LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011023\
Data File : BF131989.D
Acq On : 10 Jan 2023 10:28
Operator : CG\JU
Sample : PB150116BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB150116BL

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-BF010923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131989.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.004	492	496	513	rBV	224369	380391	7.20%	1.402%
2	5.410	560	565	568	rBV	2738558	2950827	55.88%	10.874%
3	6.434	733	739	742	rBV	2609326	2989064	56.61%	11.015%
4	6.787	795	799	802	rBV	714796	604471	11.45%	2.228%
5	7.363	890	897	900	rBV	1807344	2010893	38.08%	7.410%
6	8.075	1013	1018	1021	rBV	920037	797512	15.10%	2.939%
7	9.157	1196	1202	1205	rBV	3799811	4130876	78.23%	15.223%
8	9.833	1312	1317	1321	rBV	1130021	1028157	19.47%	3.789%
9	10.633	1446	1453	1456	rBV	2855961	2923342	55.36%	10.773%
10	11.327	1567	1571	1574	rBV	1448003	1172210	22.20%	4.320%
11	12.733	1807	1810	1814	rVB	131591	114916	2.18%	0.423%
12	12.927	1837	1843	1846	rBV	5017375	5280229	100.00%	19.458%
13	13.445	1927	1931	1934	rBV	123095	105564	2.00%	0.389%
14	13.980	2018	2022	2025	rBV	1152581	999023	18.92%	3.682%
15	14.745	2148	2152	2156	rBV	91698	83117	1.57%	0.306%
16	15.080	2205	2209	2214	rVB	103660	110266	2.09%	0.406%
17	15.445	2266	2271	2278	rBV	667636	875564	16.58%	3.227%
18	15.886	2341	2346	2353	rBV	87402	131346	2.49%	0.484%
19	16.386	2425	2431	2439	rBV2	81934	139457	2.64%	0.514%
20	16.968	2526	2530	2539	rVB3	64576	135147	2.56%	0.498%
21	17.662	2641	2648	2657	rVB3	43518	104125	1.97%	0.384%
22	18.474	2781	2786	2798	rVB6	25817	69601	1.32%	0.256%

