LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042922\
Data File : BF128002.D
Acq On : 29 Apr 2022 18:41
Operator : CG\JU
Sample : N2616-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-20S

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-BF042222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128002.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.546	549	554	557	rBV	2787275	2627109	83.22%	13.017%
2	6.551	719	725	728	rBV	2412701	2743143	86.89%	13.592%
3	6.922	784	788	791	rBV	873223	665311	21.07%	3.297%
4	7.487	879	884	887	rBV	1948806	1868769	59.19%	9.260%
5	7.557	892	896	900	rVV	74239	67034	2.12%	0.332%
6	8.204	1002	1006	1009	rBV	969479	816084	25.85%	4.044%
7	9.281	1184	1189	1192	rBV	3469967	3156993	100.00%	15.643%
8	9.351	1198	1201	1204	rVB	62407	48135	1.52%	0.239%
9	9.539	1230	1233	1239	rBV	142078	119283	3.78%	0.591%
10	9.963	1301	1305	1309	rVB	1137928	934170	29.59%	4.629%
11	10.381	1370	1376	1379	rVB2	34118	39448	1.25%	0.195%
12	10.757	1435	1440	1443	rBV	1978381	1774819	56.22%	8.794%
13	10.857	1454	1457	1465	rBV	38132	55331	1.75%	0.274%
14	11.457	1555	1559	1562	rBV	958353	831219	26.33%	4.119%
15	11.833	1621	1623	1627	rVB	231014	199418	6.32%	0.988%
16	11.969	1643	1646	1653	rBV3	137272	138199	4.38%	0.685%
17	12.545	1741	1744	1747	rVB2	155167	125381	3.97%	0.621%
18	12.633	1756	1759	1763	rBV	105273	99172	3.14%	0.491%
19	12.669	1763	1765	1768	rBV	61529	54772	1.73%	0.271%
20	12.904	1802	1805	1807	rBV	76920	66883	2.12%	0.331%
21	12.951	1807	1813	1820	rVV	138700	340919	10.80%	1.689%
22	13.045	1825	1829	1832	rVV	2534233	2185460	69.23%	10.829%
23	14.104	2005	2009	2012	rBV	652486	580300	18.38%	2.875%
24	15.615	2262	2266	2277	rVB	459147	644410	20.41%	3.193%

