LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136915.D
Acq On : 03 Jan 2024 19:16
Operator : CG\JU
Sample : 05899-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GHL-SS-10-2-4

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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136915.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	10	14	21	rVB	15992	23428	1.42%	0.199%
2	5.022	495	499	506	rVB	37885	49194	2.99%	0.418%
3	5.422	563	567	586	rVB	1299754	1276414	77.57%	10.833%
4	6.428	734	738	741	rBV	1431025	1252442	76.11%	10.629%
5	6.781	794	798	804	rVB	444933	349733	21.25%	2.968%
6	7.345	889	894	897	rBV	899140	846431	51.44%	7.184%
7	8.057	1011	1015	1018	rBV	573091	462681	28.12%	3.927%
8	9.134	1194	1198	1201	rBV	2033599	1645467	100.00%	13.965%
9	9.810	1310	1313	1317	rBV	621933	520674	31.64%	4.419%
10	10.357	1403	1406	1412	rBV3	20371	24073	1.46%	0.204%
11	10.604	1444	1448	1459	rBV	953950	928978	56.46%	7.884%
12	10.733	1465	1470	1473	rVB	30855	35887	2.18%	0.305%
13	11.304	1563	1567	1570	rBV	654513	532447	32.36%	4.519%
14	11.328	1570	1571	1575	rVV2	43710	25254	1.53%	0.214%
15	11.380	1575	1580	1583	rVV	149738	123374	7.50%	1.047%
16	11.545	1605	1608	1613	rVB	34855	32732	1.99%	0.278%
17	11.839	1654	1658	1665	rBV	383280	415914	25.28%	3.530%
18	11.986	1680	1683	1685	rBV	101528	79964	4.86%	0.679%
19	12.251	1723	1728	1732	rVB4	19555	26180	1.59%	0.222%
20	12.527	1772	1775	1777	rBV	19417	21301	1.29%	0.181%
21	12.557	1777	1780	1787	rVB8	18234	30526	1.86%	0.259%
22	12.627	1789	1792	1804	rVV	147385	171262	10.41%	1.453%
23	12.757	1811	1814	1819	rVB	95574	99834	6.07%	0.847%
24	12.898	1834	1838	1842	rBV	1426470	1316775	80.02%	11.175%
25	13.463	1931	1934	1945	rVB2	35337	70674	4.30%	0.600%
26	13.757	1981	1984	1990	rBV5	21339	29359	1.78%	0.249%
27	13.804	1990	1992	1996	rBV2	22098	22482	1.37%	0.191%
28	13.845	1996	1999	2006	rBV3	36147	75695	4.60%	0.642%
29	13.963	2015	2019	2026	rVB	344216	357646	21.74%	3.035%
30	14.127	2044	2047	2050	rBV	24497	24883	1.51%	0.211%
31	14.433	2096	2099	2103	rVB2	32778	30158	1.83%	0.256%
32	14.739	2148	2151	2156	rVB2	30346	30042	1.83%	0.255%
33	14.816	2161	2164	2168	rVB3	18502	20298	1.23%	0.172%
34	15.080	2206	2209	2213	rVB2	36966	42227	2.57%	0.358%
35	15.439	2266	2270	2282	rVB	291790	445961	27.10%	3.785%
36	15.915	2347	2351	2357	rBV	40732	65794	4.00%	0.558%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136915.D
Acq On : 03 Jan 2024 19:16
Operator : CG\JU
Sample : 05899-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-10-2-4

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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.439	2436	2440	2444	rVB2	30000	45777	2.78%	0.389%
38	16.580	2461	2464	2469	rVB7	15608	19787	1.20%	0.168%
39	17.051	2538	2544	2553	rVB2	34181	82163	4.99%	0.697%
40	17.774	2662	2667	2677	rVB4	26003	73027	4.44%	0.620%
41	18.651	2810	2816	2824	rVB3	20682	55943	3.40%	0.475%

