LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
Data File : BF135197.D
Acq On : 12 Sep 2023 23:41
Operator : CG\JU
Sample : 04338-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP3

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-BF091123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135197.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.010	492	497	507	rVB	70111	101006	3.27%	0.481%
2	5.398	558	563	566	rBV	2746756	2594192	83.89%	12.359%
3	6.404	729	734	737	rBV	2692256	2696169	87.19%	12.844%
4	6.763	791	795	798	rBV	739726	616076	19.92%	2.935%
5	7.328	885	891	894	rBV	1771441	1734161	56.08%	8.261%
6	8.039	1007	1012	1016	rBV	972425	816839	26.41%	3.891%
7	9.122	1190	1196	1199	rBV	3423731	3056380	98.84%	14.560%
8	9.798	1306	1311	1314	rBV	1083831	935890	30.26%	4.459%
9	10.592	1441	1446	1449	rBV	2170725	2042316	66.04%	9.729%
10	11.286	1560	1564	1568	rBV	1156907	1021915	33.05%	4.868%
11	11.827	1652	1656	1672	rBV2	184639	219218	7.09%	1.044%
12	12.616	1787	1790	1799	rBV	68645	83752	2.71%	0.399%
13	12.886	1831	1836	1840	rBV	3061450	3092376	100.00%	14.732%
14	13.121	1871	1876	1879	rBV	38096	33054	1.07%	0.157%
15	13.468	1931	1935	1938	rBV	69859	62085	2.01%	0.296%
16	13.798	1987	1991	1994	rBV	99136	95867	3.10%	0.457%
17	13.833	1994	1997	2011	rVV4	38591	120585	3.90%	0.574%
18	13.939	2011	2015	2023	rVB	731858	681480	22.04%	3.247%
19	14.115	2042	2045	2050	rBV	113678	94267	3.05%	0.449%
20	14.421	2094	2097	2103	rBV	81917	78431	2.54%	0.374%
21	14.710	2142	2146	2148	rBV	214519	214609	6.94%	1.022%
22	15.068	2203	2207	2211	rVB	31635	35386	1.14%	0.169%
23	15.404	2259	2264	2269	rBV	479638	565050	18.27%	2.692%

