LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092722\
Data File : BP011824.D
Acq On : 27 Sep 2022 20:05
Operator : CG/JU
Sample : N4815-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SAND-FILTER-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-BP092122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP011824.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.046	6	10	32	rVB	2020757	3133524	12.56%	2.242%
2	5.011	337	344	356	rBV	372374	613513	2.46%	0.439%
3	5.469	415	422	439	rBV	7106431	11171235	44.78%	7.995%
4	7.069	686	694	710	rBV	7109071	12134720	48.64%	8.684%
5	7.911	829	837	845	rBV	1342464	2209177	8.85%	1.581%
6	9.075	1027	1035	1054	rBV	4402511	7312794	29.31%	5.233%
7	10.716	1306	1314	1327	rBV	1970290	3405546	13.65%	2.437%
8	13.175	1725	1732	1749	rBV	11470382	17544663	70.32%	12.556%
9	14.551	1956	1966	1982	rBV	3094501	4589207	18.39%	3.284%
10	16.045	2213	2220	2239	rBV	9622744	13962405	55.96%	9.992%
11	17.310	2428	2435	2441	rBV	3699671	5343682	21.42%	3.824%
12	18.192	2580	2585	2605	rBV	1517215	3118863	12.50%	2.232%
13	19.428	2790	2795	2815	rBV	2493875	4713608	18.89%	3.373%
14	19.686	2833	2839	2852	rBV	6780360	9424186	37.77%	6.744%
15	19.869	2864	2870	2878	rVB	18734561	24949636	100.00%	17.855%
16	21.098	3075	3079	3089	rBV	945884	1635301	6.55%	1.170%
17	21.392	3124	3129	3142	rVB	4710732	6159219	24.69%	4.408%
18	21.516	3146	3150	3160	rBV	1204180	1872049	7.50%	1.340%
19	23.833	3538	3544	3555	rVB2	3103217	6442472	25.82%	4.610%

