LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
Data File : BP006537.D
Acq On : 06 Aug 2021 13:46
Operator : CG/JU
Sample : M3271-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-3

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-BP080321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP006537.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.905	304	309	317	rBV	1212760	1677964	19.12%	2.754%
2	5.358	380	386	394	rBV	3948214	5466173	62.29%	8.972%
3	5.970	485	490	495	rVB	245200	340904	3.88%	0.560%
4	6.934	647	654	667	rVB	3700781	5828834	66.42%	9.568%
5	7.752	787	793	800	rVB	931526	1459189	16.63%	2.395%
6	8.911	983	990	998	rBV	2289106	3723903	42.44%	6.113%
7	10.328	1225	1231	1241	rBV	297091	460958	5.25%	0.757%
8	10.540	1259	1267	1274	rBV	1257759	2135688	24.34%	3.506%
9	12.322	1563	1570	1581	rBV	49343	137035	1.56%	0.225%
10	13.010	1679	1687	1700	rBV	4815224	7047372	80.31%	11.568%
11	14.381	1914	1920	1929	rBV	1743108	2640990	30.10%	4.335%
12	15.875	2160	2174	2183	rBV	4033579	5629393	64.15%	9.240%
13	17.140	2381	2389	2393	rBV	2025472	2979603	33.95%	4.891%
14	17.181	2393	2396	2402	rVB	101714	138696	1.58%	0.228%
15	18.051	2538	2544	2553	rBV	1991002	2689122	30.64%	4.414%
16	19.151	2727	2731	2739	rBV	375176	550216	6.27%	0.903%
17	19.286	2750	2754	2766	rBV	821669	1155404	13.17%	1.897%
18	19.504	2787	2791	2799	rVB	381734	522927	5.96%	0.858%
19	19.716	2821	2827	2837	rVB	6979741	8775268	100.00%	14.404%
20	20.963	3035	3039	3045	rBV2	476990	555784	6.33%	0.912%
21	21.163	3069	3073	3078	rBV	566546	591979	6.75%	0.972%
22	21.233	3079	3085	3089	rBV	2416730	3442597	39.23%	5.651%
23	23.563	3475	3481	3488	rBV2	1550586	2972677	33.88%	4.879%