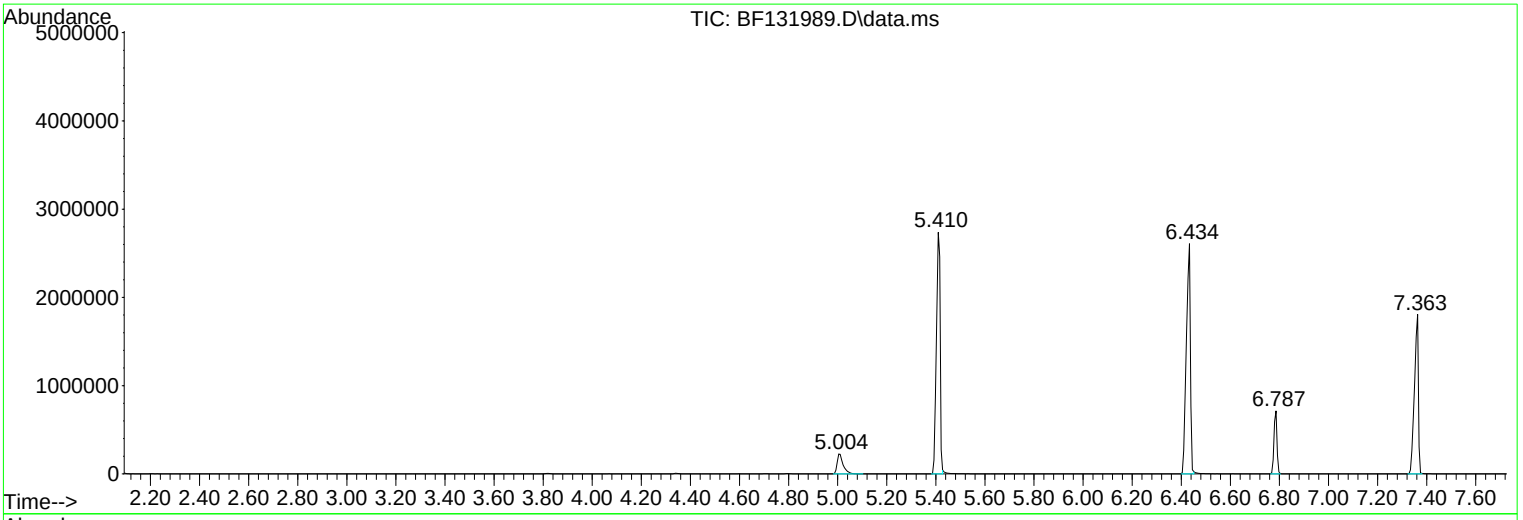
Sum of corrected areas: 27136098

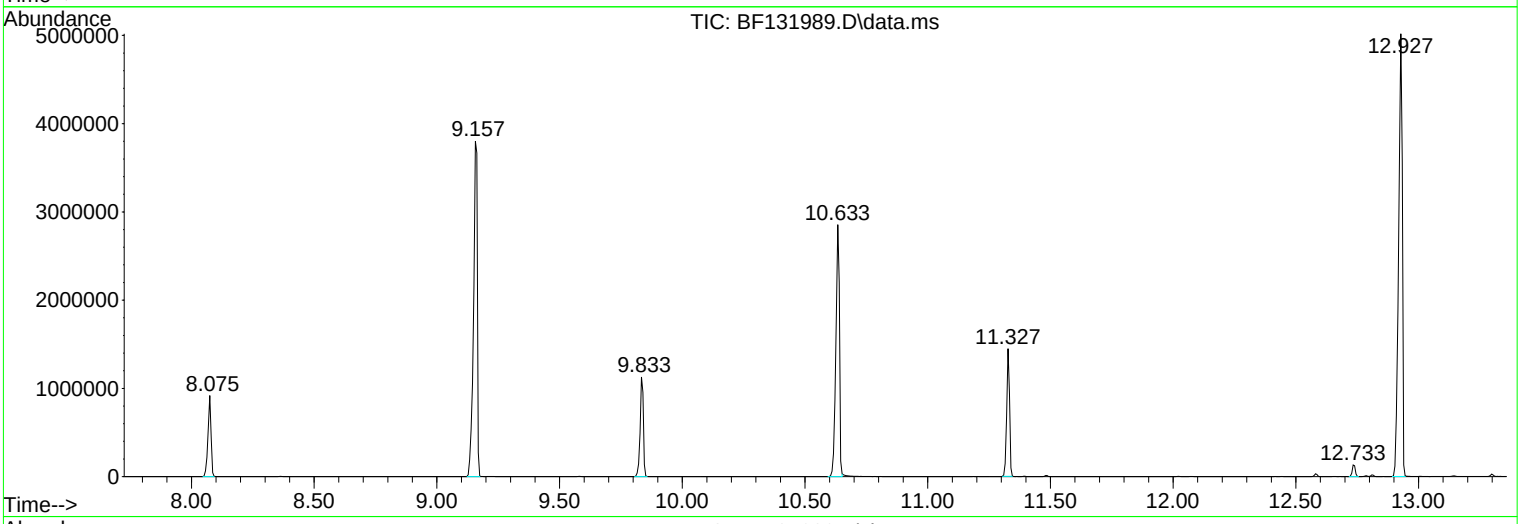
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011023\
Data File : BF131989.D
Acq On : 10 Jan 2023 10:28
Operator : CG\JU
Sample : PB150116BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

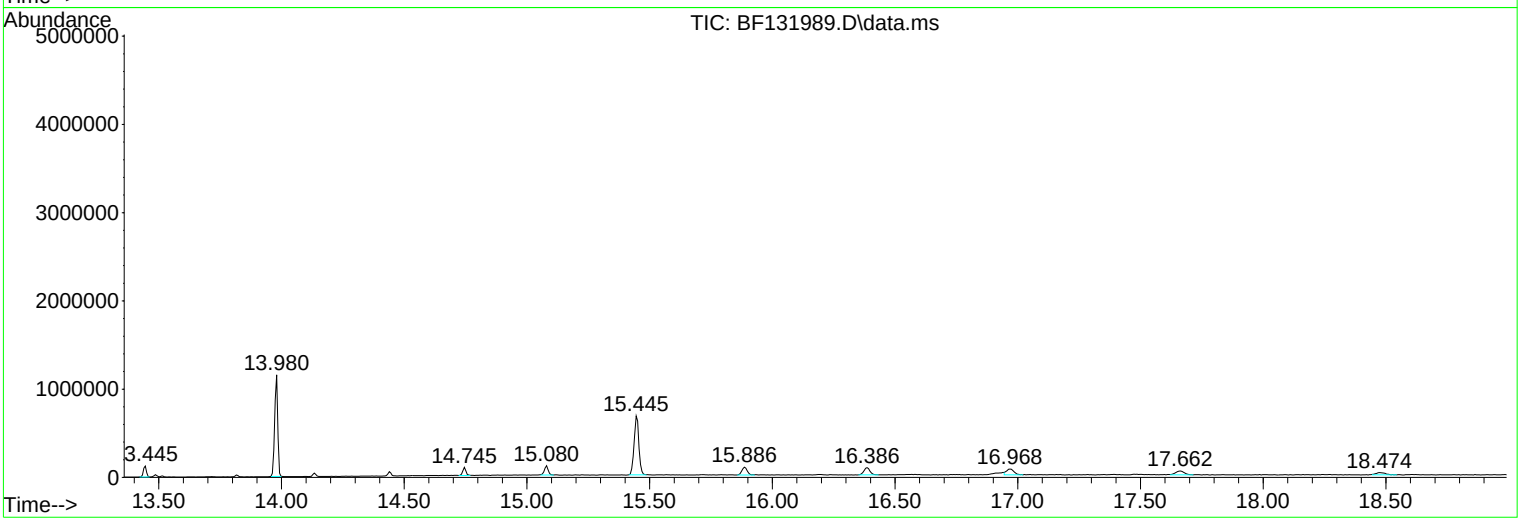
Instrument :
BNA_F
ClientSampleId :
PB150116BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.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\BF011023\
Data File : BF131989.D
Acq On : 10 Jan 2023 10:28
Operator : CG\JU
Sample : PB150116BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB150116BL