Sum of corrected areas: 20181762

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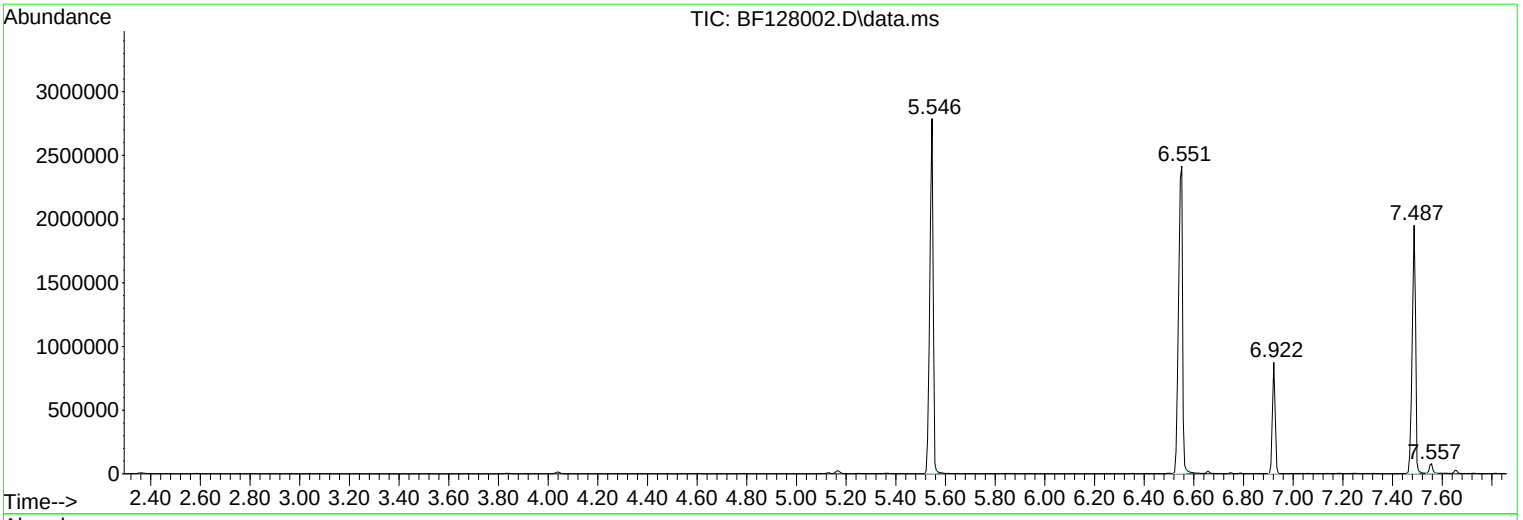
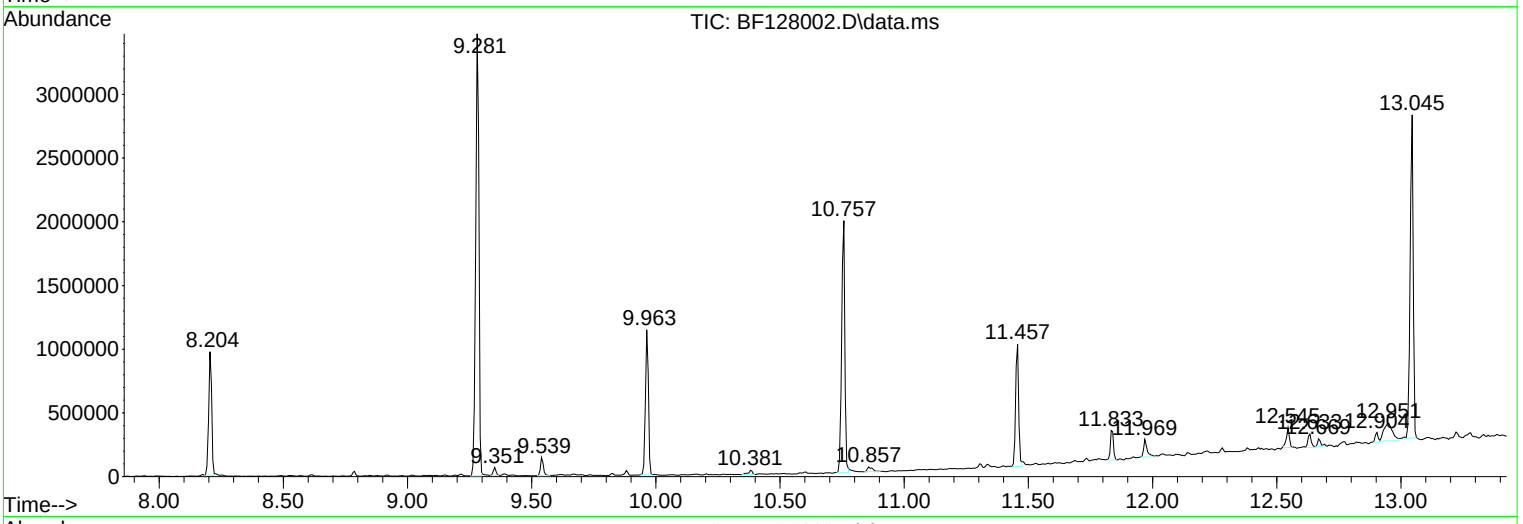
ALS Vial : 13 Sample Multiplier: 1

