LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051723\
Data File : BF133410.D
Acq On : 17 May 2023 13:33
Operator : CG\JU
Sample : PB152851BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB152851BL

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-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133410.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.922	476	482	497	rBV	2588342	4131908	47.83%	6.274%
2	5.346	548	554	557	rBV	6921734	7588320	87.85%	11.523%
3	6.369	722	728	731	rBV	6419937	7591911	87.89%	11.528%
4	6.716	783	787	790	rBV	2087519	1800352	20.84%	2.734%
5	7.287	878	884	887	rBV	5135092	5051274	58.48%	7.670%
6	7.998	1001	1005	1029	rVB	3108858	2619223	30.32%	3.977%
7	9.081	1182	1189	1192	rBV	8393738	8469247	98.04%	12.860%
8	9.751	1299	1303	1307	rBV	3474064	2970302	34.39%	4.510%
9	10.545	1433	1438	1441	rBV	4828074	5063672	58.62%	7.689%
10	11.239	1552	1556	1559	rBV	3210007	2987170	34.58%	4.536%
11	12.827	1821	1826	1829	rBV	7353552	8638267	100.00%	13.117%
12	13.357	1912	1916	1921	rBV	171196	150565	1.74%	0.229%
13	13.874	1999	2004	2012	rBV	2629936	2382930	27.59%	3.618%
14	14.045	2030	2033	2038	rVB	89546	86465	1.00%	0.131%
15	14.351	2082	2085	2090	rVB	170336	151178	1.75%	0.230%
16	14.651	2132	2136	2142	rVB	352252	351587	4.07%	0.534%
17	14.968	2186	2190	2197	rBV	409771	468040	5.42%	0.711%
18	15.298	2240	2246	2249	rBV	1519777	1886703	21.84%	2.865%
19	15.327	2249	2251	2258	rVB	502145	575341	6.66%	0.874%
20	15.739	2315	2321	2326	rBV	442852	627934	7.27%	0.954%
21	16.210	2395	2401	2406	rBV	455029	839520	9.72%	1.275%
22	16.762	2488	2495	2503	rVB	276696	562370	6.51%	0.854%
23	17.409	2598	2605	2613	rVB2	217696	508561	5.89%	0.772%
24	18.186	2729	2737	2747	rVB4	119996	352466	4.08%	0.535%