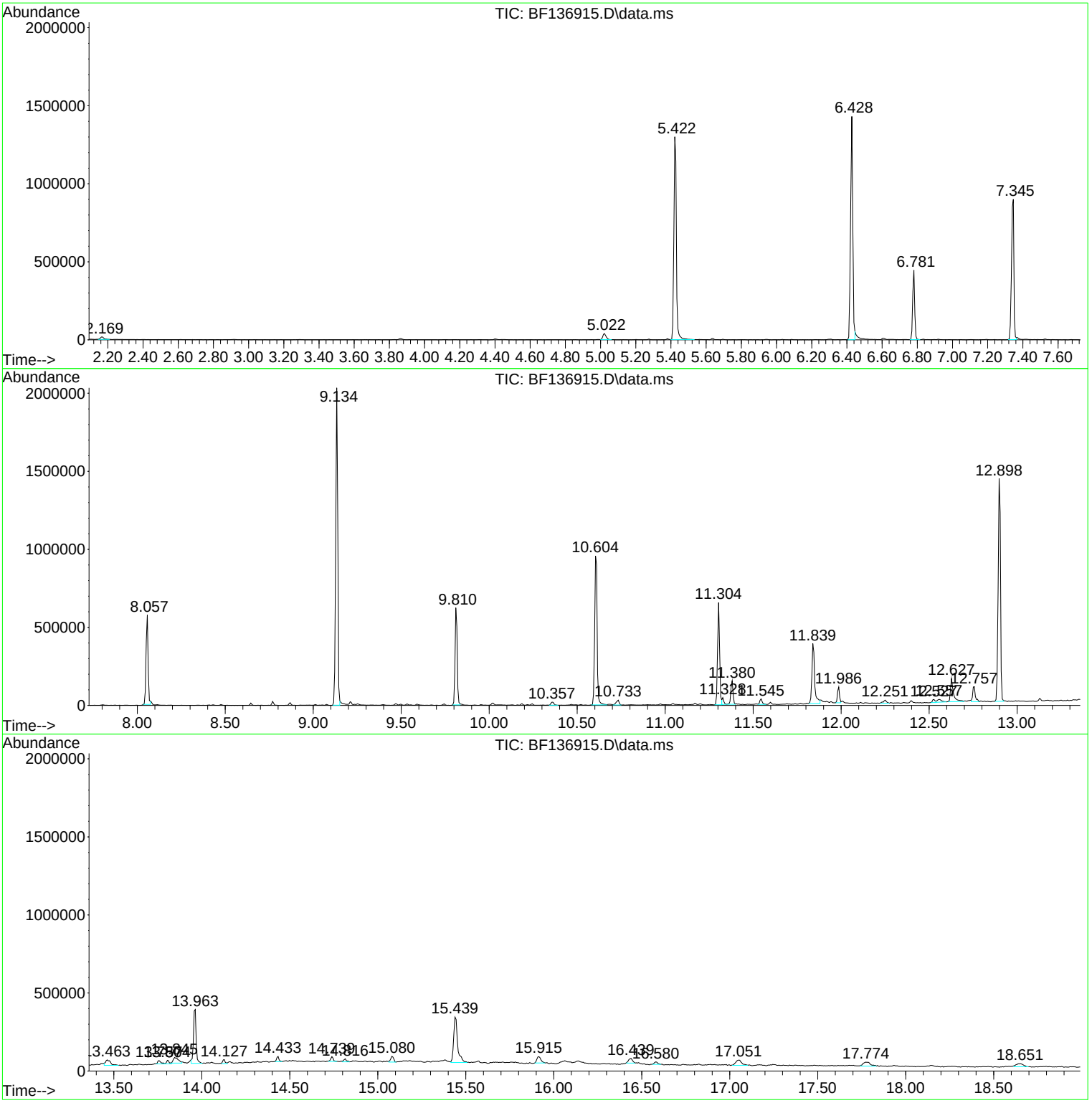
Sum of corrected areas: 11782881

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136915.D
Acq On : 03 Jan 2024 19:16
Operator : CG\JU
Sample : 05899-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-10-2-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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\BF010324\
Data File : BF136915.D
Acq On : 03 Jan 2024 19:16
Operator : CG\JU
Sample : 05899-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-10-2-4

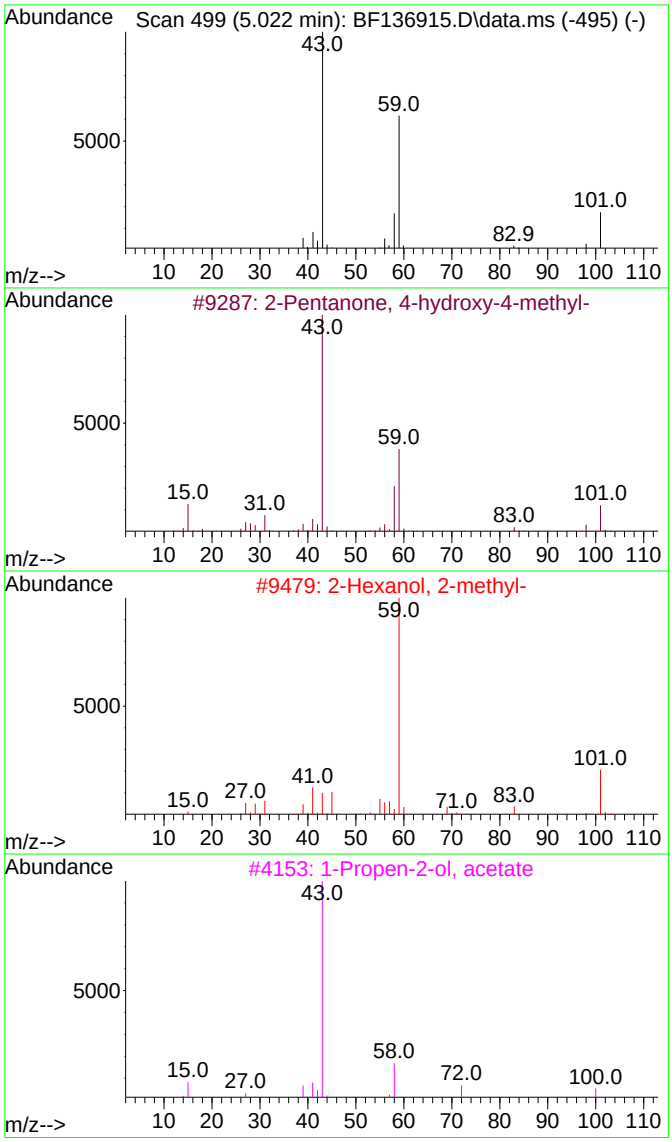
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

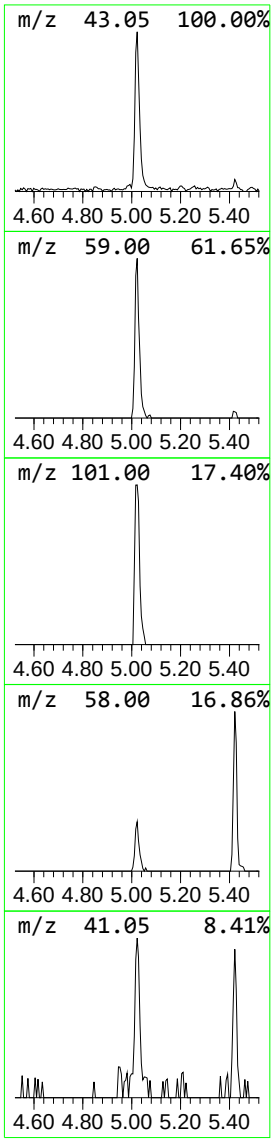
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	2.81 ng	49194	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Diacetamide	101	C4H7NO2	000625-77-4	9
5	Guanidine	59	CH5N3	000113-00-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136915.D
Acq On : 03 Jan 2024 19:16
Operator : CG\JU
Sample : 05899-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-10-2-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

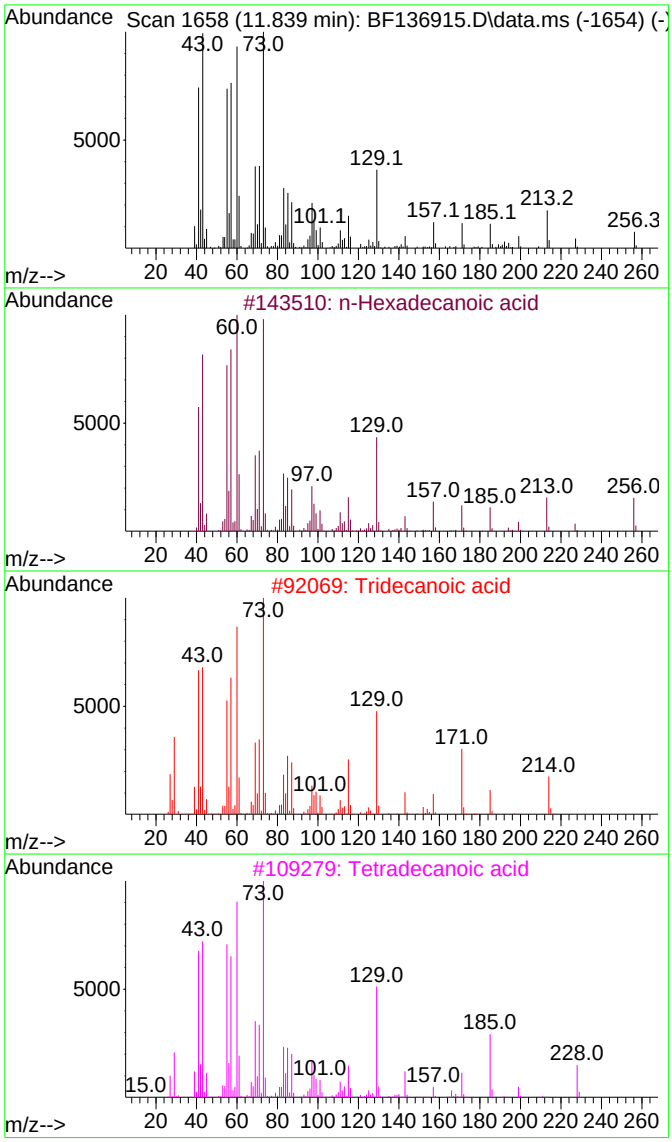
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