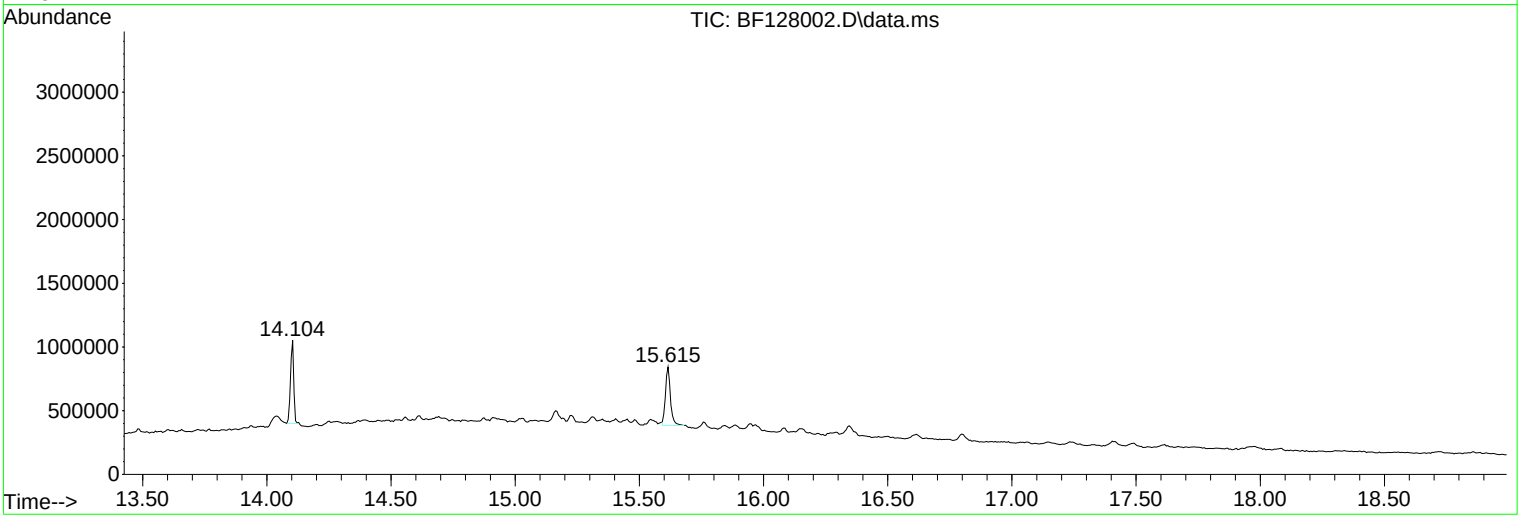
Instrument :
BNA_F
ClientSampleId :
MH-20S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.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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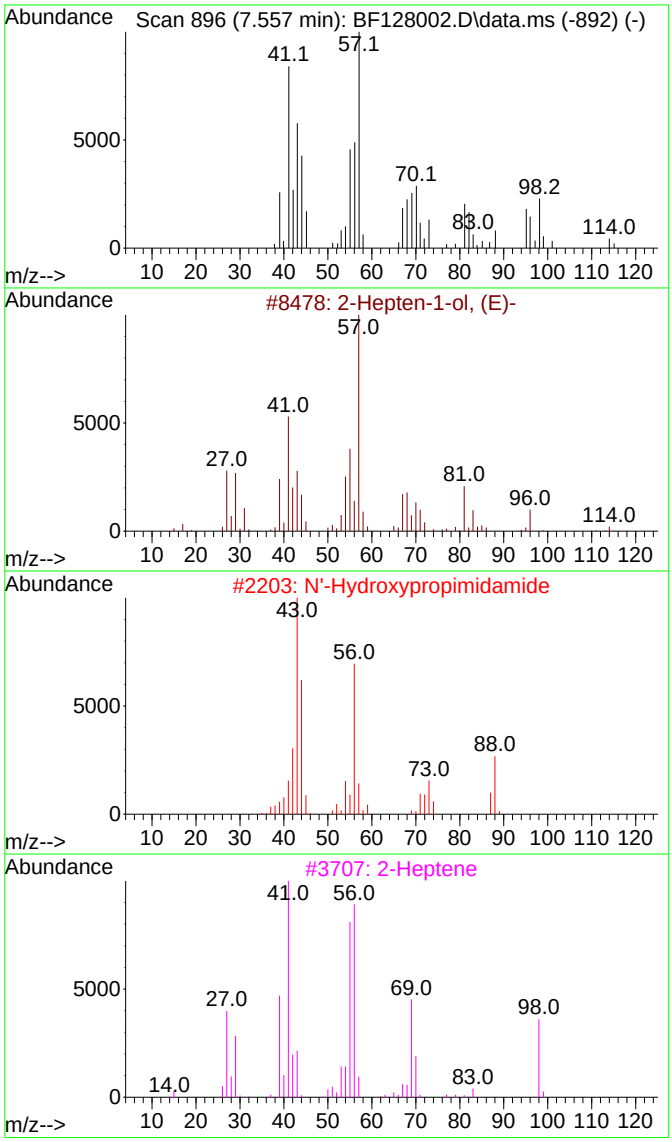
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

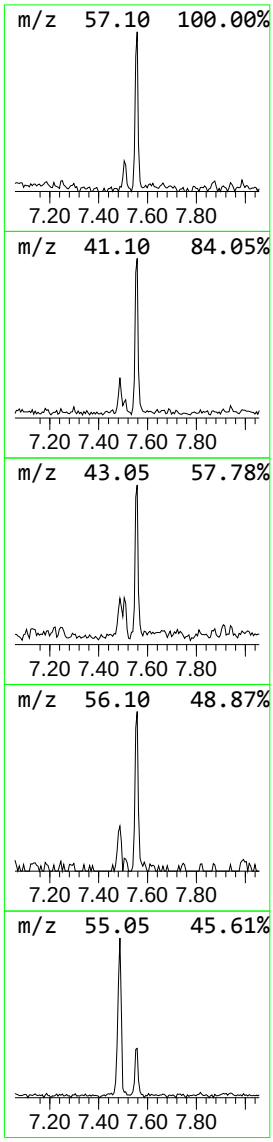
****

Peak Number 1 unknown7.557 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.557	2.02 ng	67034	1,4-Dichlorobenzene-d4	6.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hepten-1-ol, (E)-	114	C7H14O	033467-76-4	38
2	N'-Hydroxypropimidamide	88	C3H8N2O	029335-36-2	35
3	2-Heptene	98	C7H14	000592-77-8	30
4	1-Heptene	98	C7H14	000592-76-7	27
5	Cyclohexanol, 4-methyl-	114	C7H14O	000589-91-3	27





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ALS Vial : 13 Sample Multiplier: 1