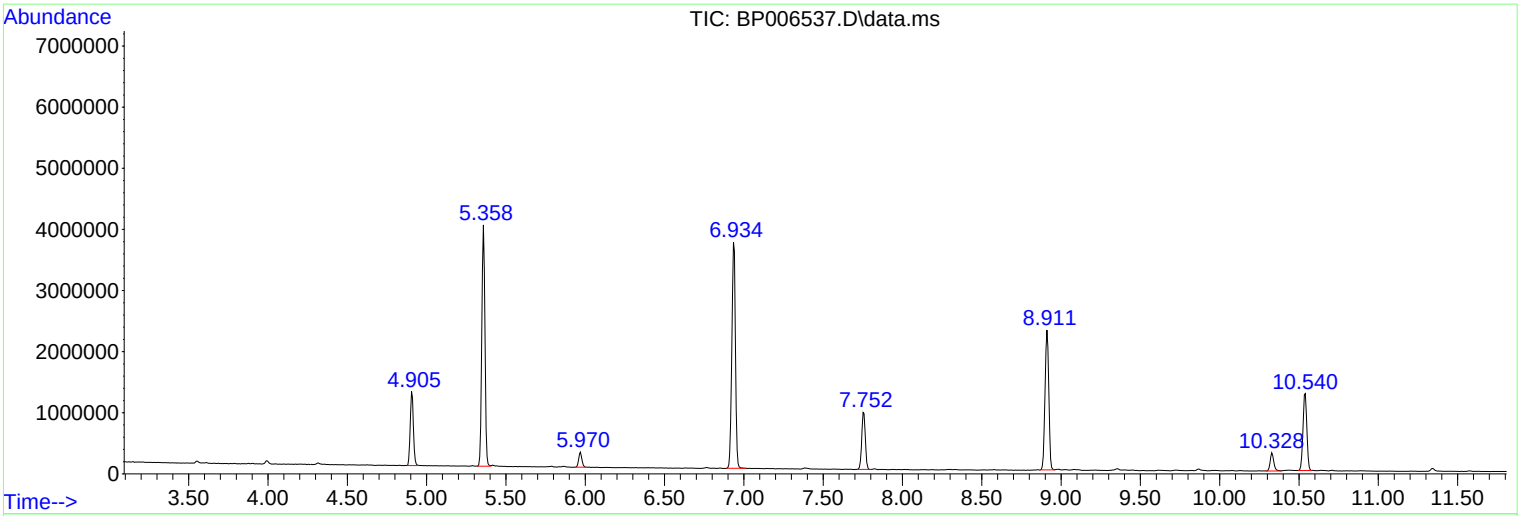
Sum of corrected areas: 60922676

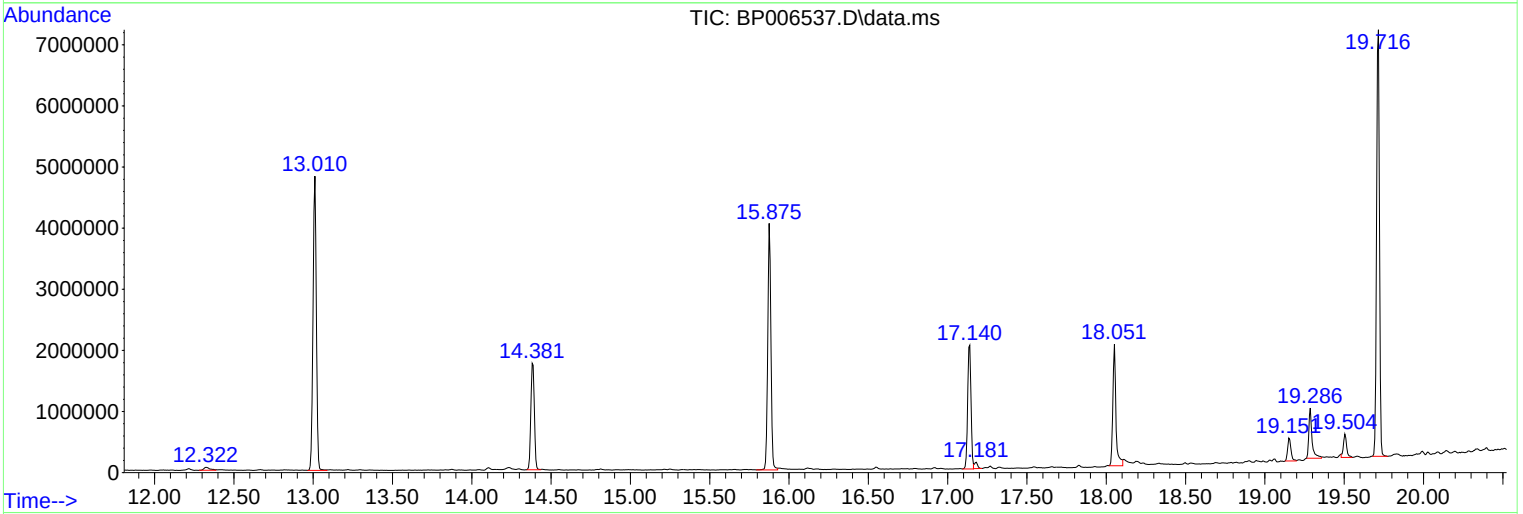
Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
Data File : BP006537.D
Acq On : 06 Aug 2021 13:46
Operator : CG/JU
Sample : M3271-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