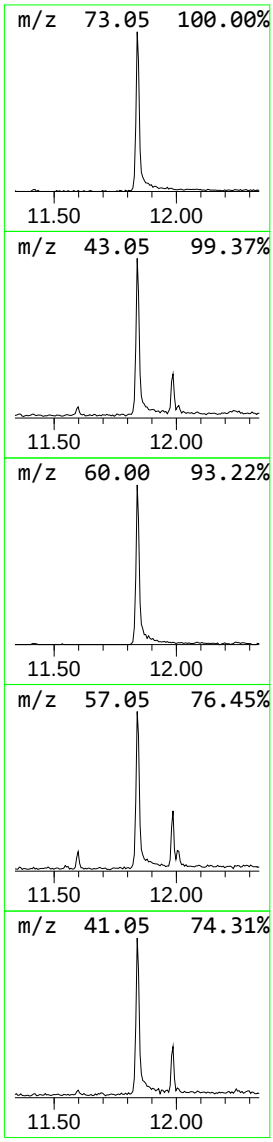
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	15.62 ng	415914	Phenanthrene-d10	11.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	96
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	55





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136915.D
Acq On : 03 Jan 2024 19:16
Operator : CG\JU
Sample : 05899-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-10-2-4

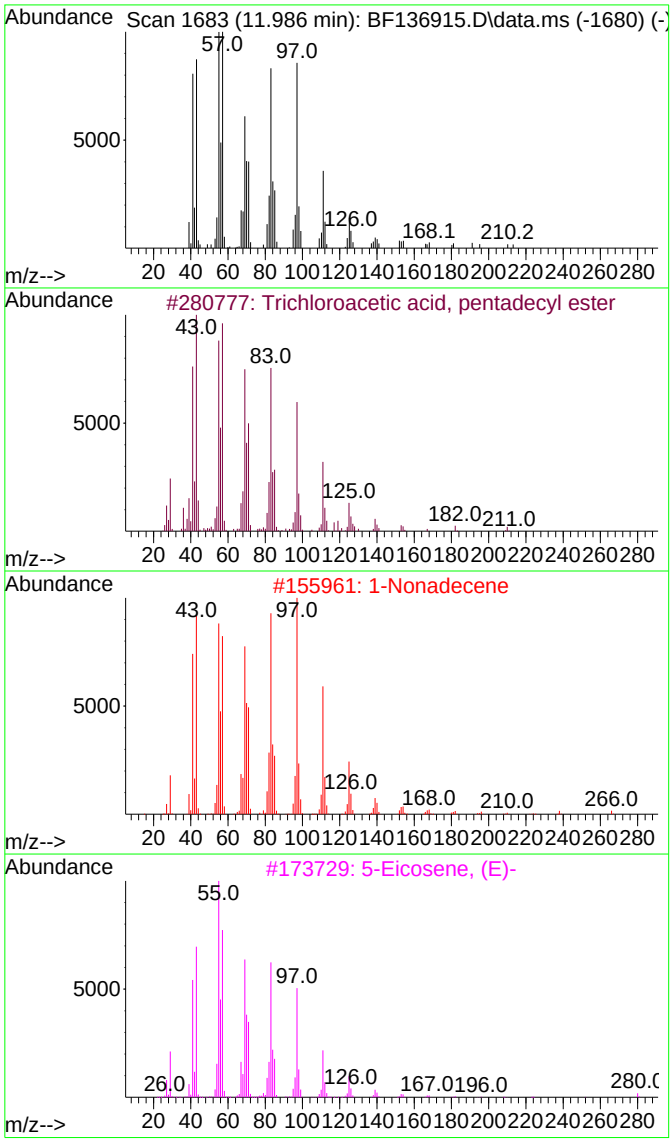
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

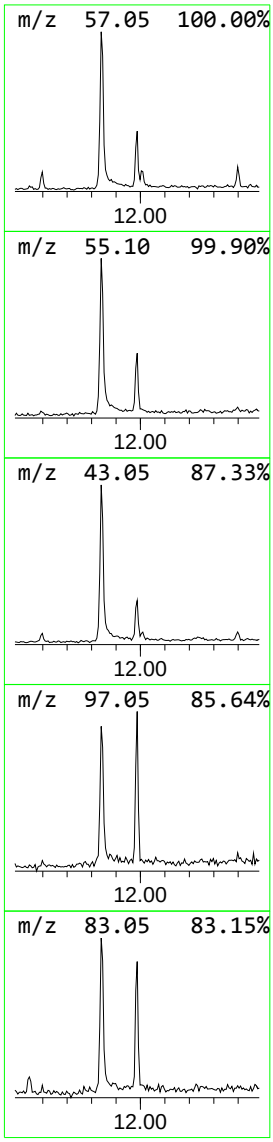
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Trichloroacetic acid, penta... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.986	3.00 ng	79964	Phenanthrene-d10	11.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	93
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
4	1-Heptadecene	238	C17H34	006765-39-5	91
5	1-Octadecene	252	C18H36	000112-88-9	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136915.D
Acq On : 03 Jan 2024 19:16
Operator : CG\JU
Sample : 05899-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-10-2-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

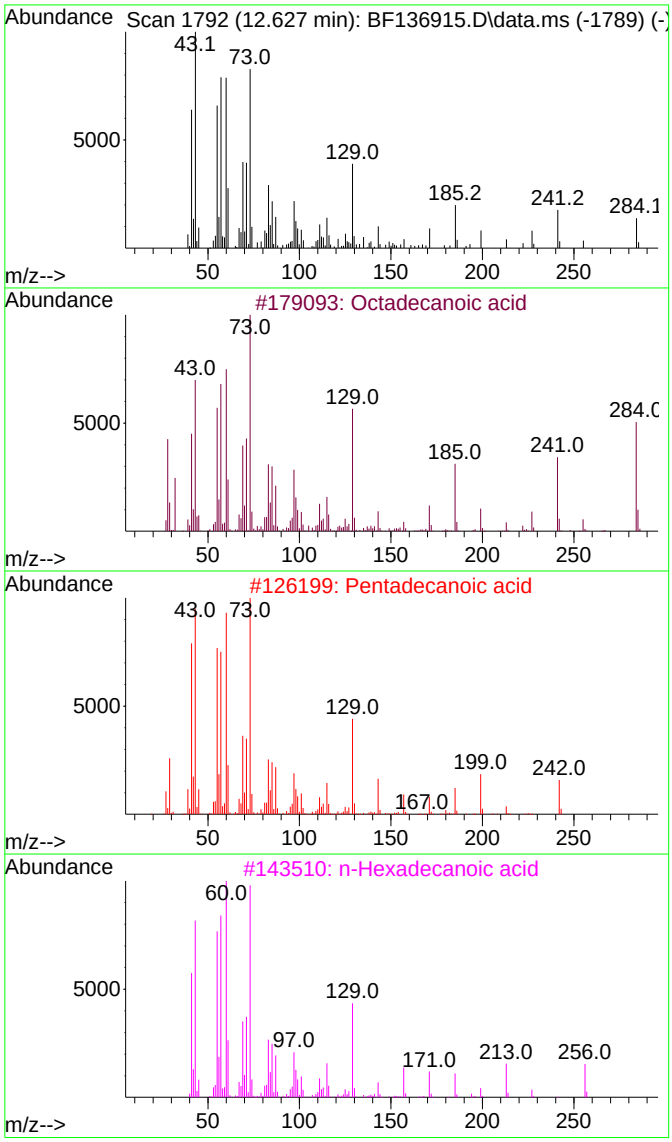
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

