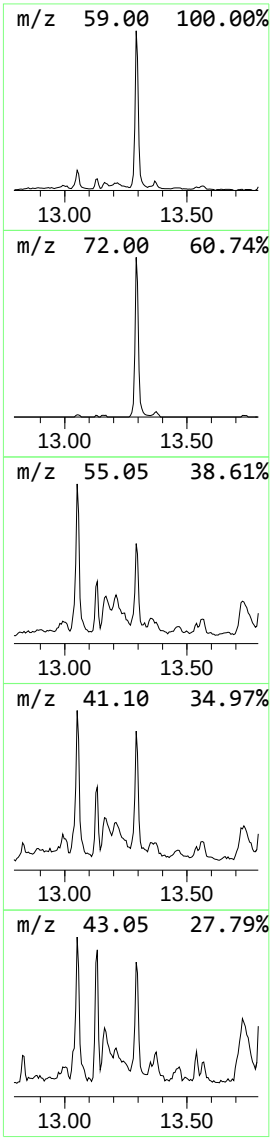
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	9.66 ng	367304	Chrysene-d12	13.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	97
2	Octanamide	143	C8H17NO	000629-01-6	59
3	Nonanamide	157	C9H19NO	001120-07-6	59
4	Hexadecanamide	255	C16H33NO	000629-54-9	56
5	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	53





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Data File : BF122270.D
Acq On : 4 Nov 2020 18:43
Operator : JU/CG
Sample : L4621-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAV-B8-110320-10-20

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.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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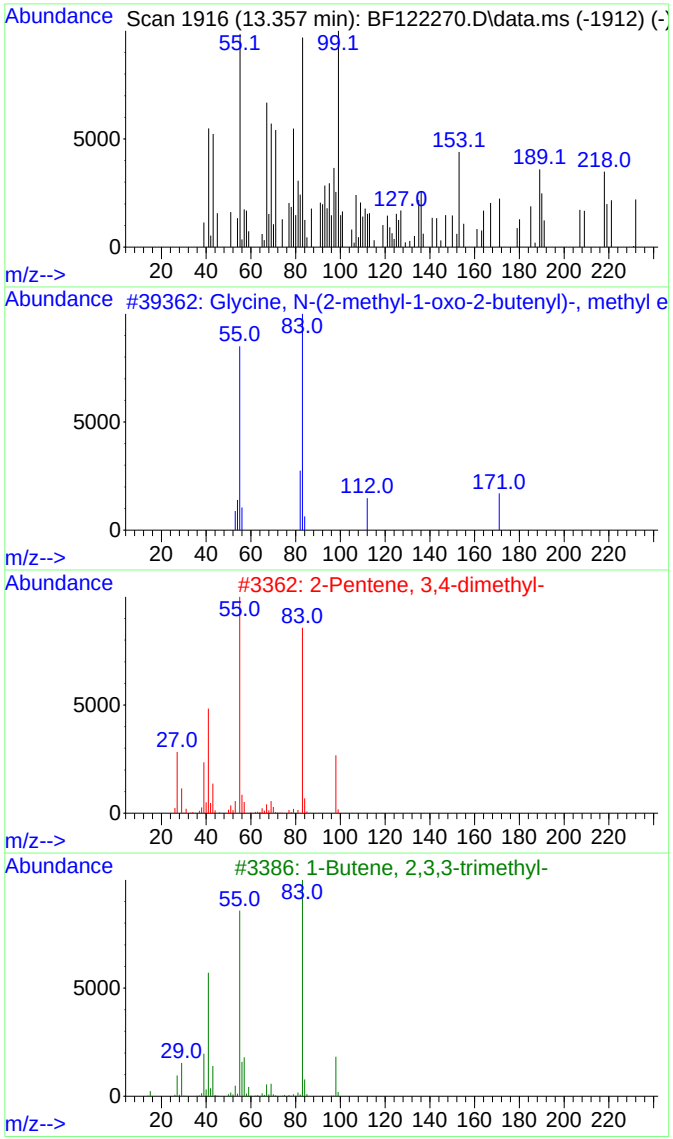
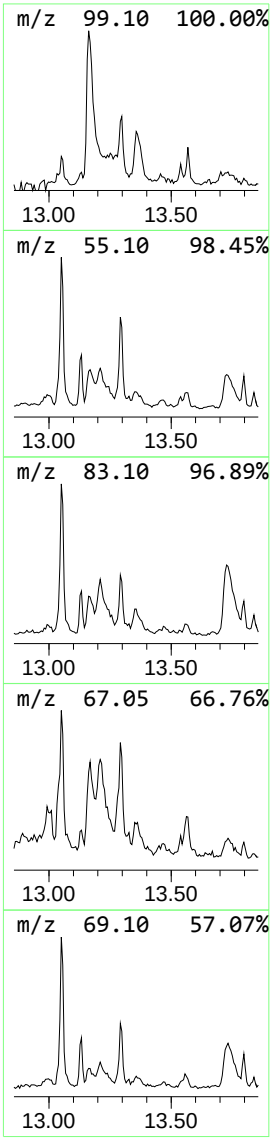
Peak Number 11 unknown13.357 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.357	3.33 ng	126672	Chrysene-d12	13.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Glycine, N-(2-methyl-1-oxo-2-but...	171	C8H13NO3	055649-53-1	14
2	2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	11
3	1-Butene, 2,3,3-trimethyl-	98	C7H14	000594-56-9	11
4	Isothiazole, 4-methyl-	99	C4H5NS	000693-90-3	11
5	2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	11





