LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101722\
Data File : BF130687.D
Acq On : 17 Oct 2022 15:23
Operator : CG\JU
Sample : N5133-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HAS-WATER-1013

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-BF101122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130687.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.740	447	451	462	rBV	171439	209546	7.07%	1.412%
2	5.175	522	525	541	rBV	867959	903181	30.49%	6.088%
3	6.222	700	703	720	rBV	551097	583317	19.69%	3.932%
4	6.569	759	762	769	rVB	616676	536632	18.11%	3.617%
5	7.145	855	860	863	rBV	1522840	1494915	50.46%	10.076%
6	7.857	976	981	984	rVB	760997	705954	23.83%	4.758%
7	8.139	1025	1029	1035	rVB	41586	39171	1.32%	0.264%
8	8.933	1158	1164	1167	rBV	3392479	2962648	100.00%	19.969%
9	9.057	1181	1185	1190	rVB	38273	45217	1.53%	0.305%
10	9.604	1273	1278	1281	rBV	935452	789103	26.64%	5.319%
11	10.392	1407	1412	1426	rBV	1791681	1868534	63.07%	12.594%
12	11.080	1526	1529	1533	rBV	823583	729767	24.63%	4.919%
13	11.627	1616	1622	1634	rBV	279929	343872	11.61%	2.318%
14	12.410	1749	1755	1767	rVB	207513	264313	8.92%	1.781%
15	12.668	1795	1799	1802	rBV	2588276	2140703	72.26%	14.429%
16	13.686	1967	1972	1973	rBV5	23753	34519	1.17%	0.233%
17	13.715	1973	1977	1984	rVB	465212	448650	15.14%	3.024%
18	14.551	2115	2119	2124	rVB	139040	126530	4.27%	0.853%
19	15.086	2206	2210	2218	rVB	398287	469186	15.84%	3.162%
20	17.309	2579	2588	2599	rVB6	43026	140808	4.75%	0.949%