Sum of corrected areas: 65855306

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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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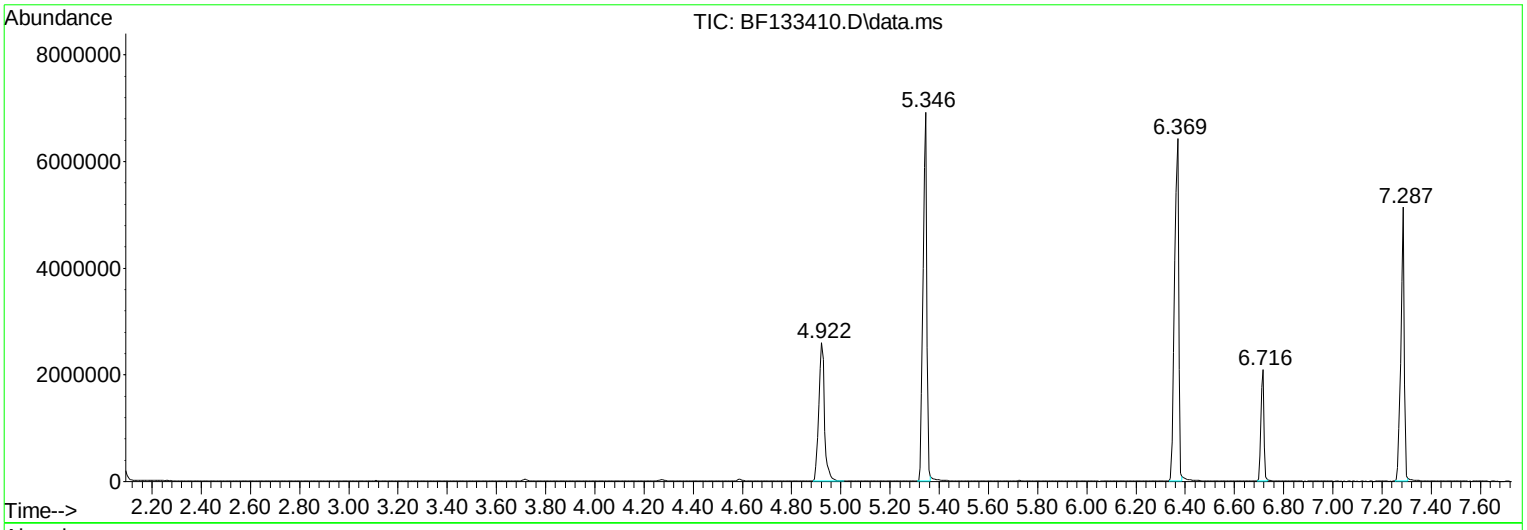
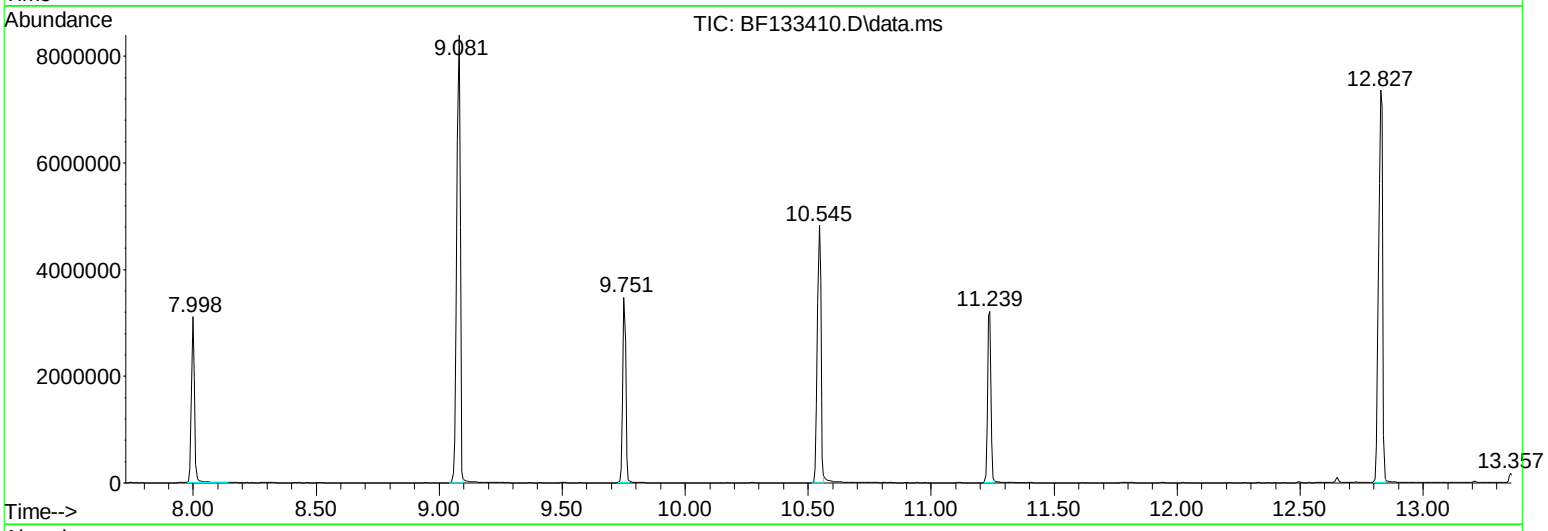
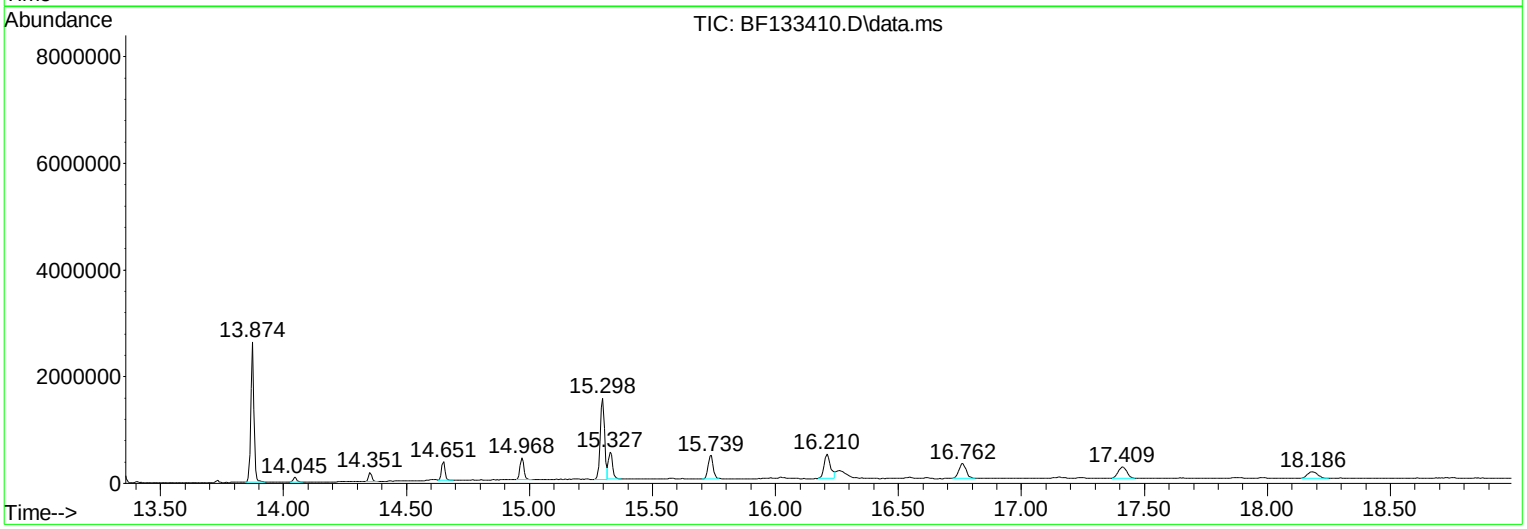
ClientSampleId :
PB152851BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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\BF051723\
Data File : BF133410.D
Acq On : 17 May 2023 13:33
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

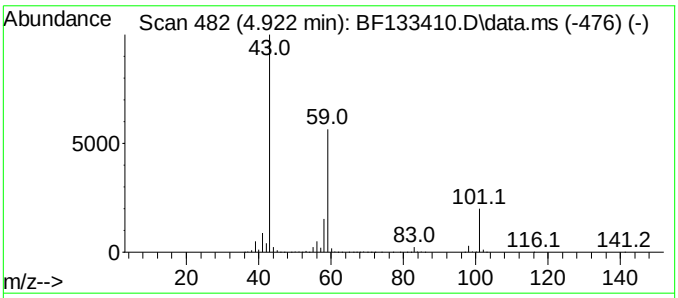
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