Sum of corrected areas: 20991104

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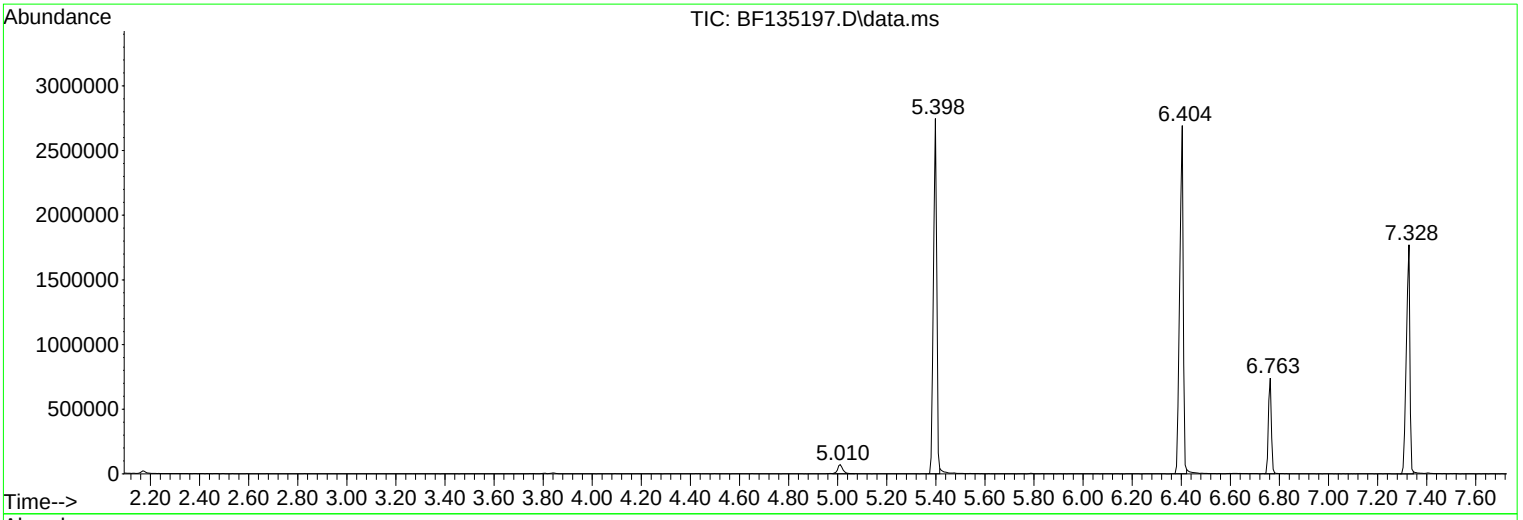
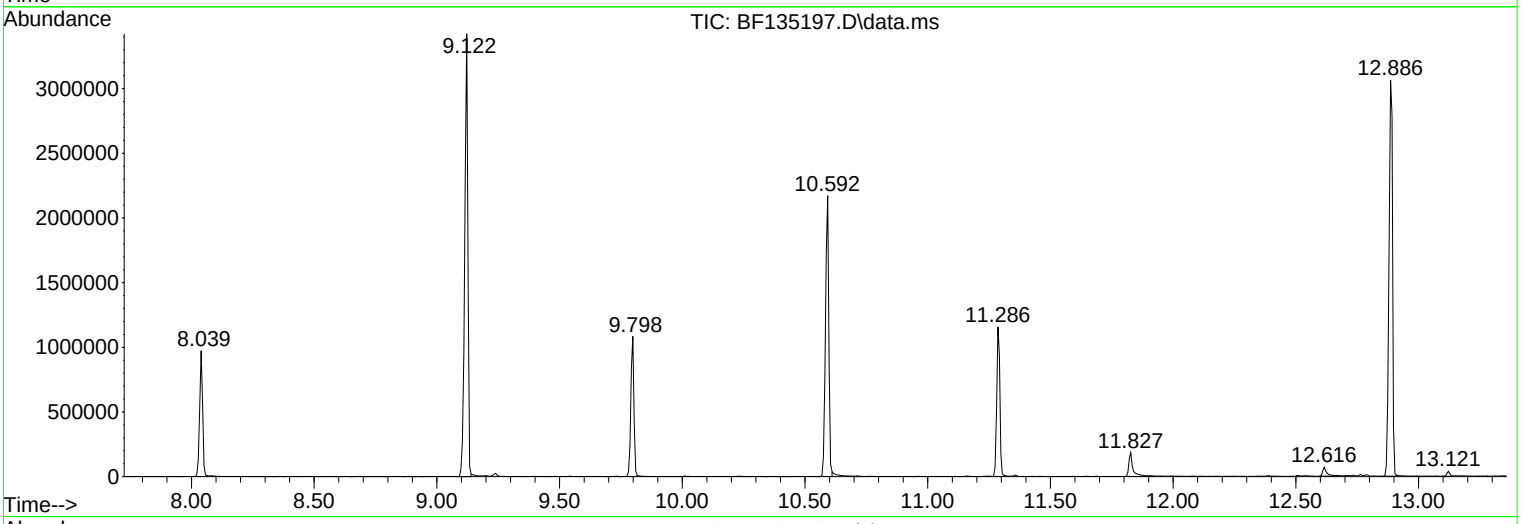
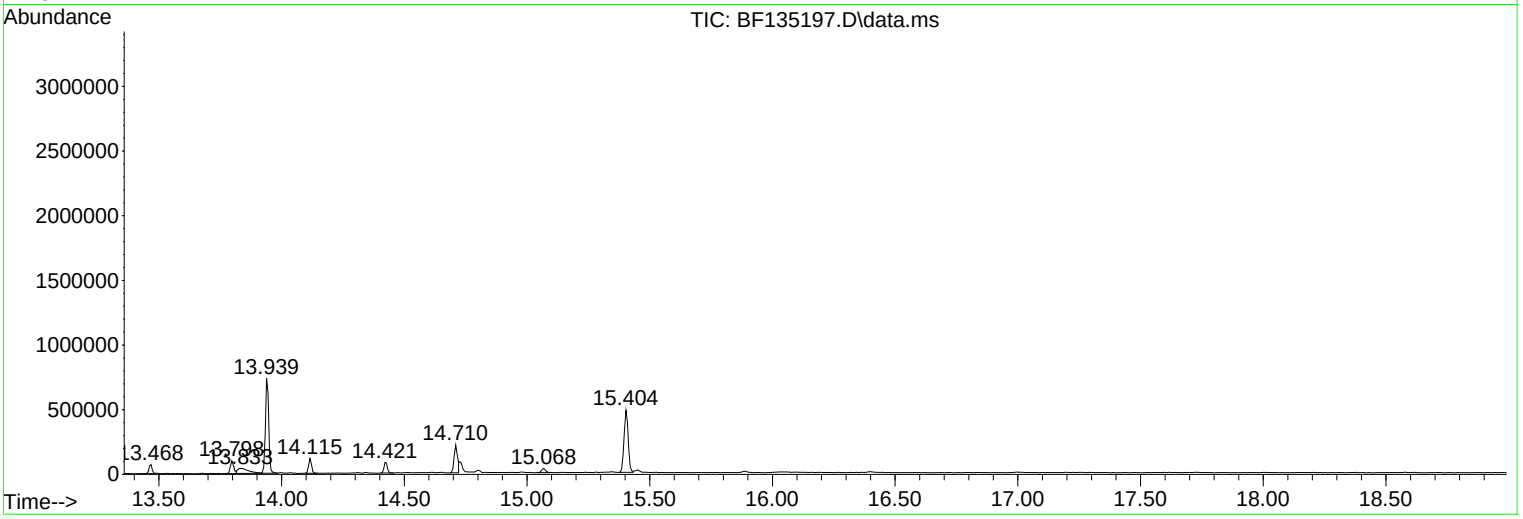
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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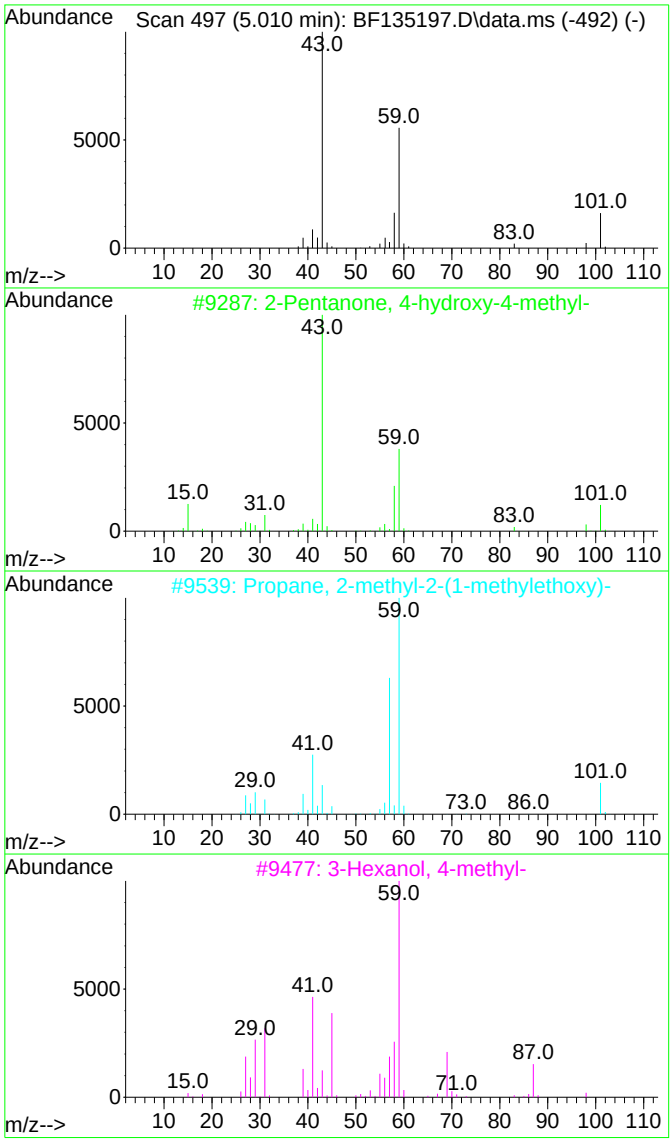
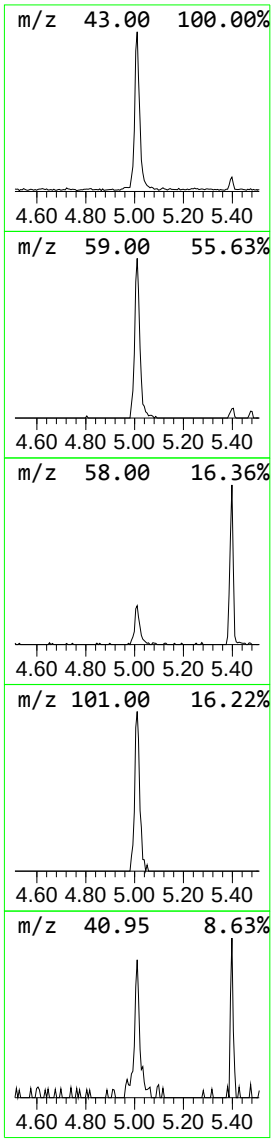
