LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111122\
Data File : BF131174.D
Acq On : 12 Nov 2022 02:34
Operator : CG\JU
Sample : N5501-01 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HS-3-110722

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-BF110922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131174.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	6.504	747	751	760	rBV	667141	660913	1.02%	0.492%
2	9.233	1212	1215	1219	rVB	896977	698669	1.08%	0.520%
3	11.821	1647	1655	1658	rBV	9635863	14857756	23.04%	11.067%
4	12.010	1675	1687	1690	rBV2	1689468	3022299	4.69%	2.251%
5	12.104	1700	1703	1710	rVB2	773873	1045408	1.62%	0.779%
6	12.586	1764	1785	1786	rBV4	12941416	64500395	100.00%	48.042%
7	12.645	1791	1795	1797	rVB	9645222	10007522	15.52%	7.454%
8	12.745	1797	1812	1818	rBV4	7491873	32509160	50.40%	24.214%
9	13.198	1886	1889	1893	rVB2	537813	768721	1.19%	0.573%
10	13.251	1893	1898	1901	rBV2	1140318	1382938	2.14%	1.030%
11	13.333	1908	1912	1914	rBV	1507727	1308823	2.03%	0.975%
12	13.445	1925	1931	1935	rBV	797363	1216222	1.89%	0.906%
13	13.762	1981	1985	1991	rVB3	542931	792938	1.23%	0.591%
14	13.998	2021	2025	2028	rBV	1771881	1485552	2.30%	1.106%

Sum of corrected areas: 134257316

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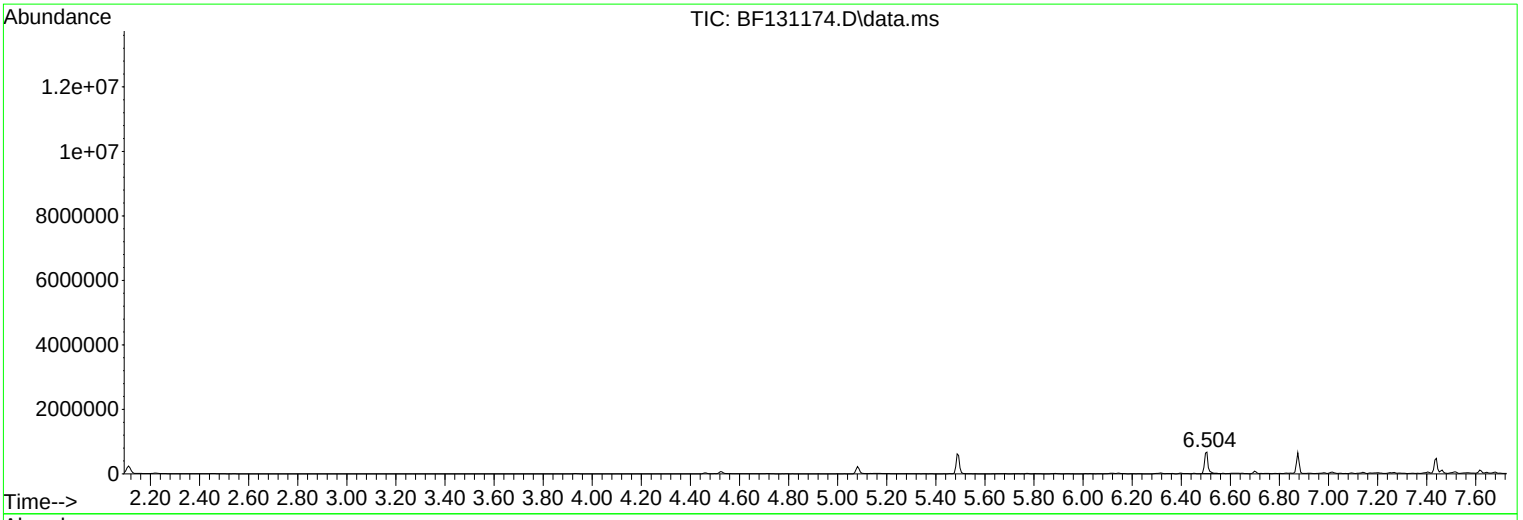
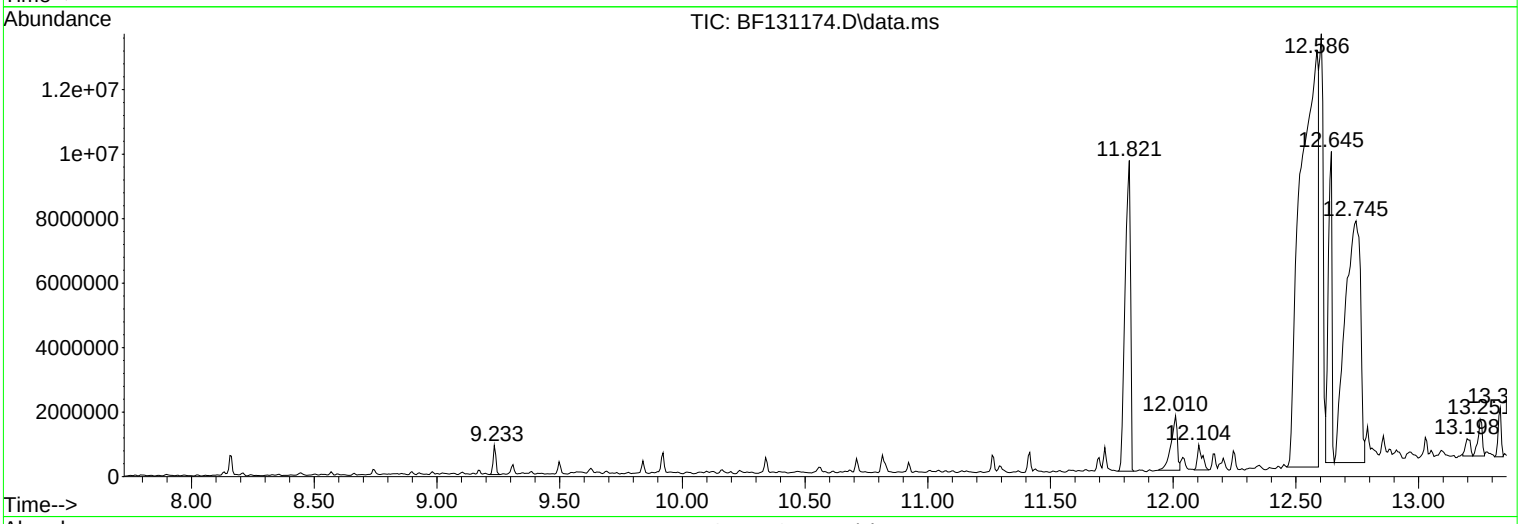
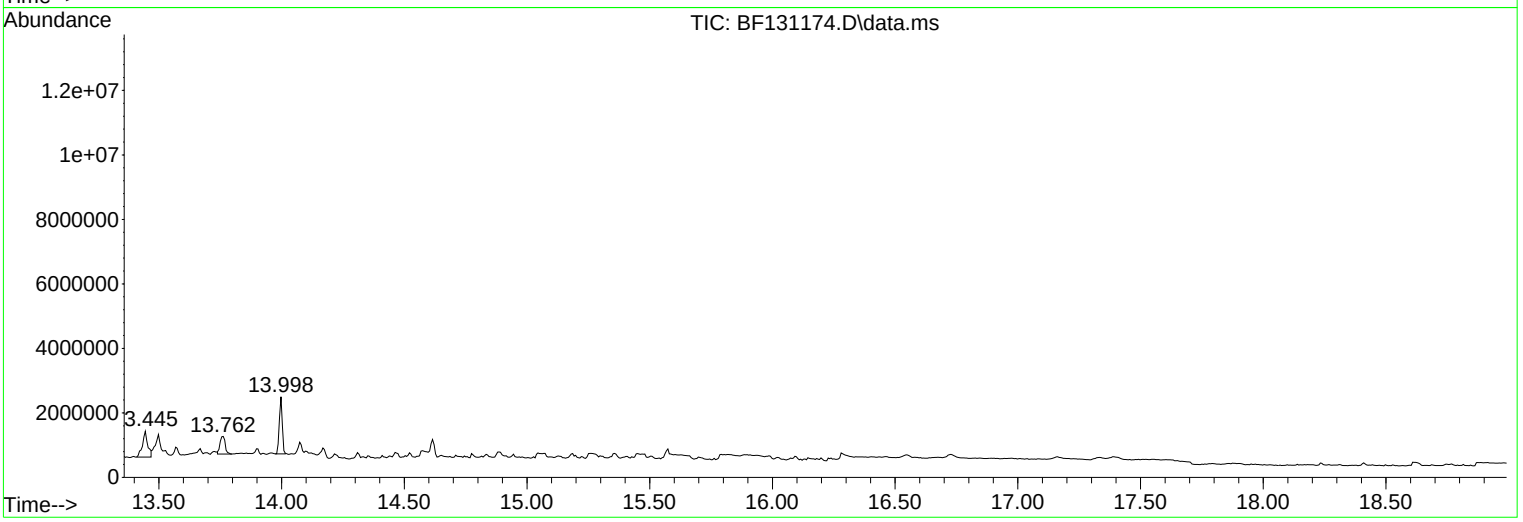
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