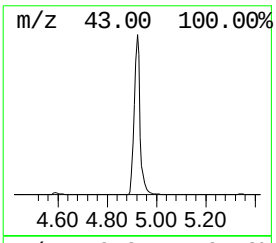
****

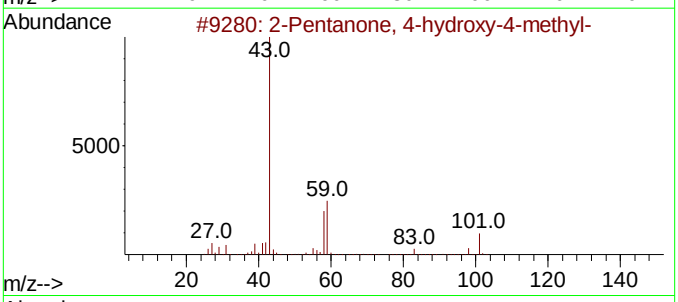
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

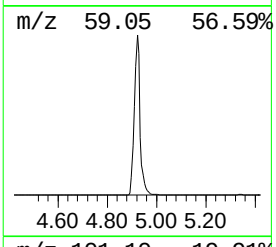
R.T.	EstConc	Area	Relative to ISTD	R.T.
4.922	45.90 ng	4131910	1,4-Dichlorobenzene-d4	6.716

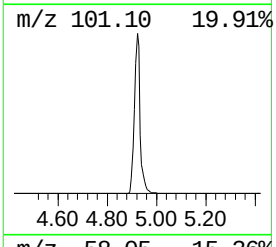
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9

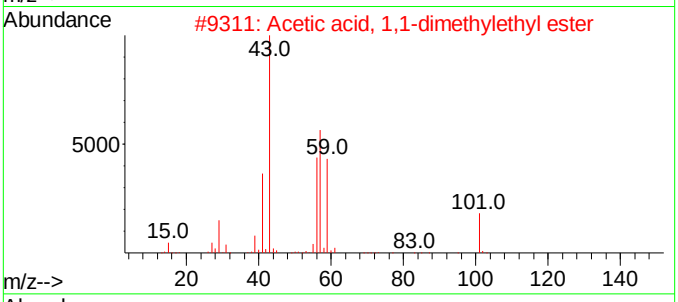


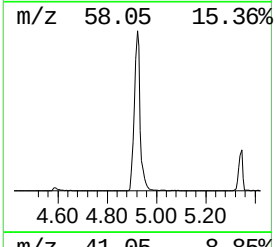


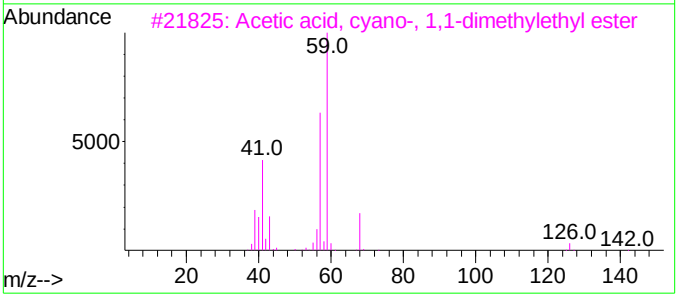


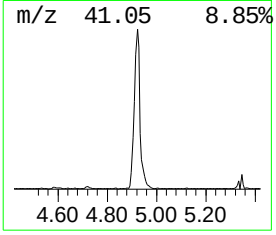












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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB152851BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

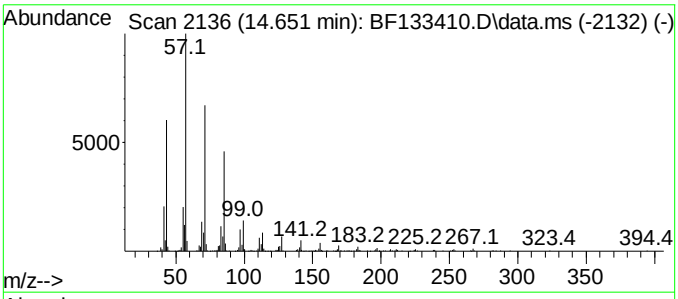
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

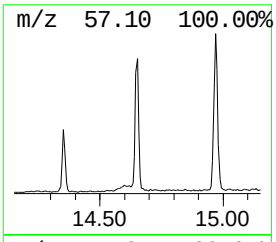
****

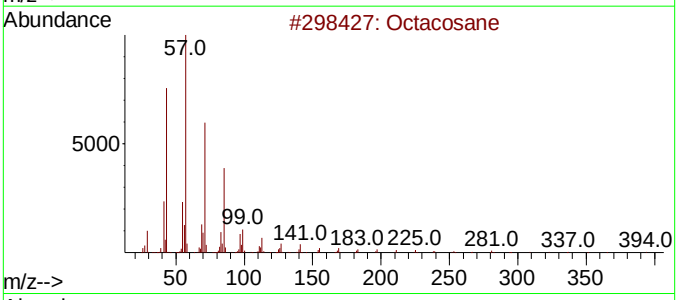
Peak Number 2 Octacosane Concentration Rank 8

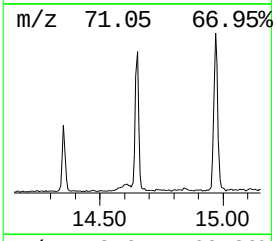
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.651	3.73 ng	351587	Perylene-d12	15.298

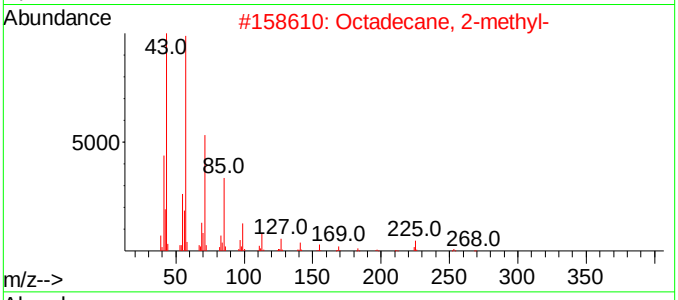
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	97
2	Octadecane, 2-methyl-	268	C19H40	001560-88-9	94
3	Octadecane	254	C18H38	000593-45-3	94
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Hexacosane	366	C26H54	000630-01-3	91

