LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010722\
Data File : BP008732.D
Acq On : 07 Jan 2022 18:29
Operator : CG/JU
Sample : N1039-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S-1

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_P\Methods\8270E-BP010622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008732.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.070	9	14	27	rVB	2774897	3521433	16.57%	3.235%
2	4.987	334	340	348	rBV2	166204	261079	1.23%	0.240%
3	5.452	412	419	437	rBV	5532784	8291042	39.01%	7.618%
4	7.046	681	690	708	rBV	4982771	8486884	39.94%	7.797%
5	7.869	822	830	838	rBV	1355505	2168563	10.20%	1.992%
6	9.028	1019	1027	1039	rBV	3269713	5549869	26.11%	5.099%
7	10.457	1262	1270	1283	rBV	294798	604128	2.84%	0.555%
8	10.675	1297	1307	1320	rBV	1711237	3071479	14.45%	2.822%
9	13.134	1717	1725	1740	rBV	9456917	14159561	66.63%	13.009%
10	14.504	1952	1958	1973	rBV	2580724	4216245	19.84%	3.874%
11	15.998	2205	2212	2236	rBV	7134533	11242317	52.90%	10.329%
12	17.257	2420	2426	2440	rBV	3500050	5349348	25.17%	4.915%
13	18.157	2574	2579	2598	rBV	677793	1213824	5.71%	1.115%
14	19.392	2784	2789	2797	rBV	570764	1002325	4.72%	0.921%
15	19.822	2856	2862	2871	rBV	17001020	21251727	100.00%	19.525%
16	21.063	3069	3073	3079	rBV	999438	1271022	5.98%	1.168%
17	21.345	3117	3121	3127	rVB	4338294	5646099	26.57%	5.187%
18	21.469	3137	3142	3161	rBV	3788438	6228823	29.31%	5.723%
19	21.992	3228	3231	3243	rVB2	556281	920999	4.33%	0.846%
20	23.774	3528	3534	3541	rBV2	2234053	4384789	20.63%	4.029%