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BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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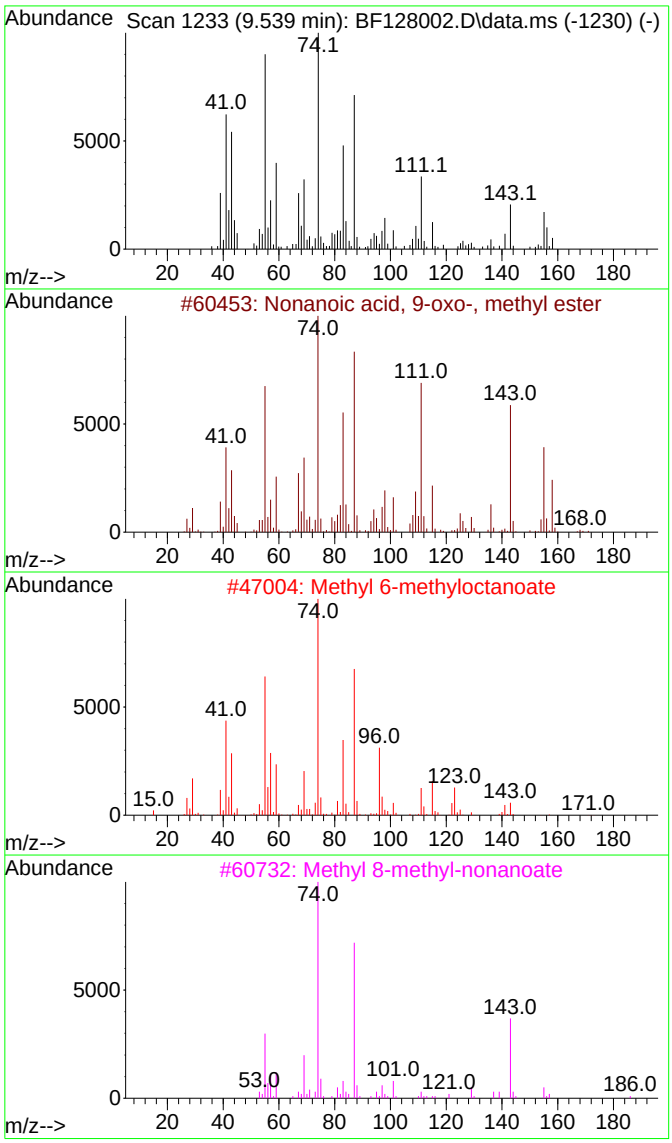
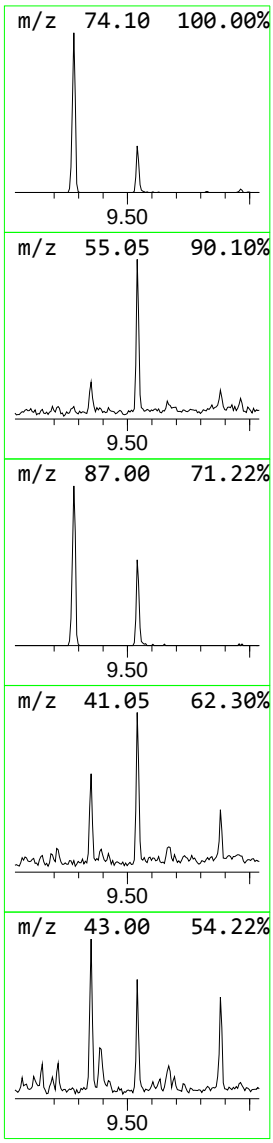
****
Peak Number 2 Nonanoic acid, 9-oxo-, meth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.539	2.55 ng	119283	Acenaphthene-d10	9.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanoic acid, 9-oxo-, methyl ester	186	C10H18O3	001931-63-1	90
2	Methyl 6-methyloctanoate	172	C10H20O2	005129-62-4	53
3	Methyl 8-methyl-nonanoate	186	C11H22O2	1000452-00-9	43
4	Hexanoic acid, methyl ester	130	C7H14O2	000106-70-7	38
5	Cyclopentanol, 3-(carbmethoxy)me...	158	C8H14O3	339363-86-9	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042922\
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Sample : N2616-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-20S