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.010	3.28 ng	101006	1,4-Dichlorobenzene-d4	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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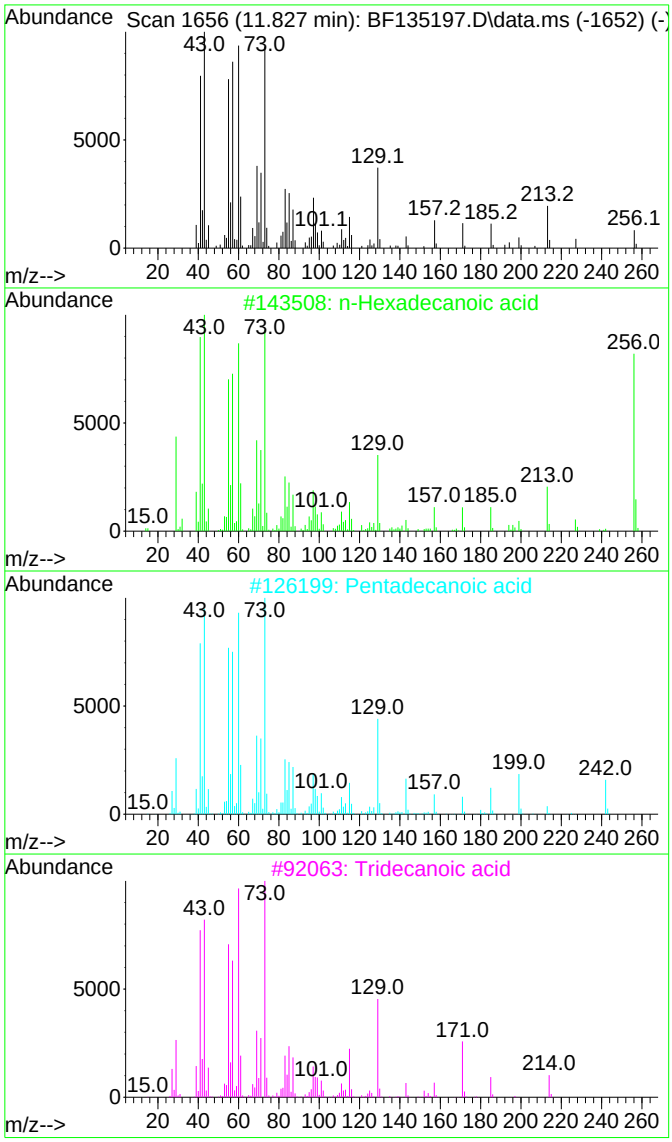
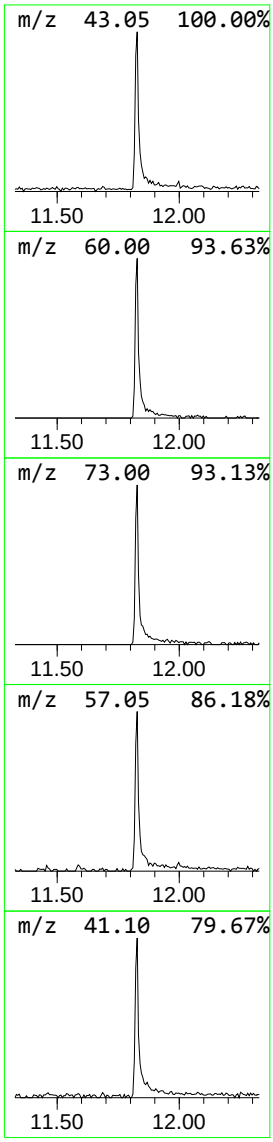
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.827	4.29 ng	219218	Phenanthrene-d10	11.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