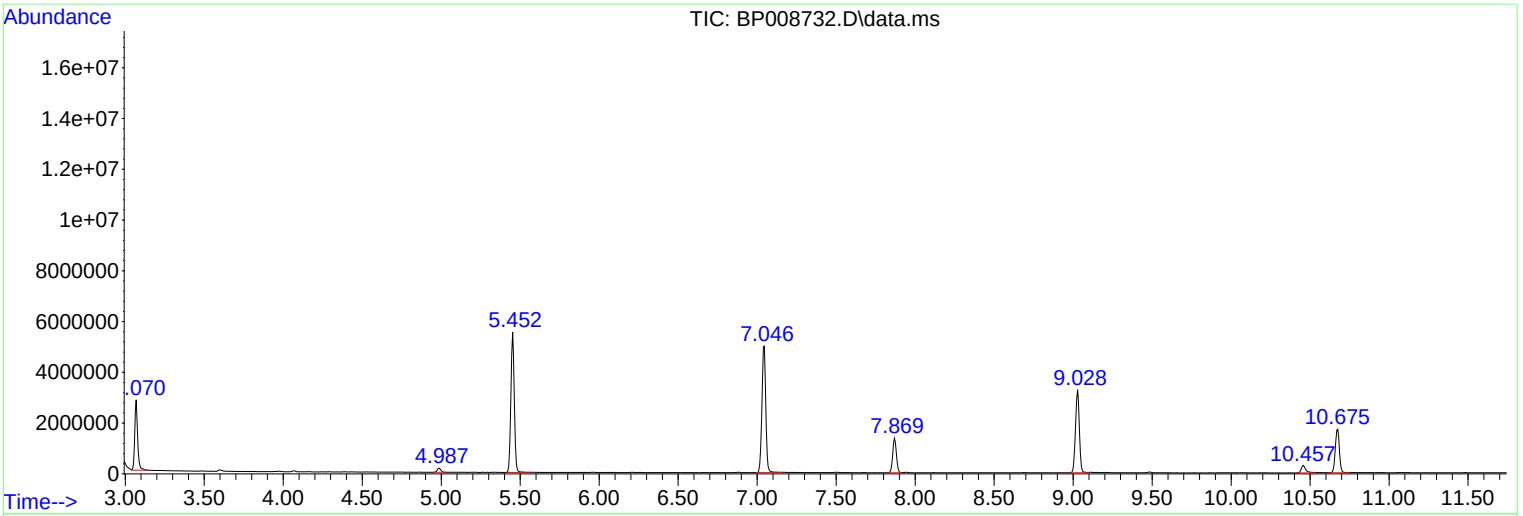
Sum of corrected areas: 108841556

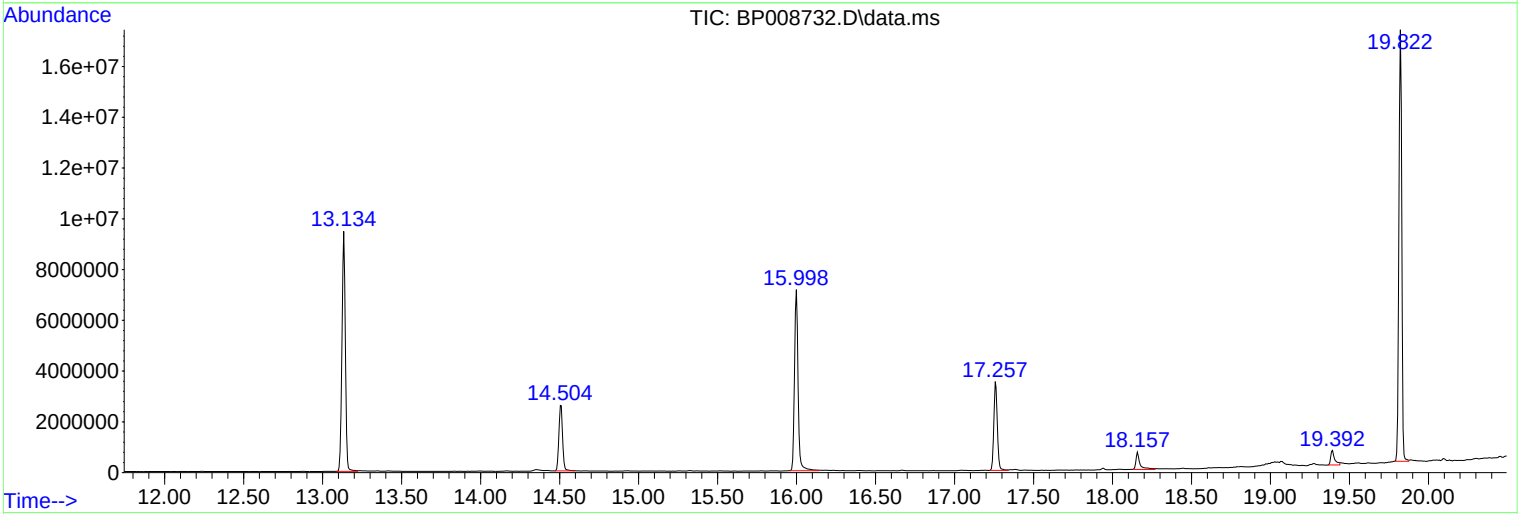
Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010722\
Data File : BP008732.D
Acq On : 07 Jan 2022 18:29
Operator : CG/JU
Sample : N1039-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

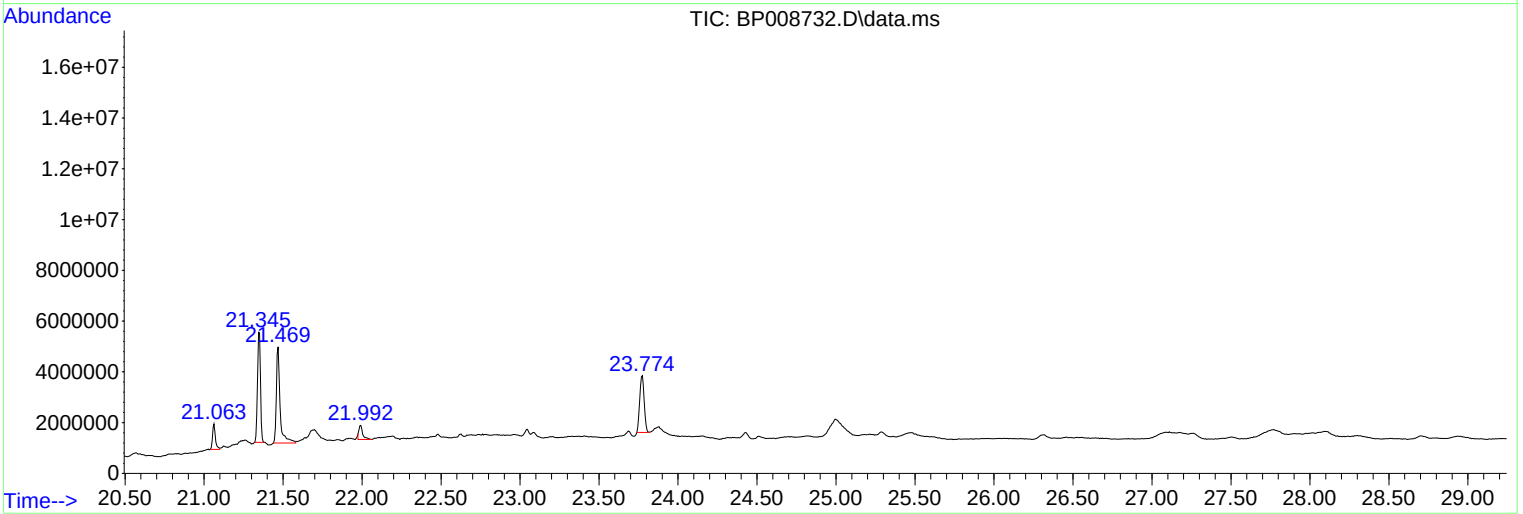
Instrument :
BNA_P
ClientSampleId :
S-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.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_P\Data\BP010722\
Data File : BP008732.D
Acq On : 07 Jan 2022 18:29
Operator : CG/JU
Sample : N1039-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S-1

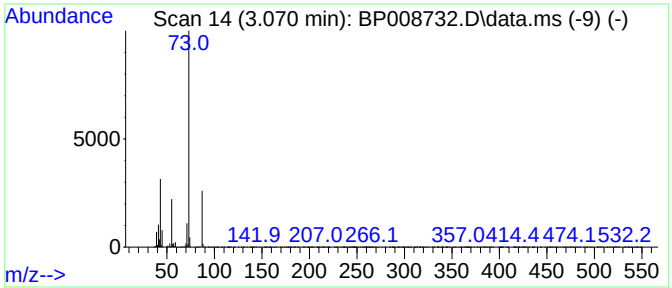
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