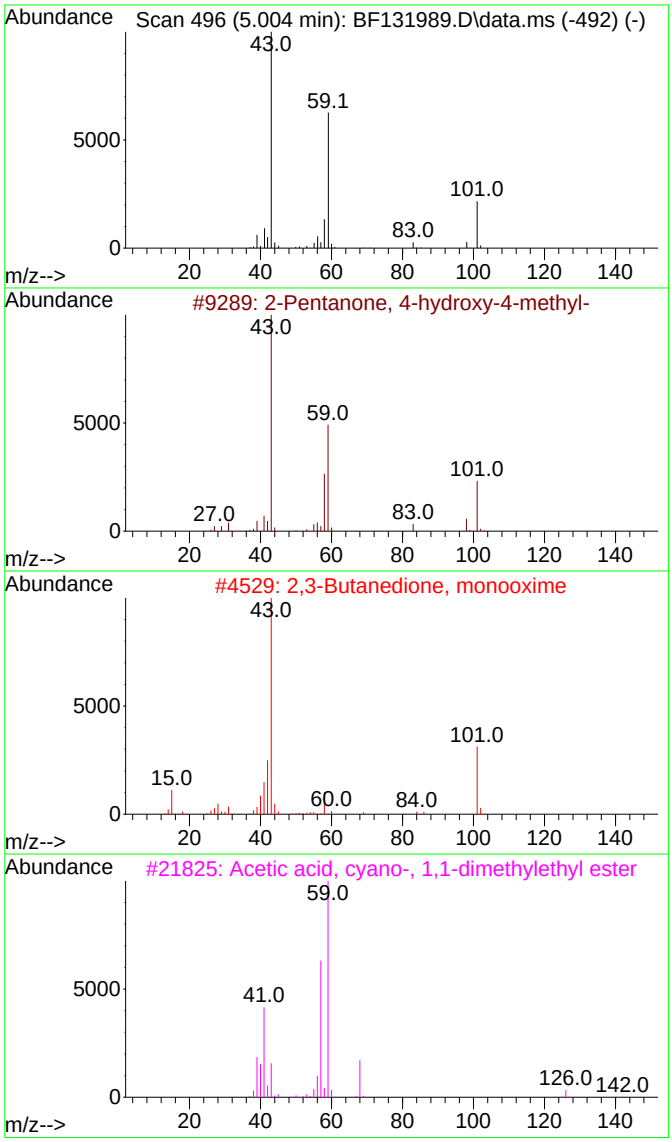
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

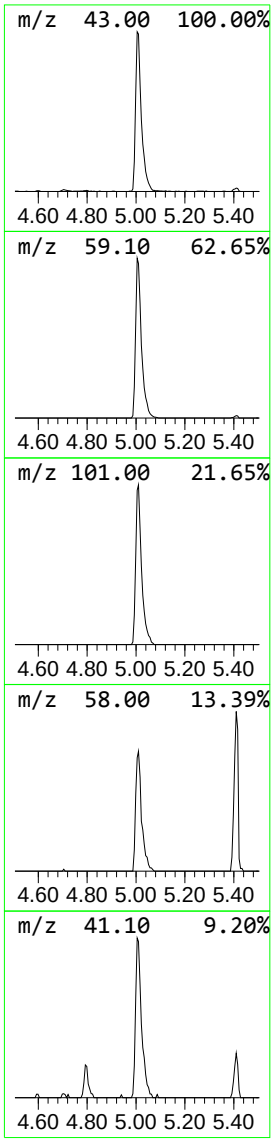
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.004	12.59 ng	380391	1,4-Dichlorobenzene-d4	6.787

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011023\
Data File : BF131989.D
Acq On : 10 Jan 2023 10:28
Operator : CG\JU
Sample : PB150116BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB150116BL

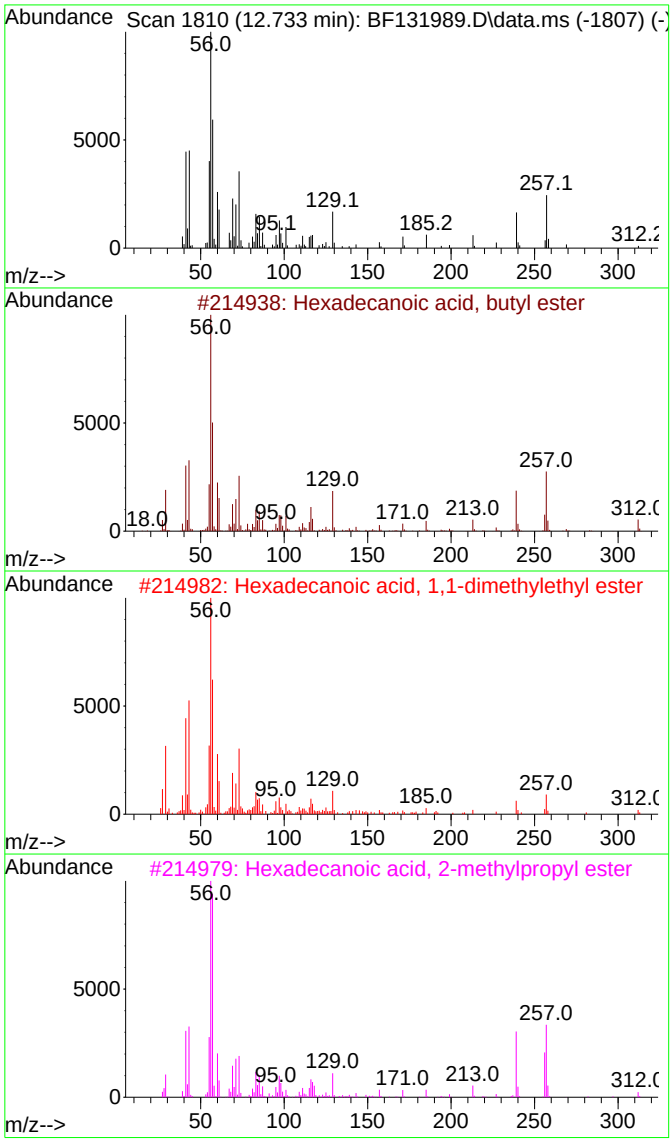
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