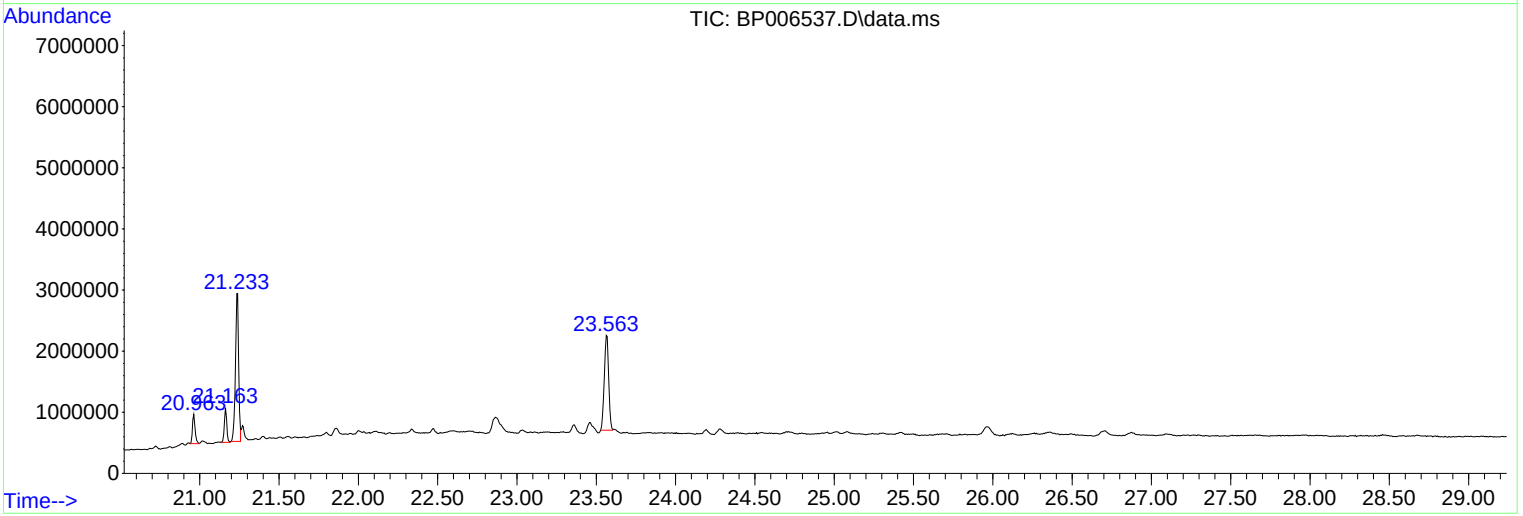
Instrument :
BNA_P
ClientSampleId :
TP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.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\BP080621\
Data File : BP006537.D
Acq On : 06 Aug 2021 13:46
Operator : CG/JU
Sample : M3271-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-3

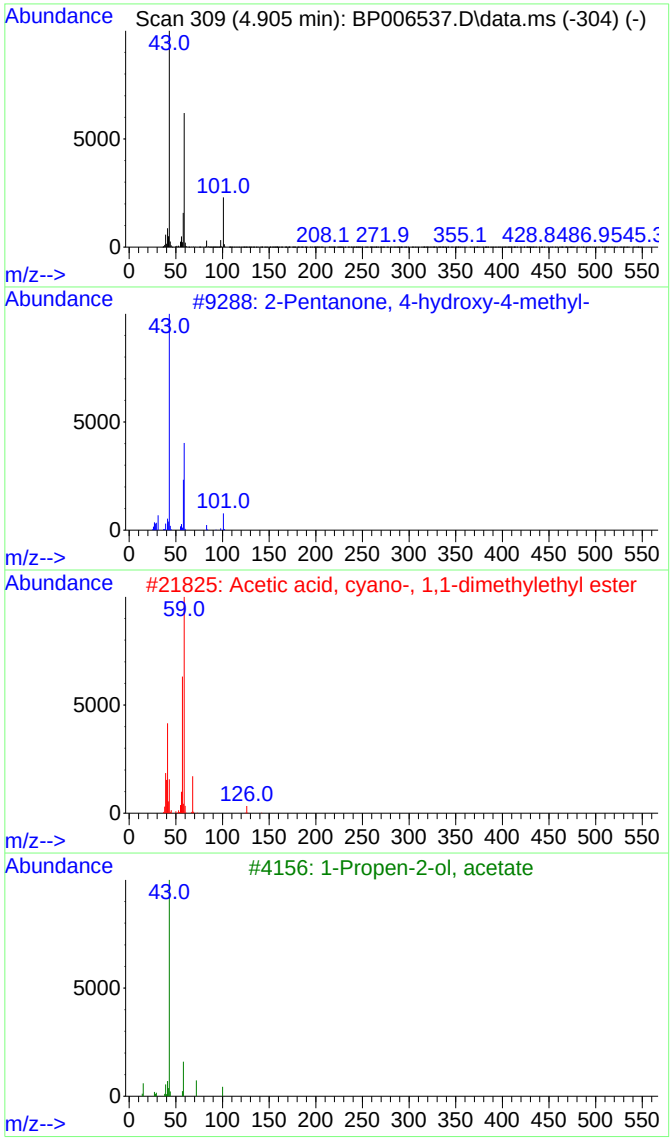
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