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Operator : CG\JU
Sample : 04338-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

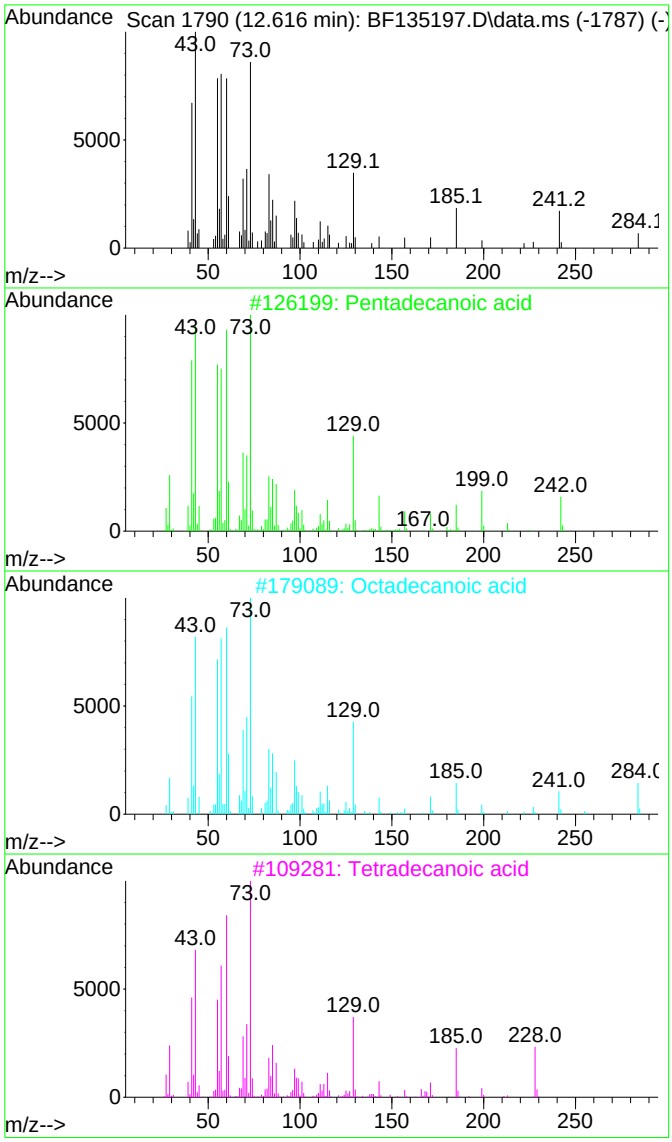
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

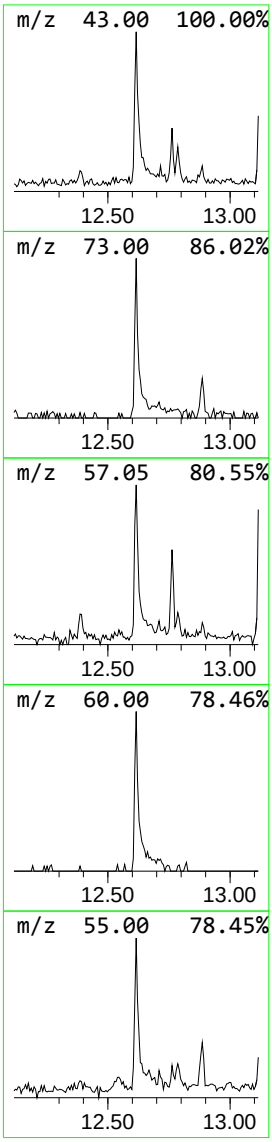
****

Peak Number 3 Pentadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	2.46 ng	83752	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
2	Octadecanoic acid	284	C18H36O2	000057-11-4	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	47