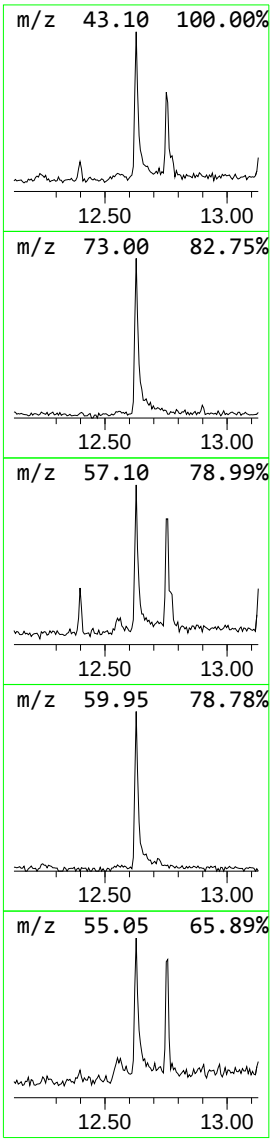
****

Peak Number 4 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.627	6.43 ng	171262	Phenanthrene-d10	11.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Undecanoic acid	186	C11H22O2	000112-37-8	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136915.D
Acq On : 03 Jan 2024 19:16
Operator : CG\JU
Sample : 05899-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-10-2-4

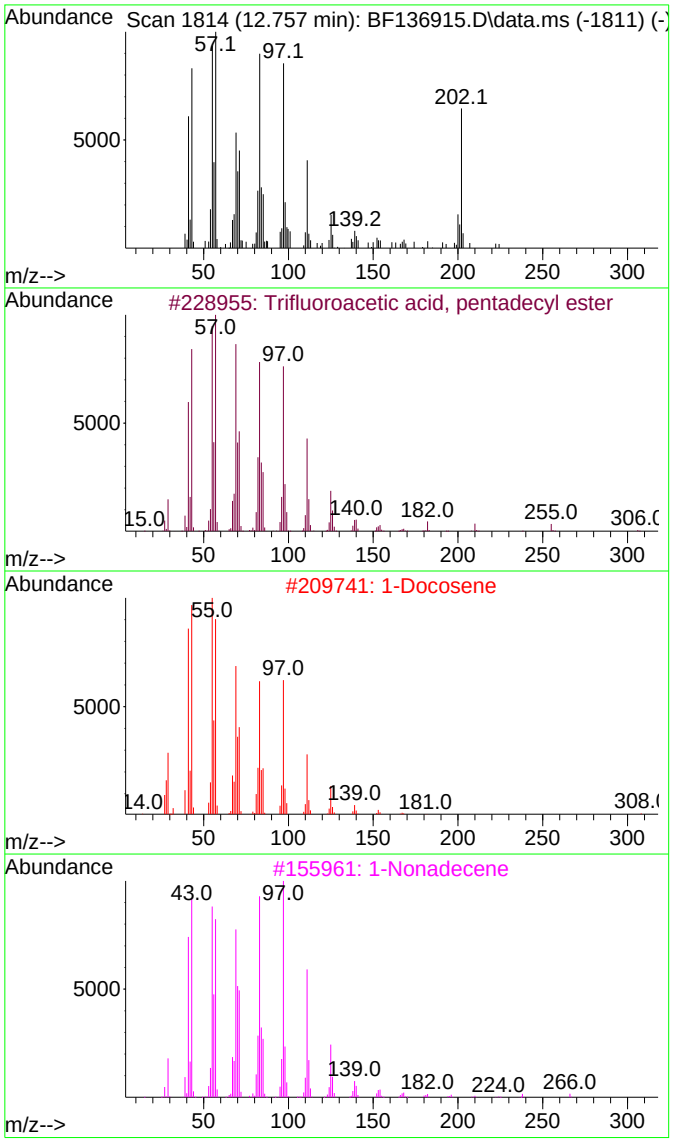
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

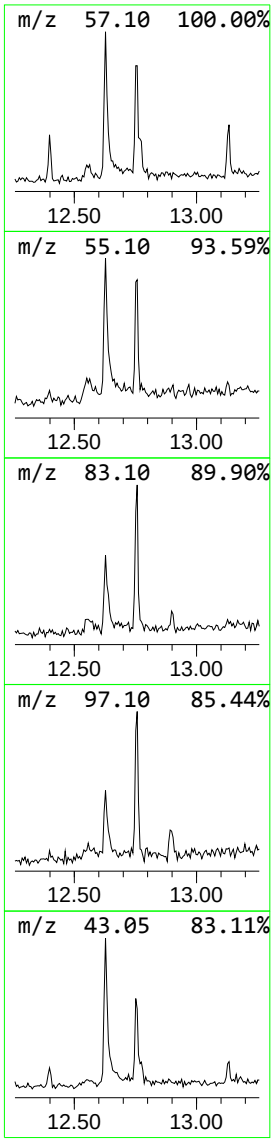
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Trifluoroacetic acid, penta... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.757	5.58 ng	99834	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	80
2	1-Docosene	308	C22H44	001599-67-3	80
3	1-Nonadecene	266	C19H38	018435-45-5	68
4	11-Tricosene	322	C23H46	052078-56-5	64
5	1-Octadecene	252	C18H36	000112-88-9	62





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Acq On : 03 Jan 2024 19:16
Operator : CG\JU
Sample : 05899-04
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ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-10-2-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