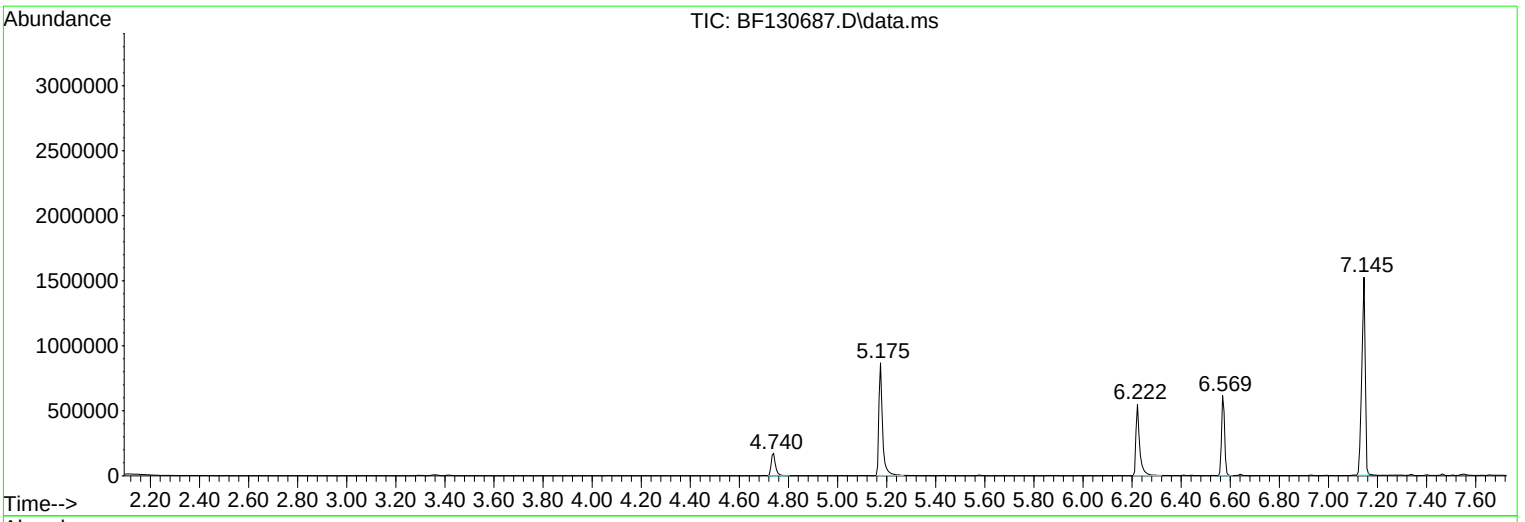
Sum of corrected areas: 14836566

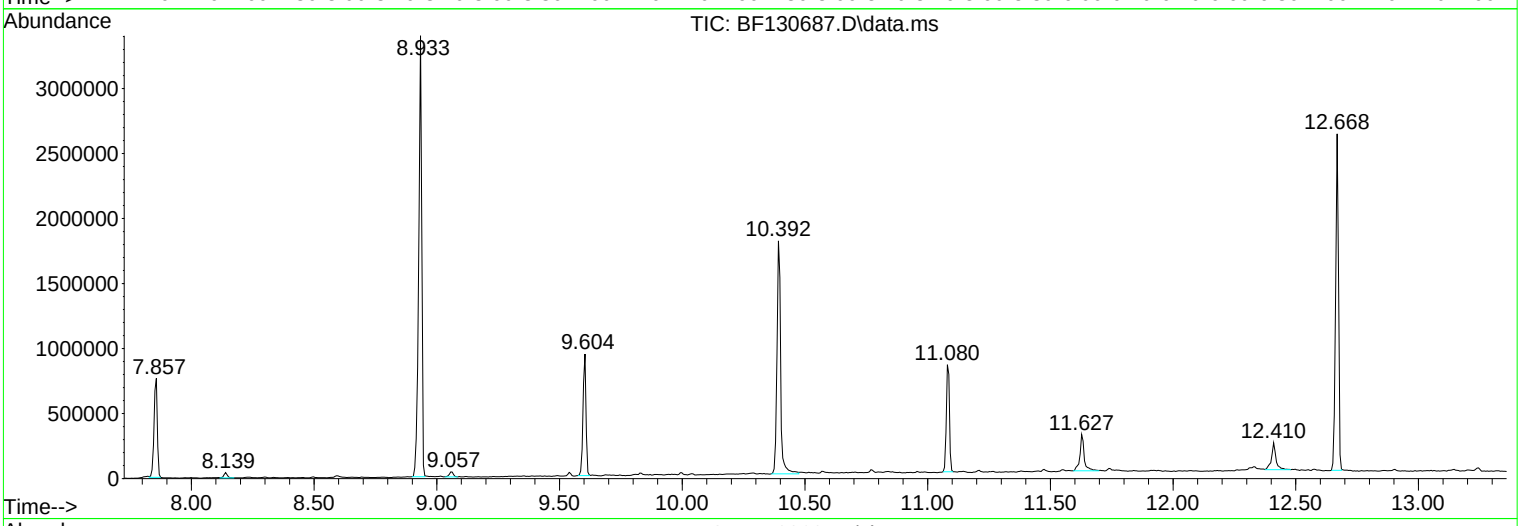
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101722\
Data File : BF130687.D
Acq On : 17 Oct 2022 15:23
Operator : CG\JU
Sample : N5133-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

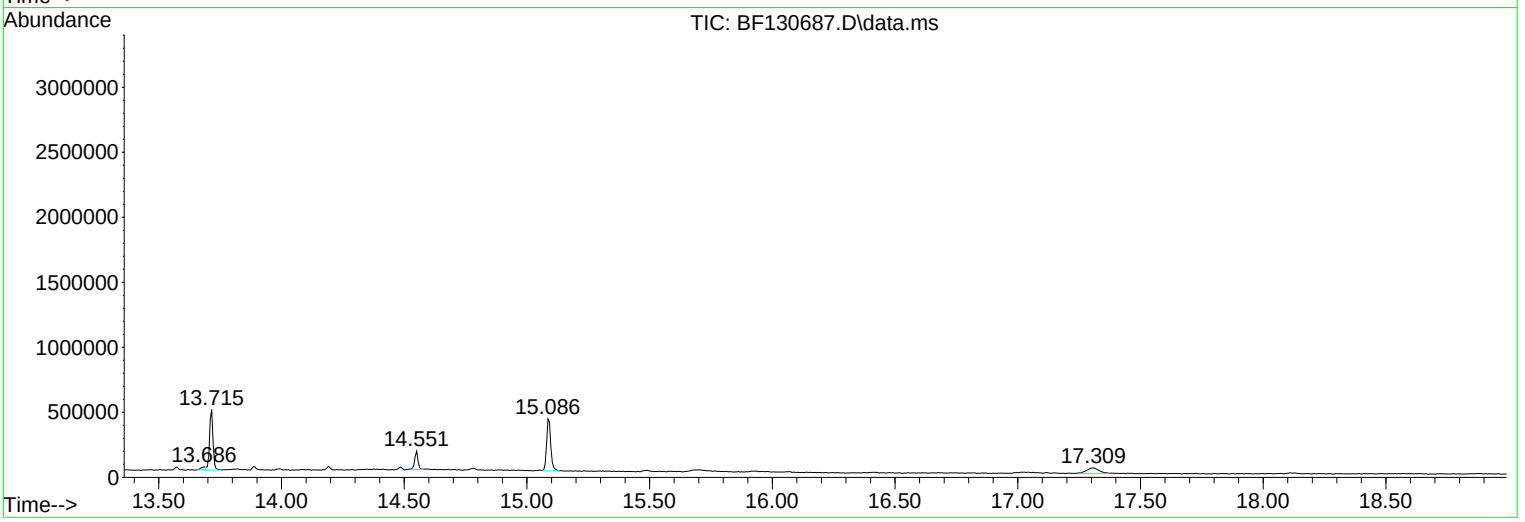
Instrument :
BNA_F
ClientSampleId :
HAS-WATER-1013