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Data File : BF135197.D
Acq On : 12 Sep 2023 23:41
Operator : CG\JU
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

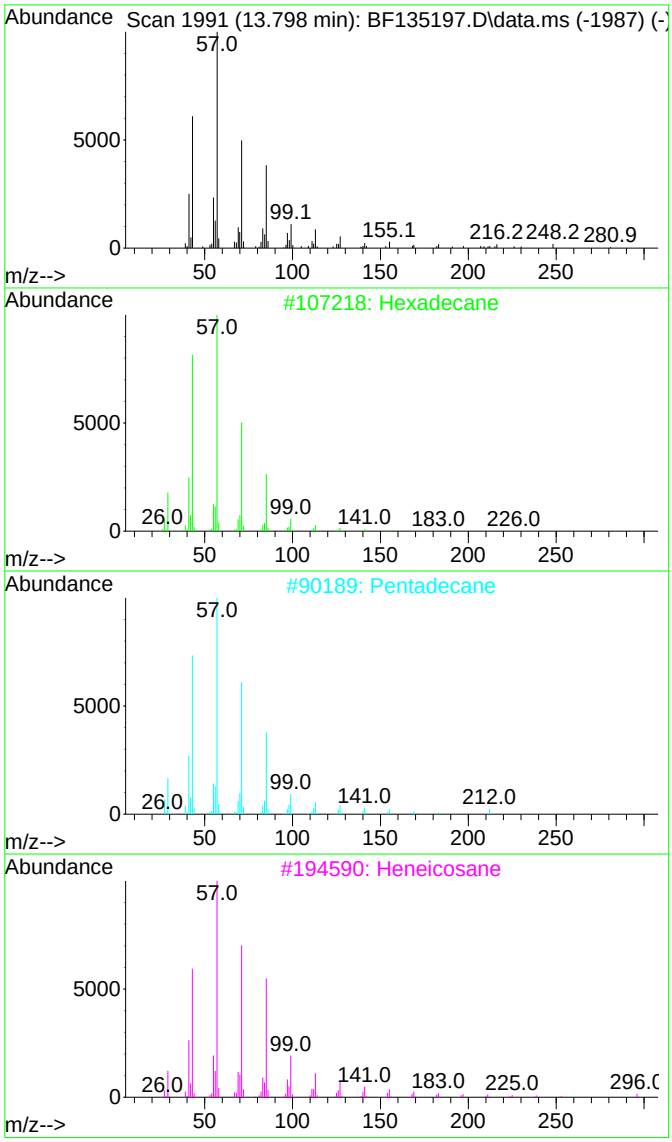
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

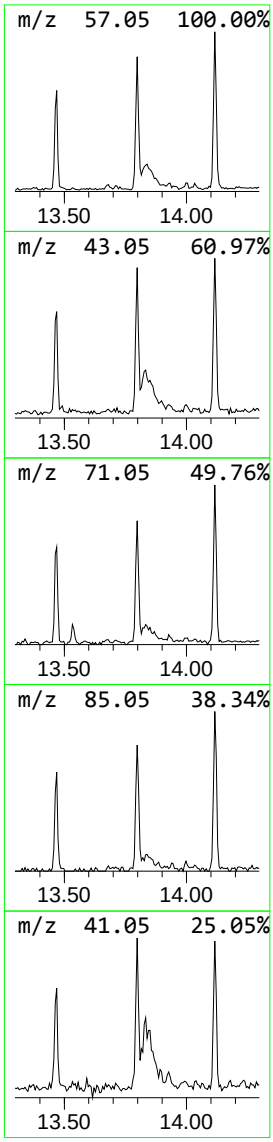
****

Peak Number 4 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.798	2.81 ng	95867	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	97
2	Pentadecane	212	C15H32	000629-62-9	95
3	Heneicosane	296	C21H44	000629-94-7	90
4	Nonadecane	268	C19H40	000629-92-5	90
5	Hexacosane	366	C26H54	000630-01-3	87