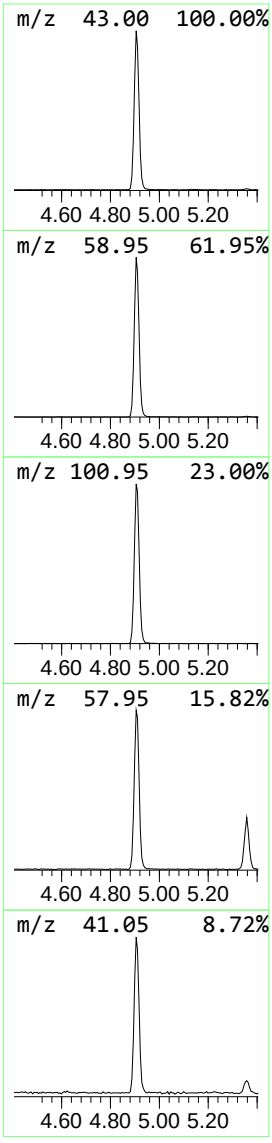
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.905	23.00 ng	1677960	1,4-Dichlorobenzene-d4	7.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
Data File : BP006537.D
Acq On : 06 Aug 2021 13:46
Operator : CG/JU
Sample : M3271-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-3

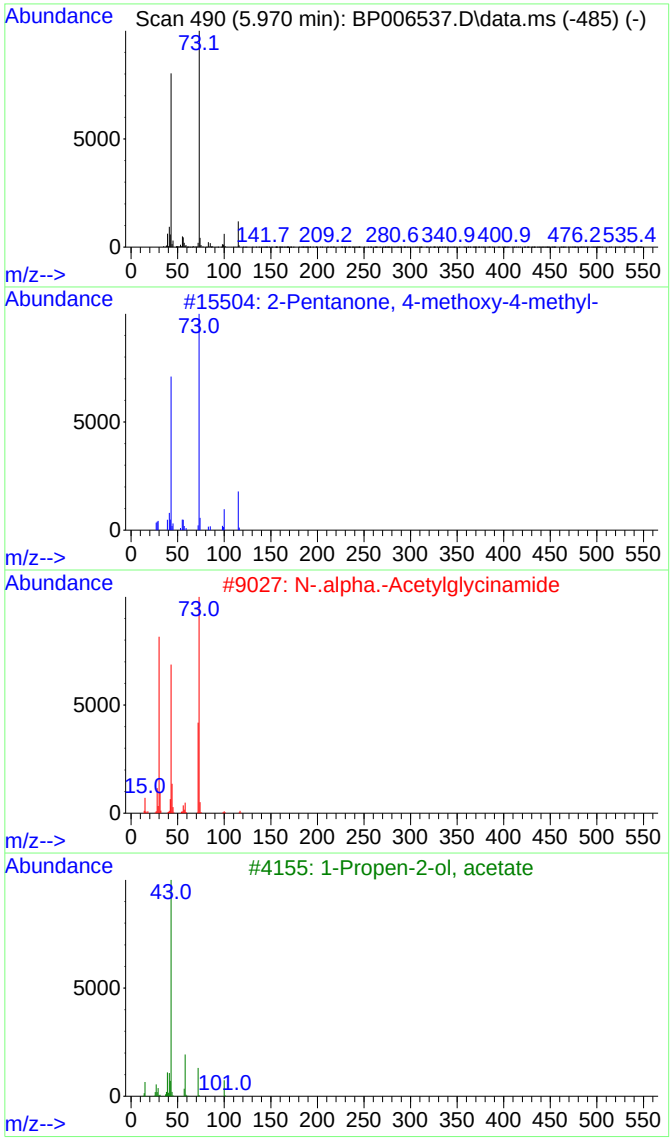
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