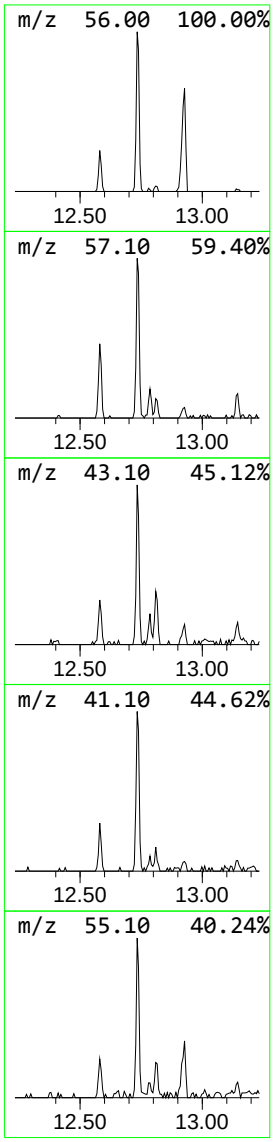
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Hexadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.733	2.30 ng	114916	Chrysene-d12	13.980

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	80
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	35
4	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	35
5	2-Methyl-1-octadecene	266	C19H38	061868-20-0	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011023\
Data File : BF131989.D
Acq On : 10 Jan 2023 10:28
Operator : CG\JU
Sample : PB150116BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB150116BL

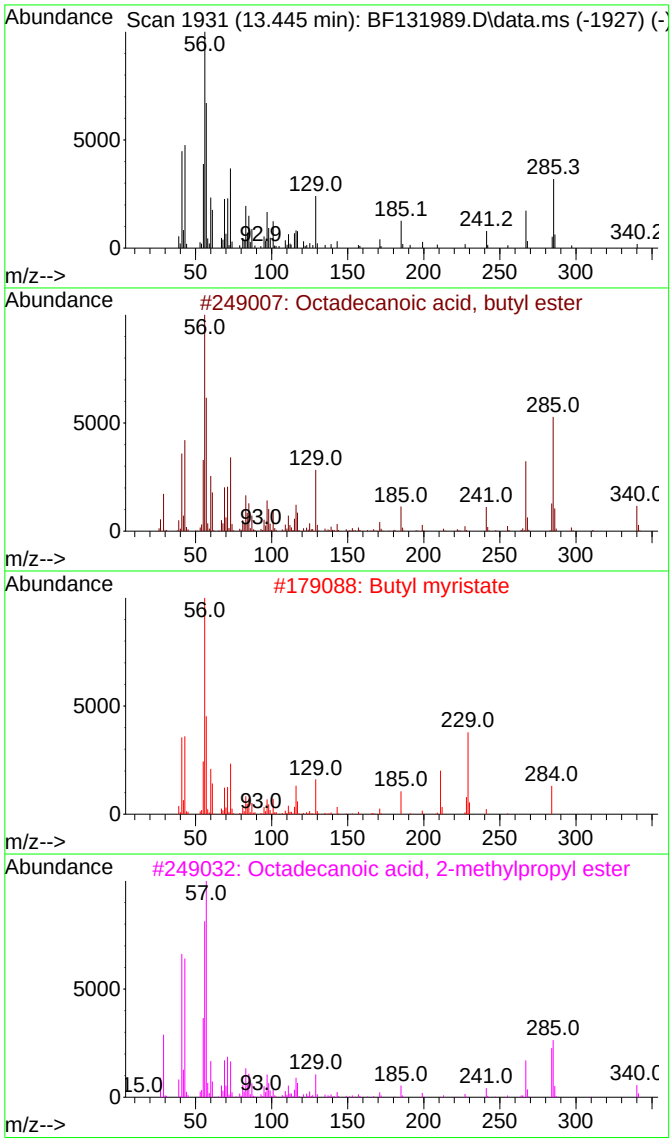
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

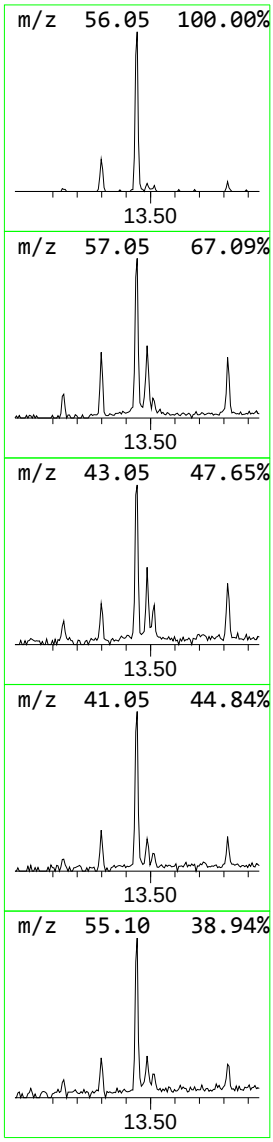
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Octadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.445	2.11 ng	105564	Chrysene-d12	13.980