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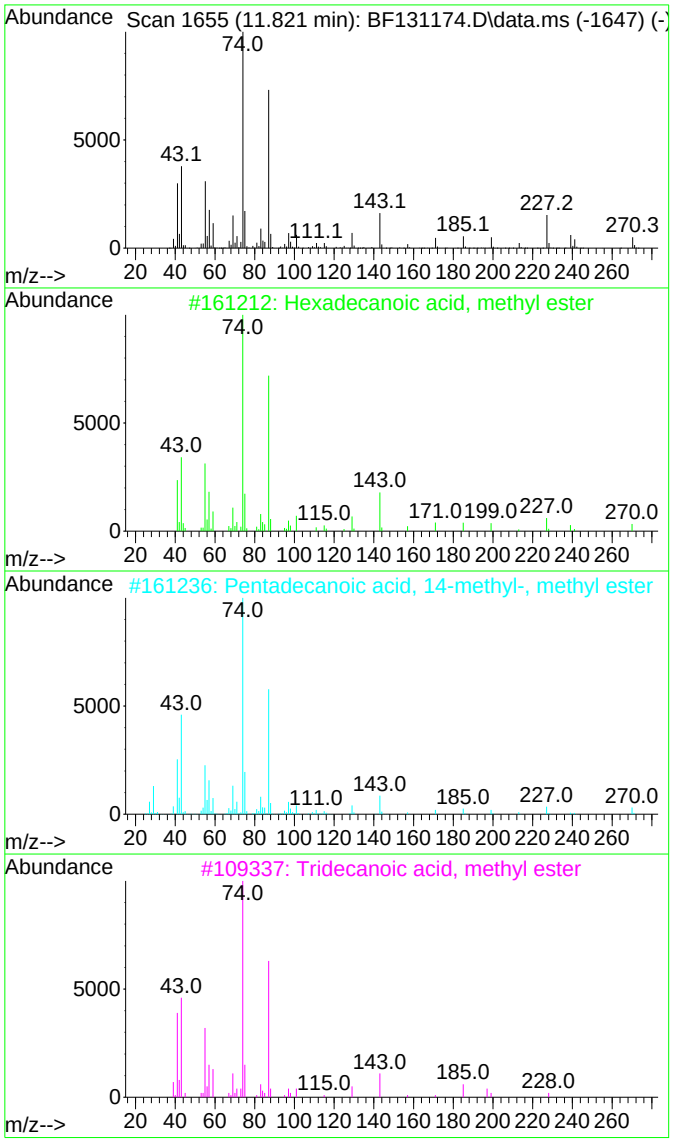
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

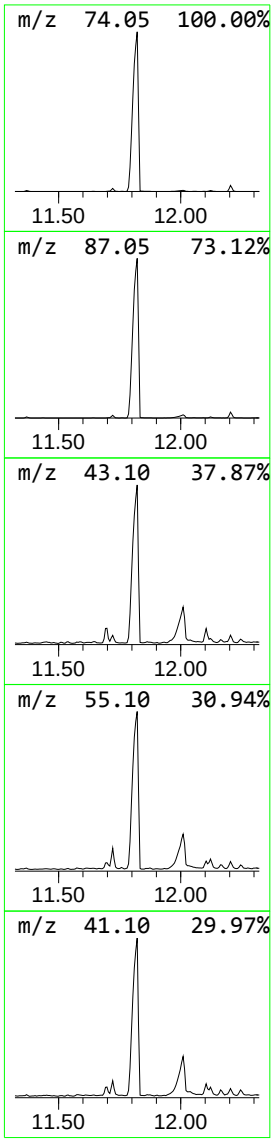
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.821	20.00 ng	14857800	Phenanthrene-d10	11.416

