LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136833.D
Acq On : 29 Dec 2023 17:13
Operator : CG\JU
Sample : 05909-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-48

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: BF136833.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.028	497	500	512	rVB	21937	30324	1.84%	0.253%
2	5.428	564	568	571	rBV	1839992	1594179	96.96%	13.314%
3	6.428	733	738	741	rBV	1651257	1628202	99.03%	13.599%
4	6.781	794	798	802	rBV	510440	394719	24.01%	3.297%
5	7.345	889	894	897	rBV	1110381	1052914	64.04%	8.794%
6	8.057	1011	1015	1018	rBV	648013	520584	31.66%	4.348%
7	9.133	1193	1198	1201	rBV	1917637	1644177	100.00%	13.732%
8	9.816	1310	1314	1317	rBV	688030	582783	35.45%	4.867%
9	10.610	1445	1449	1452	rBV	1284991	1121444	68.21%	9.366%
10	11.304	1564	1567	1571	rBV	670425	625095	38.02%	5.221%
11	11.839	1655	1658	1675	rBV	90551	145284	8.84%	1.213%
12	12.092	1698	1701	1704	rBV2	33232	28671	1.74%	0.239%
13	12.633	1791	1793	1805	rBV7	12209	27058	1.65%	0.226%
14	12.904	1834	1839	1842	rBV	1524983	1329802	80.88%	11.106%
15	13.810	1986	1993	1999	rBV	57203	51704	3.14%	0.432%
16	13.963	2015	2019	2029	rVB	474237	437090	26.58%	3.651%
17	14.433	2096	2099	2104	rVB	53395	53902	3.28%	0.450%
18	14.745	2146	2152	2155	rBV3	16796	22986	1.40%	0.192%
19	14.892	2174	2177	2180	rBV2	22423	20420	1.24%	0.171%
20	15.086	2206	2210	2217	rVB	96013	110625	6.73%	0.924%
21	15.445	2266	2271	2282	rBV	268960	374787	22.79%	3.130%
22	15.686	2307	2312	2317	rVB2	24785	36678	2.23%	0.306%
23	15.921	2347	2352	2357	rBV2	34423	51508	3.13%	0.430%
24	16.745	2487	2492	2499	rBV8	20179	39364	2.39%	0.329%
25	18.239	2739	2746	2756	rVB8	9339	27136	1.65%	0.227%
26	18.603	2800	2808	2813	rBV10	8814	21841	1.33%	0.182%