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	83
2	Butyl myristate	284	C18H36O2	000110-36-1	72
3	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	64
4	Cyclohexane, (1,1-dimethylethyl)-	140	C10H20	003178-22-1	27
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011023\
Data File : BF131989.D
Acq On : 10 Jan 2023 10:28
Operator : CG\JU
Sample : PB150116BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB150116BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

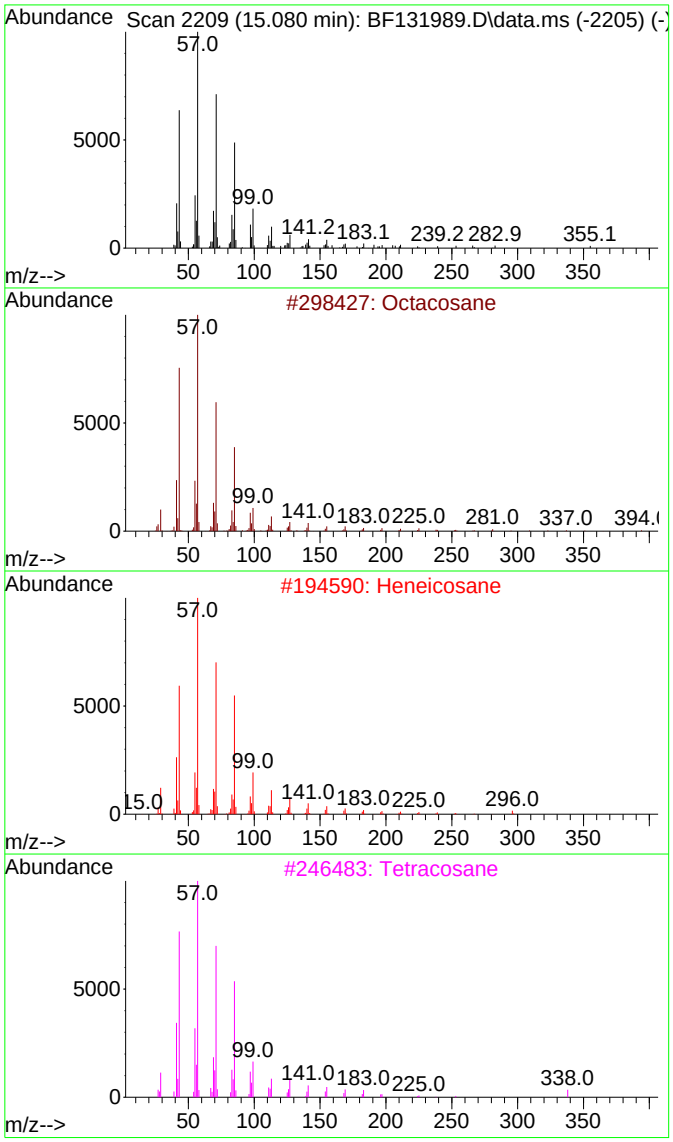
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

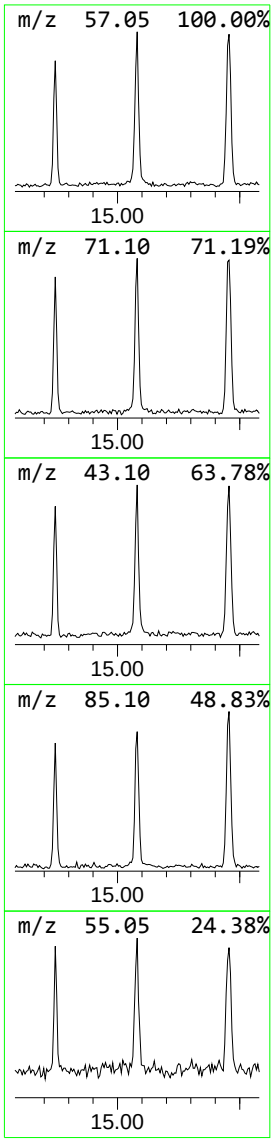
****

Peak Number 4 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.080	2.52 ng	110266	Perylene-d12	15.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5	Hexacosane	366	C26H54	000630-01-3	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011023\
Data File : BF131989.D
Acq On : 10 Jan 2023 10:28
Operator : CG\JU
Sample : PB150116BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB150116BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