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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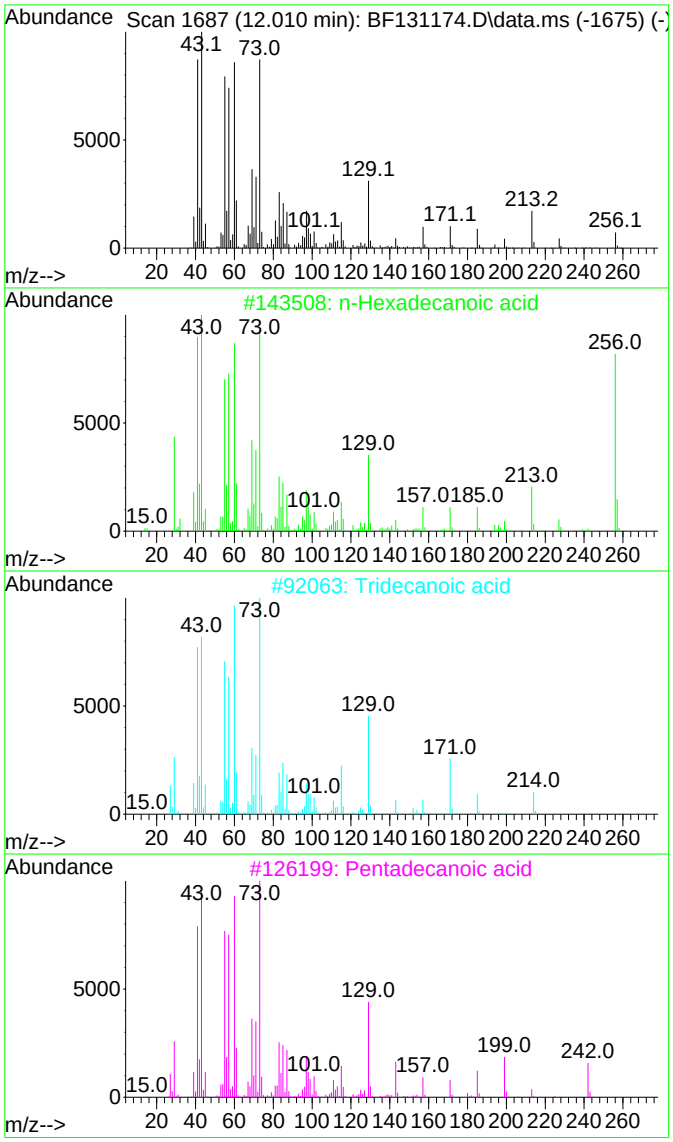
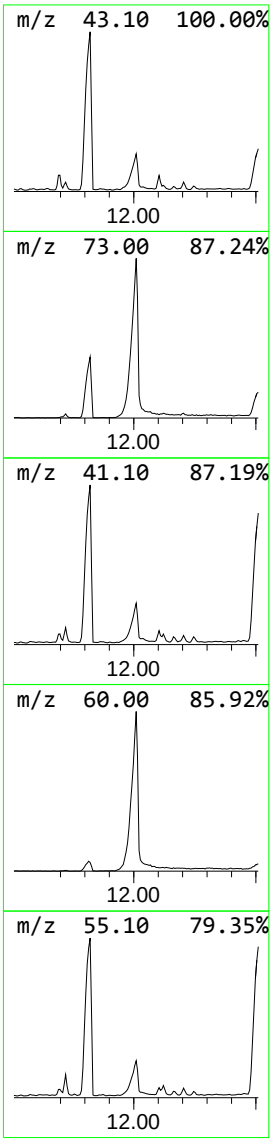
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.010	4.07 ng	3022300	Phenanthrene-d10	11.416

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	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	72





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Sample : N5501-01 2X
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Instrument :
BNA_F
ClientSampleId :
HS-3-110722

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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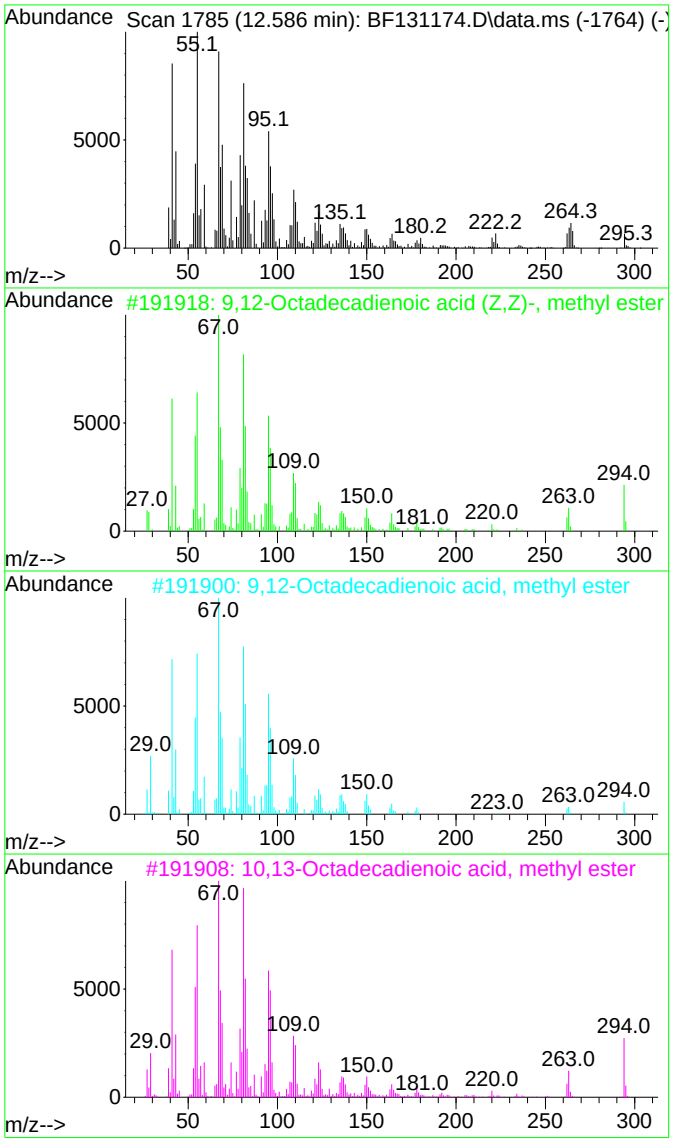
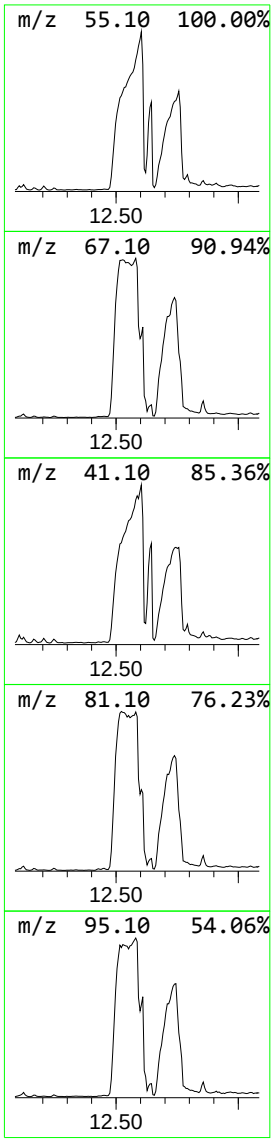
Peak Number 3 9,12-Octadecadienoic acid (... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.586	86.82 ng	64500400	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
3	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	98
4	Methyl 7,12-octadecadienoate	294	C19H34O2	1000336-43-8	97
5	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	95