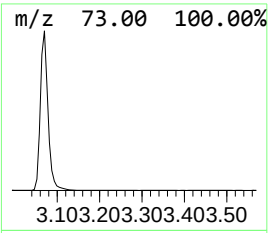
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

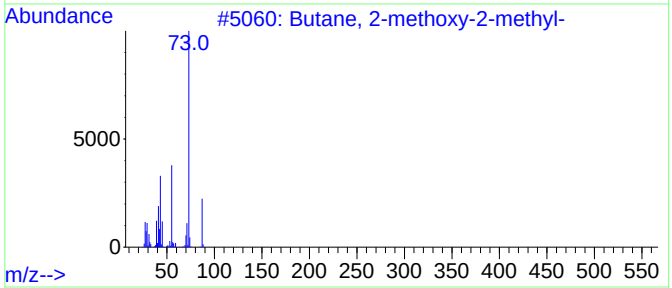
****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

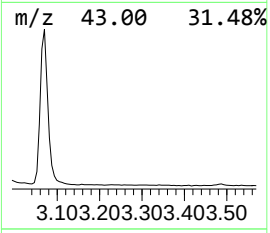
R.T.	EstConc	Area	Relative to ISTD	R.T.
3.070	32.48 ng	3521430	1,4-Dichlorobenzene-d4	7.869

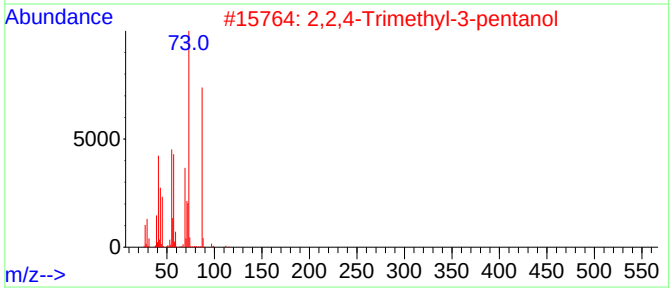
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9

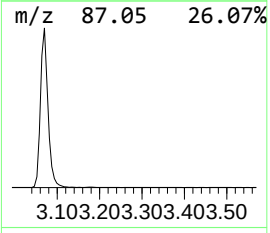


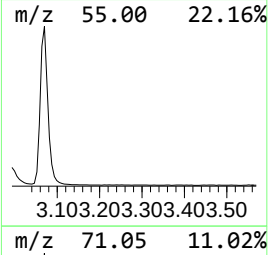


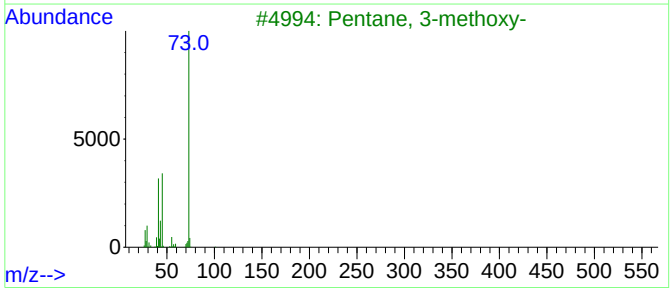


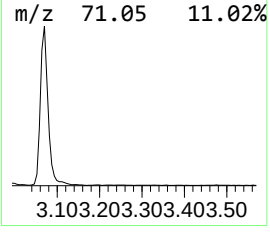












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010722\
Data File : BP008732.D
Acq On : 07 Jan 2022 18:29
Operator : CG/JU
Sample : N1039-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S-1

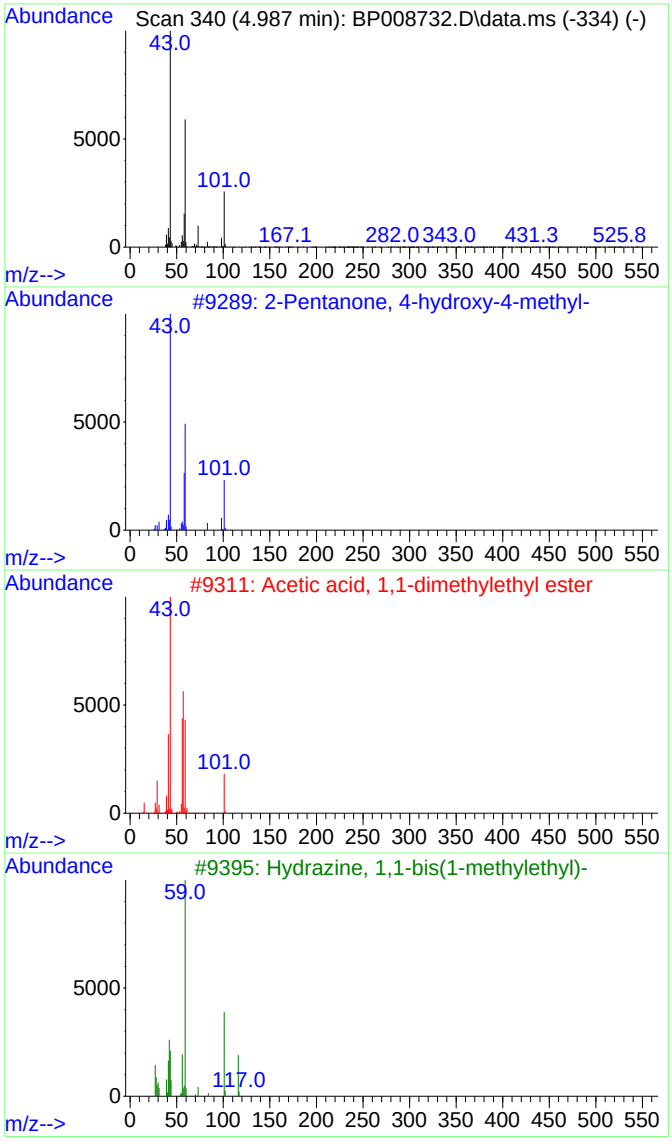
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