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Data File : BF122270.D
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Operator : JU/CG
Sample : L4621-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAV-B8-110320-10-20

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.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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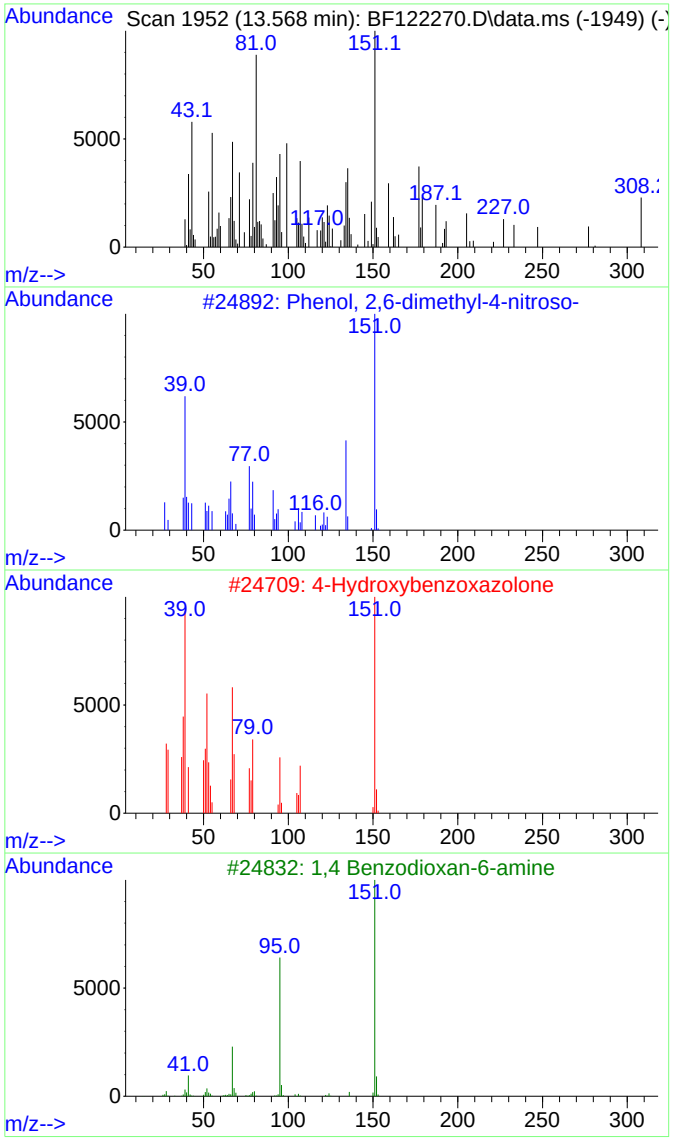
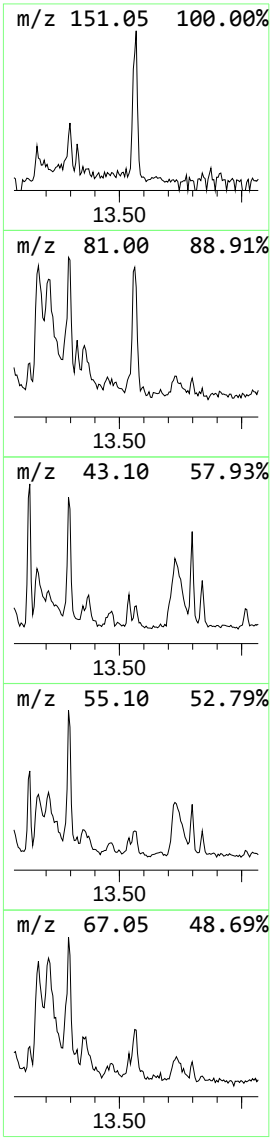
Peak Number 12 unknown13.568 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.568	3.52 ng	133915	Chrysene-d12	13.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-dimethyl-4-nitroso-	151	C8H9NO2	013331-93-6	42
2	4-Hydroxybenzoxazolone	151	C7H5NO3	028955-70-6	18
3	1,4 Benzodioxan-6-amine	151	C8H9NO2	022013-33-8	14
4	2,6-Dimethylbenzoquinone-4-oxime	151	C8H9NO2	004965-29-1	11
5	5-Nitro-m-xylene	151	C8H9NO2	000099-12-7	11





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110420\
Data File : BF122270.D
Acq On : 4 Nov 2020 18:43
Operator : JU/CG
Sample : L4621-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAV-B8-110320-10-20