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Operator : CG\JU
Sample : 04338-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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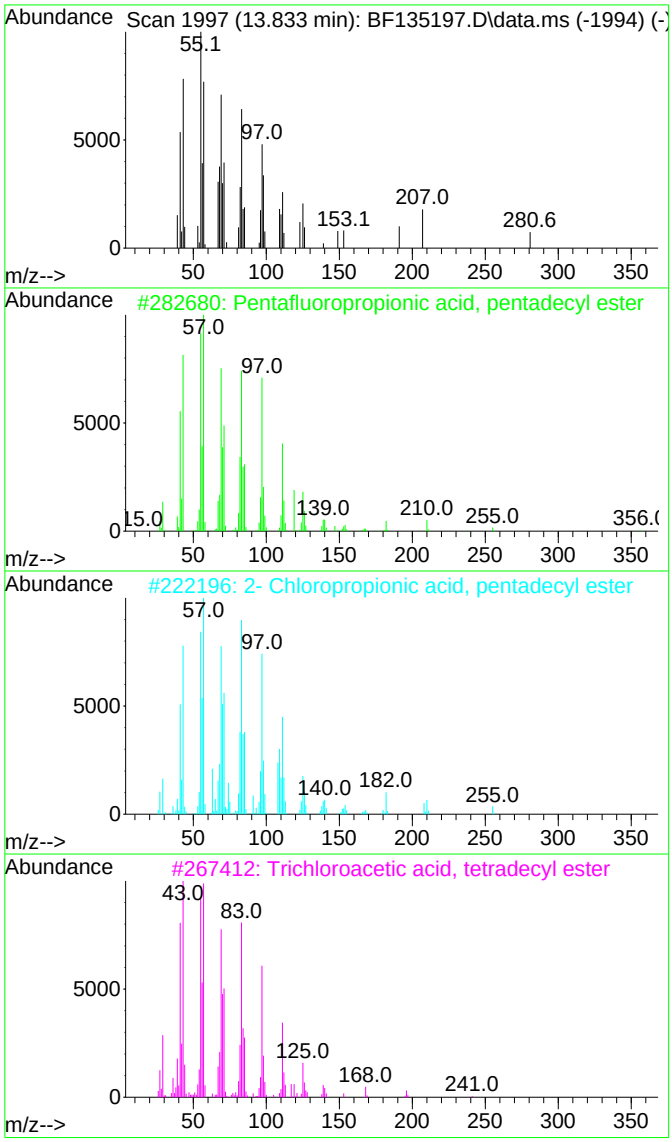
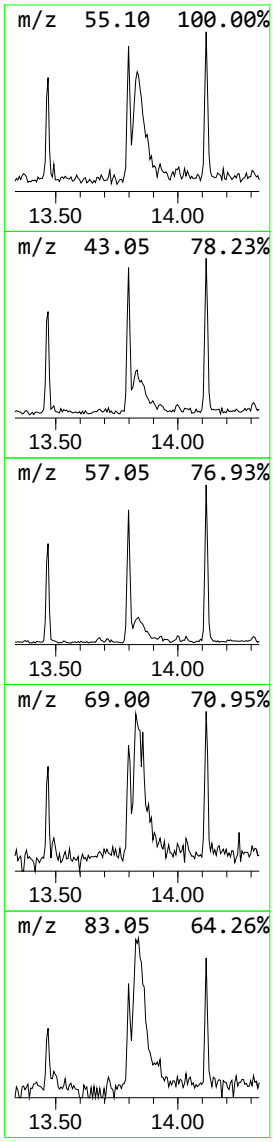
****
Peak Number 5 Pentafluoropropionic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.833	3.54 ng	120585	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	81
2	2- Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	74
3	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	74
4	11-Tricosene	322	C23H46	052078-56-5	74
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	74





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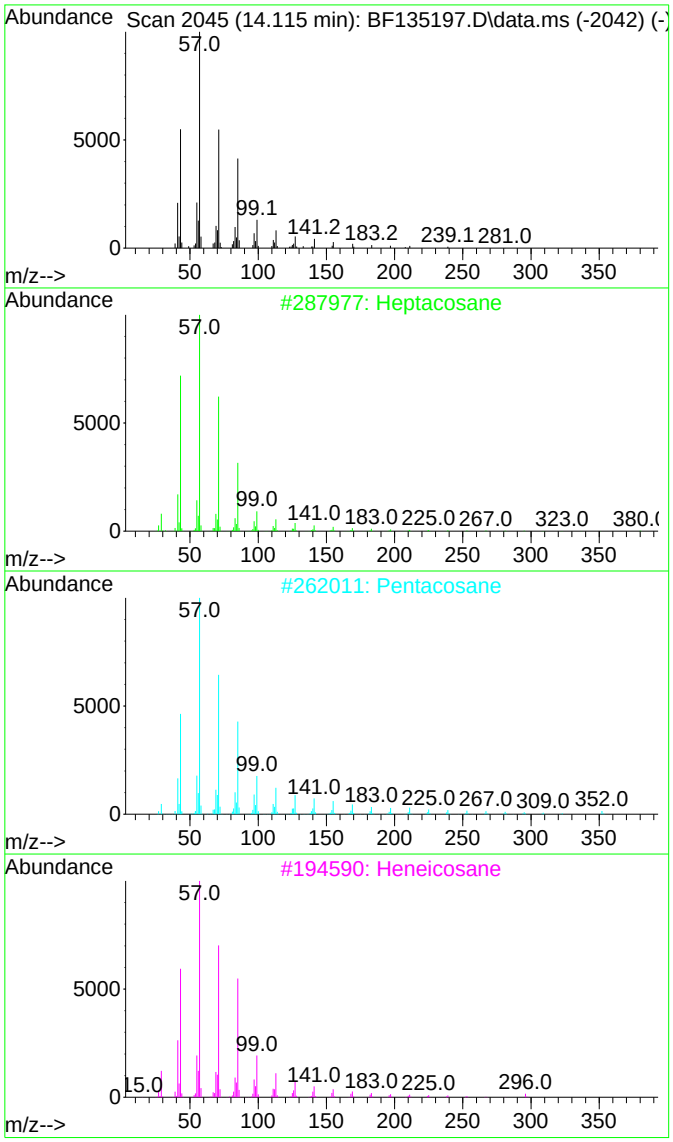
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