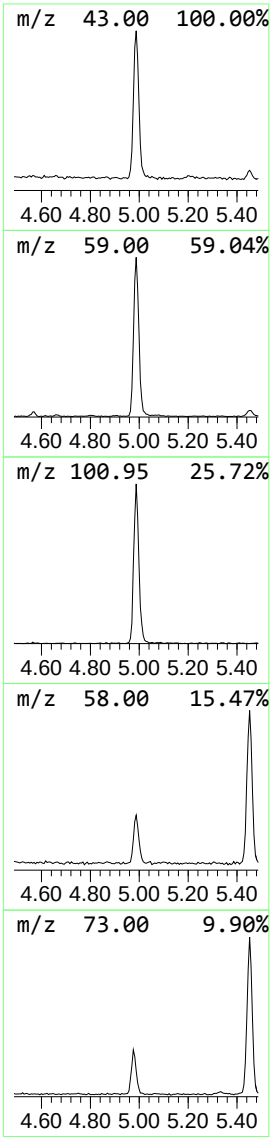
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.987	2.41 ng	261079	1,4-Dichlorobenzene-d4	7.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	36
3	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	25
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010722\
Data File : BP008732.D
Acq On : 07 Jan 2022 18:29
Operator : CG/JU
Sample : N1039-01
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Instrument :
BNA_P
ClientSampleId :
S-1

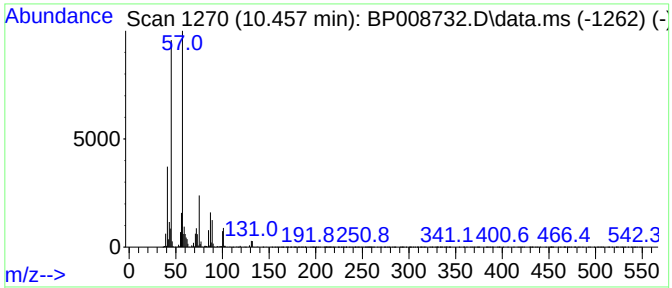
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

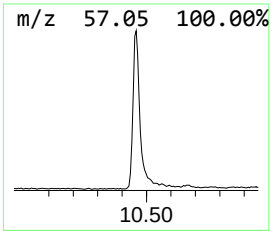
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

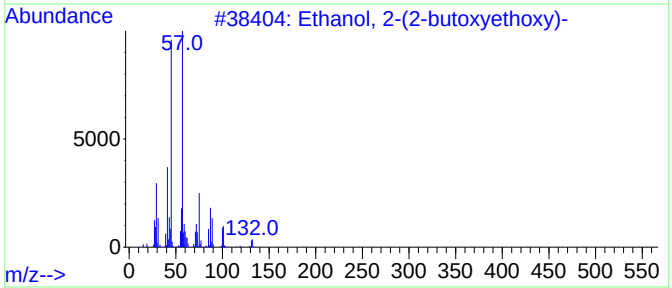
****
Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

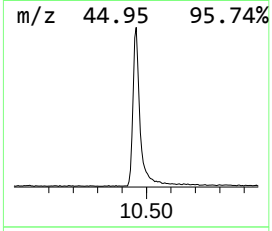
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.457	3.93 ng	604128	Naphthalene-d8	10.675

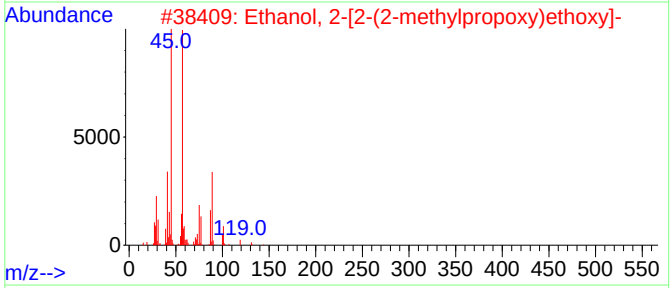
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	91
2	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	Di-sec-Butyl ether	130	C8H18O	006863-58-7	50
5	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50