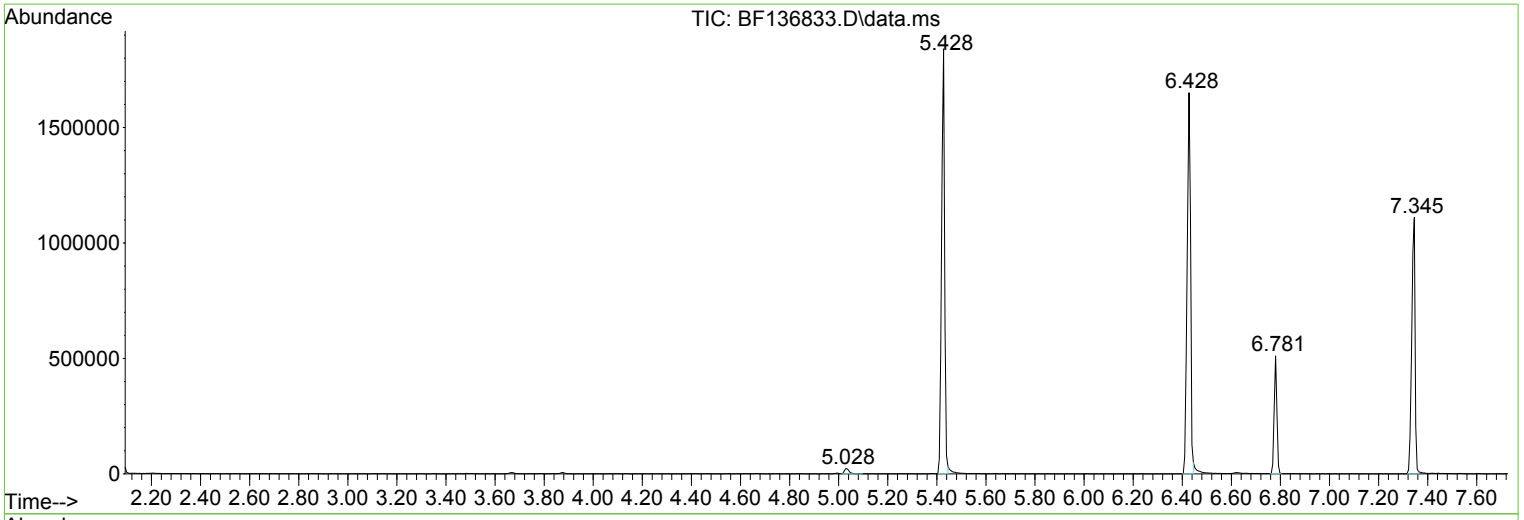
Sum of corrected areas: 11973277

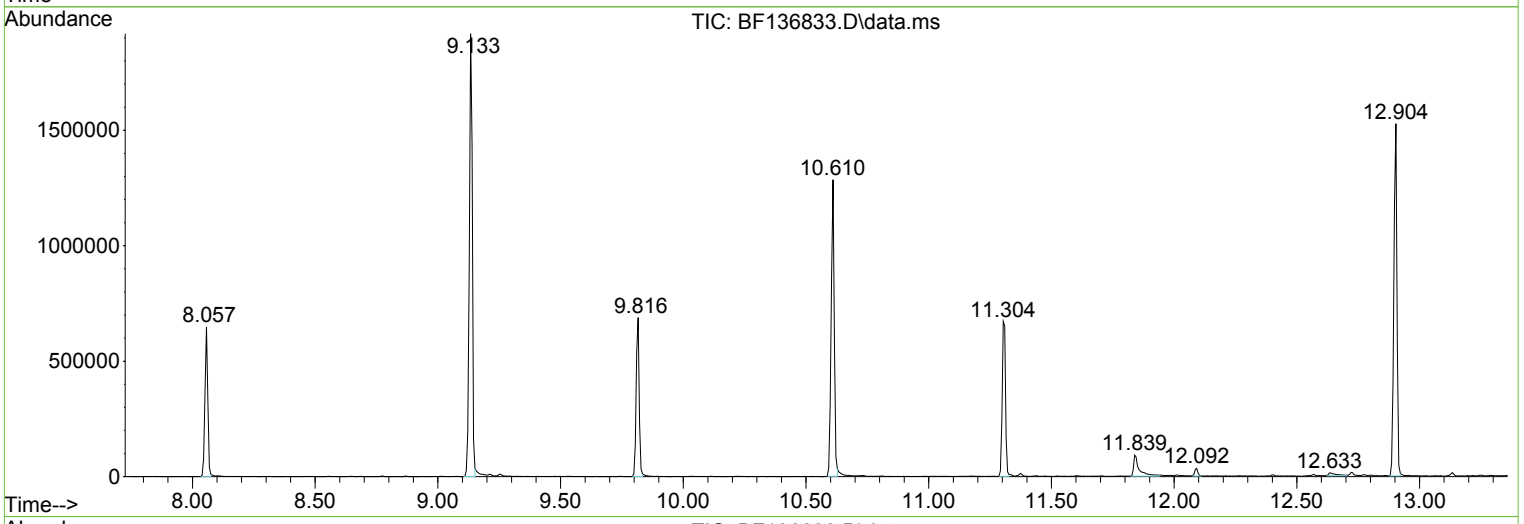
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136833.D
Acq On : 29 Dec 2023 17:13
Operator : CG\JU
Sample : 05909-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