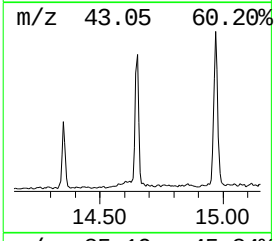


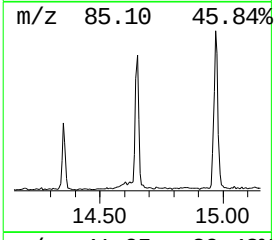


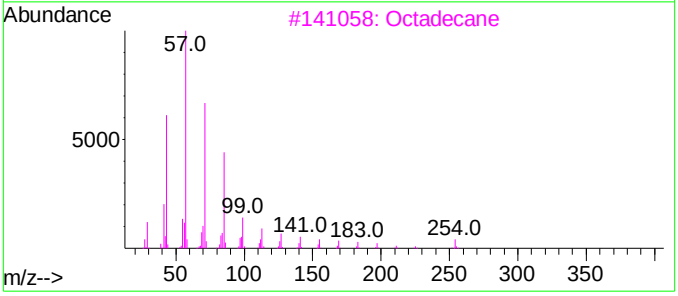


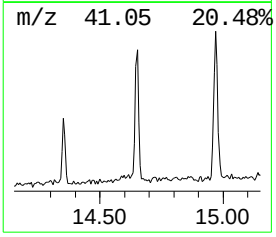












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Misc :
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Instrument :
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ClientSampleId :
PB152851BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

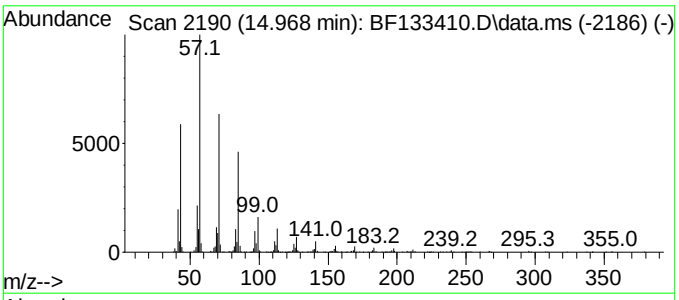
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

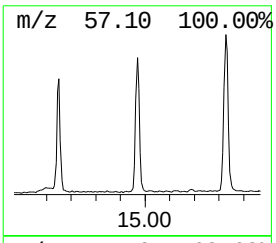
****

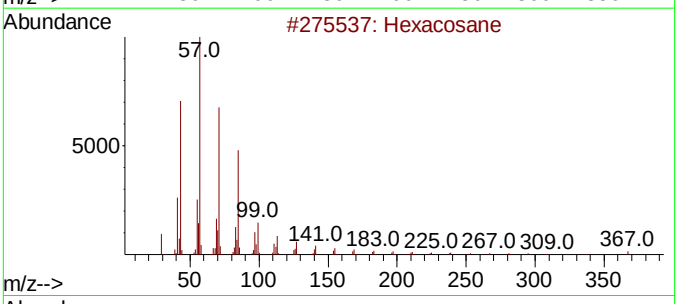
Peak Number 3 Hexacosane Concentration Rank 6

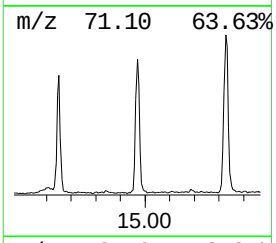
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.969	4.96 ng	468040	Perylene-d12	15.298

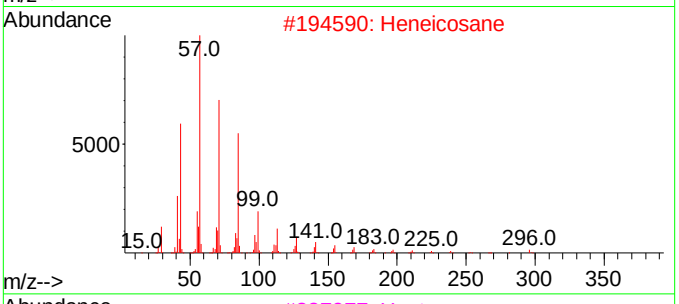
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	4-Methylheneicosane	310	C22H46	025117-29-7	91
5	Tetracosane	338	C24H50	000646-31-1	90

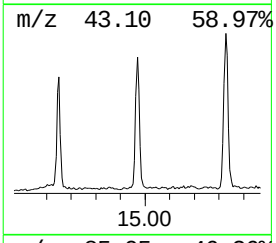


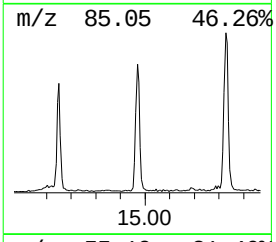


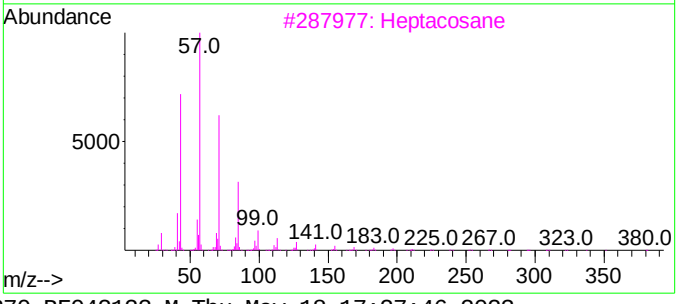


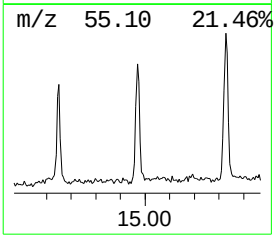












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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