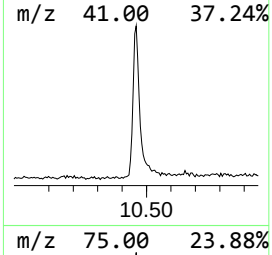


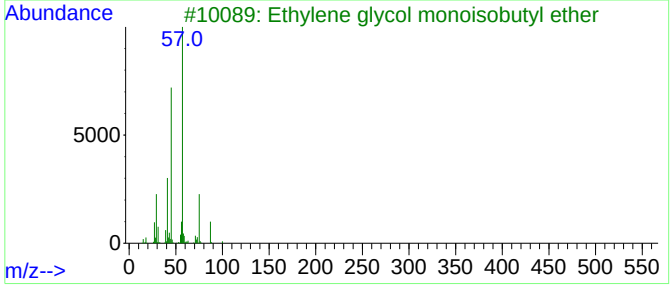


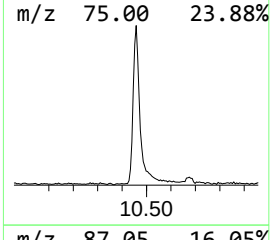


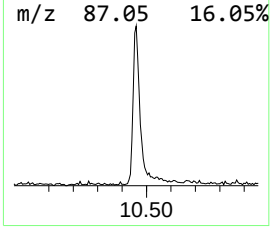












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010722\
Data File : BP008732.D
Acq On : 07 Jan 2022 18:29
Operator : CG/JU
Sample : N1039-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

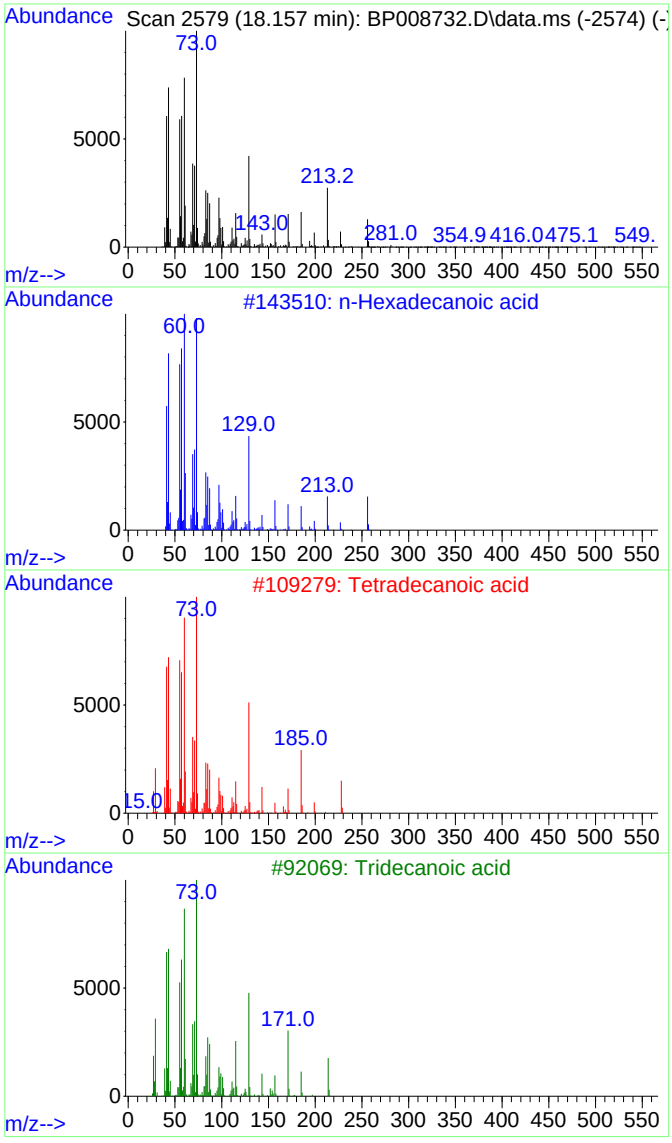
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

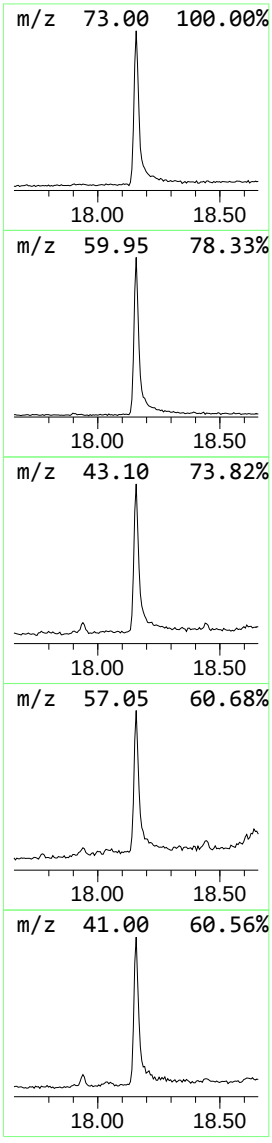
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.157	4.54 ng	1213820	Phenanthrene-d10	17.257

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Undecanoic acid	186	C11H22O2	000112-37-8	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010722\
Data File : BP008732.D
Acq On : 07 Jan 2022 18:29
Operator : CG/JU
Sample : N1039-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