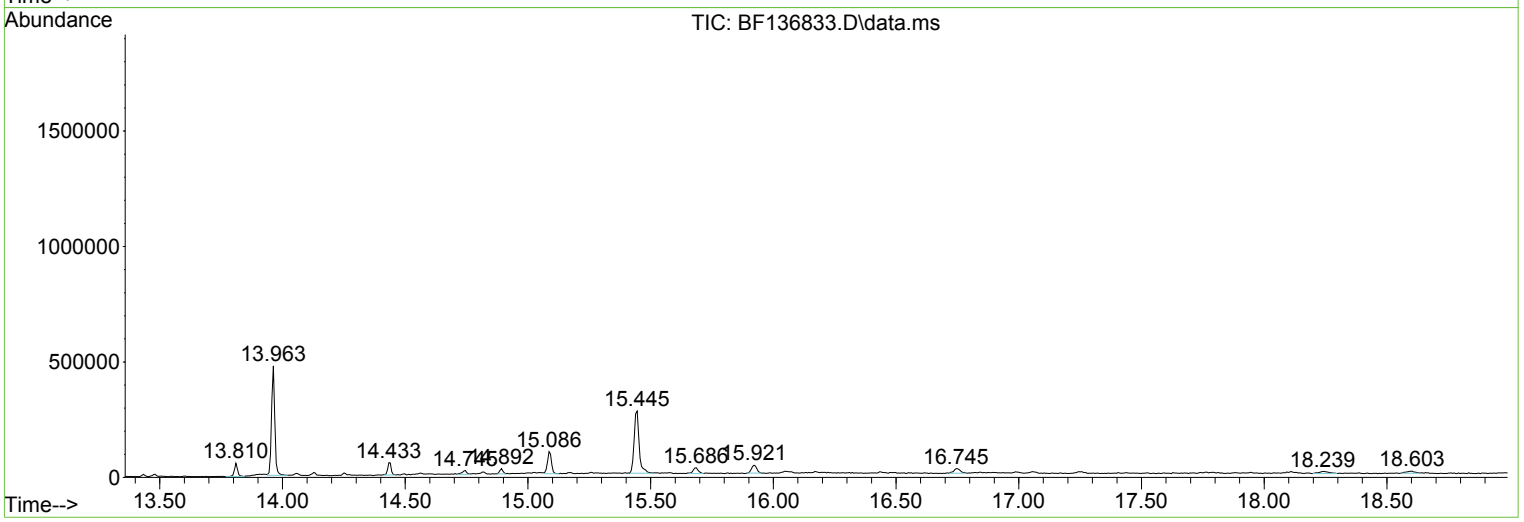
Instrument :
BNA_F
ClientSampleId :
GHL-SS-48

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\BF122923\
Data File : BF136833.D
Acq On : 29 Dec 2023 17:13
Operator : CG\JU
Sample : 05909-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-48

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

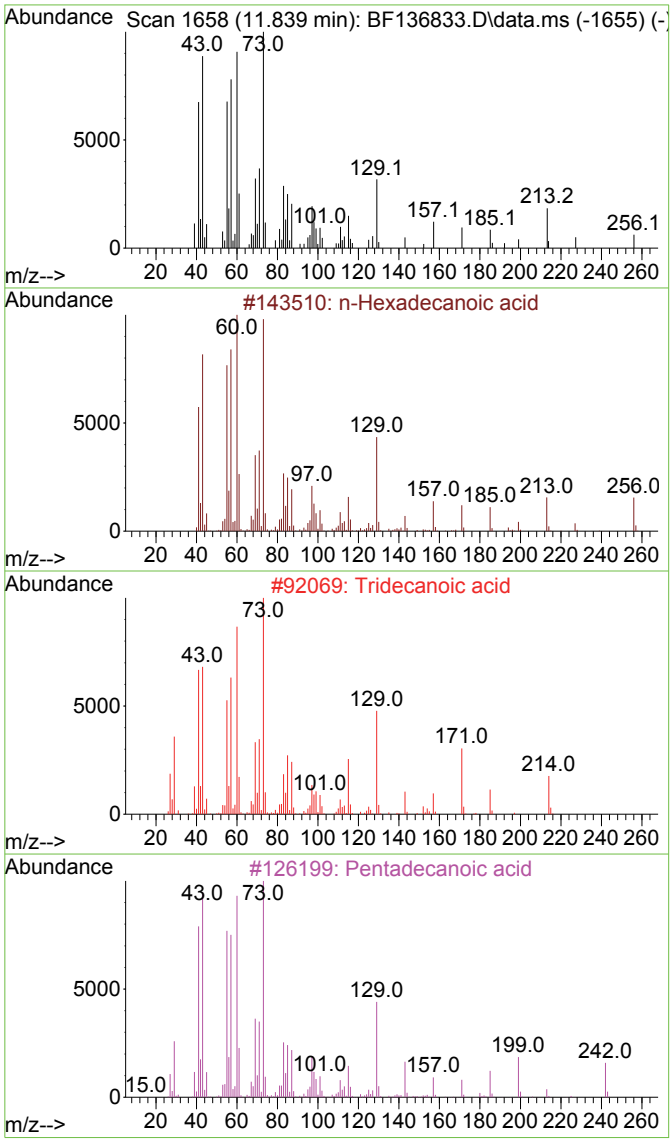
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