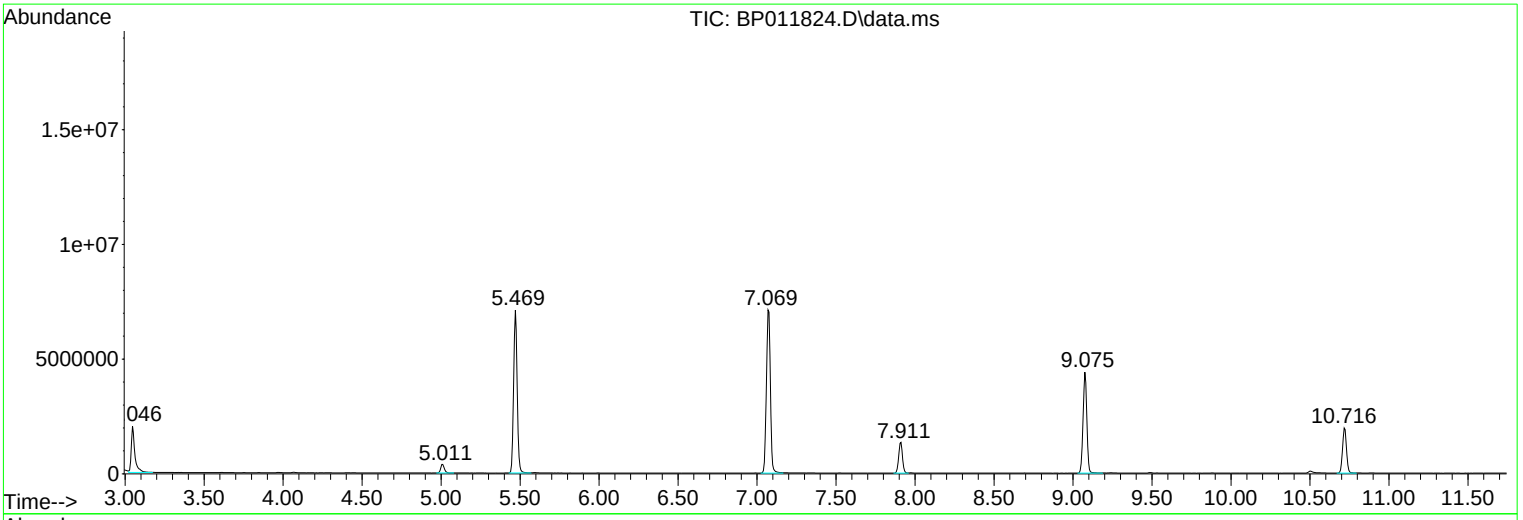
Sum of corrected areas: 139735800

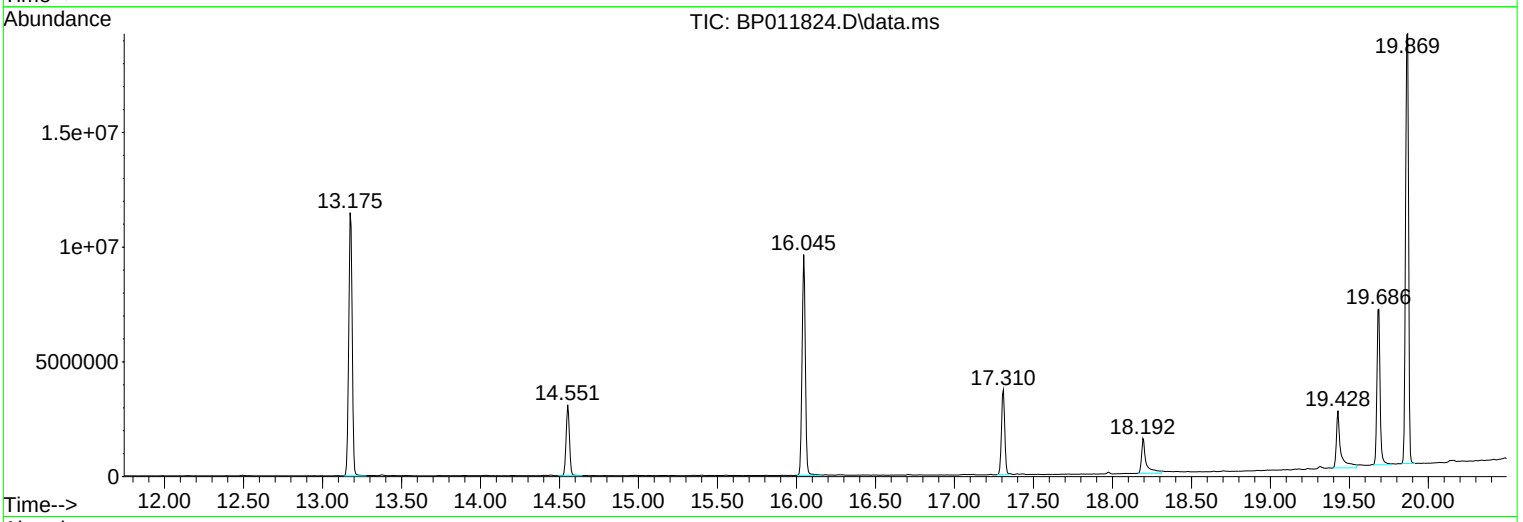
Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092722\
Data File : BP011824.D
Acq On : 27 Sep 2022 20:05
Operator : CG/JU
Sample : N4815-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