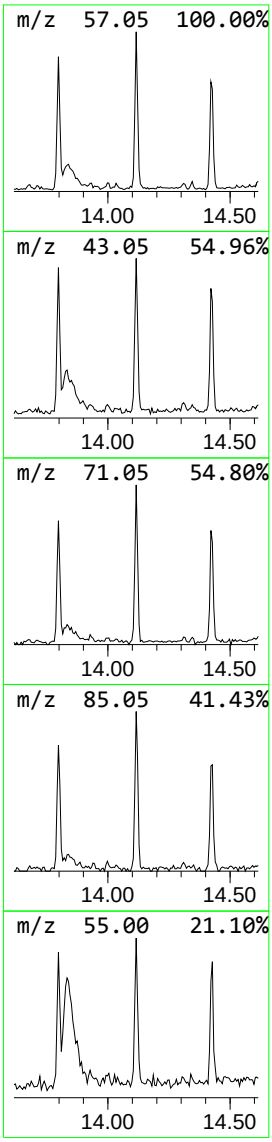
****

Peak Number 6 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.116	2.77 ng	94267	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Pentacosane	352	C25H52	000629-99-2	91
3	Heneicosane	296	C21H44	000629-94-7	90
4	Hexacosane	366	C26H54	000630-01-3	90
5	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	90





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ALS Vial : 14 Sample Multiplier: 1

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BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

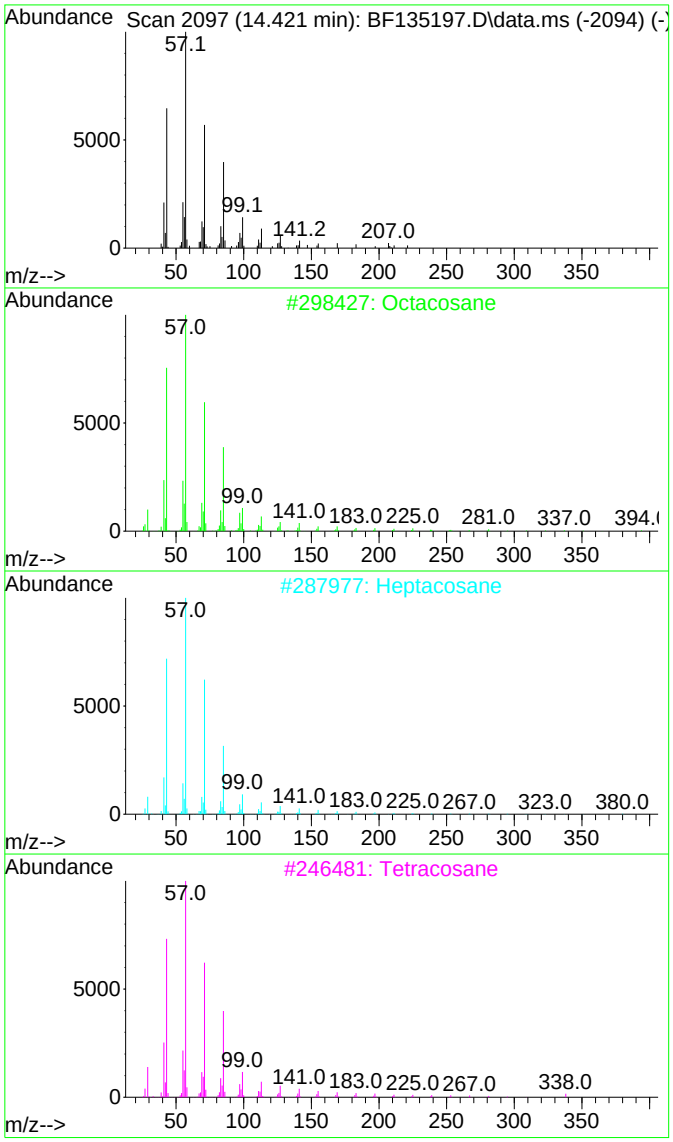
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

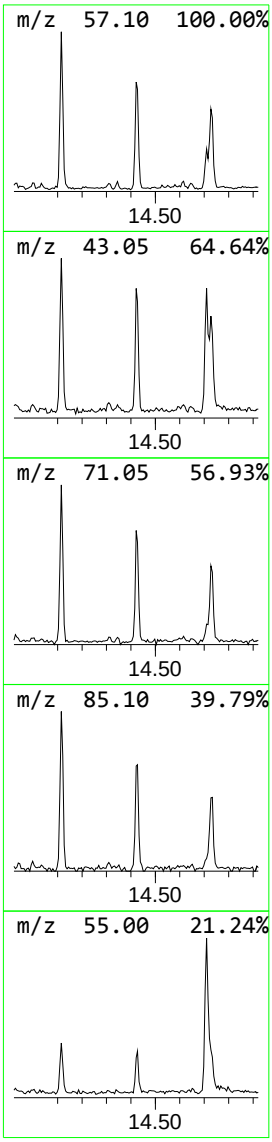
****

Peak Number 7 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.421	2.30 ng	78431	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Heptadecane	240	C17H36	000629-78-7	91
5	Heneicosane	296	C21H44	000629-94-7	91