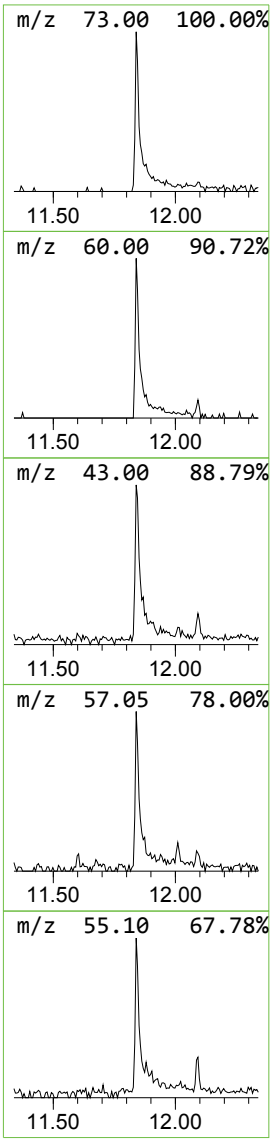
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	4.65 ng	145284	Phenanthrene-d10	11.310

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	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Dodecanoic acid	200	C12H24O2	000143-07-7	59
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136833.D
Acq On : 29 Dec 2023 17:13
Operator : CG\JU
Sample : 05909-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-48

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

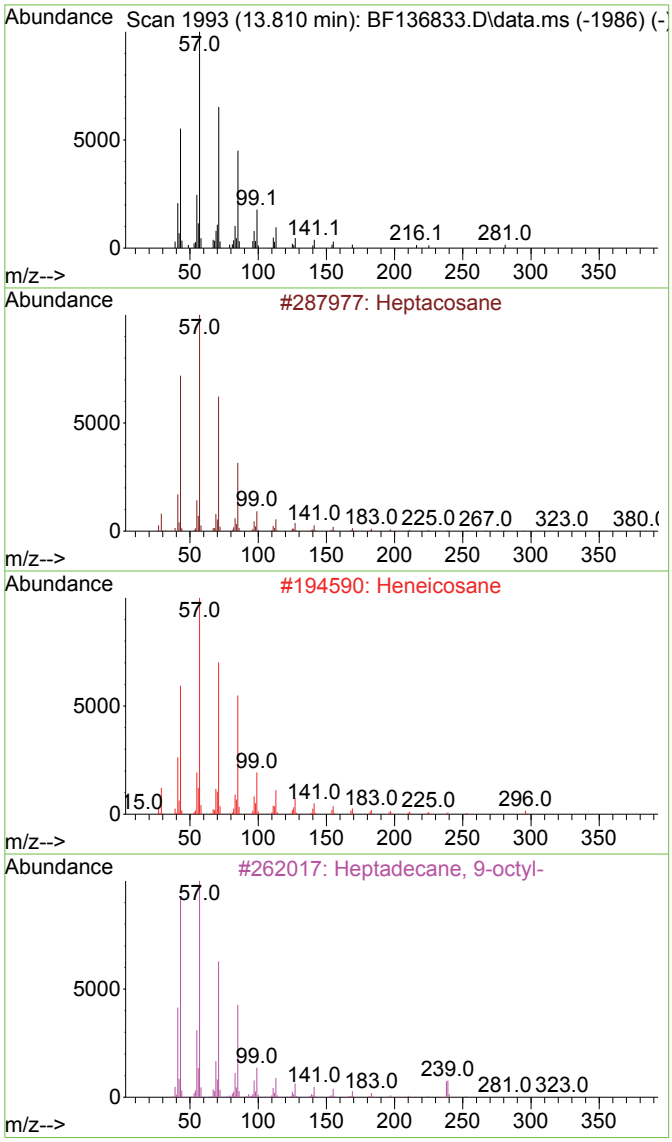
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