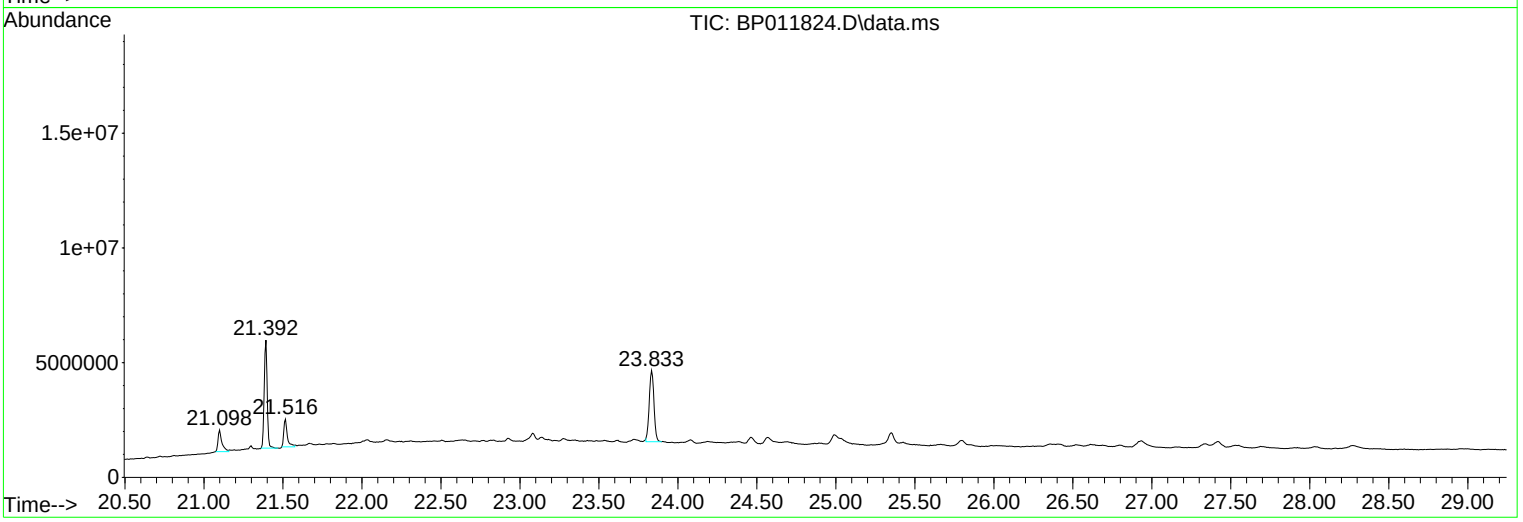
Instrument :
BNA_P
ClientSampleId :
SAND-FILTER-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.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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Data File : BP011824.D
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

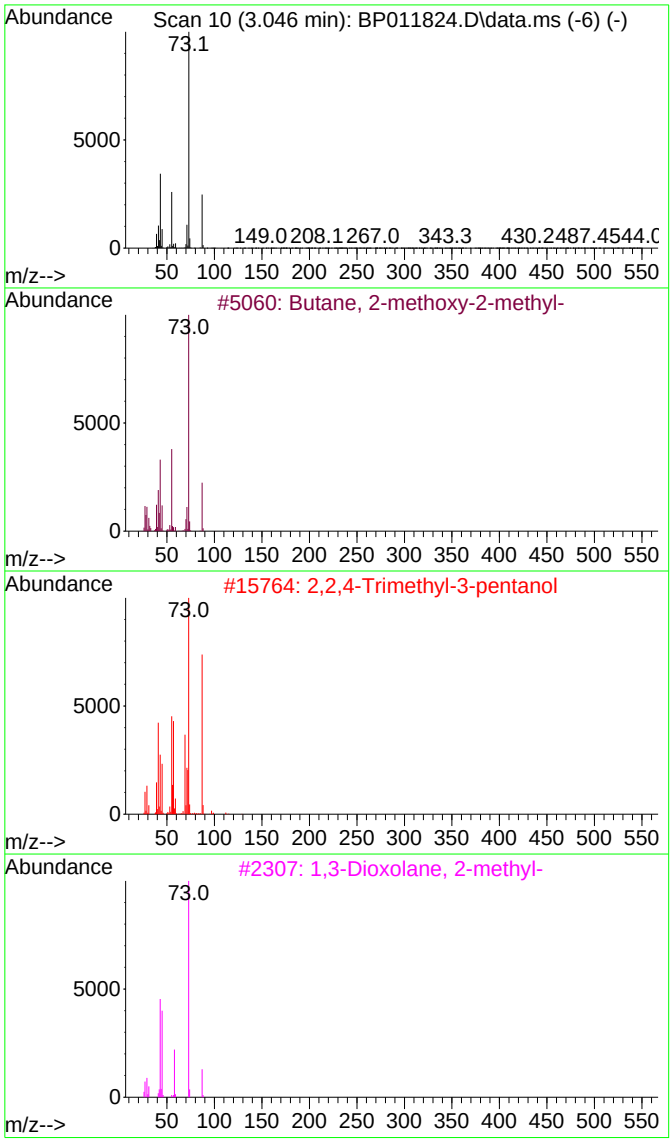
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