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101722\
Data File : BF130687.D
Acq On : 17 Oct 2022 15:23
Operator : CG\JU
Sample : N5133-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HAS-WATER-1013

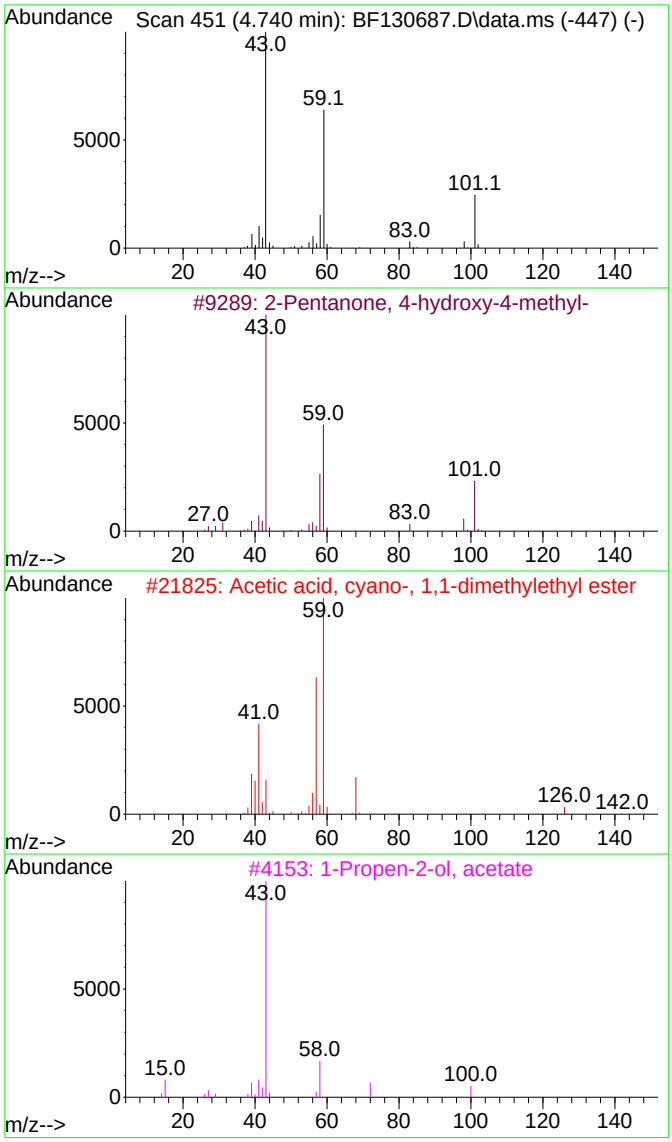
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