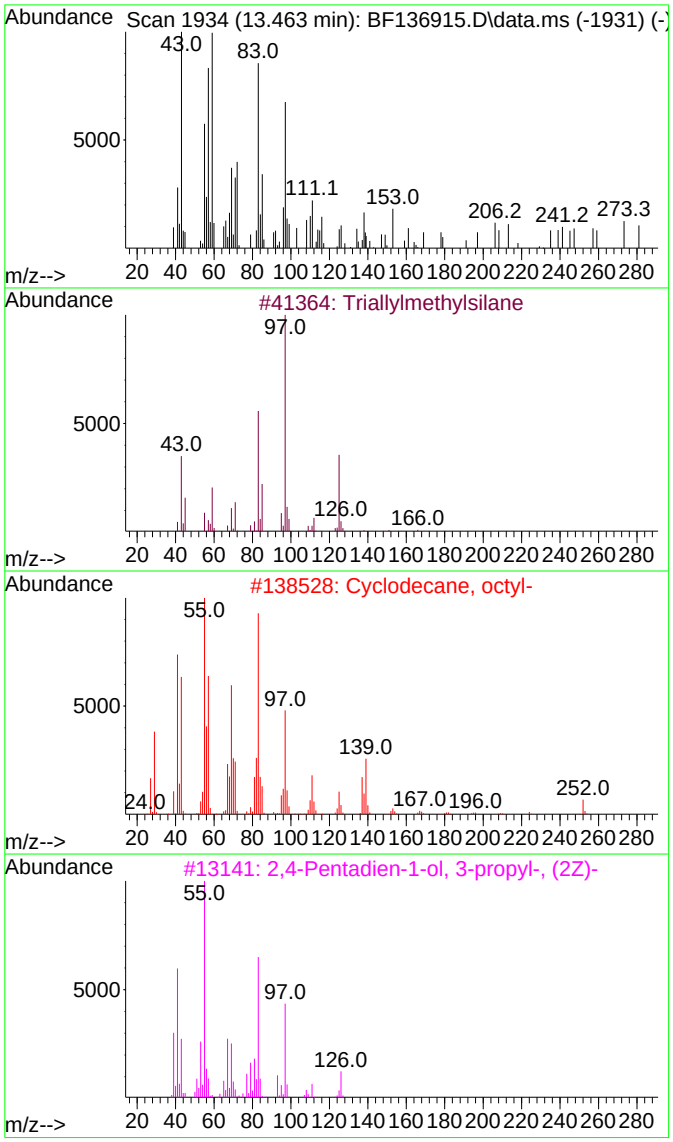
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

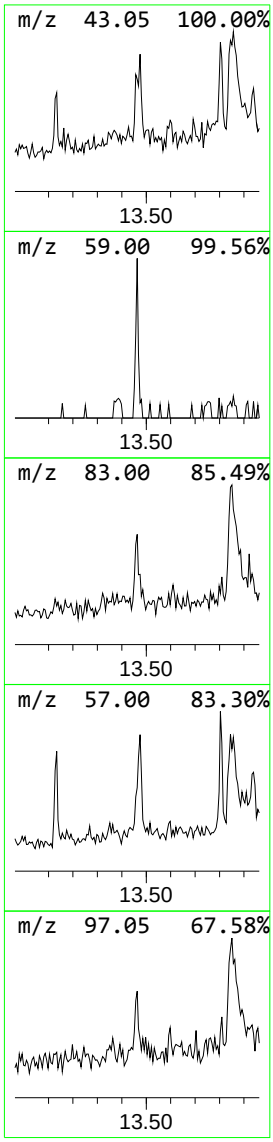
****

Peak Number 6 Triallylmethylsilane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.463	3.95 ng	70674	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triallylmethylsilane	166	C10H18Si	001112-91-0	50
2	Cyclodecane, octyl-	252	C18H36	016539-09-6	35
3	2,4-Pentadien-1-ol, 3-propyl-, (...	126	C8H14O	1000142-17-9	27
4	Cycloheptanol, 2-methylene	126	C8H14O	016240-38-3	25
5	1-Nonadecene	266	C19H38	018435-45-5	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136915.D
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Sample : 05899-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-10-2-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

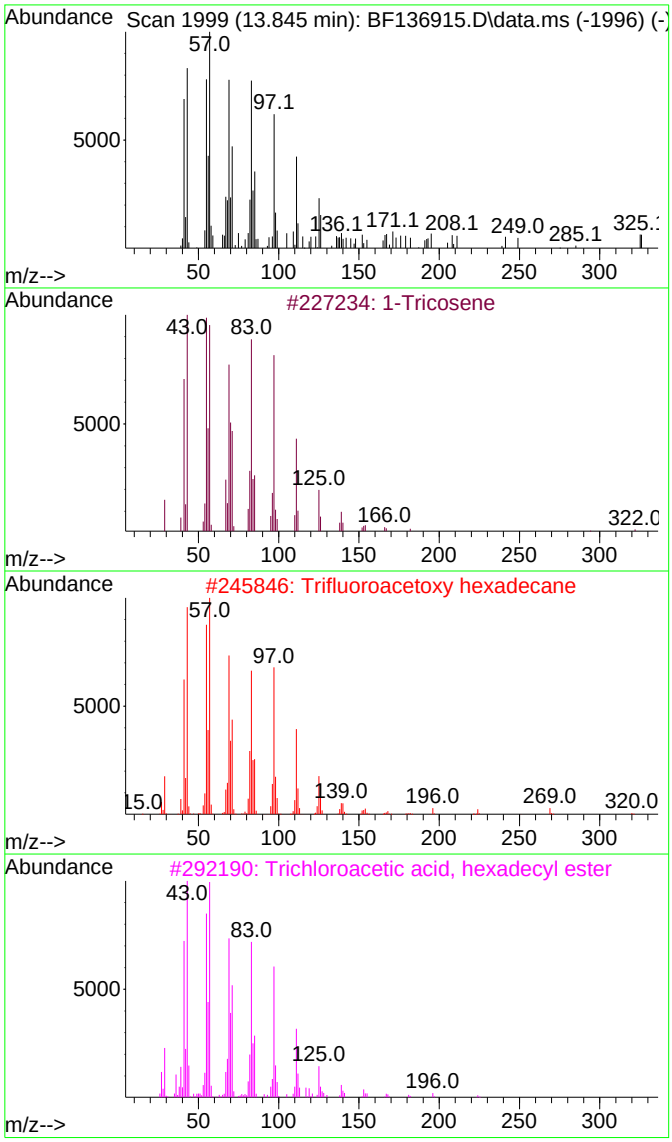
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

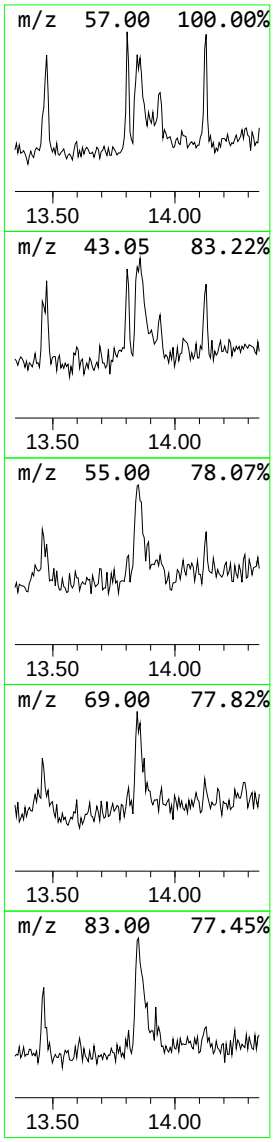
****

Peak Number 7 1-Tricosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.845	4.23 ng	75695	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene	322	C23H46	018835-32-0	91
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136915.D
Acq On : 03 Jan 2024 19:16
Operator : CG\JU
Sample : 05899-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-10-2-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