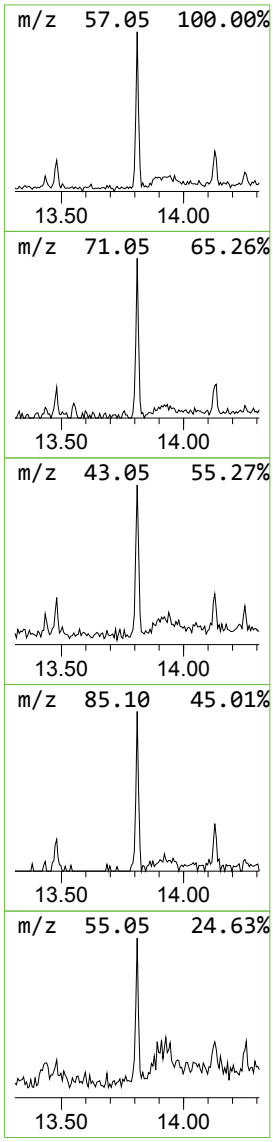
****

Peak Number 2 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.810	2.37 ng	51704	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Heneicosane	296	C21H44	000629-94-7	90
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
4	Hexadecane	226	C16H34	000544-76-3	86
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136833.D
Acq On : 29 Dec 2023 17:13
Operator : CG\JU
Sample : 05909-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-48

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

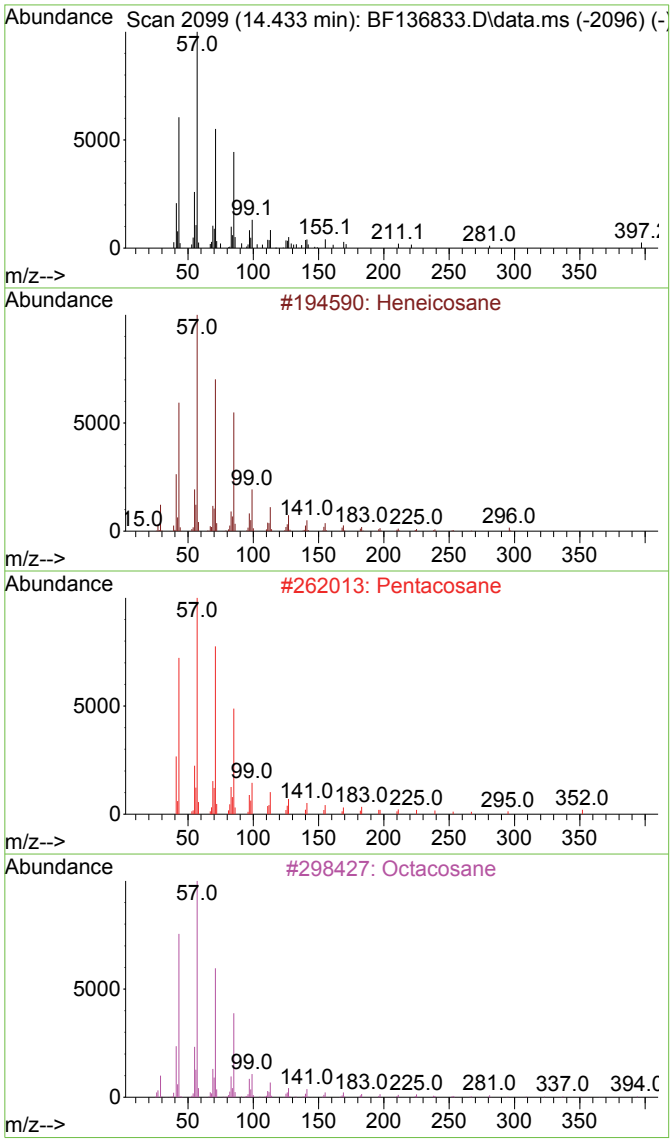
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