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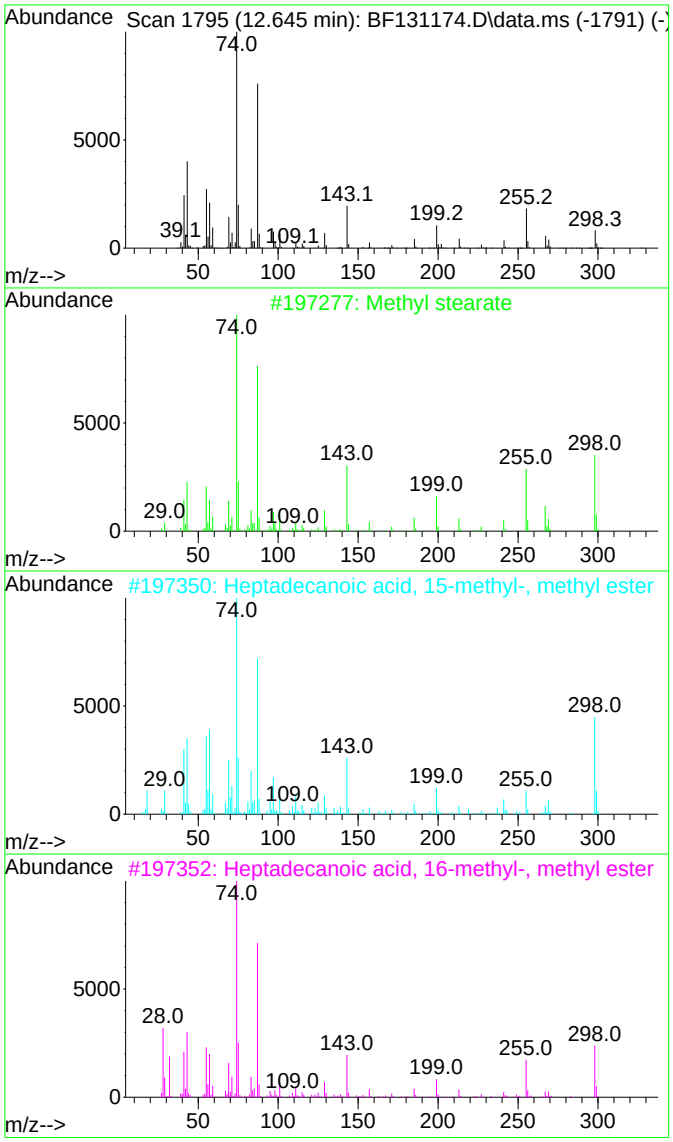
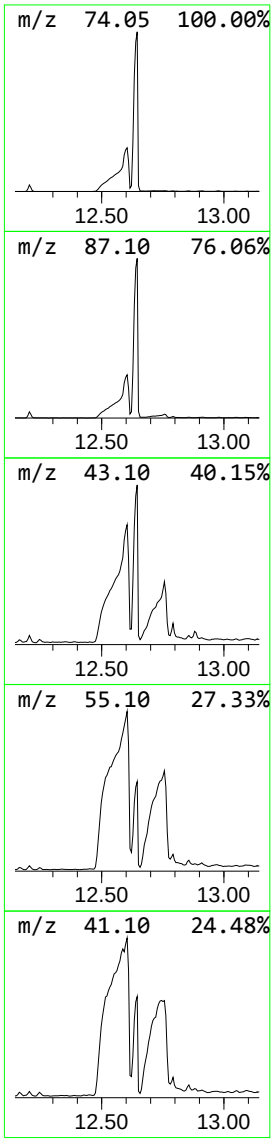
****

Peak Number 4 Methyl stearate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.645	13.47 ng	10007500	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	98
2	Heptadecanoic acid, 15-methyl-, ...	298	C19H38O2	054833-55-5	94
3	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	90
4	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	87
5	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	87





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Operator : CG\JU
Sample : N5501-01 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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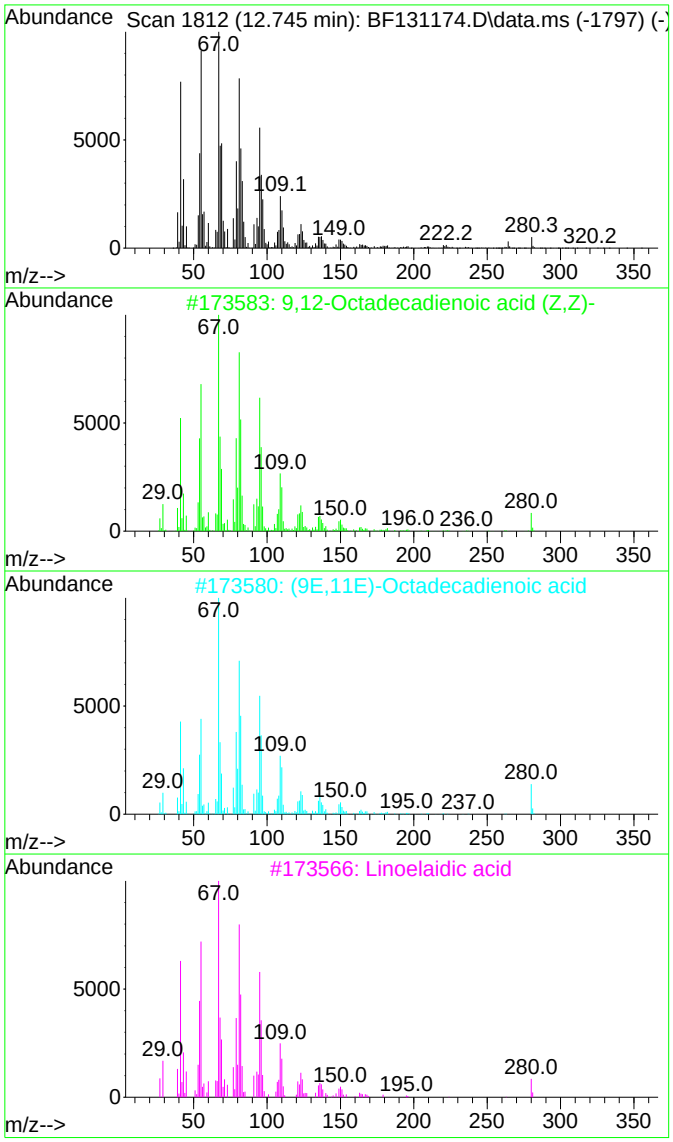
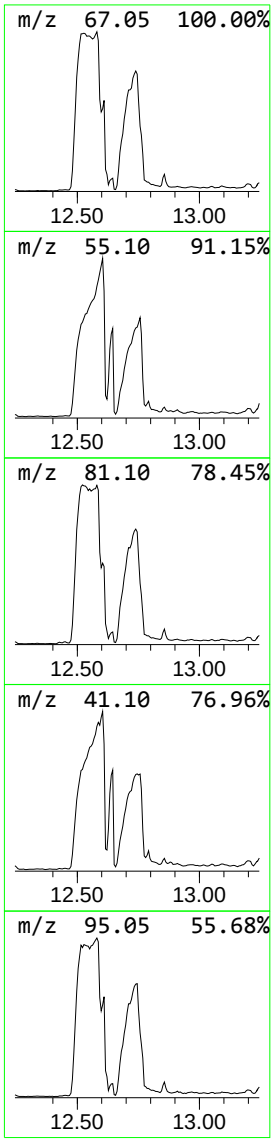
****
Peak Number 5 9,12-Octadecadienoic acid (... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.745	437.67 ng	32509200	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	99
2	(9E,11E)-Octadecadienoic acid	280	C18H32O2	000544-71-8	98
3	Linoelaidic acid	280	C18H32O2	000506-21-8	98
4	10E,12Z-Octadecadienoic acid	280	C18H32O2	002420-56-6	98
5	9,17-Octadecadienal, (Z)-	264	C18H32O	056554-35-9	93