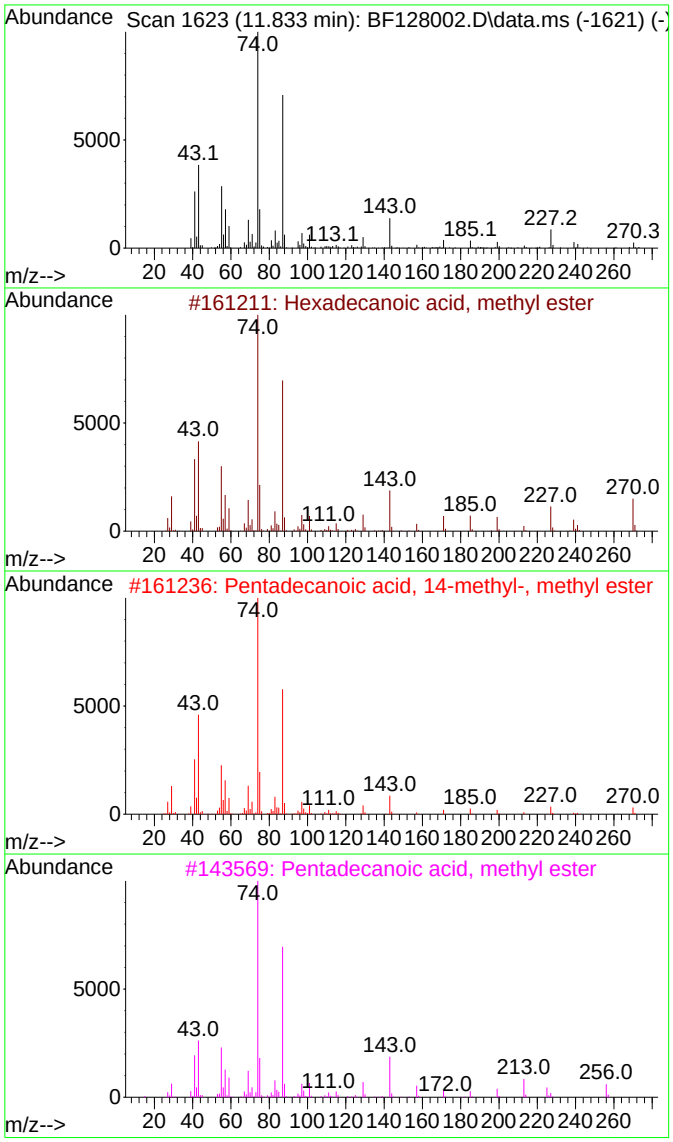
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

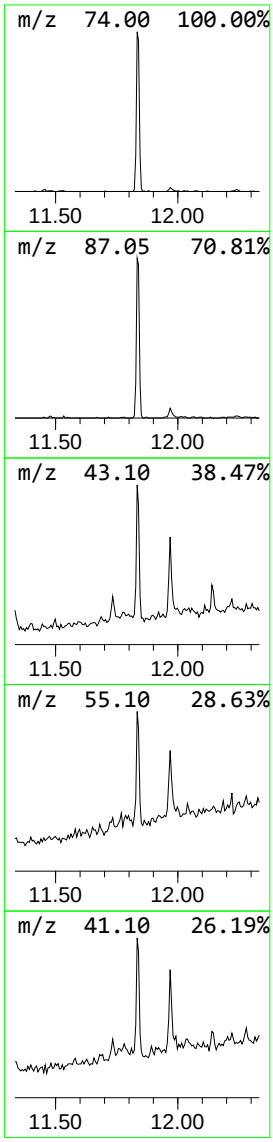
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.833	4.80 ng	199418	Phenanthrene-d10	11.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	97
3	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	93
4	Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	90
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	90





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Operator : CG\JU
Sample : N2616-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-20S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

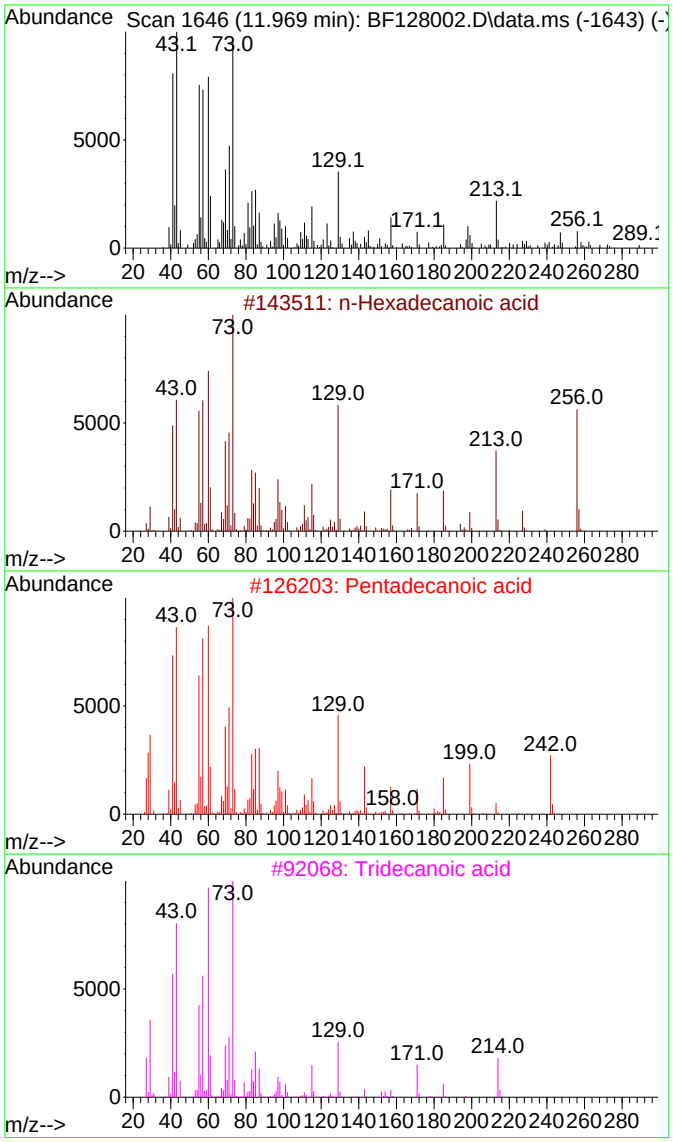
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