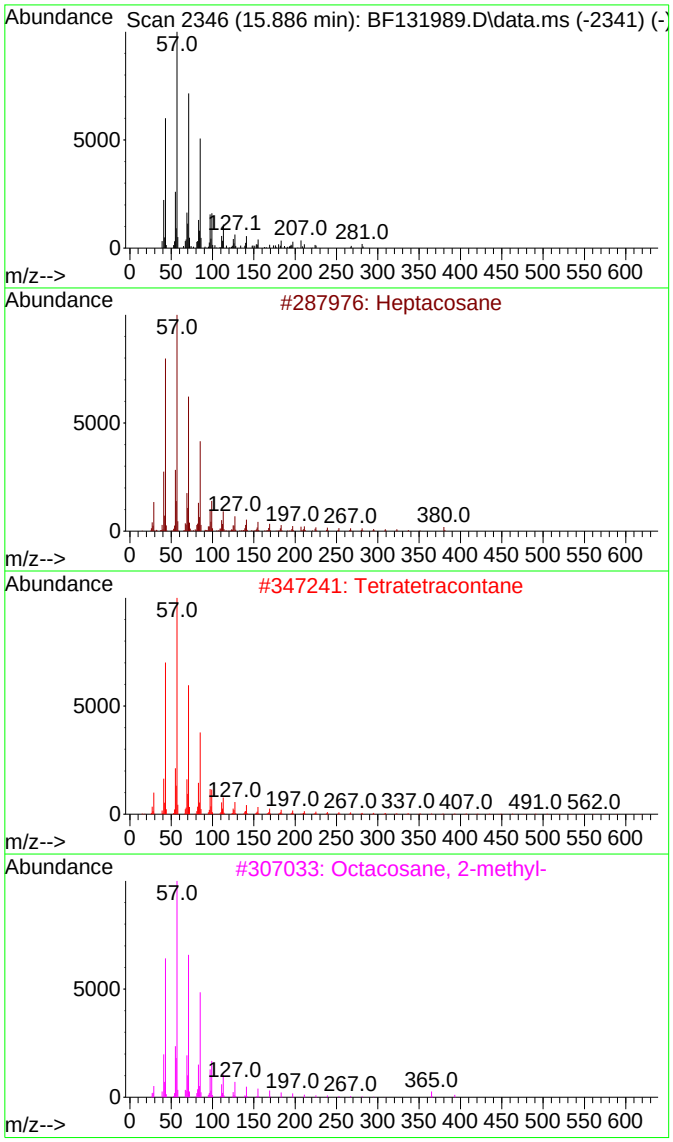
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

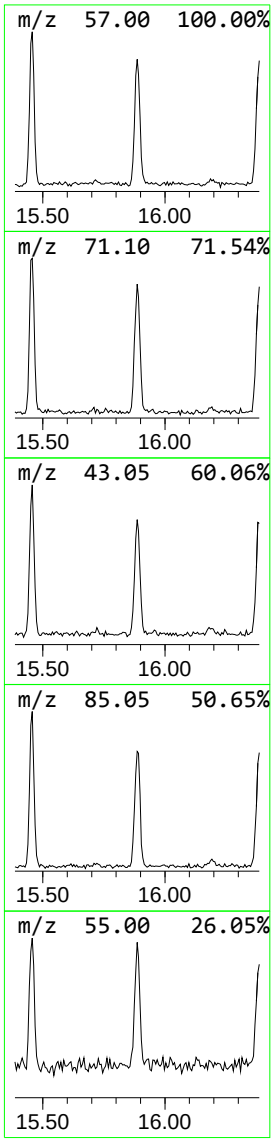
****

Peak Number 5 Heptacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.886	3.00 ng	131346	Perylene-d12	15.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Tetratetracontane	619	C44H90	007098-22-8	90
3	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
4	Nonadecane	268	C19H40	000629-92-5	87
5	Heneicosane	296	C21H44	000629-94-7	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011023\
Data File : BF131989.D
Acq On : 10 Jan 2023 10:28
Operator : CG\JU
Sample : PB150116BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB150116BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

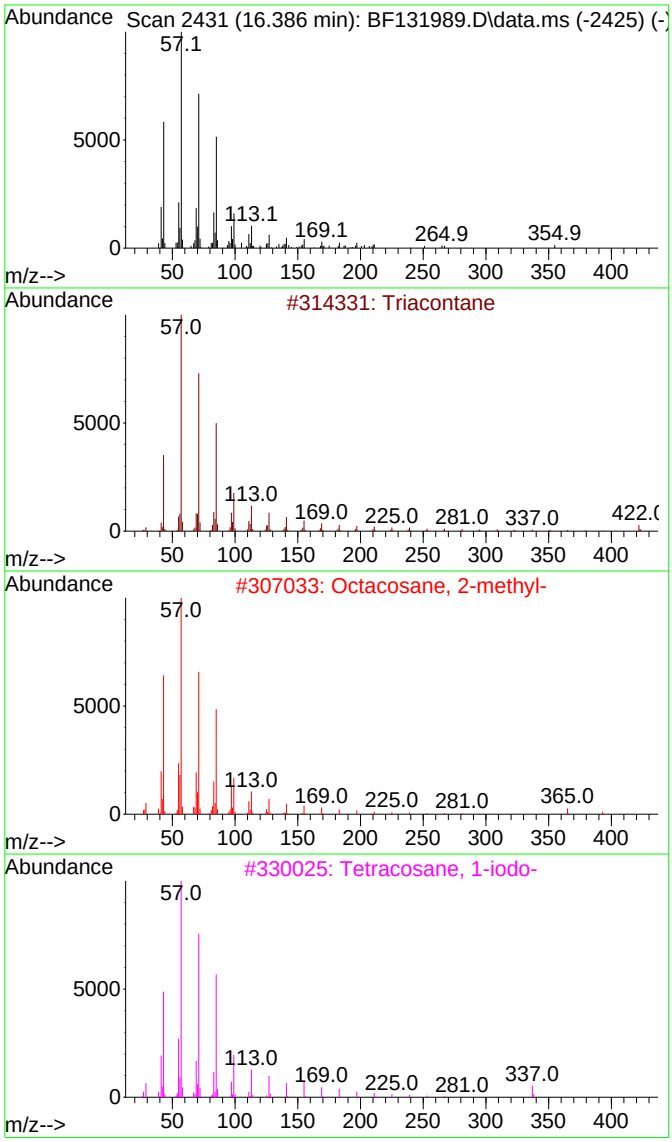
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