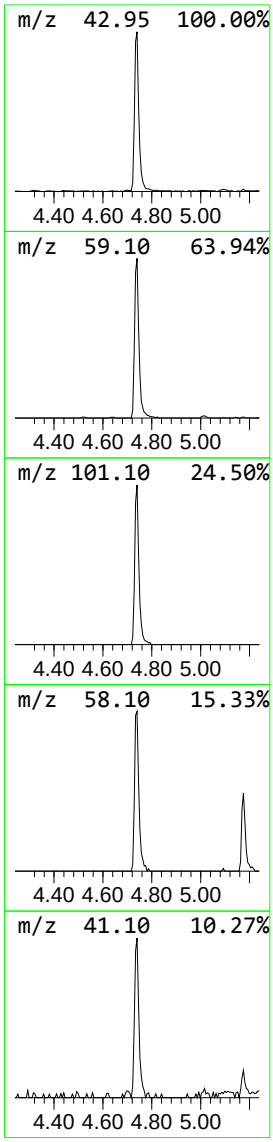
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.740	7.81 ng	209546	1,4-Dichlorobenzene-d4	6.569

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101722\
Data File : BF130687.D
Acq On : 17 Oct 2022 15:23
Operator : CG\JU
Sample : N5133-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HAS-WATER-1013

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

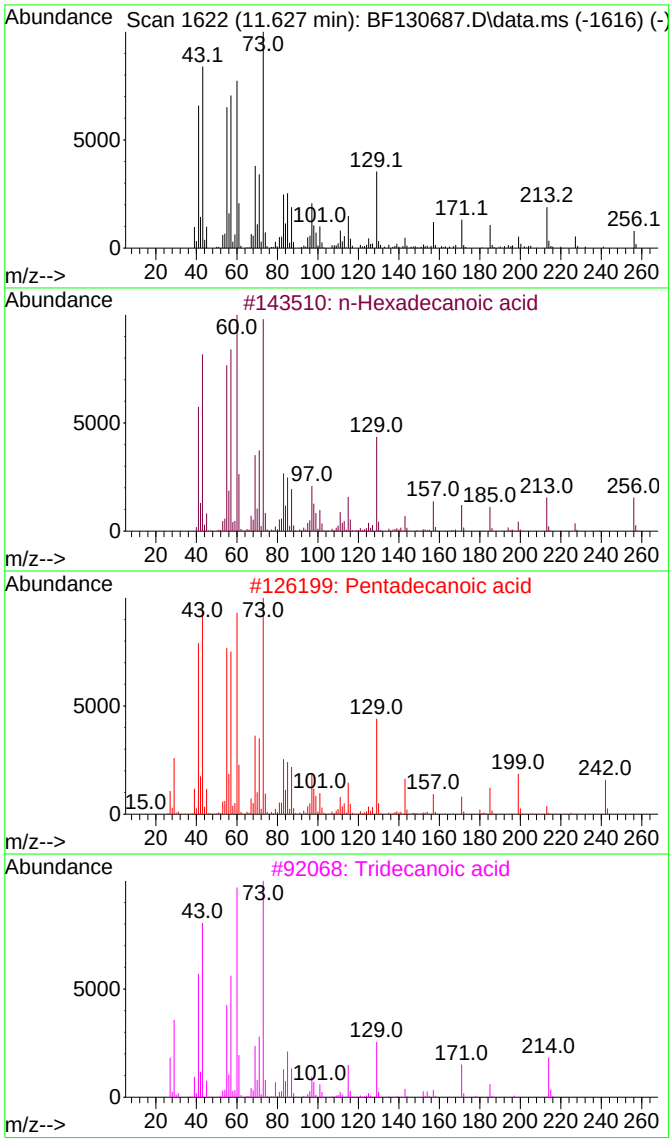
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

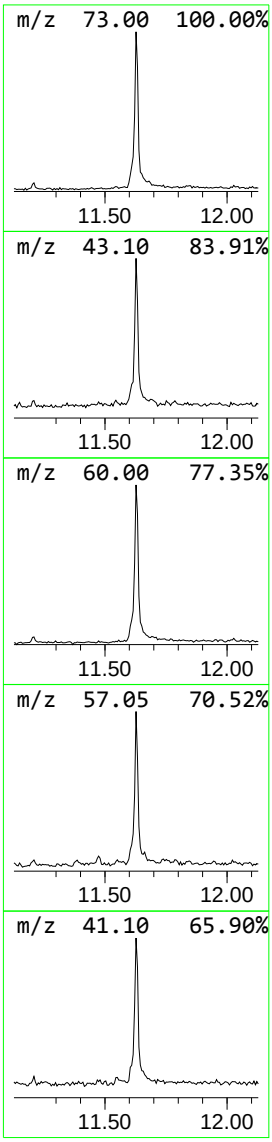
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.627	9.42 ng	343872	Phenanthrene-d10	11.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101722\
Data File : BF130687.D
Acq On : 17 Oct 2022 15:23
Operator : CG\JU
Sample : N5133-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HAS-WATER-1013