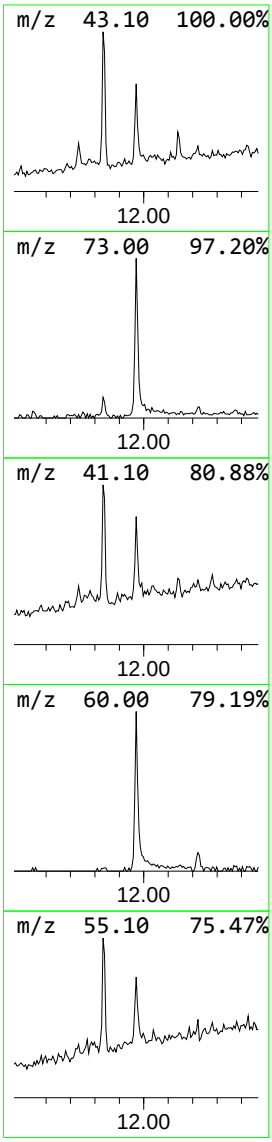
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.969	3.33 ng	138199	Phenanthrene-d10	11.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042922\
Data File : BF128002.D
Acq On : 29 Apr 2022 18:41
Operator : CG\JU
Sample : N2616-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-20S

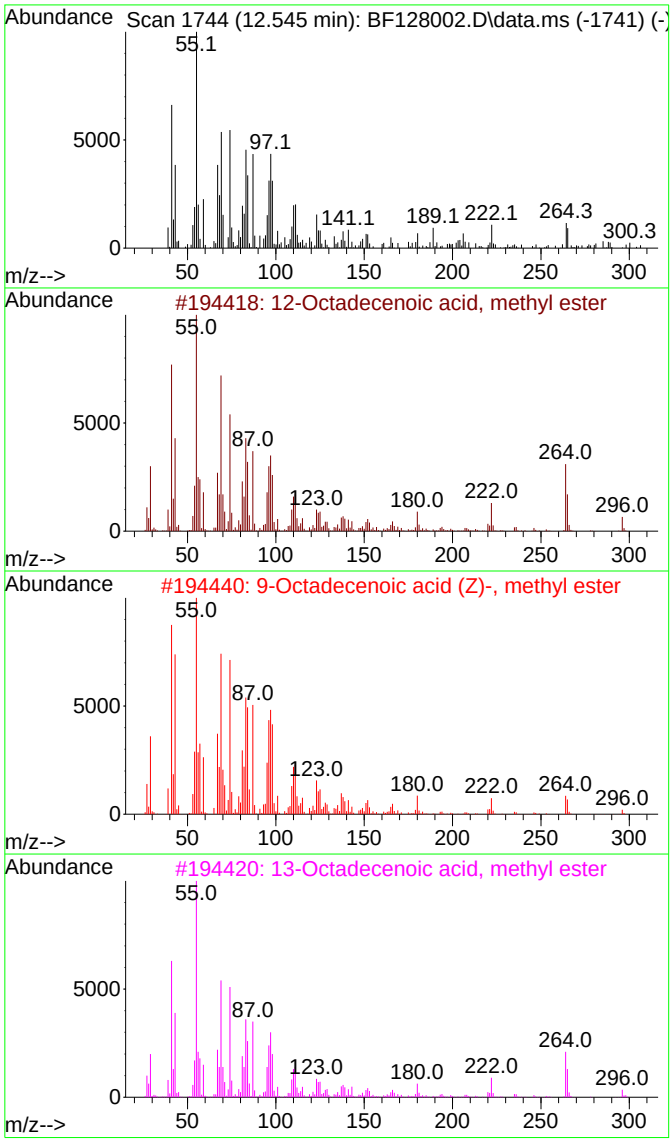
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