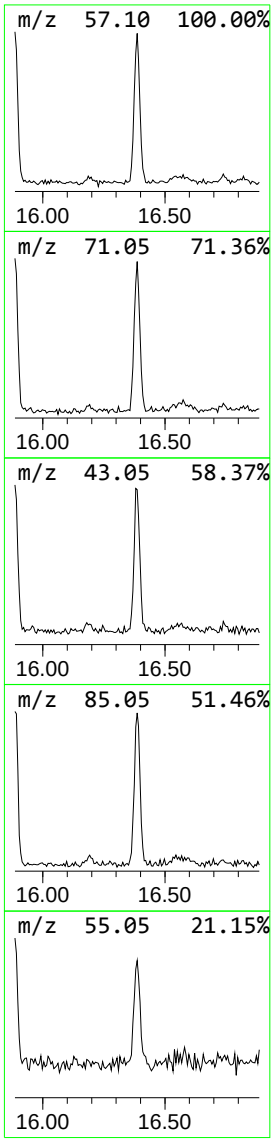
****

Peak Number 6 Triacontane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.386	3.19 ng	139457	Perylene-d12	15.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	90
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
3	Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	87
4	Octacosane	394	C28H58	000630-02-4	87
5	Heptacosane	380	C27H56	000593-49-7	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011023\
Data File : BF131989.D
Acq On : 10 Jan 2023 10:28
Operator : CG\JU
Sample : PB150116BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB150116BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

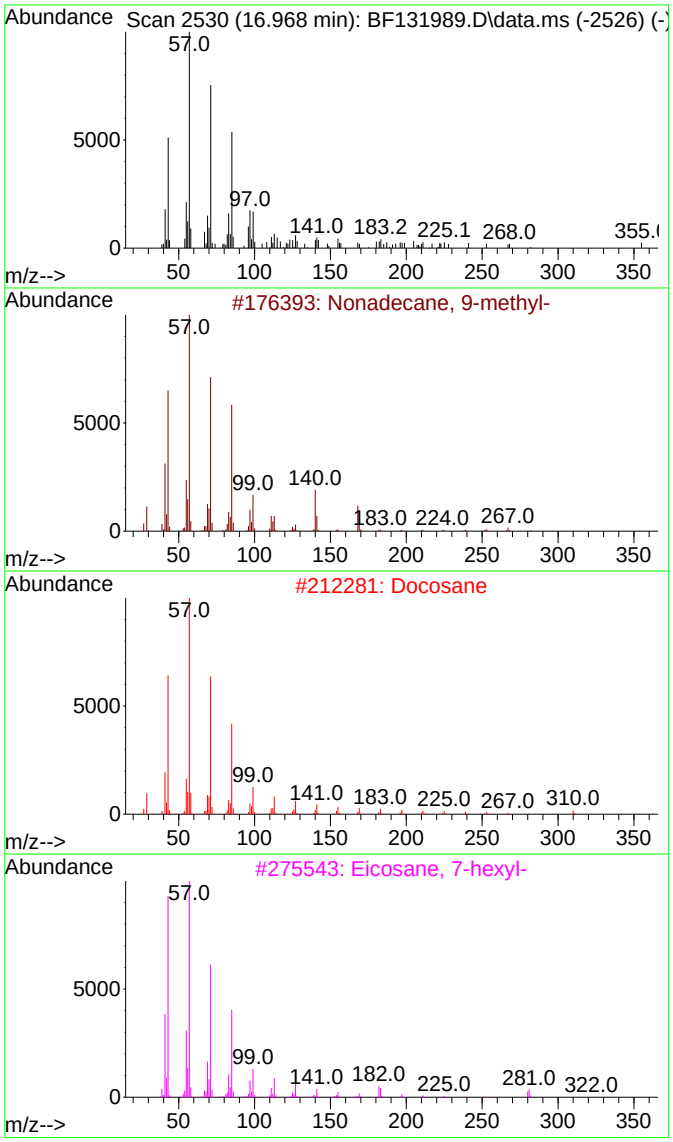
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

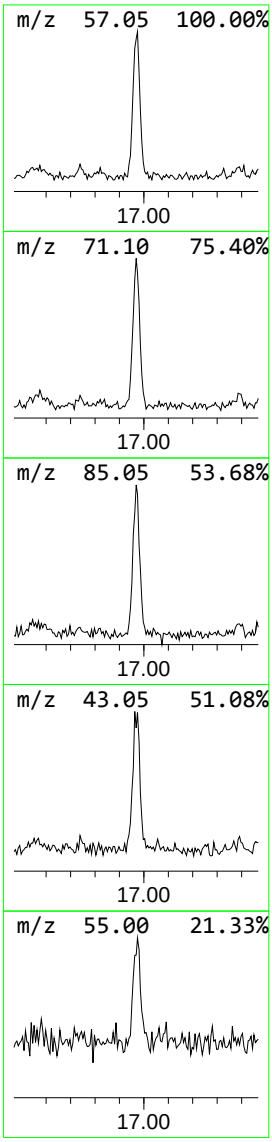
****

Peak Number 7 Nonadecane, 9-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.968	3.09 ng	135147	Perylene-d12	15.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	87
2	Docosane	310	C22H46	000629-97-0	83
3	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	80
4	Pentadecane	212	C15H32	000629-62-9	72
5	Nonadecane	268	C19H40	000629-92-5	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011023\
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Acq On : 10 Jan 2023 10:28
Operator : CG\JU
Sample : PB150116BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB150116BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