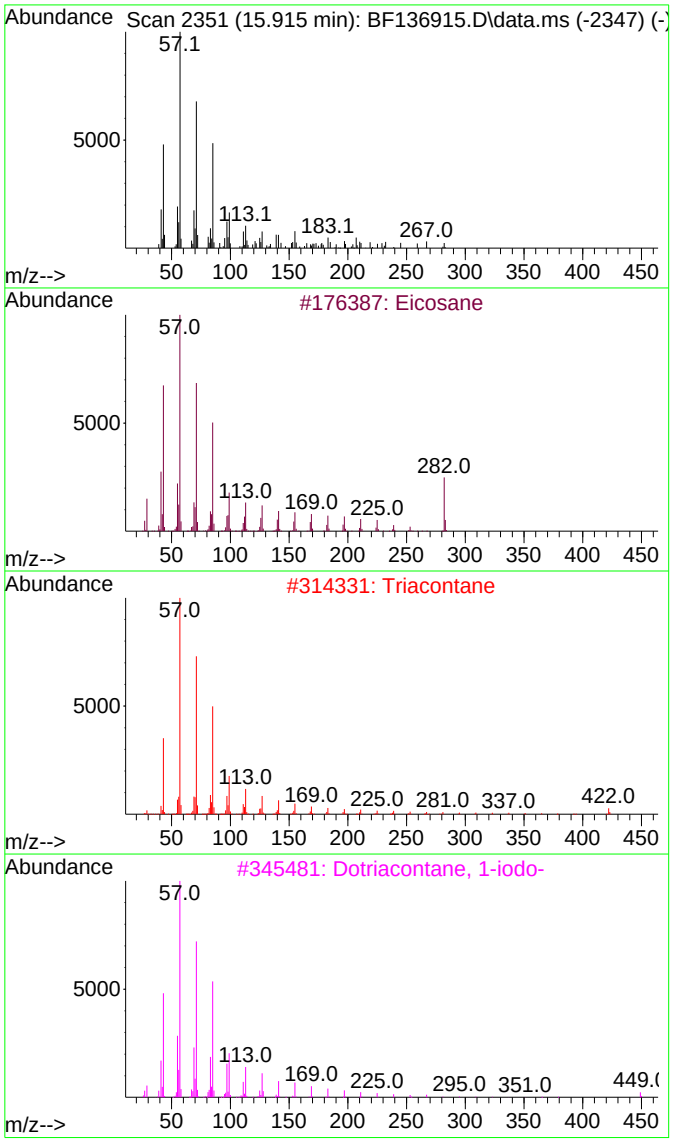
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

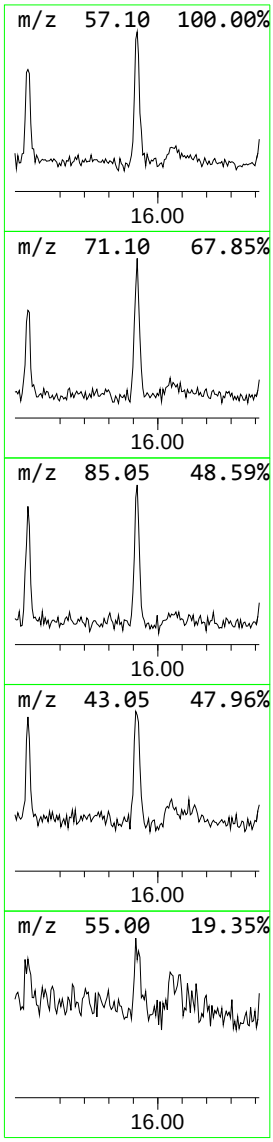
****

Peak Number 8 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.916	2.95 ng	65794	Perylene-d12	15.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Triacontane	422	C30H62	000638-68-6	87
3	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	87
4	Octacosane	394	C28H58	000630-02-4	87
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136915.D
Acq On : 03 Jan 2024 19:16
Operator : CG\JU
Sample : 05899-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-10-2-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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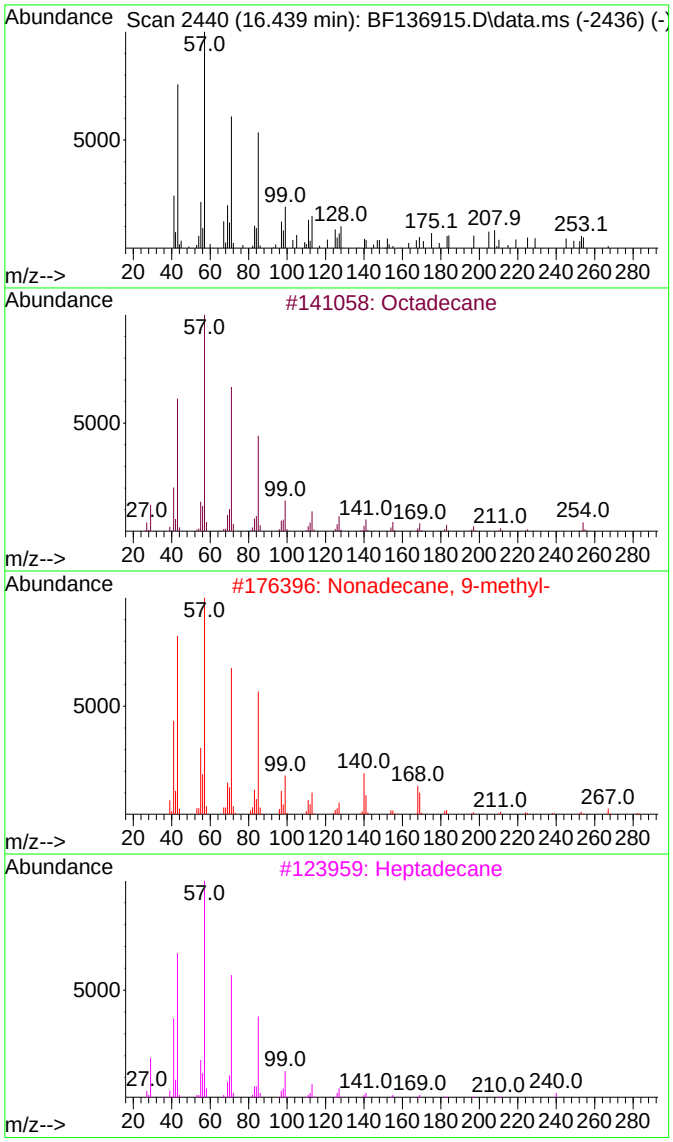
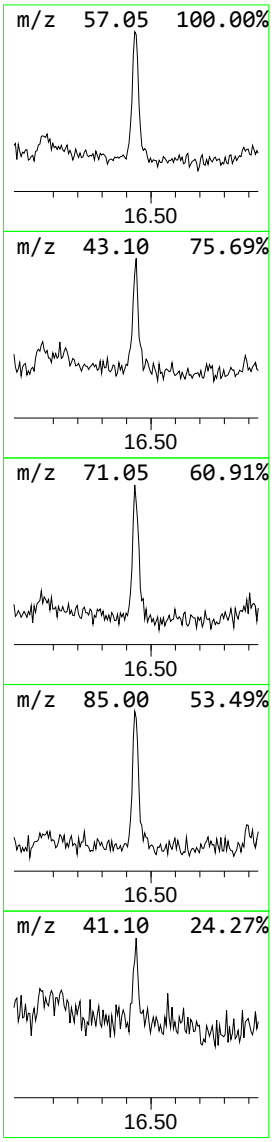
Peak Number 9 Octadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.439	2.05 ng	45777	Perylene-d12	15.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	64
2	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	58
3	Heptadecane	240	C17H36	000629-78-7	58
4	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	53
5	Tridecane	184	C13H28	000629-50-5	52