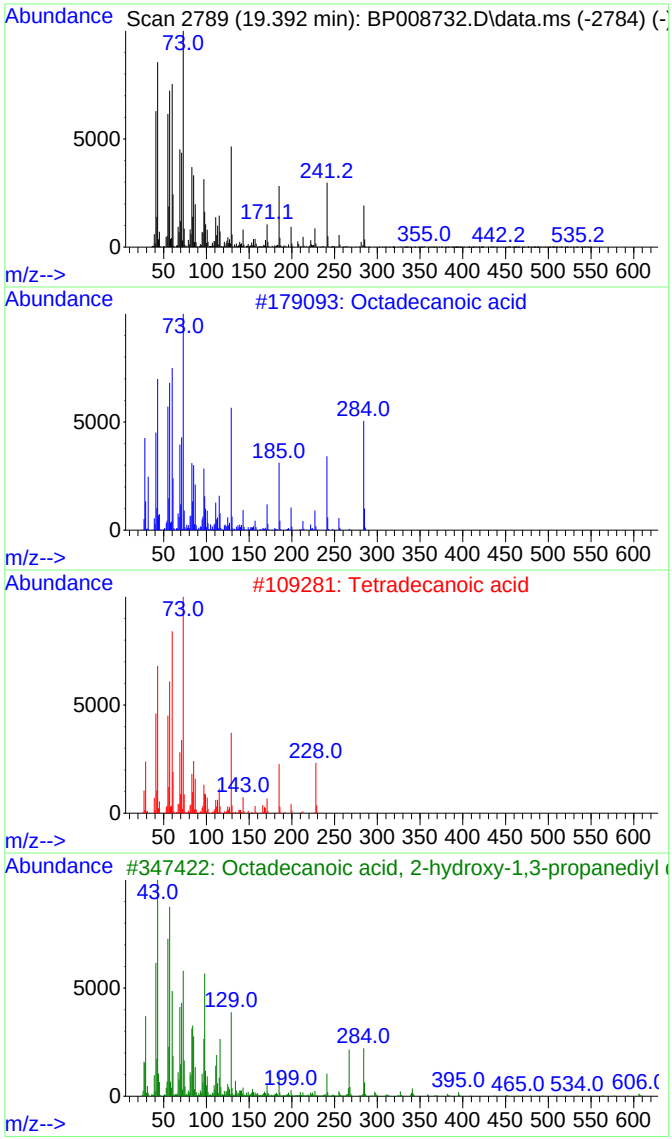
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

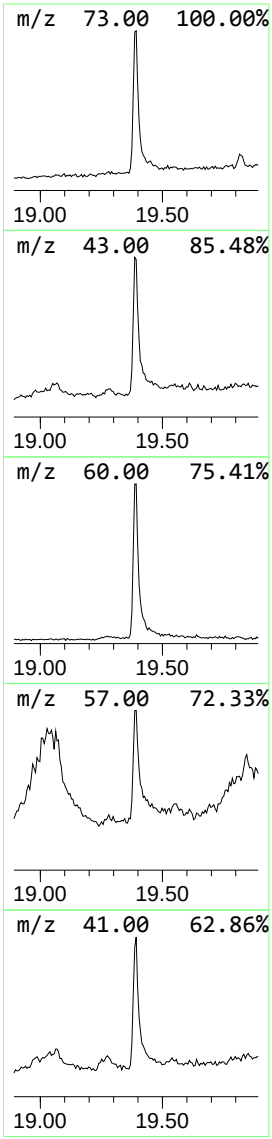
****

Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.392	3.55 ng	1002330	Chrysene-d12	21.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
3	Octadecanoic acid, 2-hydroxy-1,3...	625	C39H76O5	000504-40-5	58
4	n-Decanoic acid	172	C10H20O2	000334-48-5	58
5	Tridecanoic acid	214	C13H26O2	000638-53-9	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010722\
Data File : BP008732.D
Acq On : 07 Jan 2022 18:29
Operator : CG/JU
Sample : N1039-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

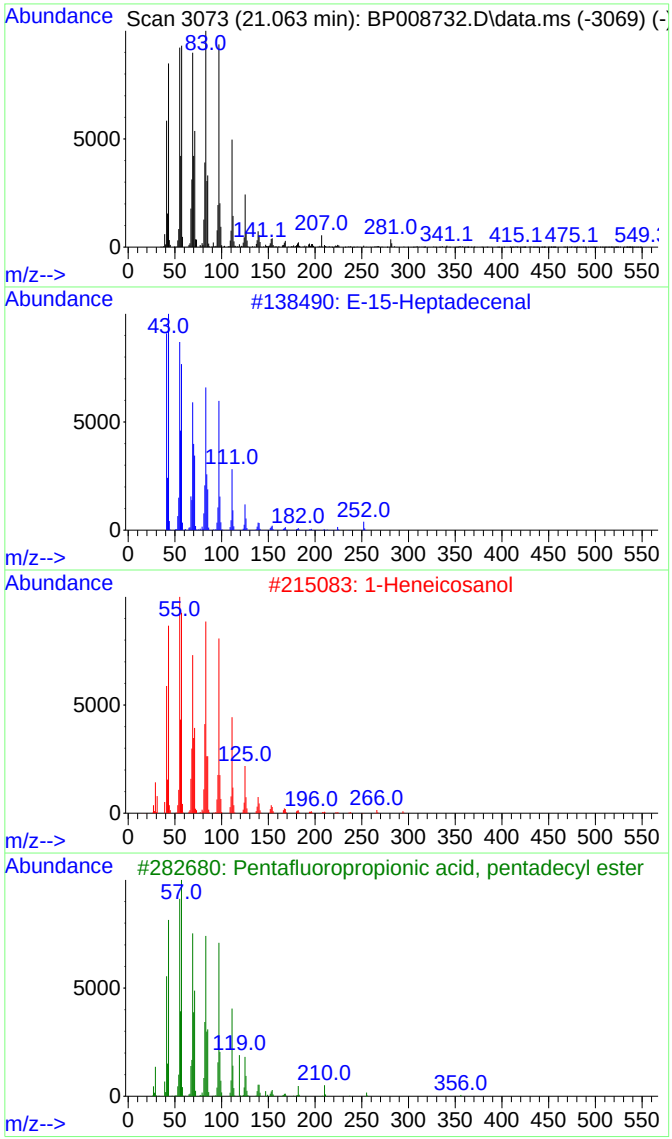
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