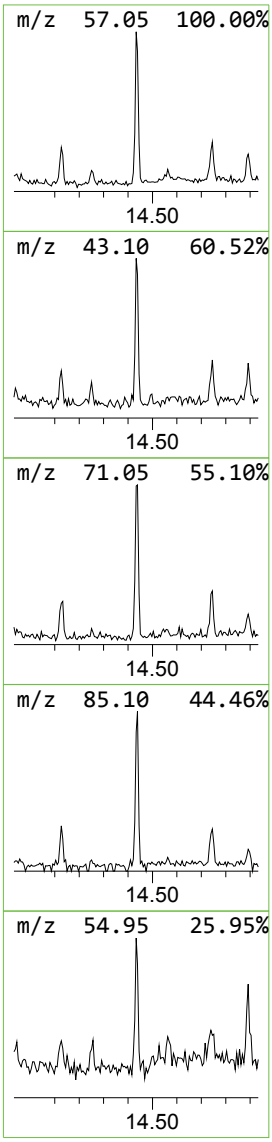
****

Peak Number 3 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.433	2.47 ng	53902	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Pentacosane	352	C25H52	000629-99-2	90
3	Octacosane	394	C28H58	000630-02-4	90
4	Pentadecane	212	C15H32	000629-62-9	90
5	Octadecane	254	C18H38	000593-45-3	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136833.D
Acq On : 29 Dec 2023 17:13
Operator : CG\JU
Sample : 05909-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-48

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

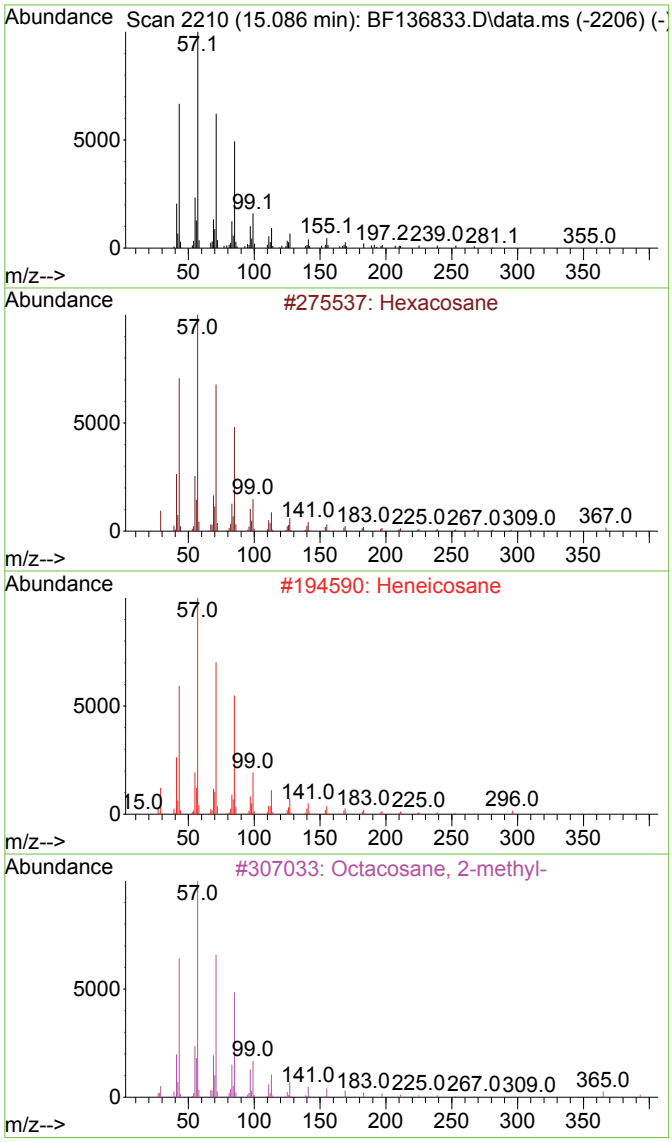
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

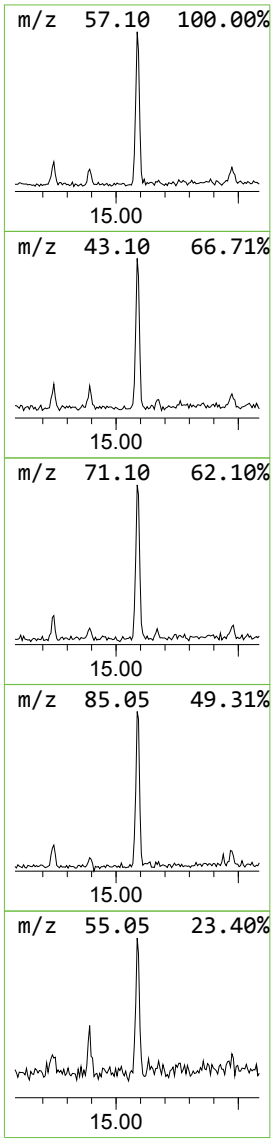
****

Peak Number 4 Hexacosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.086	5.90 ng	110625	Perylene-d12	15.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	93
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136833.D
Acq On : 29 Dec 2023 17:13
Operator : CG\JU
Sample : 05909-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-48