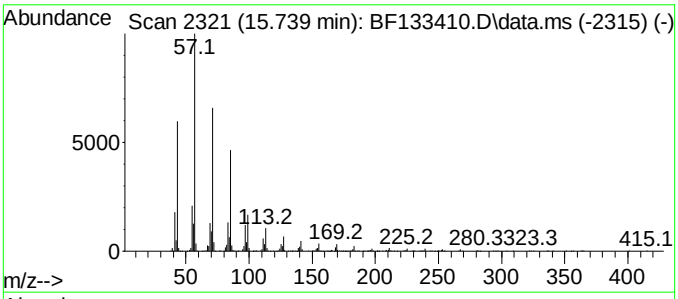
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

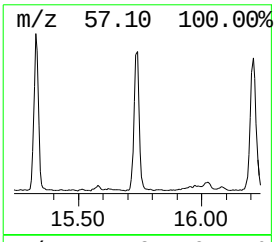
****

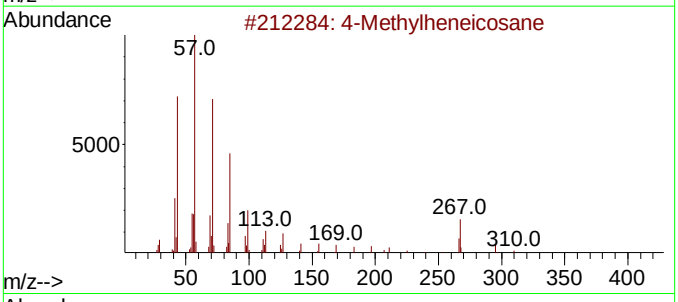
Peak Number 4 4-Methylheneicosane Concentration Rank 3

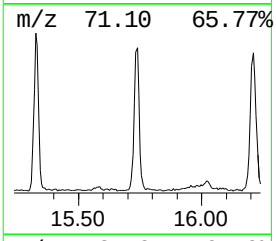
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.739	6.66 ng	627934	Perylene-d12	15.298

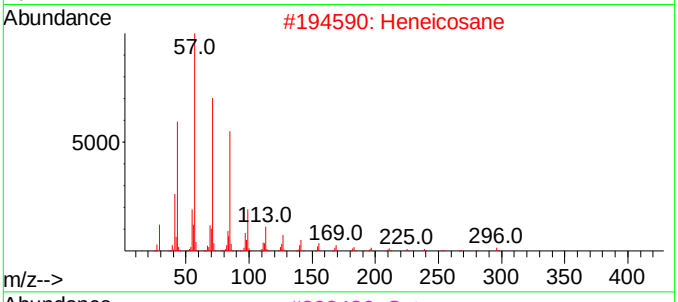
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methylheneicosane	310	C22H46	025117-29-7	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Hentriacontane	437	C31H64	000630-04-6	91

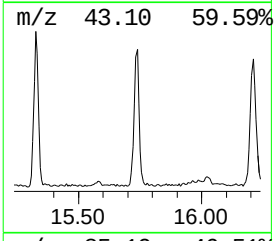


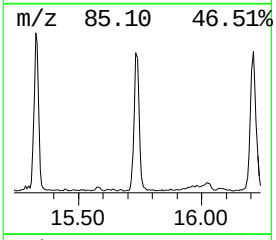


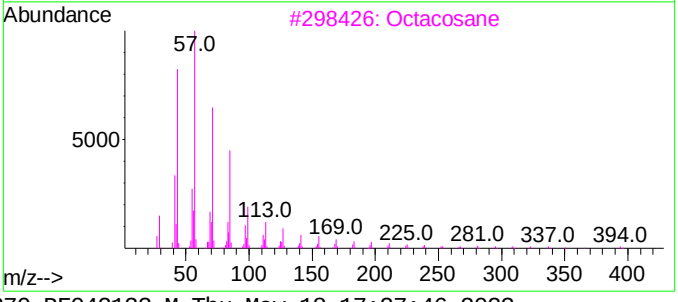


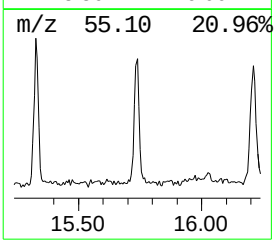












Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051723\
Data File : BF133410.D
Acq On : 17 May 2023 13:33
Operator : CG\JU
Sample : PB152851BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB152851BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

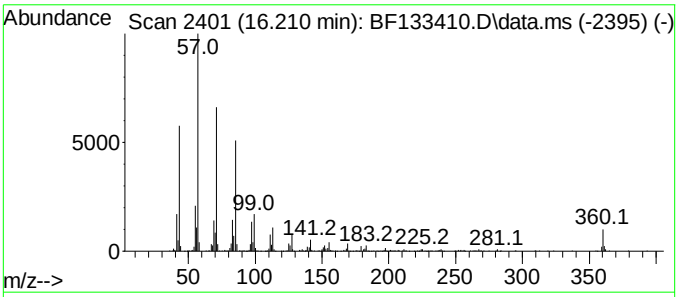
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

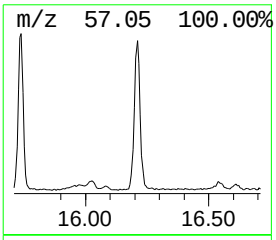
****

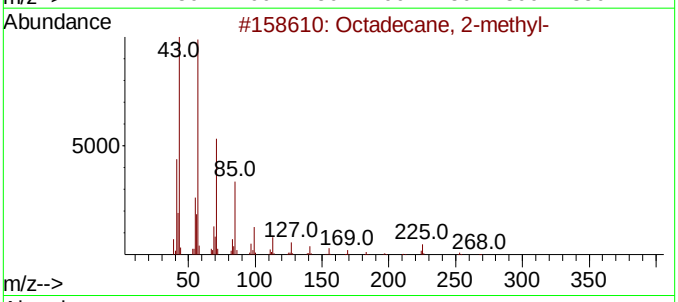
Peak Number 5 Octadecane, 2-methyl- Concentration Rank 2