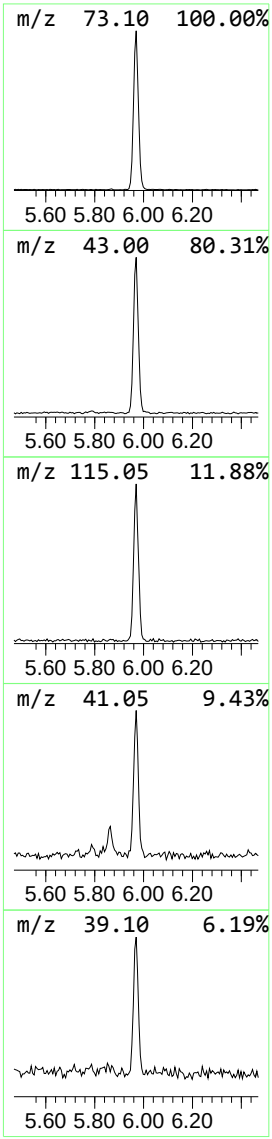
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.970	4.67 ng	340904	1,4-Dichlorobenzene-d4	7.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	10
5	N-Formylmorpholine	115	C5H9NO2	004394-85-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
Data File : BP006537.D
Acq On : 06 Aug 2021 13:46
Operator : CG/JU
Sample : M3271-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-3

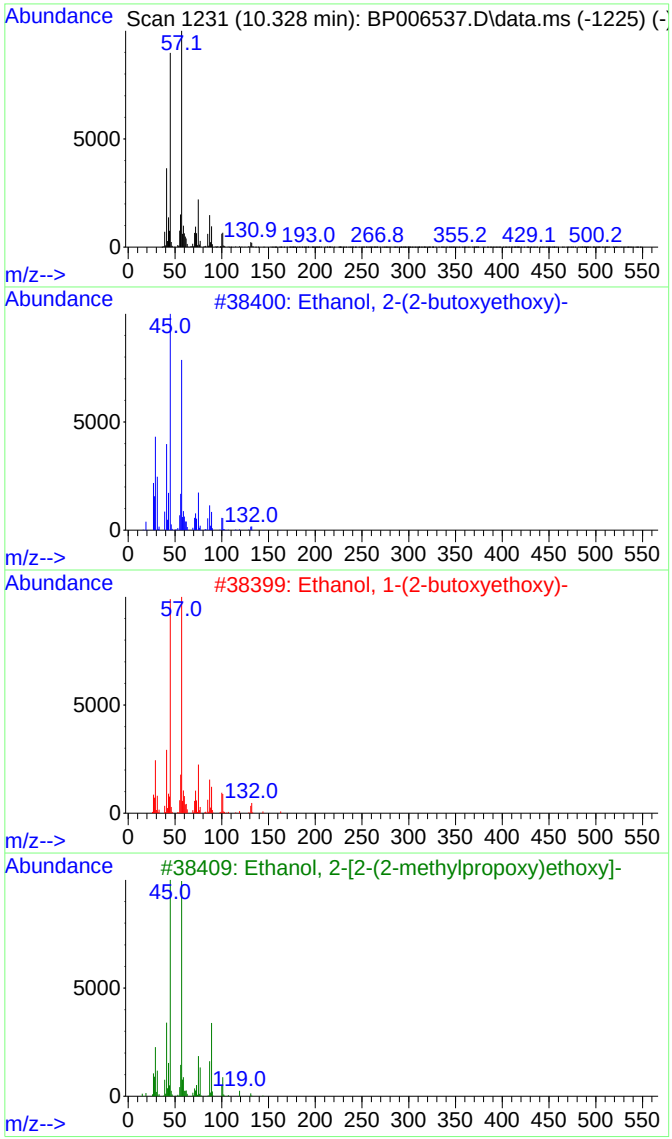
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

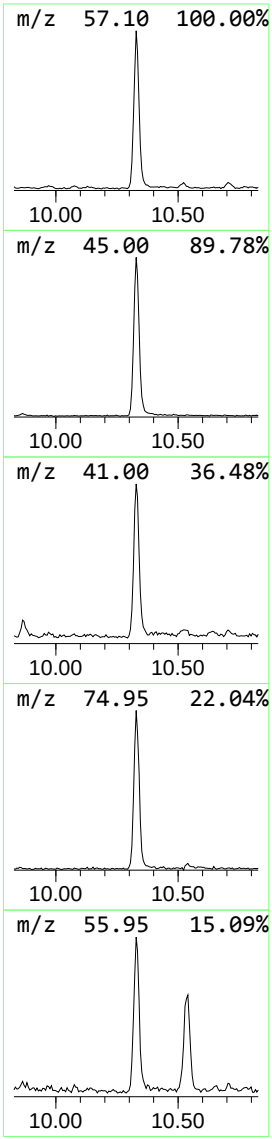
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.328	4.32 ng	460958	Naphthalene-d8	10.540