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

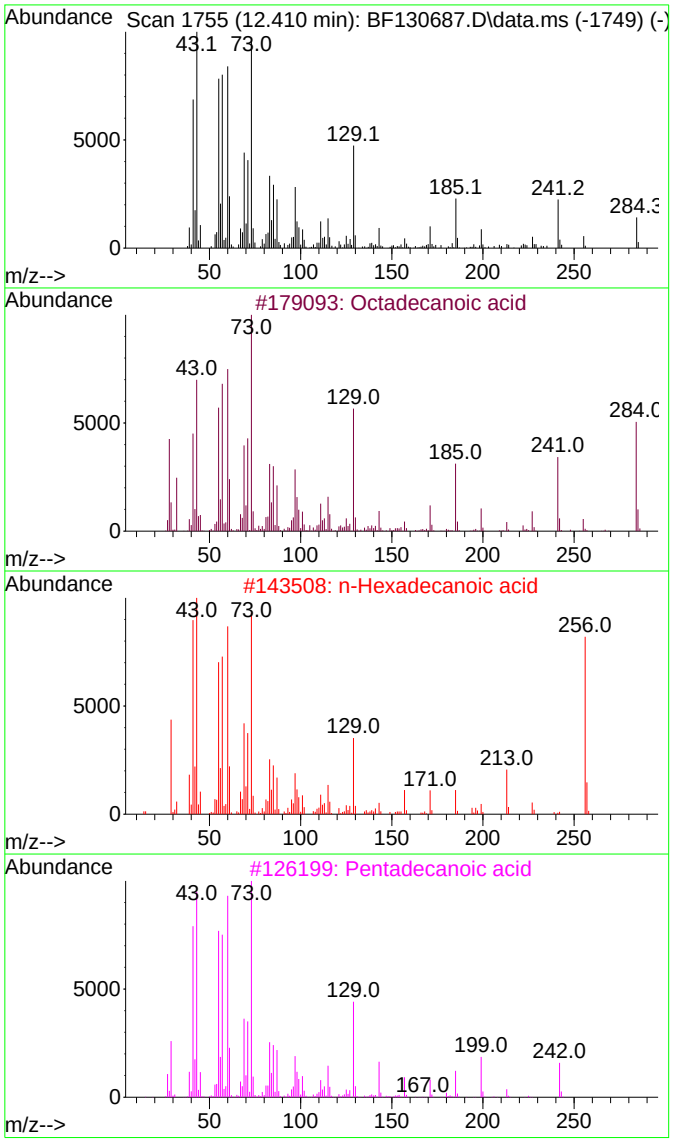
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

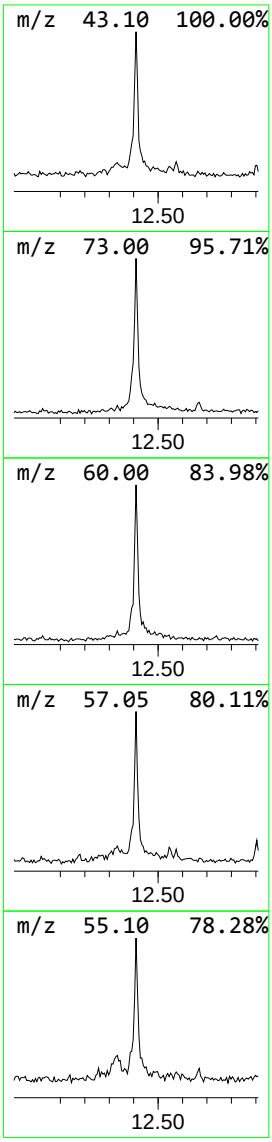
****

Peak Number 3 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.410	11.78 ng	264313	Chrysene-d12	13.715

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101722\
Data File : BF130687.D
Acq On : 17 Oct 2022 15:23
Operator : CG\JU
Sample : N5133-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HAS-WATER-1013