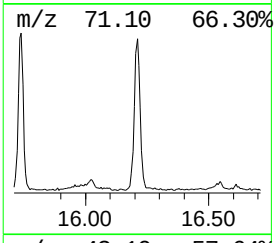
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.210	8.90 ng	839520	Perylene-d12	15.298

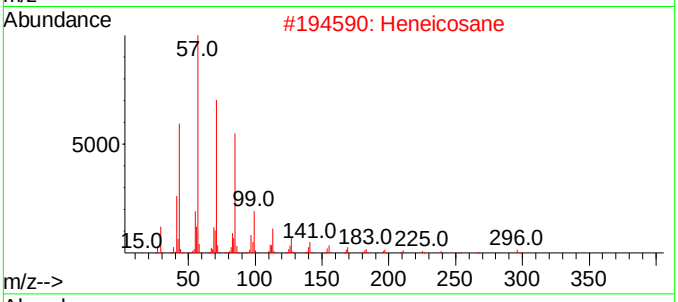
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 2-methyl-	268	C19H40	001560-88-9	91
2	Heneicosane	296	C21H44	000629-94-7	87
3	Hexacosane, 1-iodo-	492	C26H53I	1000406-32-1	87
4	Docosane, 1-iodo-	436	C22H45I	1000406-31-9	83
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83

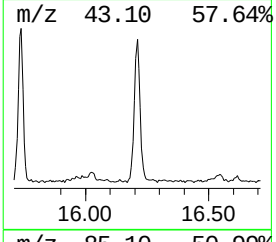


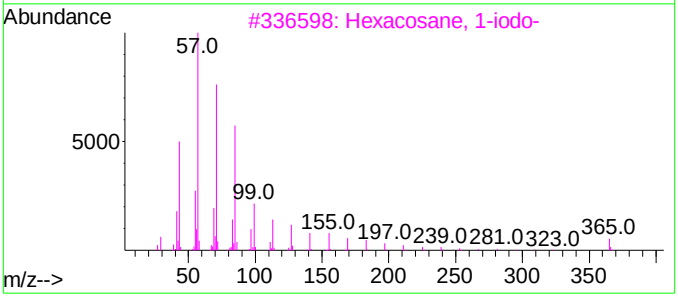


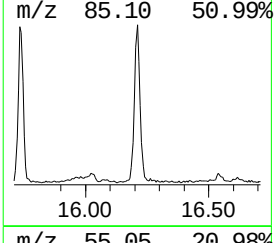


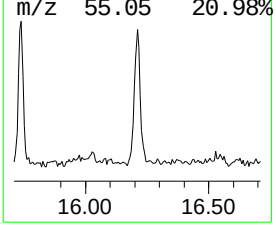












Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051723\
Data File : BF133410.D
Acq On : 17 May 2023 13:33
Operator : CG\JU
Sample : PB152851BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB152851BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

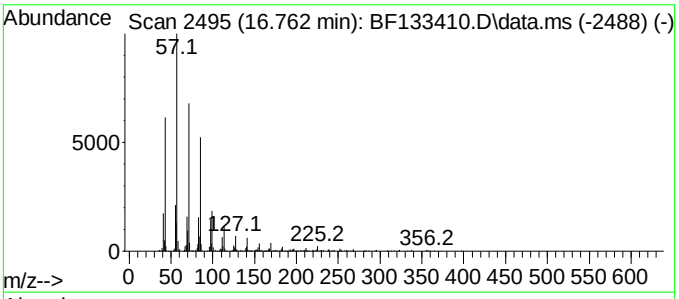
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

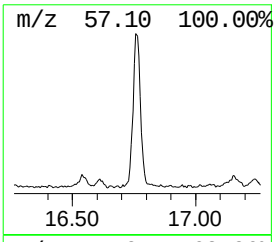
****

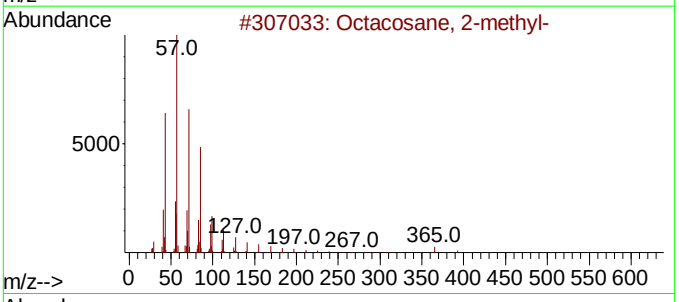
Peak Number 6 Octacosane, 2-methyl- Concentration Rank 4

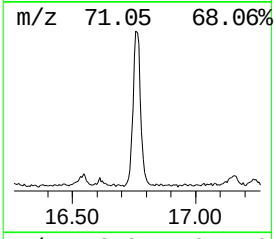
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.762	5.96 ng	562370	Perylene-d12	15.298

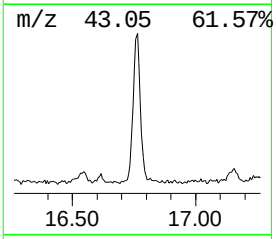
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
2	Tetratetracontane	619	C44H90	007098-22-8	91
3	Octadecane	254	C18H38	000593-45-3	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Hexacosane, 1-iodo-	492	C26H53I	1000406-32-1	91