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
4	Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	43
5	1,4,7,10,13,16-Hexaoxacyclooctad...	264	C12H24O6	017455-13-9	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
Data File : BP006537.D
Acq On : 06 Aug 2021 13:46
Operator : CG/JU
Sample : M3271-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

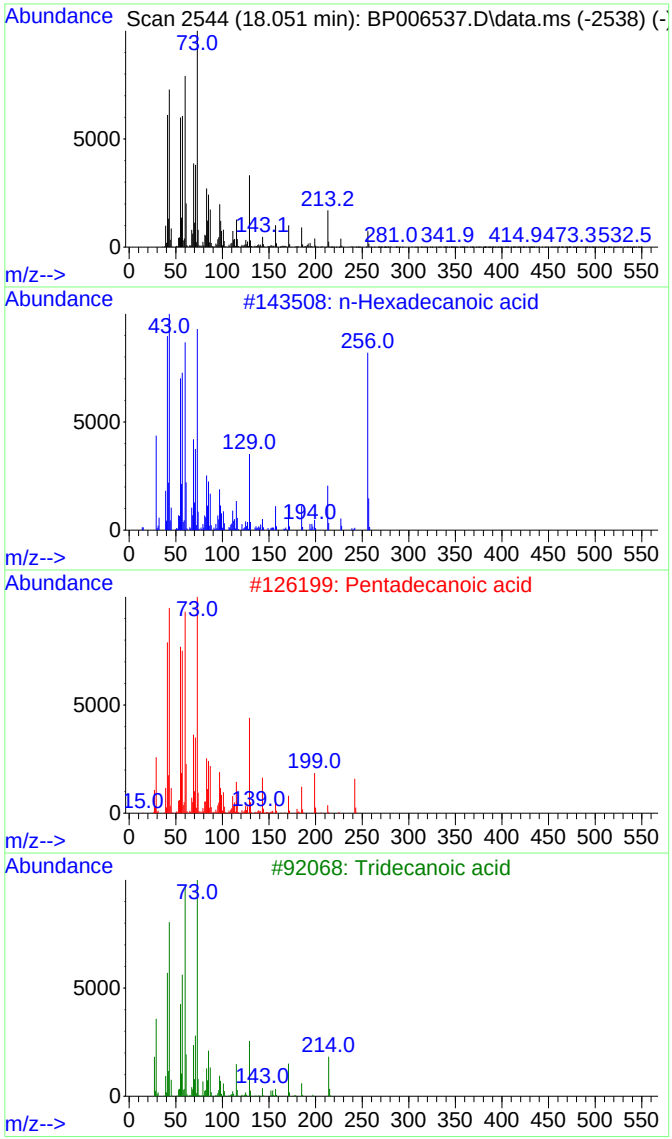
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

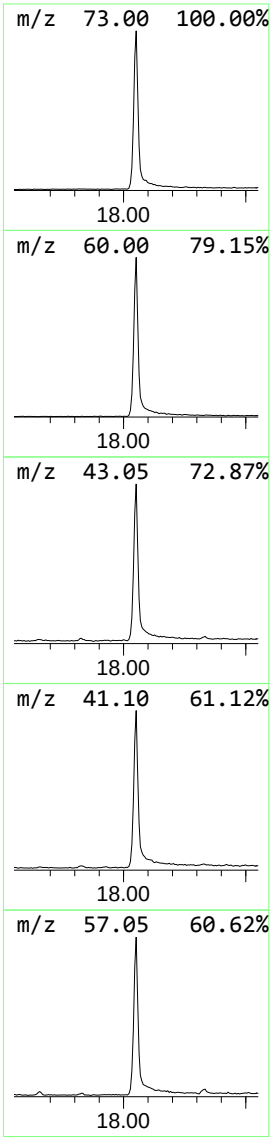
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.051	18.05 ng	2689120	Phenanthrene-d10	17.140