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

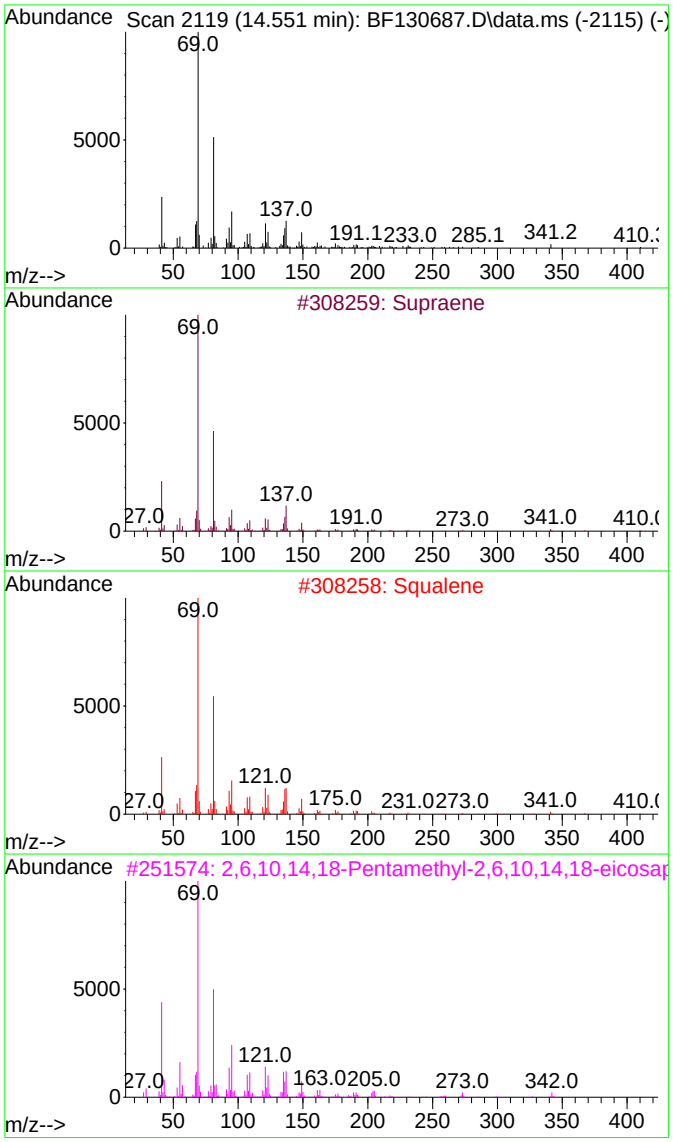
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

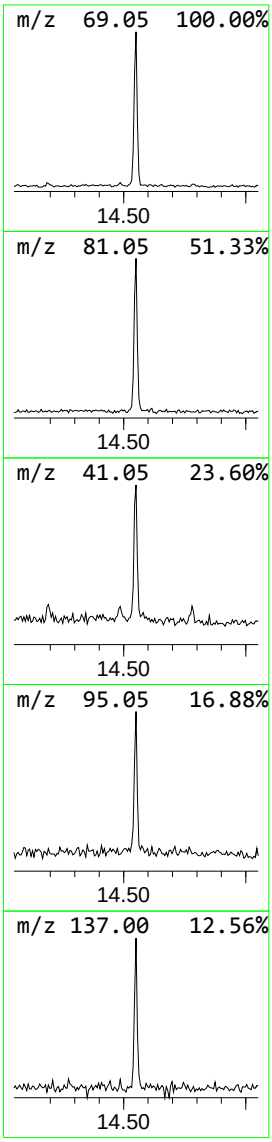
****

Peak Number 4 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.551	5.39 ng	126530	Perylene-d12	15.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	98
2	Squalene	410	C30H50	000111-02-4	95
3	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	78
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	59
5	Cyclopropanecarboxylic acid, 4-i...	204	C13H16O2	1000331-01-9	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101722\
Data File : BF130687.D
Acq On : 17 Oct 2022 15:23
Operator : CG\JU
Sample : N5133-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HAS-WATER-1013