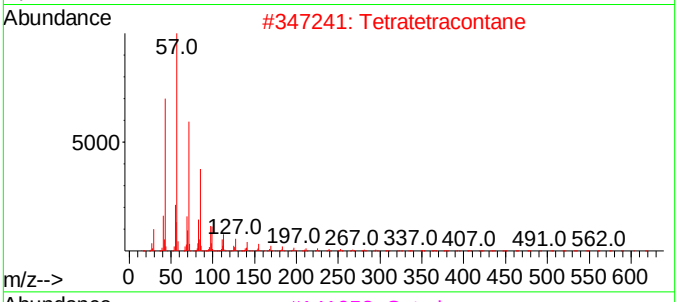


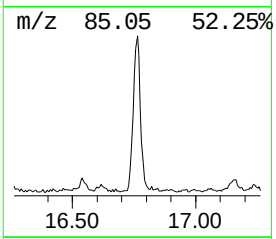


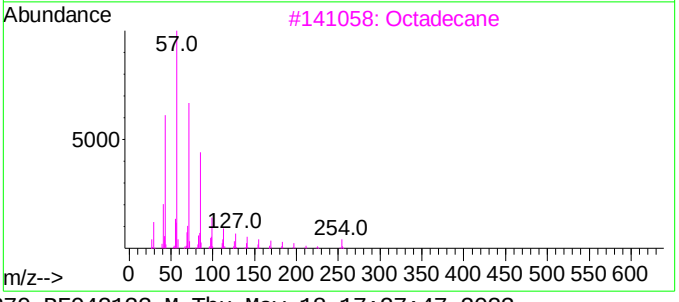


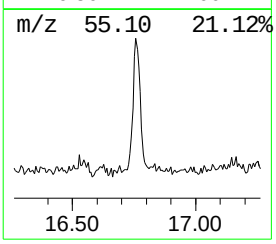












Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051723\
Data File : BF133410.D
Acq On : 17 May 2023 13:33
Operator : CG\JU
Sample : PB152851BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB152851BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

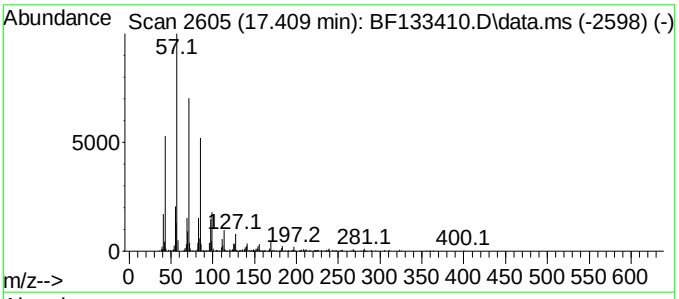
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

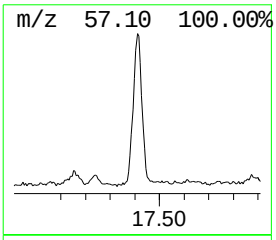
****

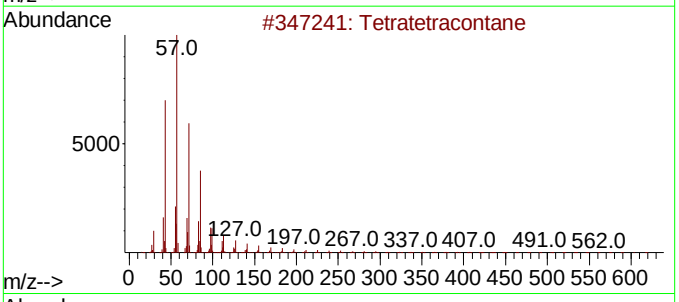
Peak Number 7 Tetratetracontane Concentration Rank 5

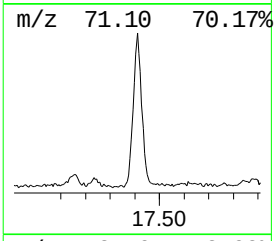
R.T.	EstConc	Area	Relative to ISTD	R.T.
17.410	5.39 ng	508561	Perylene-d12	15.298

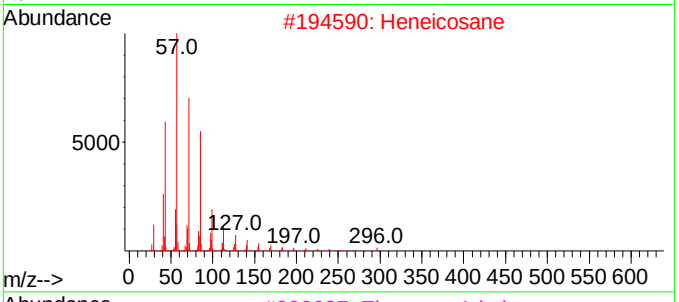
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	91
2	Heneicosane	296	C21H44	000629-94-7	90
3	Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	90
4	Heptadecane	240	C17H36	000629-78-7	87
5	Docosane	310	C22H46	000629-97-0	87

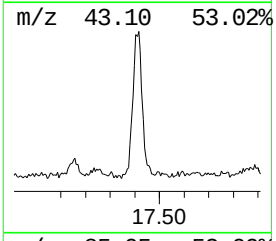


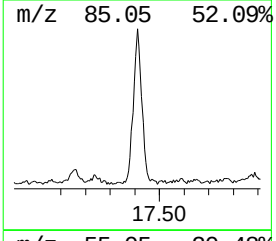


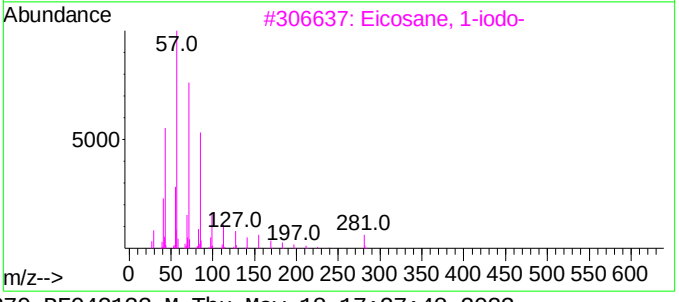


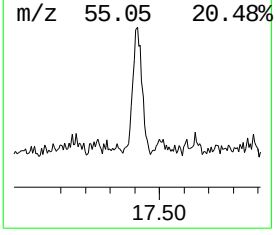












Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051723\
Data File : BF133410.D
Acq On : 17 May 2023 13:33
Operator : CG\JU
Sample : PB152851BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB152851BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