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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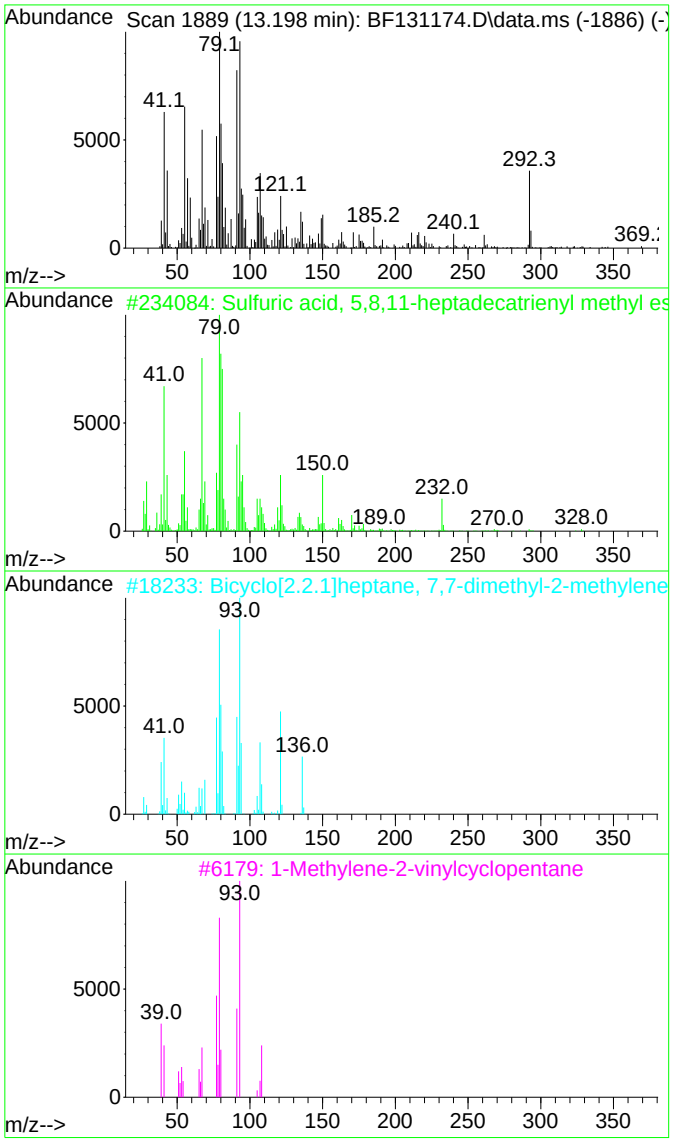
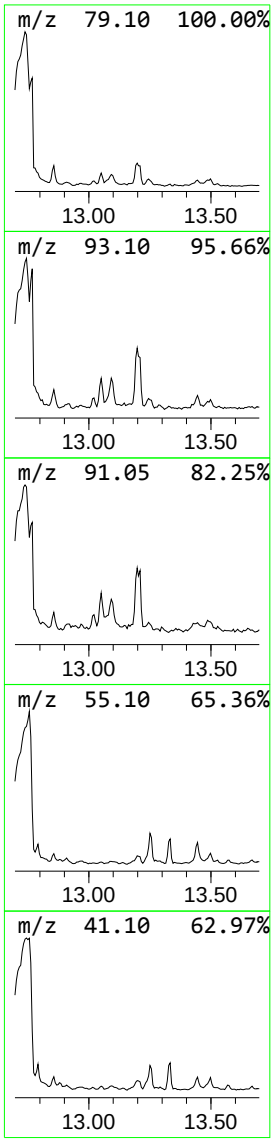
****

Peak Number 6 Sulfuric acid, 5,8,11-hepta... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.198	10.35 ng	768721	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfuric acid, 5,8,11-heptadecat...	328	C18H32O3S	056554-67-7	83
2	Bicyclo[2.2.1]heptane, 7,7-dimet...	136	C10H16	000471-84-1	70
3	1-Methylene-2-vinylcyclopentane	108	C8H12	006196-78-7	64
4	Cyclohexene, 5-methyl-3-(1-methy...	136	C10H16	056816-08-1	62
5	m-Mentha-4,8-diene, (1S,3S)-(+)-	136	C10H16	005208-51-5	62