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	74
4	Dodecanoic acid	200	C12H24O2	000143-07-7	72
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
Data File : BP006537.D
Acq On : 06 Aug 2021 13:46
Operator : CG/JU
Sample : M3271-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

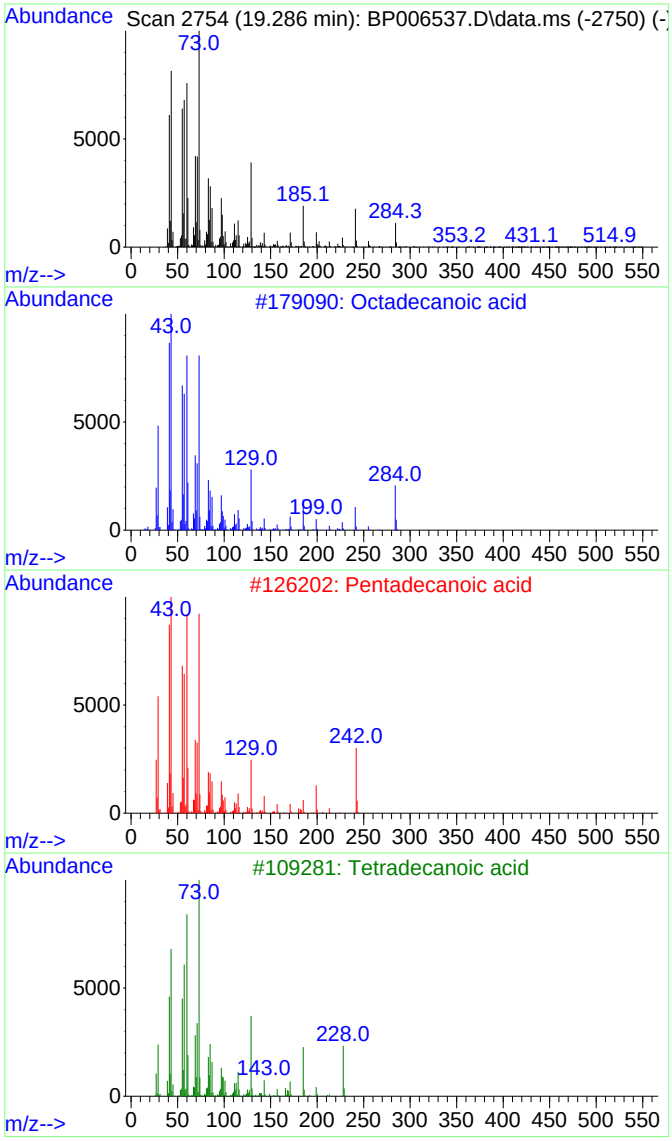
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

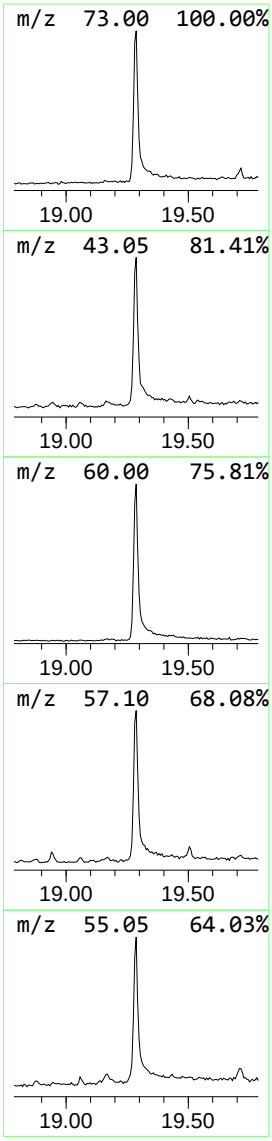
****

Peak Number 5 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.287	6.71 ng	1155400	Chrysene-d12	21.239

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
Data File : BP006537.D
Acq On : 06 Aug 2021 13:46
Operator : CG/JU
Sample : M3271-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-3