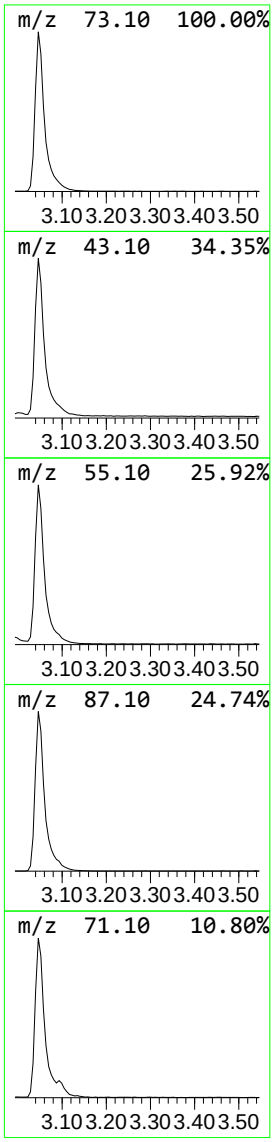
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.046	28.37 ng	3133520	1,4-Dichlorobenzene-d4	7.911

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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





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Operator : CG/JU
Sample : N4815-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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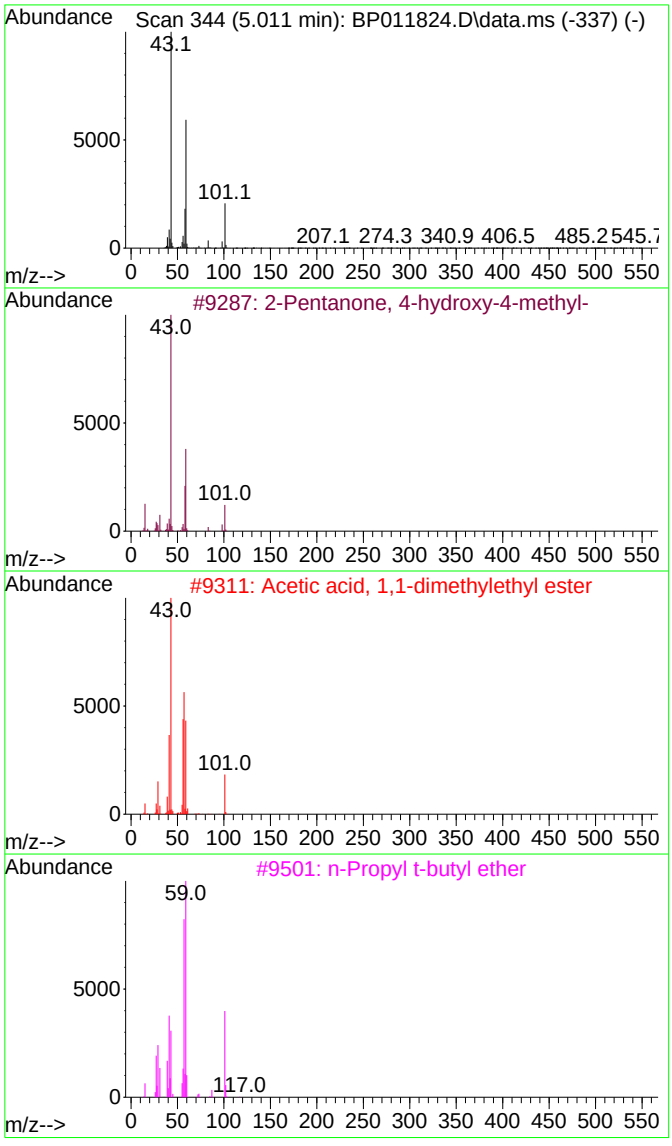
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

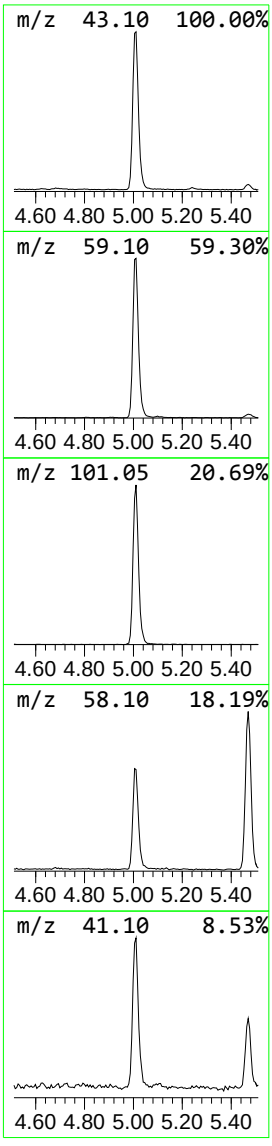
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.011	5.55 ng	613513	1,4-Dichlorobenzene-d4	7.911