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136915.D
Acq On : 03 Jan 2024 19:16
Operator : CG\JU
Sample : 05899-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-10-2-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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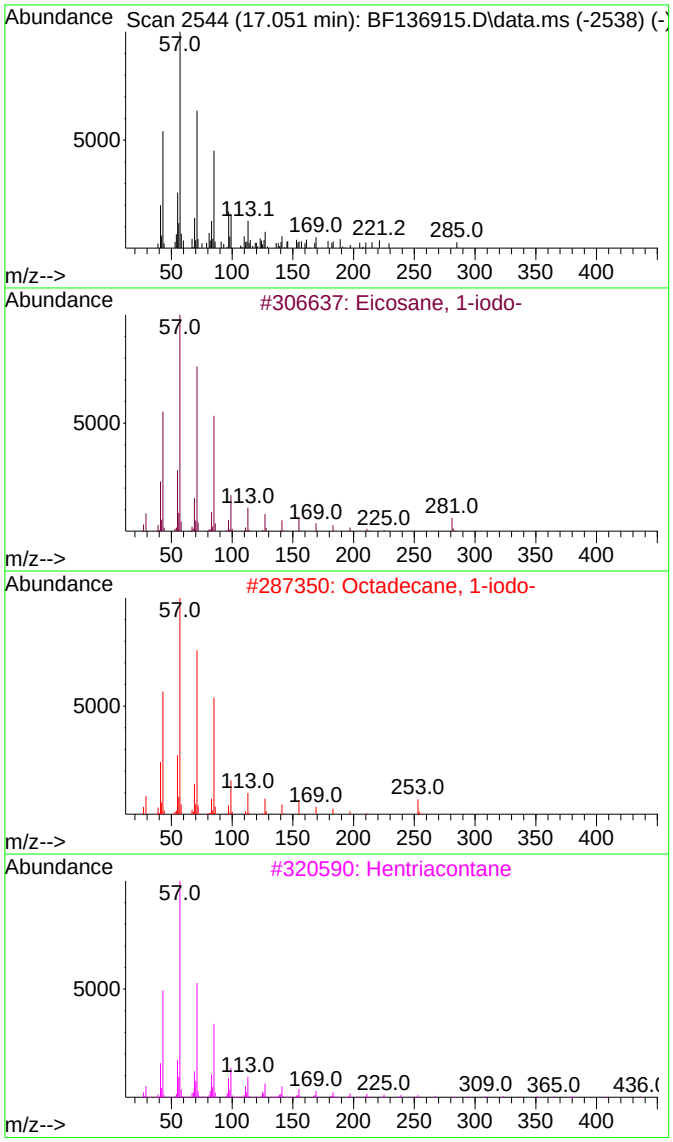
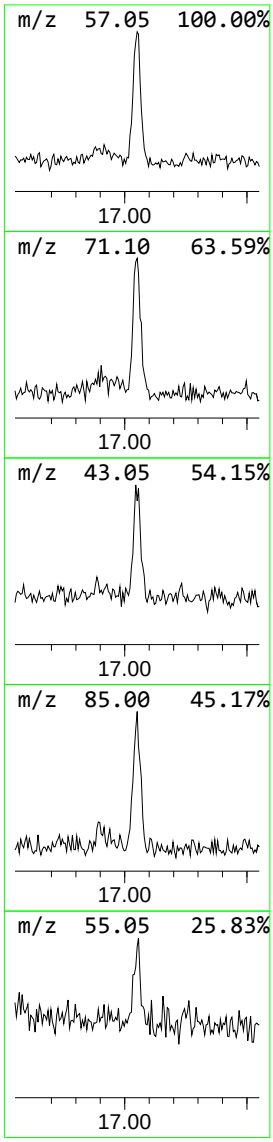
Peak Number 10 Eicosane, 1-iodo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.051	3.68 ng	82163	Perylene-d12	15.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	83
2	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	83
3	Hentriacontane	437	C31H64	000630-04-6	80
4	Octacosane	394	C28H58	000630-02-4	80
5	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136915.D
Acq On : 03 Jan 2024 19:16
Operator : CG\JU
Sample : 05899-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-10-2-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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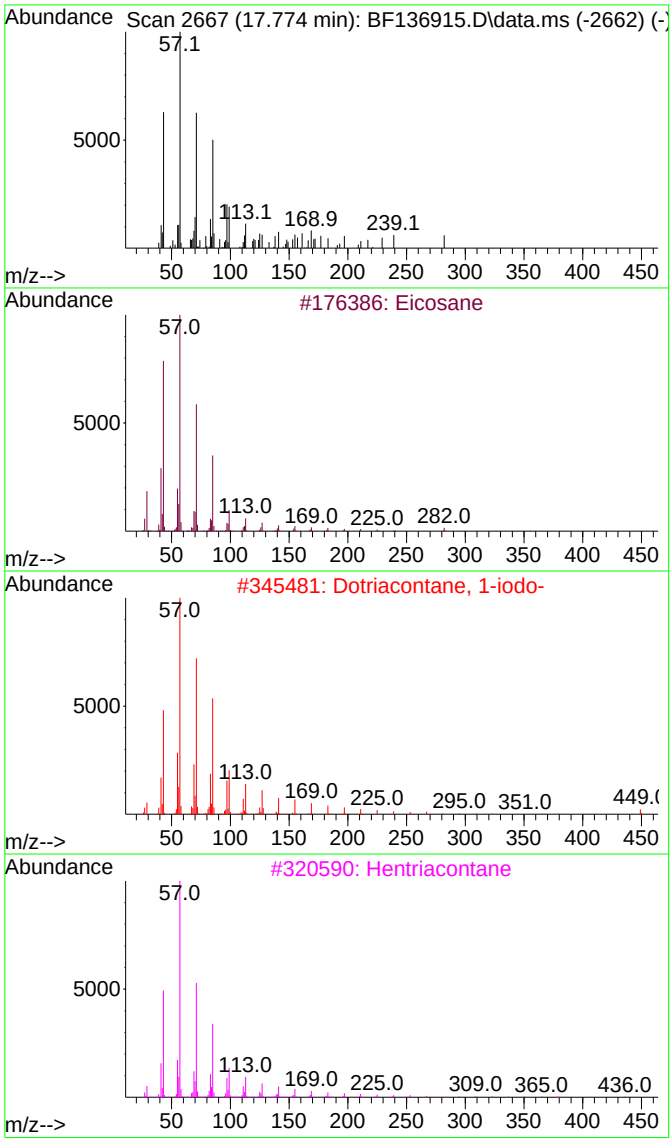
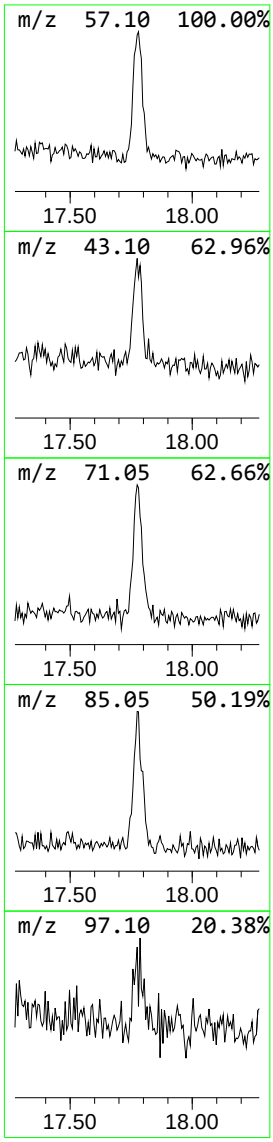
Peak Number 11 Dotriacontane, 1-iodo- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.774	3.28 ng	73027	Perylene-d12	15.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	72
3	Hentriacontane	437	C31H64	000630-04-6	72
4	Hexadecane	226	C16H34	000544-76-3	72
5	Octacosane	394	C28H58	000630-02-4	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136915.D
Acq On : 03 Jan 2024 19:16
Operator : CG\JU