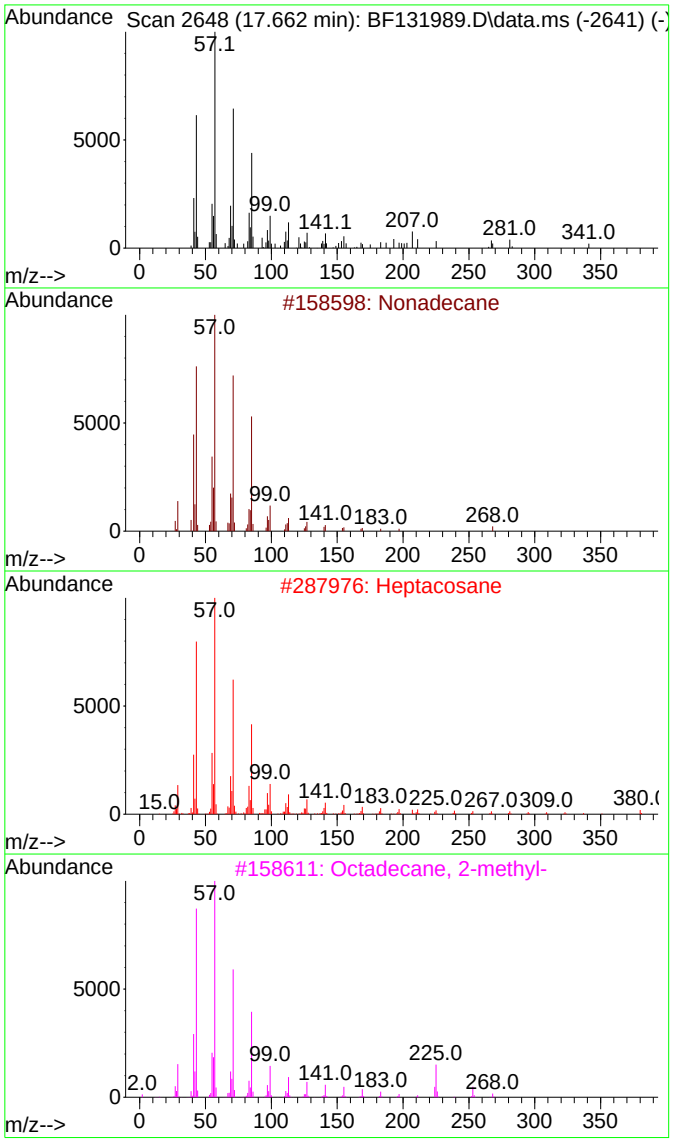
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

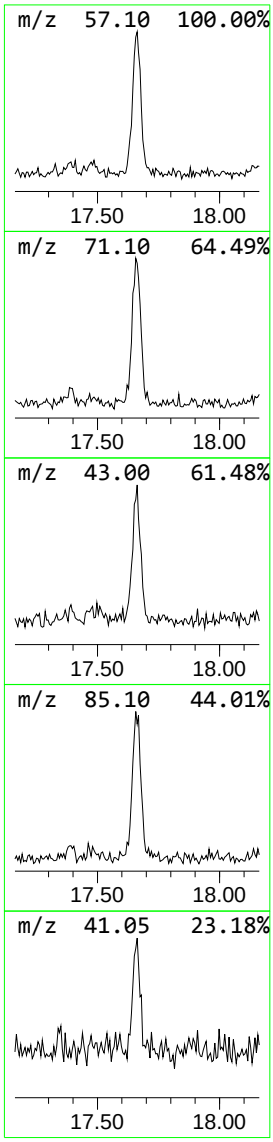
****

Peak Number 8 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.662	2.38 ng	104125	Perylene-d12	15.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	95
2	Heptacosane	380	C27H56	000593-49-7	90
3	Octadecane, 2-methyl-	268	C19H40	001560-88-9	90
4	Heneicosane	296	C21H44	000629-94-7	87
5	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011023\
Data File : BF131989.D
Acq On : 10 Jan 2023 10:28
Operator : CG\JU
Sample : PB150116BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB150116BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.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-...	5.004	12.6	ng	380391	1	6.787	604471	20.0
Hexadecanoic ac...	12.733	2.3	ng	114916	5	13.980	999023	20.0
Octadecanoic ac...	13.445	2.1	ng	105564	5	13.980	999023	20.0
Octacosane	15.080	2.5	ng	110266	6	15.445	875564	20.0
Heptacosane	15.886	3.0	ng	131346	6	15.445	875564	20.0
Triacontane	16.386	3.2	ng	139457	6	15.445	875564	20.0
Nonadecane, 9-m...	16.968	3.1	ng	135147	6	15.445	875564	20.0
Nonadecane	17.662	2.4	ng	104125	6	15.445	875564	20.0