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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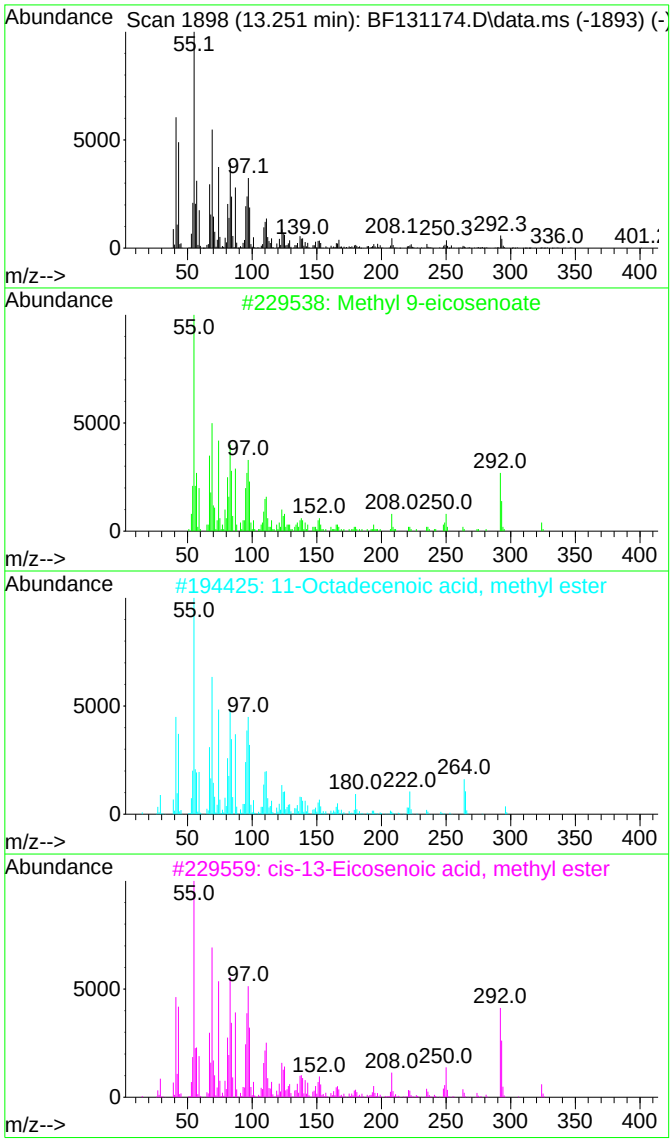
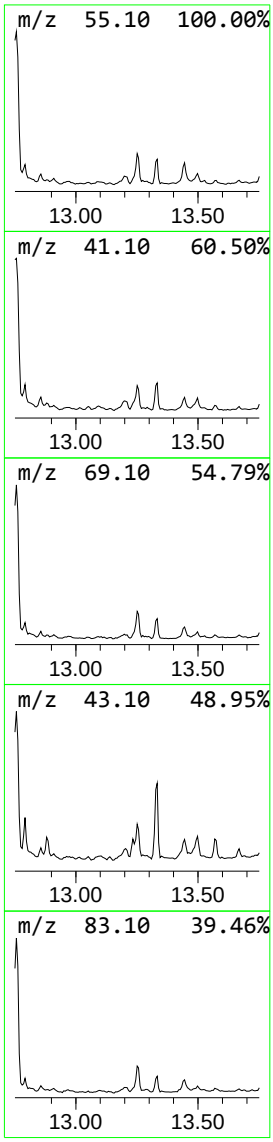
Peak Number 7 Methyl 9-eicosenoate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.251	18.62 ng	1382940	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 9-eicosenoate	324	C21H40O2	1000336-50-5	99
2	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	95
3	cis-13-Eicosenoic acid, methyl e...	324	C21H40O2	069120-02-1	91
4	11-Eicosenoic acid, methyl ester	324	C21H40O2	003946-08-5	91
5	cis-Methyl 11-eicosenoate	324	C21H40O2	002390-09-2	91





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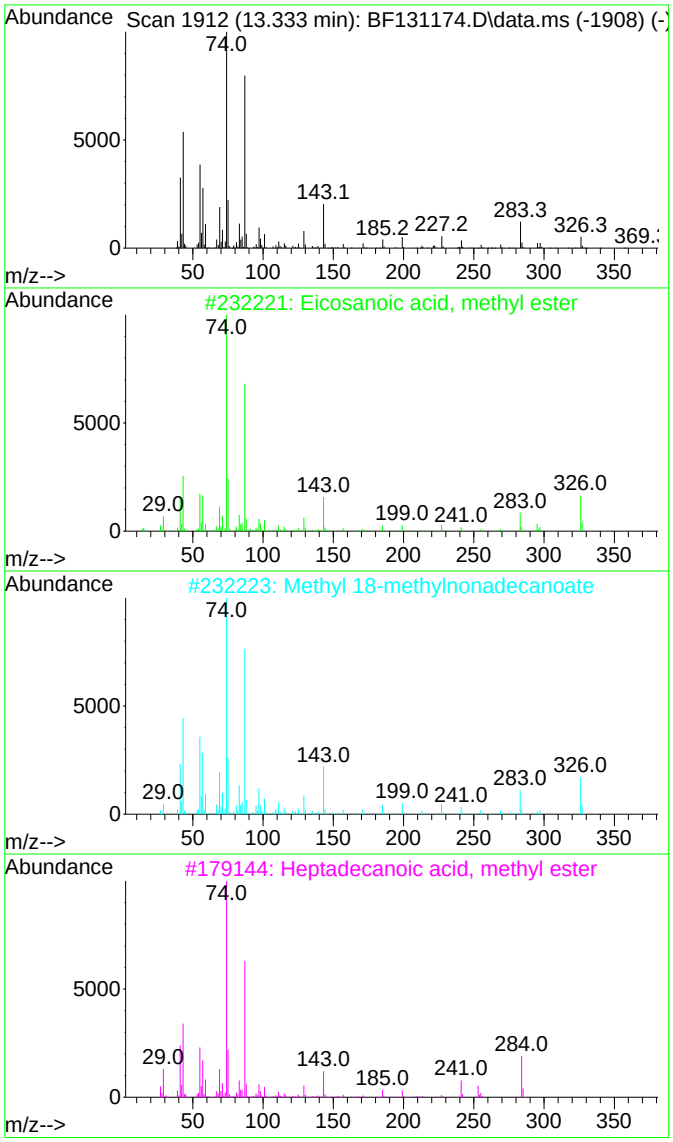
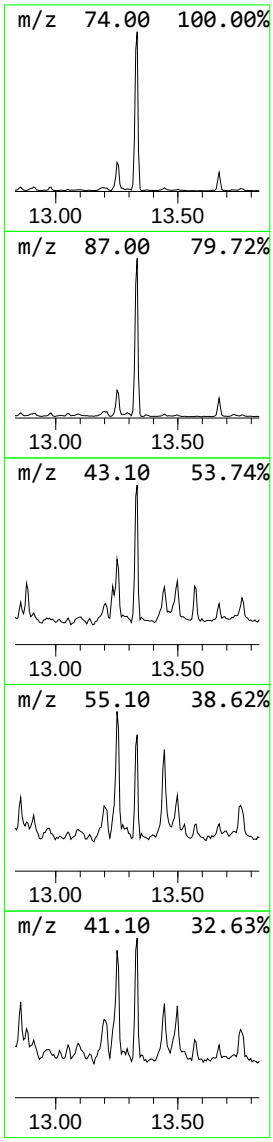
Peak Number 8 Eicosanoic acid, methyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.333	17.62 ng	1308820	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	98
2	Methyl 18-methylnonadecanoate	326	C21H42O2	1000424-52-4	94
3	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	93
4	Methyl stearate	298	C19H38O2	000112-61-8	93
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	90