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

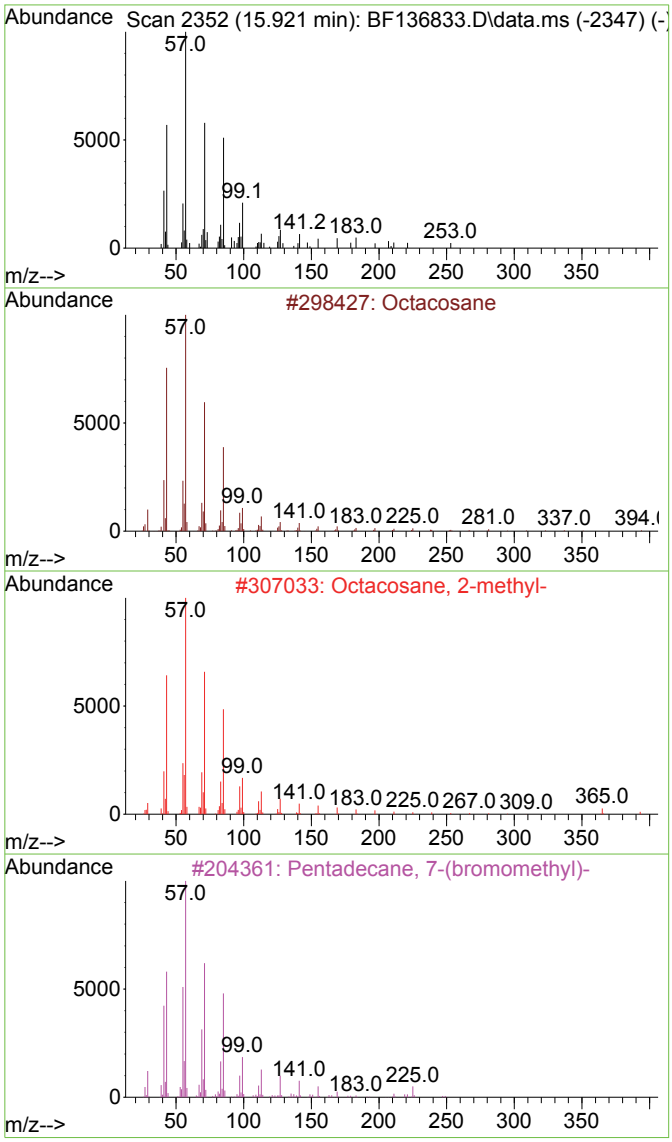
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

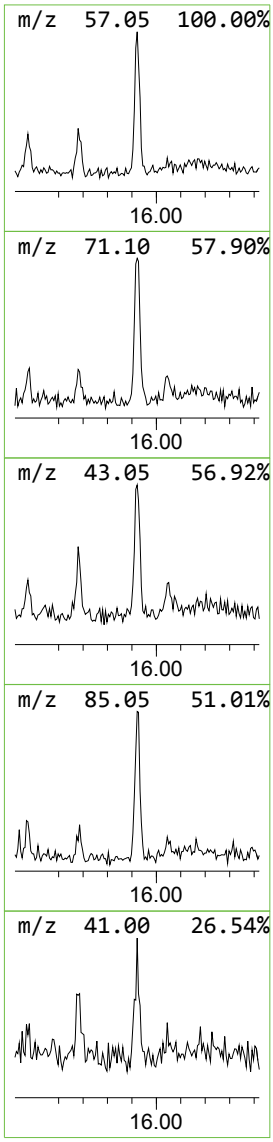
****

Peak Number 5 Octacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.921	2.75 ng	51508	Perylene-d12	15.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	87
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	83
3	Pentadecane, 7-(bromomethyl)-	304	C16H33Br	052997-43-0	83
4	Undecane, 2,9-dimethyl-	184	C13H28	017301-26-7	64
5	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136833.D
Acq On : 29 Dec 2023 17:13
Operator : CG\JU
Sample : 05909-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-48