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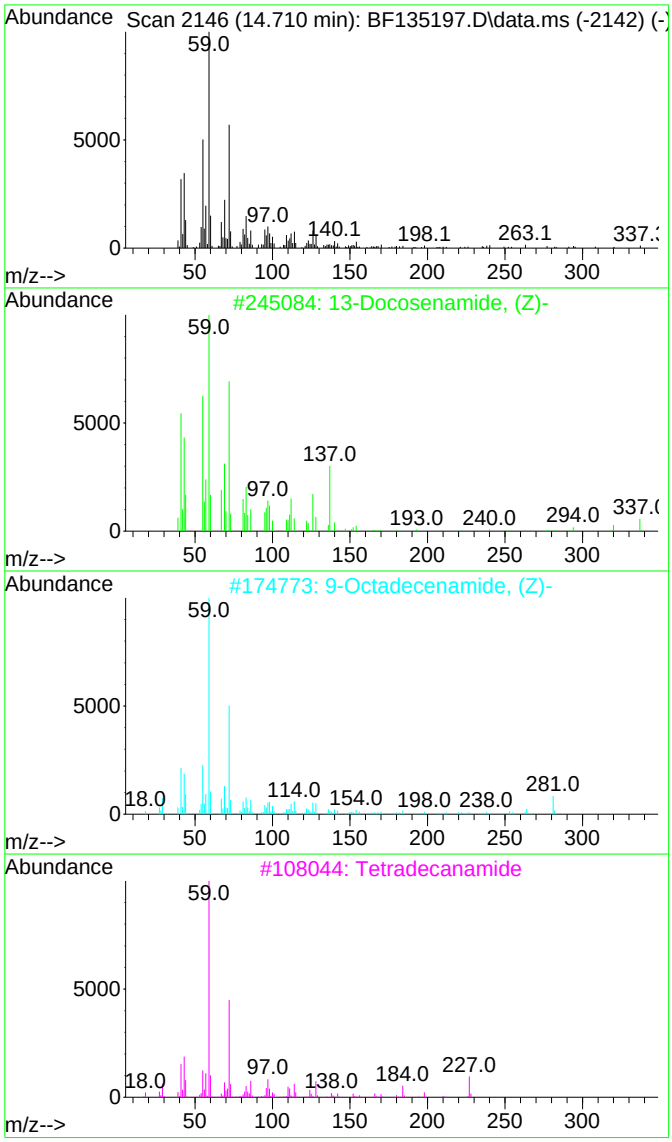
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

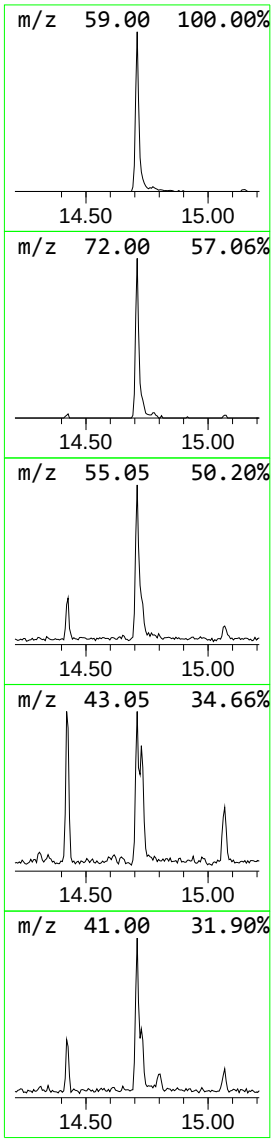
****

Peak Number 8 13-Docosenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.710	7.60 ng	214609	Perylene-d12	15.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	93
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
3	Tetradecanamide	227	C14H29NO	000638-58-4	78
4	Hexadecanamide	255	C16H33NO	000629-54-9	72
5	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	64





Tentatively Identified Compound (LSC) summary

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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-...	5.010	3.3	ng	101006	1	6.763	616076	20.0
n-Hexadecanoic ...	11.827	4.3	ng	219218	4	11.286	1021920	20.0
Pentadecanoic acid	12.616	2.5	ng	83752	5	13.939	681480	20.0
Hexadecane	13.798	2.8	ng	95867	5	13.939	681480	20.0
Pentafluoroprop...	13.833	3.5	ng	120585	5	13.939	681480	20.0
Heptacosane	14.116	2.8	ng	94267	5	13.939	681480	20.0
Octacosane	14.421	2.3	ng	78431	5	13.939	681480	20.0
13-Docosenamide...	14.710	7.6	ng	214609	6	15.404	565050	20.0