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TIC Library : C:\Database\NIST20.L
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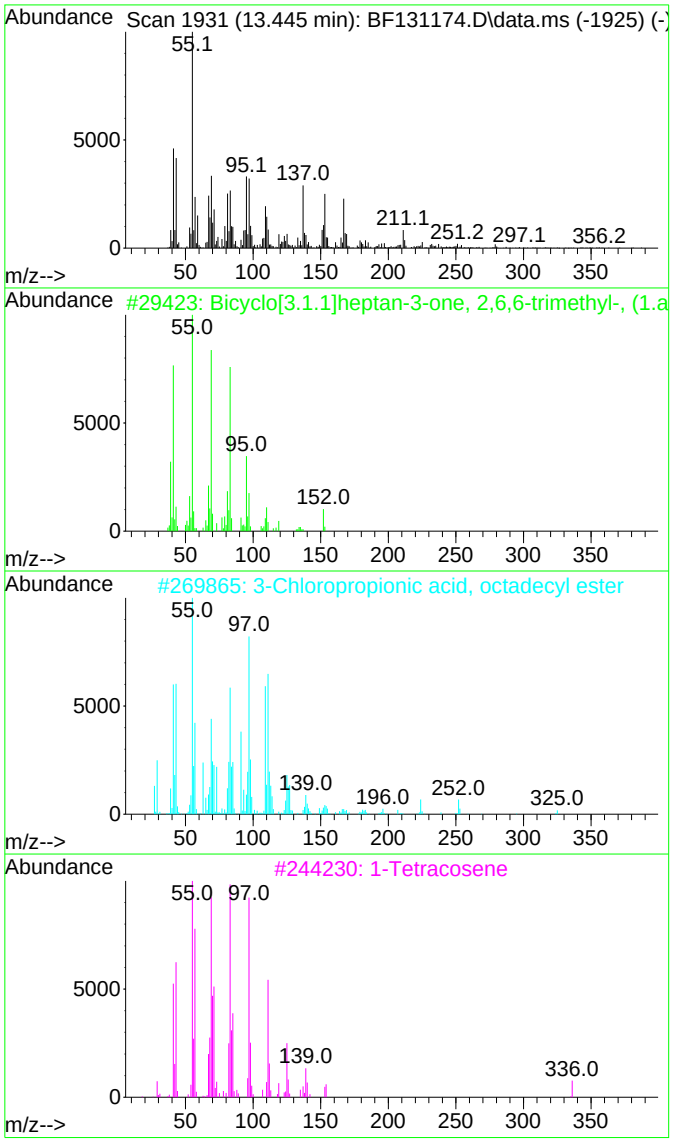
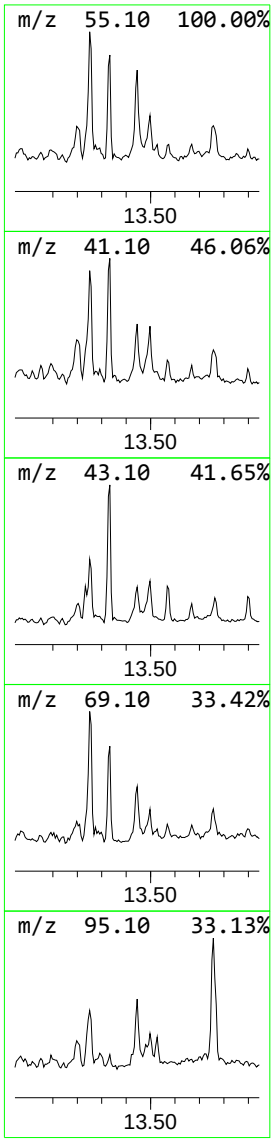
Peak Number 9 unknown13.445 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.445	16.37 ng	1216220	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	22
2	3-Chloropropionic acid, octadecy...	360	C21H41ClO2	088168-99-4	22
3	1-Tetracosene	336	C24H48	010192-32-2	15
4	6-Nonenal, 3,7-dimethyl-	168	C11H20O	1000132-43-9	14
5	2-Allyl-2-methylcyclohexanone	152	C10H16O	1000424-66-1	14





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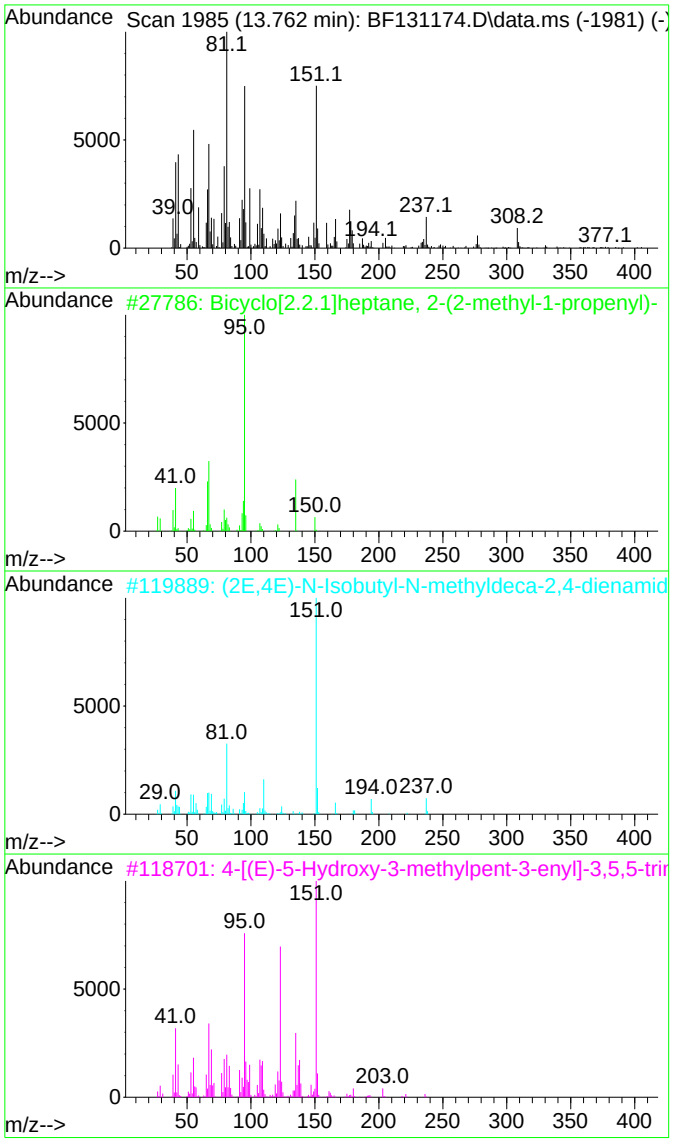
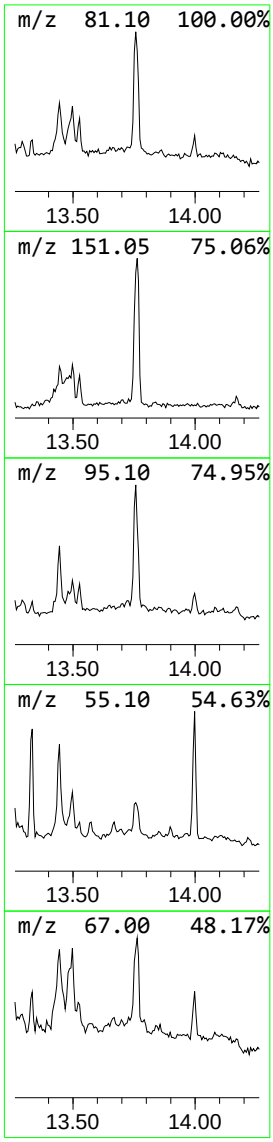
Peak Number 10 unknown13.762 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.762	10.68 ng	792938	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptane, 2-(2-meth...	150	C11H18	061142-27-6	43
2	(2E,4E)-N-Isobutyl-N-methyldeca-...	237	C15H27NO	1472057-16-1	38
3	4-[(E)-5-Hydroxy-3-methylpent-3-...	236	C15H24O2	1083195-46-3	25
4	2,6-Dimethyl-3-aminobenzoquinone	151	C8H9NO2	090005-56-4	15
5	1,4-Cyclohexanedimethanol	144	C8H16O2	000105-08-8	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111122\
Data File : BF131174.D
Acq On : 12 Nov 2022 02:34
Operator : CG\JU
Sample : N5501-01 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HS-3-110722