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

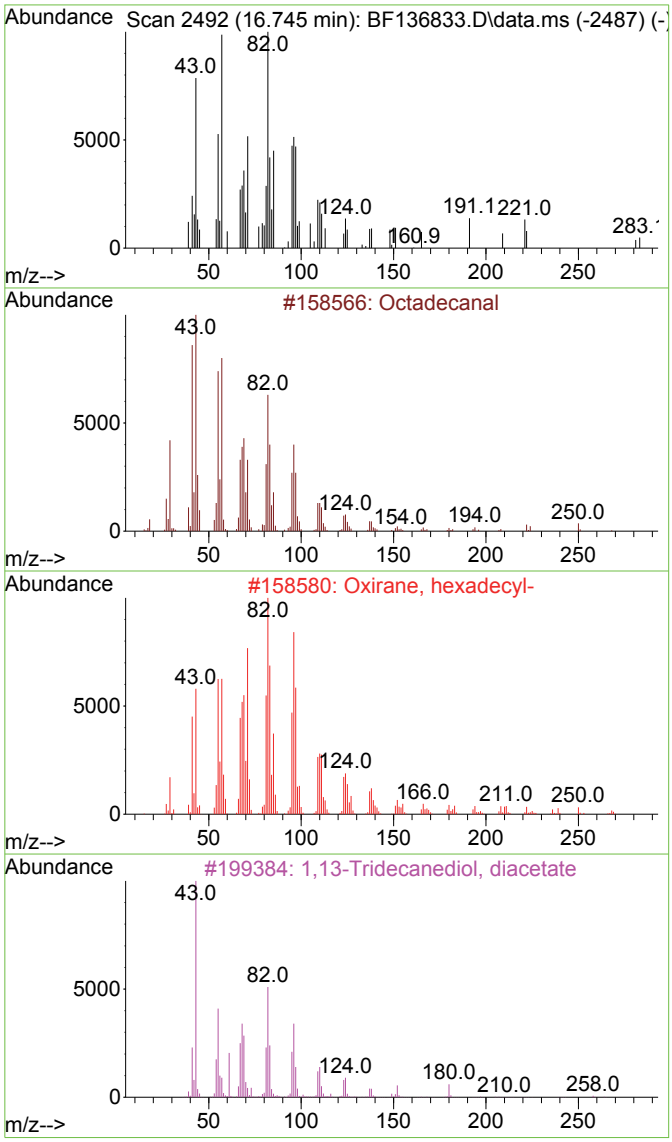
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

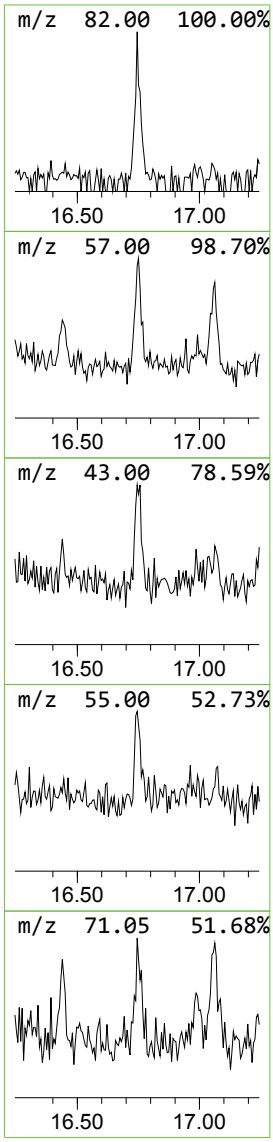
****

Peak Number 6 Octadecanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.745	2.10 ng	39364	Perylene-d12	15.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	72
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	62
3	1,13-Tridecanediol, diacetate	300	C17H32O4	042236-70-4	58
4	E-11(13-Methyl)tetradecen-1-ol a...	268	C17H32O2	1000130-80-4	58
5	7-Azabicyclo[4.1.0]heptane, 1-me...	111	C7H13N	025022-25-7	42





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136833.D
Acq On : 29 Dec 2023 17:13
Operator : CG\JU
Sample : 05909-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-48

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
n-Hexadecanoic ...	11.839	4.7	ng	145284	4	11.310	625095	20.0
Heptacosane	13.810	2.4	ng	51704	5	13.963	437090	20.0
Heneicosane	14.433	2.5	ng	53902	5	13.963	437090	20.0
Hexacosane	15.086	5.9	ng	110625	6	15.445	374787	20.0
Octacosane	15.921	2.8	ng	51508	6	15.445	374787	20.0
Octadecanal	16.745	2.1	ng	39364	6	15.445	374787	20.0