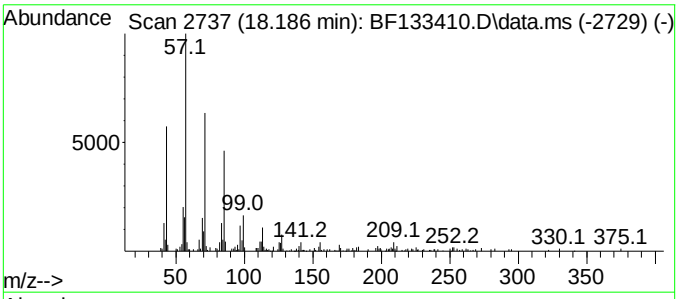
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

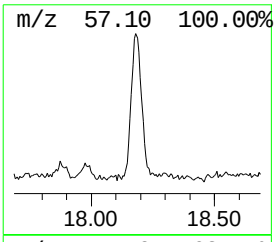
****

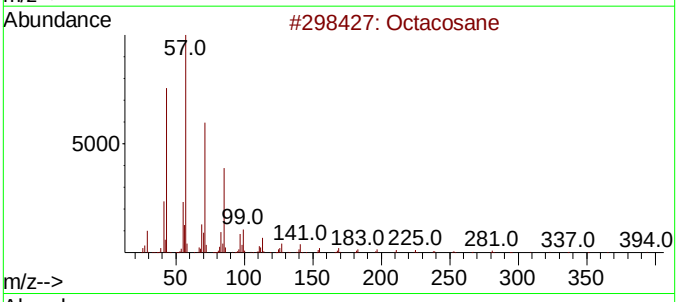
Peak Number 8 Eicosane Concentration Rank 7

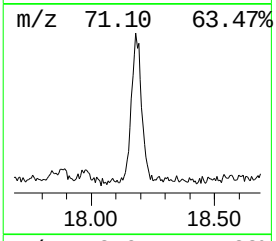
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.186	3.74 ng	352466	Perylene-d12	15.298

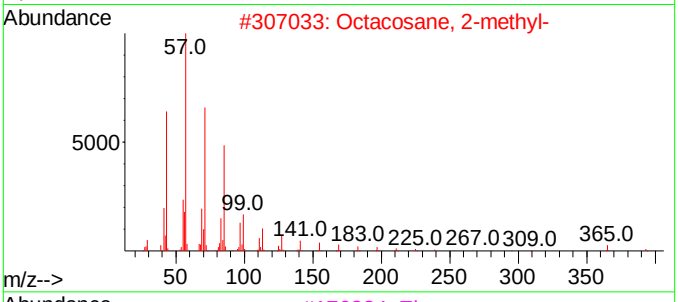
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
3	Eicosane	282	C20H42	000112-95-8	87
4	4-Methylheneicosane	310	C22H46	025117-29-7	87
5	Hexatriacontane	507	C36H74	000630-06-8	87

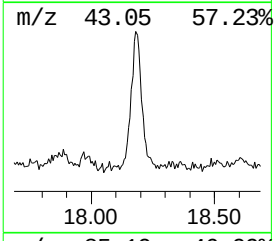


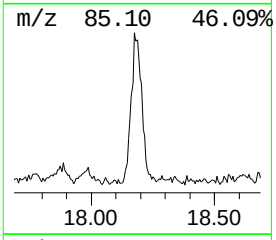


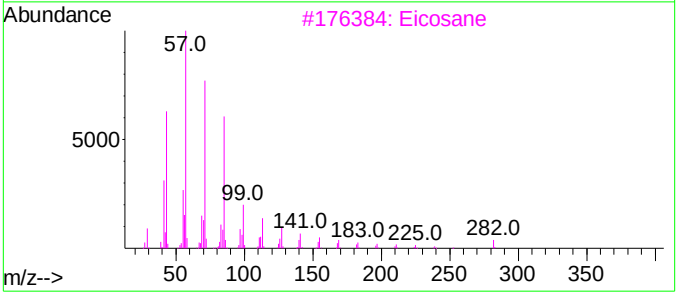


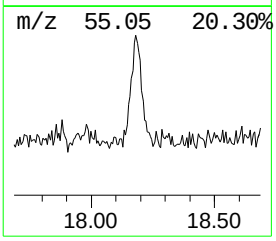












Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051723\
Data File : BF133410.D
Acq On : 17 May 2023 13:33
Operator : CG\JU
Sample : PB152851BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB152851BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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-...	4.922	45.9	ng	4131910	1	6.716	1800350	20.0
Octacosane	14.651	3.7	ng	351587	6	15.298	1886700	20.0
Hexacosane	14.969	5.0	ng	468040	6	15.298	1886700	20.0
4-Methylheneico...	15.739	6.7	ng	627934	6	15.298	1886700	20.0
Octadecane, 2-m...	16.210	8.9	ng	839520	6	15.298	1886700	20.0
Octacosane, 2-m...	16.762	6.0	ng	562370	6	15.298	1886700	20.0
Tetratetracontane	17.410	5.4	ng	508561	6	15.298	1886700	20.0
Eicosane	18.186	3.7	ng	352466	6	15.298	1886700	20.0