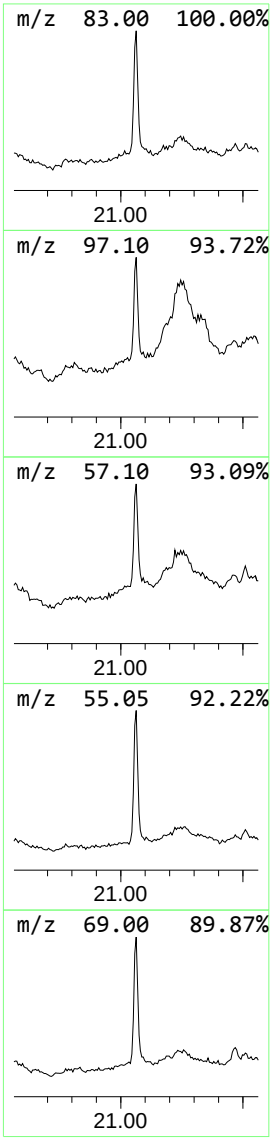
****

Peak Number 6 E-15-Heptadecenal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.063	4.50 ng	1271020	Chrysene-d12	21.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal	252	C17H32O	1000130-97-9	99
2	1-Heneicosanol	312	C21H44O	015594-90-8	94
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
5	Behenic alcohol	326	C22H46O	000661-19-8	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010722\
Data File : BP008732.D
Acq On : 07 Jan 2022 18:29
Operator : CG/JU
Sample : N1039-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S-1

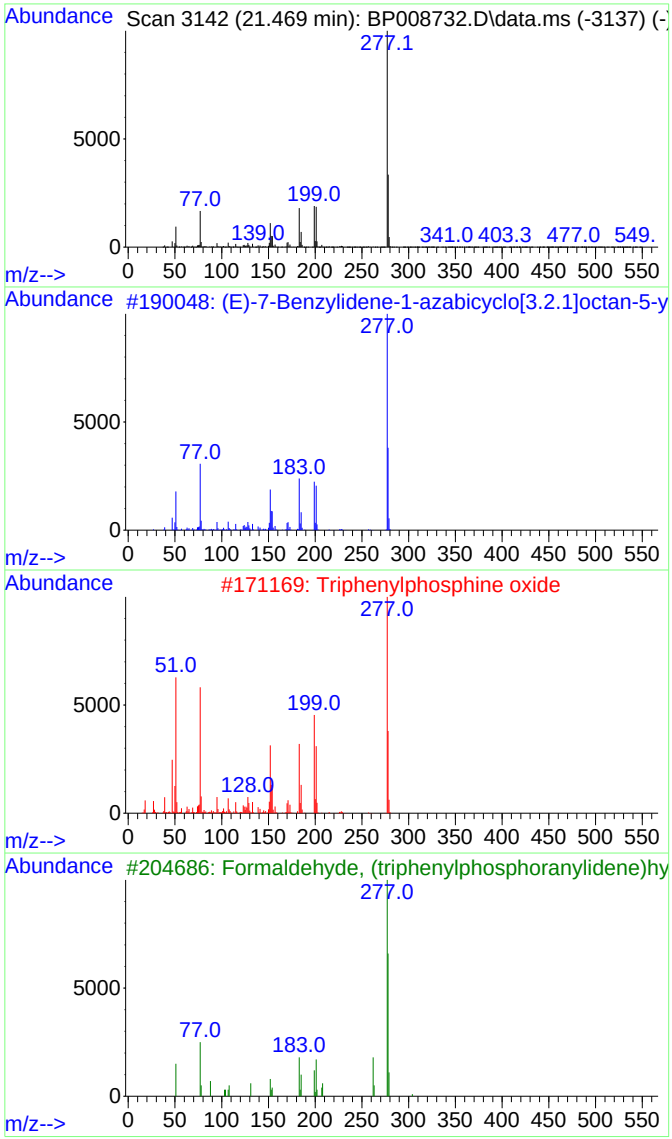
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

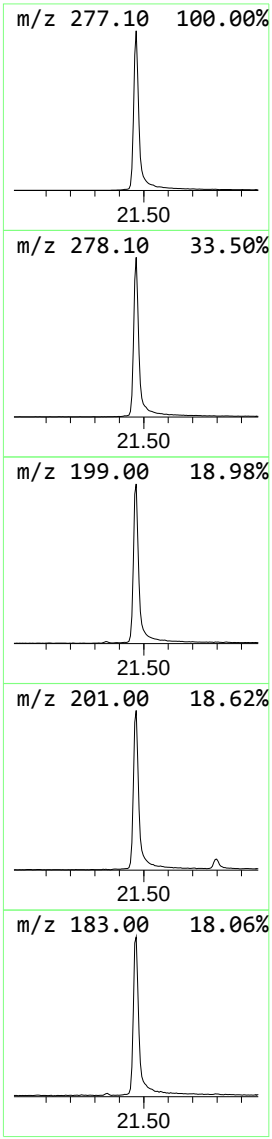
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (E)-7-Benzylidene-1-azabicy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.469	22.06 ng	6228820	Chrysene-d12	21.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	91
2	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	87
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	38
4	5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	28
5	Oxoprophines	277	C17H11NO3	1000128-51-1	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010722\
Data File : BP008732.D
Acq On : 07 Jan 2022 18:29
Operator : CG/JU
Sample : N1039-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