Sample : 05899-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-10-2-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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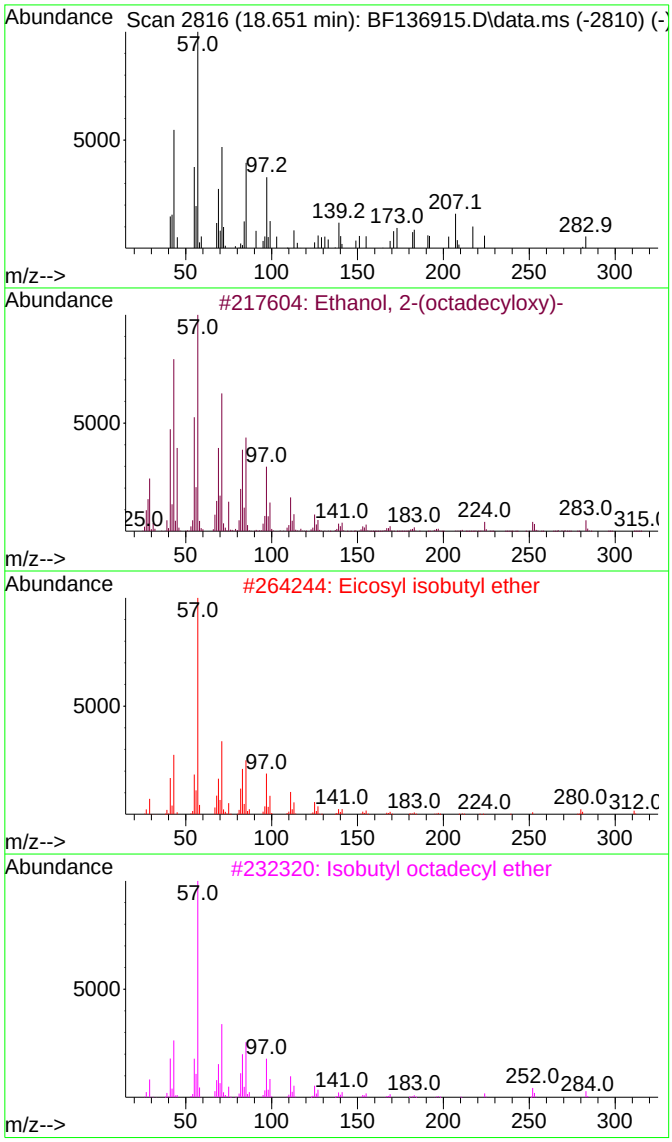
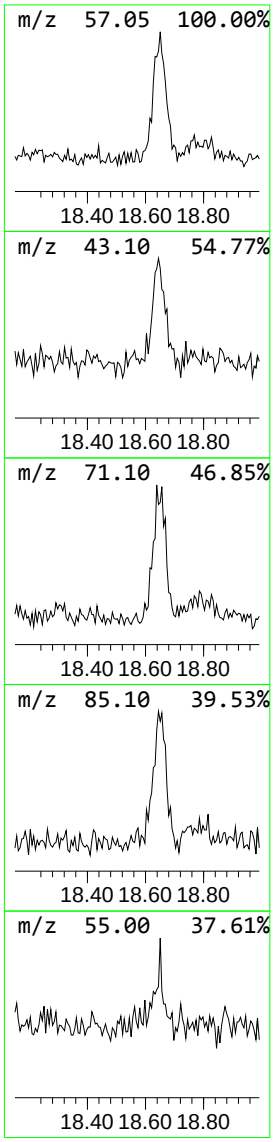
Peak Number 12 Ethanol, 2-(octadecyloxy)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.651	2.51 ng	55943	Perylene-d12	15.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	53
2	Eicosyl isobutyl ether	354	C24H50O	1000406-33-0	52
3	Isobutyl octadecyl ether	326	C22H46O	1000406-32-9	52
4	Docosyl isobutyl ether	382	C26H54O	1000406-33-1	52
5	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1010309-18-1	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136915.D
Acq On : 03 Jan 2024 19:16
Operator : CG\JU
Sample : 05899-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-10-2-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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-...	5.022	2.8	ng	49194	1	6.781	349733	20.0
n-Hexadecanoic ...	11.839	15.6	ng	415914	4	11.304	532447	20.0
Trichloroacetic...	11.986	3.0	ng	79964	4	11.304	532447	20.0
Octadecanoic acid	12.627	6.4	ng	171262	4	11.304	532447	20.0
Trifluoroacetic...	12.757	5.6	ng	99834	5	13.963	357646	20.0
Triallylmethyls...	13.463	4.0	ng	70674	5	13.963	357646	20.0
1-Tricosene	13.845	4.2	ng	75695	5	13.963	357646	20.0
Eicosane	15.916	3.0	ng	65794	6	15.439	445961	20.0
Octadecane	16.439	2.0	ng	45777	6	15.439	445961	20.0
Eicosane, 1-iodo-	17.051	3.7	ng	82163	6	15.439	445961	20.0
Dotriacontane, ...	17.774	3.3	ng	73027	6	15.439	445961	20.0
Ethanol, 2-(oct...	18.651	2.5	ng	55943	6	15.439	445961	20.0