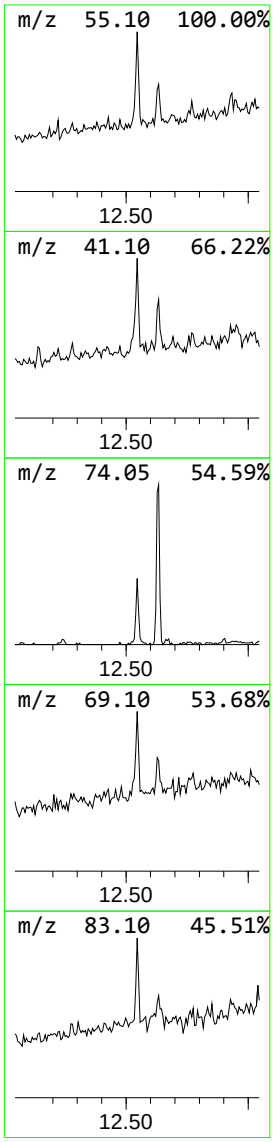
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 12-Octadecenoic acid, methy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.545	3.02 ng	125381	Phenanthrene-d10	11.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	95
2	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	94
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	94
4	(Z)-15-Octadecenoic acid methyl ...	296	C19H36O2	1000427-69-3	91
5	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	91





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

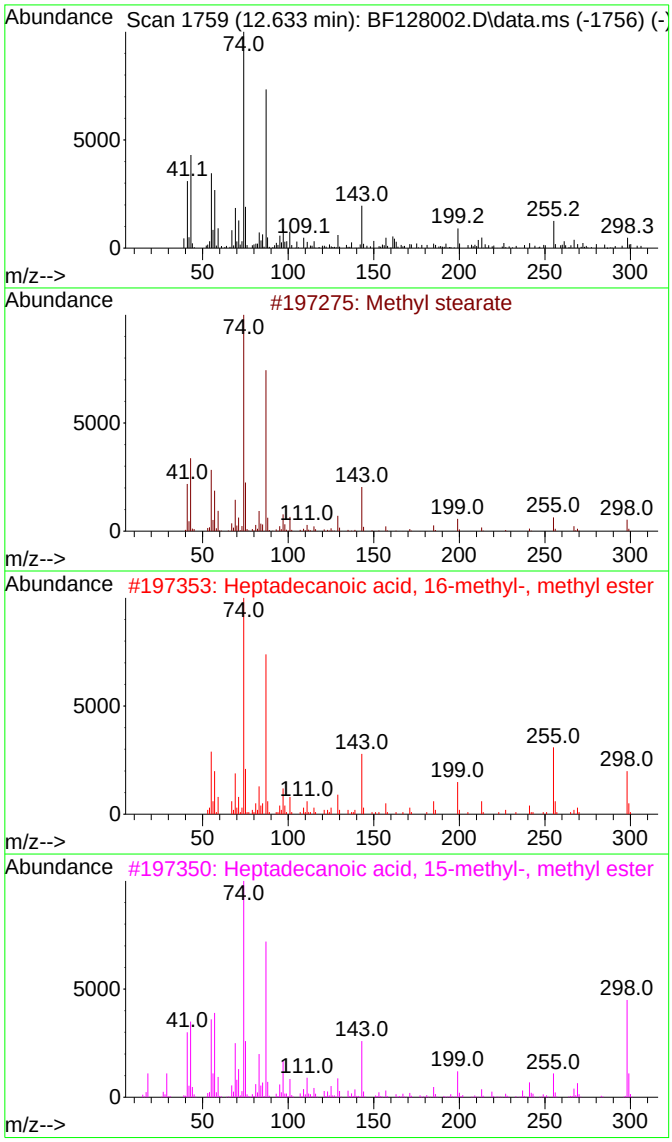
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

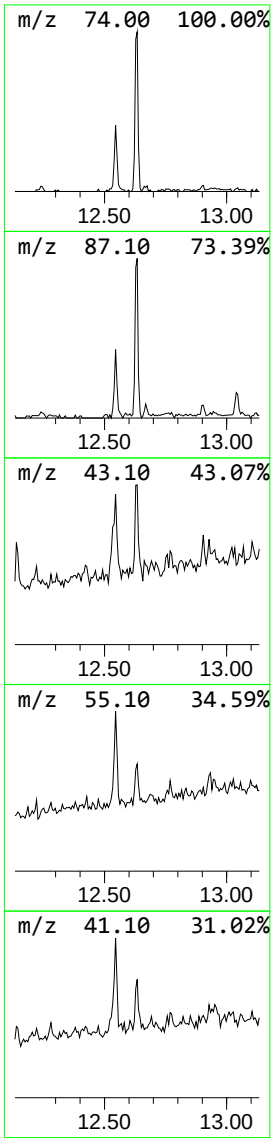
****

Peak Number 6 Methyl stearate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.633	2.39 ng	99172	Phenanthrene-d10	11.457