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

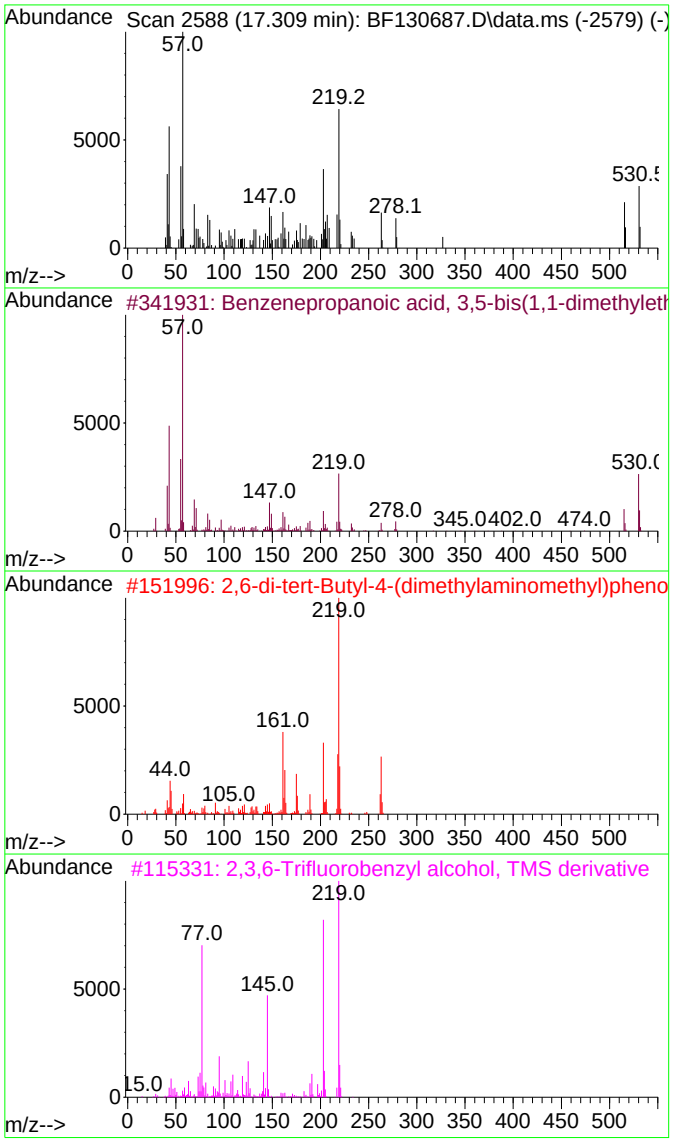
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

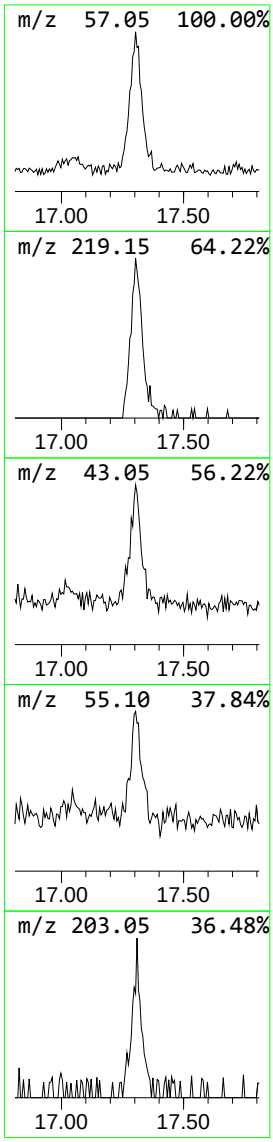
****

Peak Number 5 Benzenepropanoic acid, 3,5-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.309	6.00 ng	140808	Perylene-d12	15.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenepropanoic acid, 3,5-bis(1...	530	C35H62O3	002082-79-3	89
2	2,6-di-tert-Butyl-4-(dimethylami...	263	C17H29NO	000088-27-7	83
3	2,3,6-Trifluorobenzyl alcohol, T...	234	C10H13F3OSi	1010364-21-5	35
4	(2-Nitro-4-trifluoromethyl-pheno...	279	C9H8F3N3O4	1000294-73-1	27
5	Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	22





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101722\
Data File : BF130687.D
Acq On : 17 Oct 2022 15:23
Operator : CG\JU
Sample : N5133-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HAS-WATER-1013

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101122.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
2-Pentanone, 4-...	4.740	7.8	ng	209546	1	6.569	536632	20.0
n-Hexadecanoic ...	11.627	9.4	ng	343872	4	11.080	729767	20.0
Octadecanoic acid	12.410	11.8	ng	264313	5	13.715	448650	20.0
Supraene	14.551	5.4	ng	126530	6	15.086	469186	20.0
Benzenepropanoi...	17.309	6.0	ng	140808	6	15.086	469186	20.0