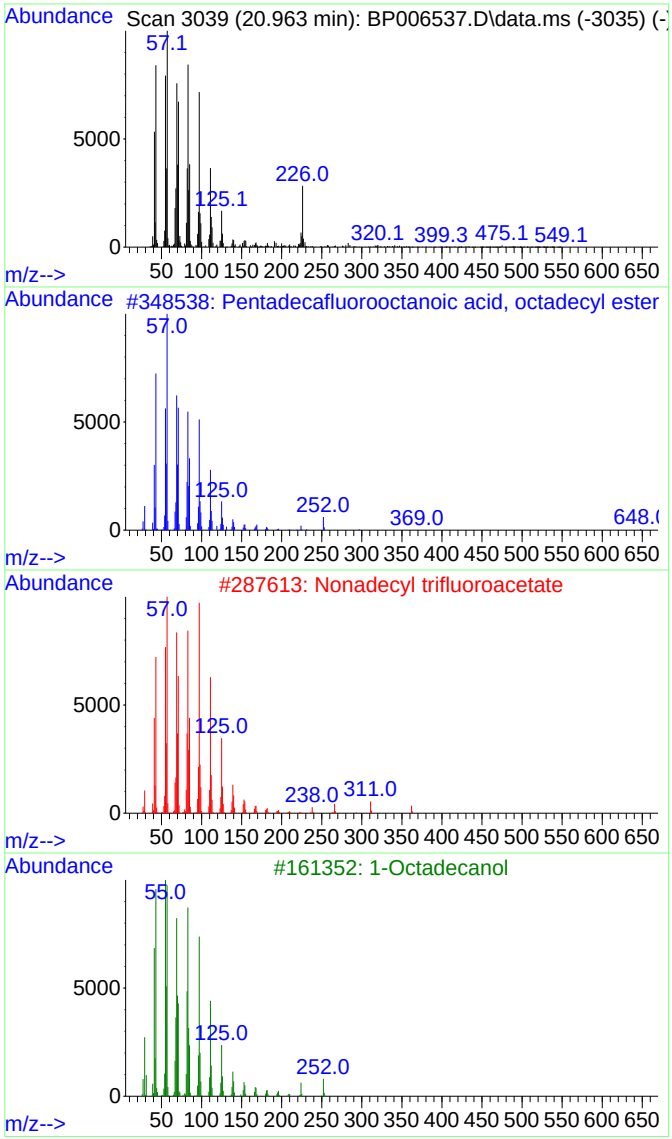
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

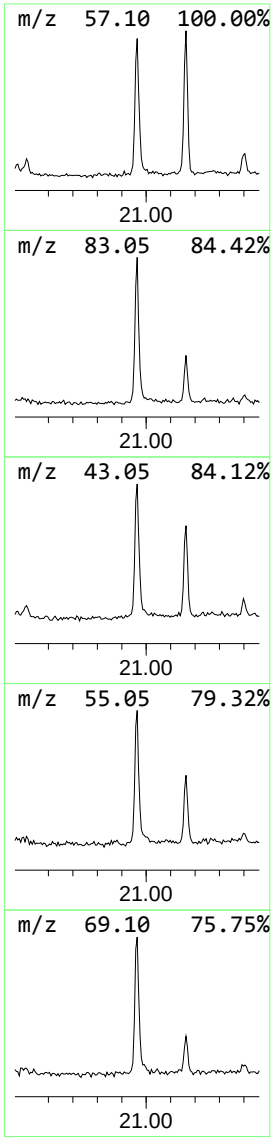
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Pentadecafluorooctanoic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.963	3.23 ng	555784	Chrysene-d12	21.239

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
2	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	90
3	1-Octadecanol	270	C18H38O	000112-92-5	90
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	90
5	Octacosanol	410	C28H58O	000557-61-9	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
Data File : BP006537.D
Acq On : 06 Aug 2021 13:46
Operator : CG/JU
Sample : M3271-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.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-...	4.905	23.0	ng	1677960	1	7.752	1459190	20.0
2-Pentanone, 4-...	5.970	4.7	ng	340904	1	7.752	1459190	20.0
Ethanol, 2-(2-b...	10.328	4.3	ng	460958	2	10.540	2135690	20.0
n-Hexadecanoic ...	18.051	18.1	ng	2689120	4	17.140	2979600	20.0
Octadecanoic acid	19.287	6.7	ng	1155400	5	21.239	3442600	20.0
Pentadecafluoro...	20.963	3.2	ng	555784	5	21.239	3442600	20.0