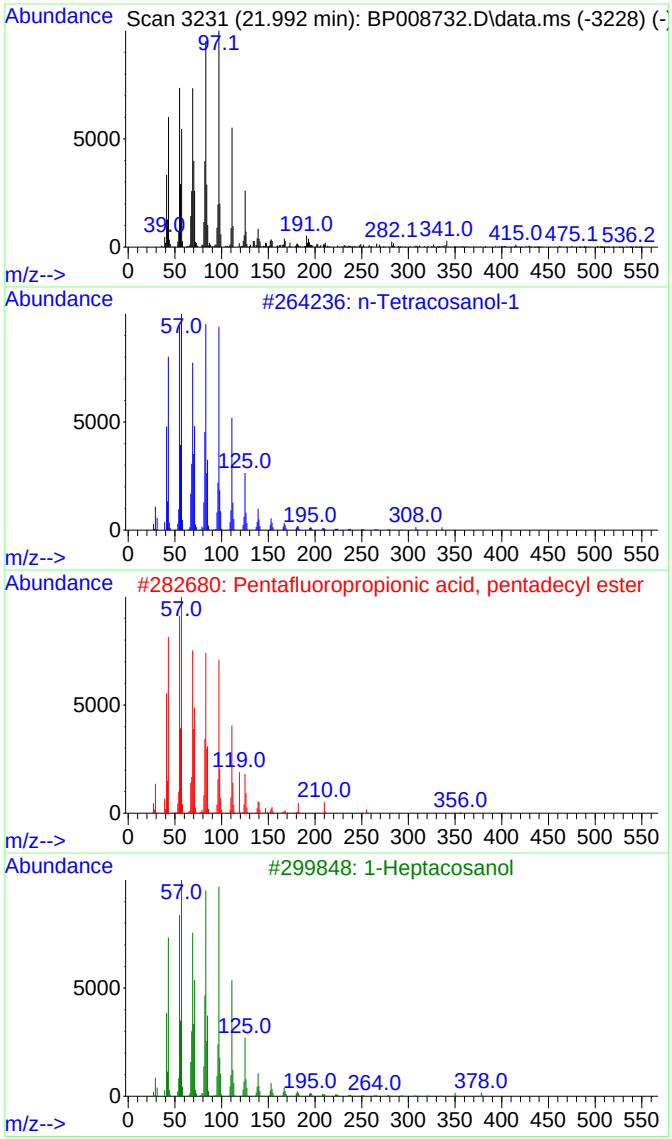
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

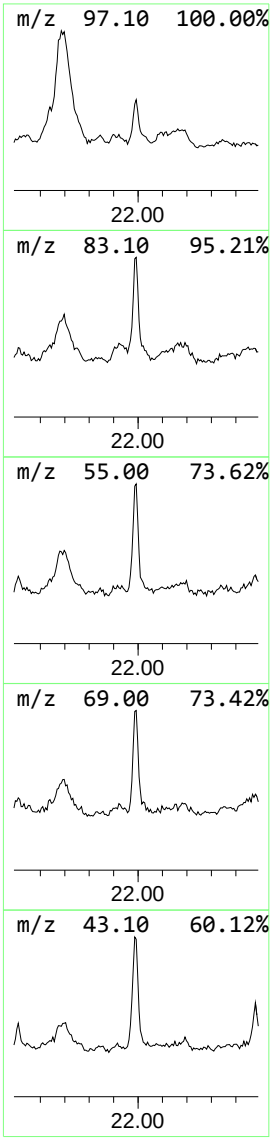
****

Peak Number 8 n-Tetracosanol-1 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.992	3.26 ng	920999	Chrysene-d12	21.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
3	1-Heptacosanol	396	C27H56O	002004-39-9	90
4	9-Nonadecene	266	C19H38	031035-07-1	89
5	1-Nonadecene	266	C19H38	018435-45-5	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010722\
Data File : BP008732.D
Acq On : 07 Jan 2022 18:29
Operator : CG/JU
Sample : N1039-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.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
Butane, 2-metho...	3.070	32.5	ng	3521430	1	7.869	2168560	20.0
2-Pentanone, 4-...	4.987	2.4	ng	261079	1	7.869	2168560	20.0
Ethanol, 2-(2-b...	10.457	3.9	ng	604128	2	10.675	3071480	20.0
n-Hexadecanoic ...	18.157	4.5	ng	1213820	4	17.257	5349350	20.0
Octadecanoic acid	19.392	3.5	ng	1002330	5	21.351	5646100	20.0
E-15-Heptadecenal	21.063	4.5	ng	1271020	5	21.351	5646100	20.0
(E)-7-Benzylide...	21.469	22.1	ng	6228820	5	21.351	5646100	20.0
n-Tetracosanol-1	21.992	3.3	ng	920999	5	21.351	5646100	20.0