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

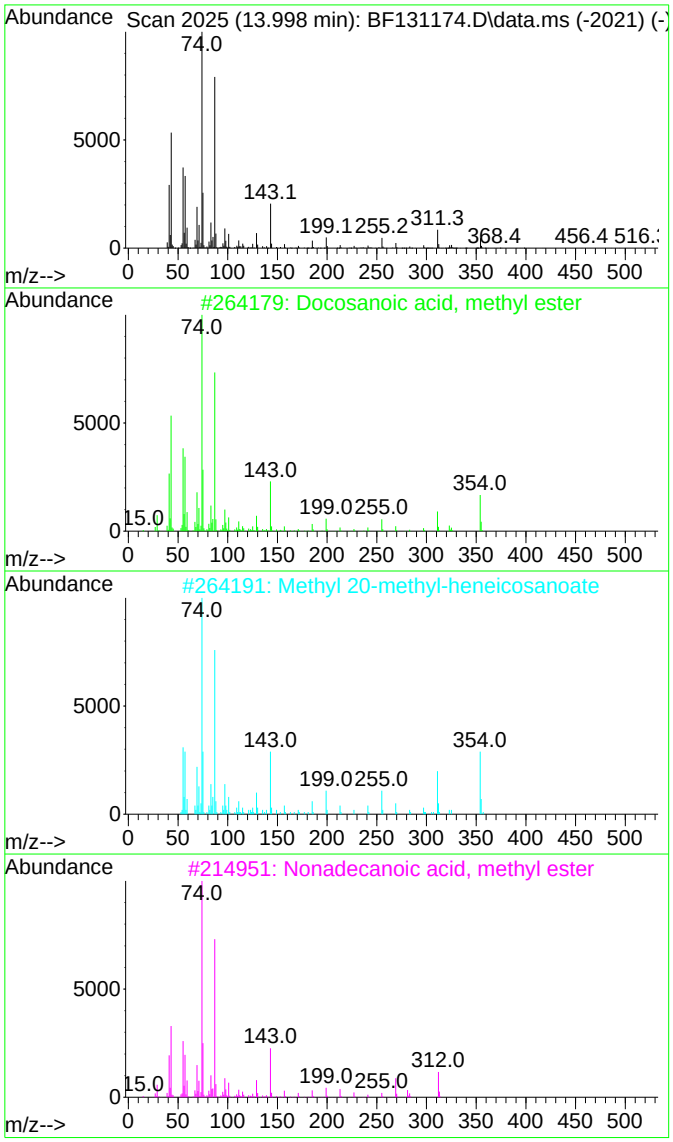
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

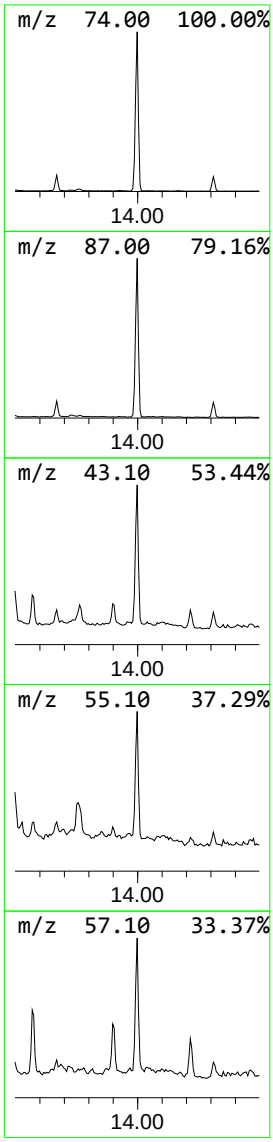
****

Peak Number 11 Docosanoic acid, methyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.998	20.00 ng	1485550	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosanoic acid, methyl ester	354	C23H46O2	000929-77-1	98
2	Methyl 20-methyl-heneicosanoate	354	C23H46O2	1000336-47-4	96
3	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	87
4	Methyl stearate	298	C19H38O2	000112-61-8	87
5	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111122\
Data File : BF131174.D
Acq On : 12 Nov 2022 02:34
Operator : CG\JU
Sample : N5501-01 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HS-3-110722

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Hexadecanoic ac...	11.821	20.0	ng	14857800	4	11.416	14857800	20.0
n-Hexadecanoic ...	12.010	4.1	ng	3022300	4	11.416	14857800	20.0
9,12-Octadecadi...	12.586	86.8	ng	64500400	4	11.416	14857800	20.0
Methyl stearate	12.645	13.5	ng	10007500	4	11.416	14857800	20.0
9,12-Octadecadi...	12.745	437.7	ng	32509200	5	14.074	1485550	20.0
Sulfuric acid, ...	13.198	10.4	ng	768721	5	14.074	1485550	20.0
Methyl 9-eicose...	13.251	18.6	ng	1382940	5	14.074	1485550	20.0
Eicosanoic acid...	13.333	17.6	ng	1308820	5	14.074	1485550	20.0
unknown13.445	13.445	16.4	ng	1216220	5	14.074	1485550	20.0
unknown13.762	13.762	10.7	ng	792938	5	14.074	1485550	20.0
Docosanoic acid...	13.998	20.0	ng	1485550	5	14.074	1485550	20.0