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	94
3	Heptadecanoic acid, 15-methyl-, ...	298	C19H38O2	054833-55-5	90
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	87
5	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	80





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BNA_F
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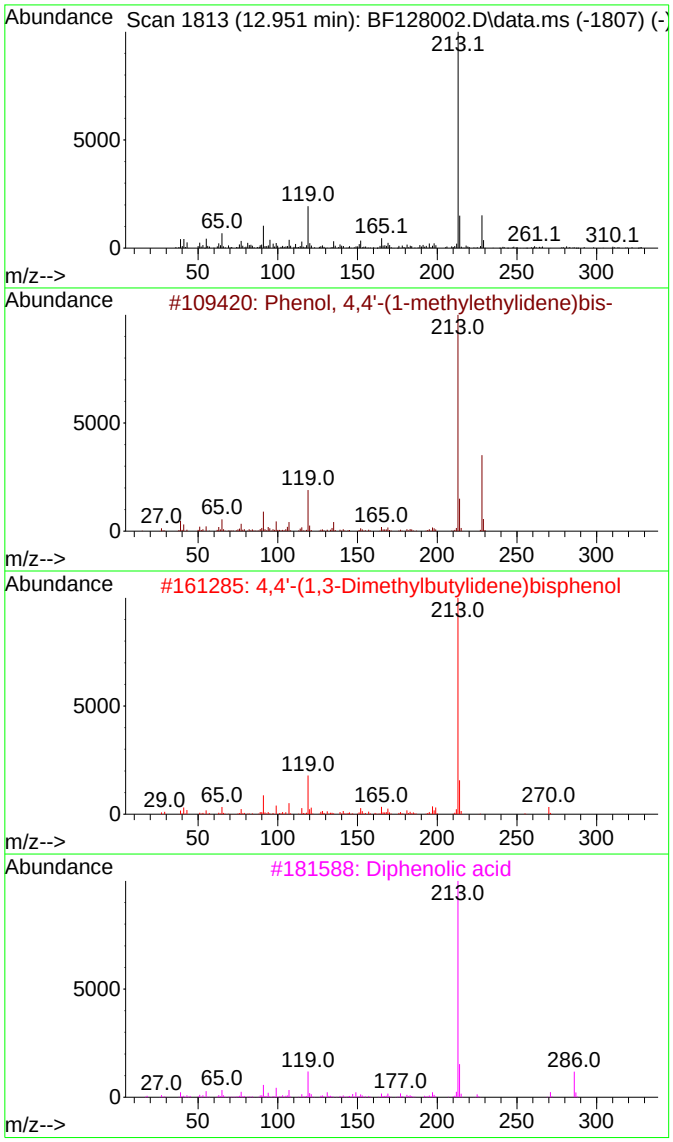
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

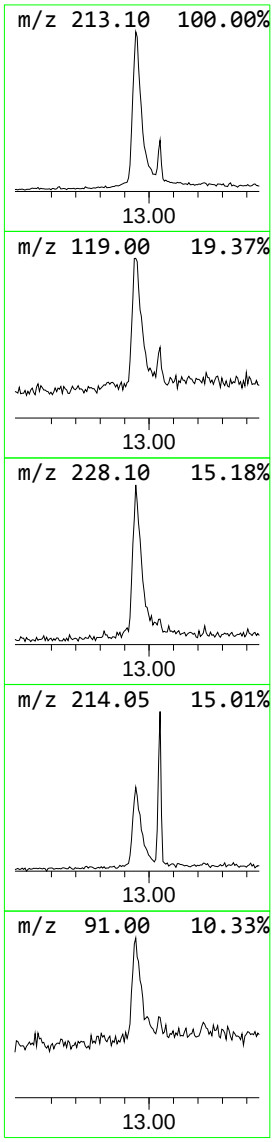
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Phenol, 4,4'-(1-methylethyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.951	11.75 ng	340919	Chrysene-d12	14.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	94
2	4,4'-(1,3-Dimethylbutylidene)bis...	270	C18H22O2	006807-17-6	72
3	Diphenolic acid	286	C17H18O4	000126-00-1	72
4	2,2-Bis-(4-hyxroxyphenyl)-butane	242	C16H18O2	000077-40-7	56
5	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	53





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown7.557	7.557	2.0	ng	67034	1	6.922	665311	20.0
Nonanoic acid, ...	9.539	2.5	ng	119283	3	9.963	934170	20.0
Hexadecanoic ac...	11.833	4.8	ng	199418	4	11.457	831219	20.0
n-Hexadecanoic ...	11.969	3.3	ng	138199	4	11.457	831219	20.0
12-Octadecenoic...	12.545	3.0	ng	125381	4	11.457	831219	20.0
Methyl stearate	12.633	2.4	ng	99172	4	11.457	831219	20.0
Phenol, 4,4'-(1...	12.951	11.8	ng	340919	5	14.104	580300	20.0