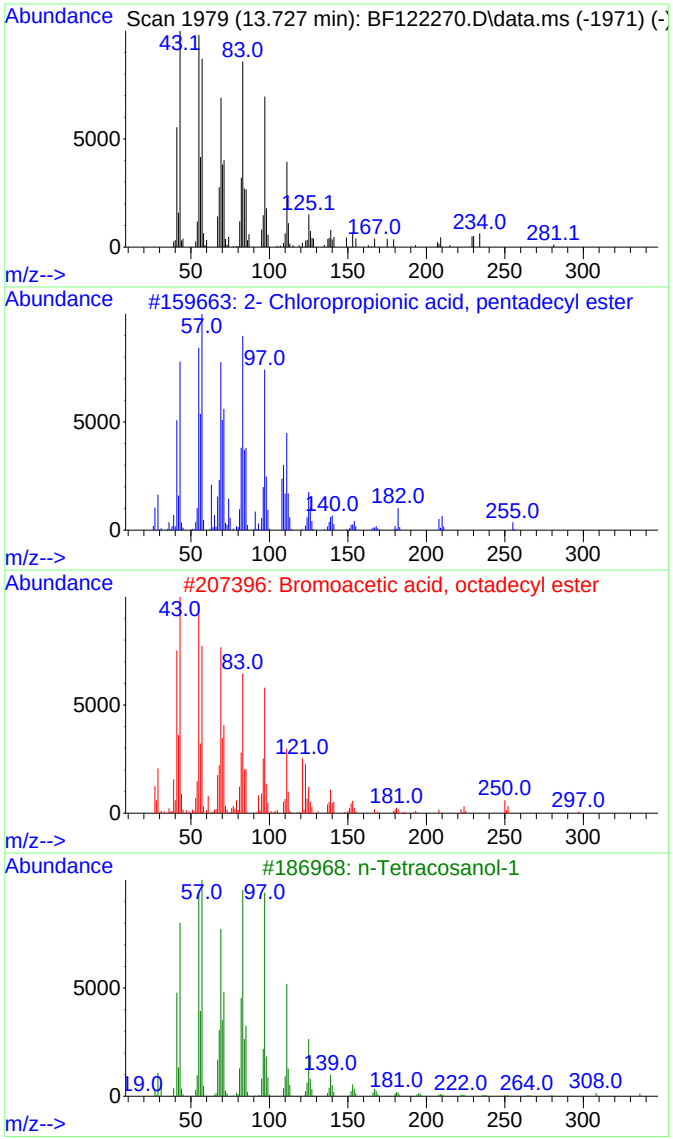
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

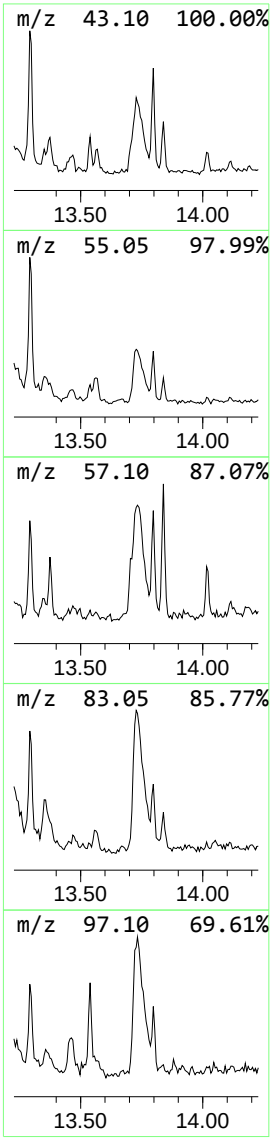
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 2- Chloropropionic acid, pe... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.727	8.91 ng	338986	Chrysene-d12	13.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	94
2	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
5	1-Heneicosanol	312	C21H44O	015594-90-8	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110420\
Data File : BF122270.D
Acq On : 4 Nov 2020 18:43
Operator : JU/CG
Sample : L4621-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAV-B8-110320-10-20

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
2,4,7,9-Tetrame...	9.186	5.9	ng	226867	3	9.745	769021	20.0
Methyl tetradec...	10.745	6.5	ng	211917	4	11.233	648770	20.0
9-Hexadecenoic ...	11.539	9.6	ng	312111	4	11.233	648770	20.0
Hexadecanoic ac...	11.621	125.6	ng	4072640	4	11.233	648770	20.0
10,13-Octadecad...	12.310	203.3	ng	6595150	4	11.233	648770	20.0
16-Octadecenoic...	12.351	378.4	ng	12276400	4	11.233	648770	20.0
Methyl 13-eicos...	13.051	14.2	ng	541822	5	13.886	760728	20.0
Eicosanoic acid...	13.133	6.4	ng	243876	5	13.886	760728	20.0
11-Hexadecynal	13.168	6.6	ng	251028	5	13.886	760728	20.0
9-Octadecenamid...	13.292	9.7	ng	367304	5	13.886	760728	20.0
unknown13.357	13.357	3.3	ng	126672	5	13.886	760728	20.0
unknown13.568	13.568	3.5	ng	133915	5	13.886	760728	20.0
2- Chloropropio...	13.727	8.9	ng	338986	5	13.886	760728	20.0