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
4	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25





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Data File : BP011824.D
Acq On : 27 Sep 2022 20:05
Operator : CG/JU
Sample : N4815-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SAND-FILTER-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

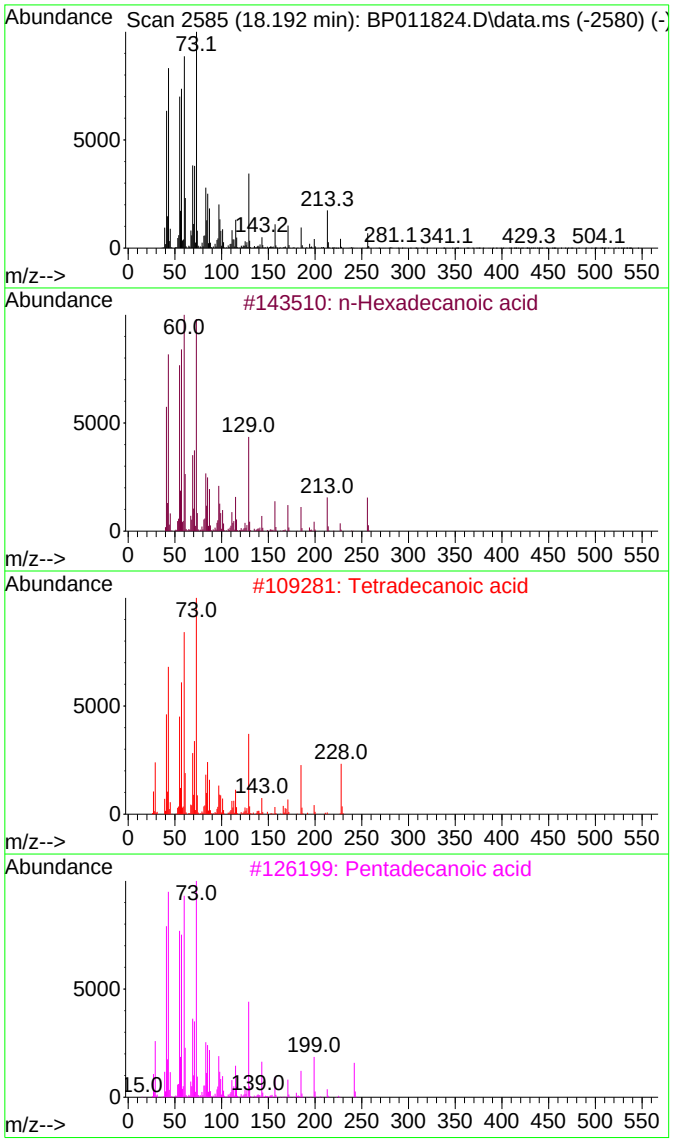
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

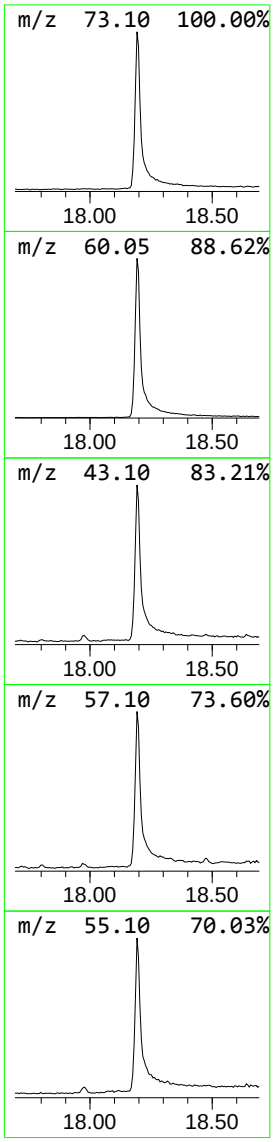
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.192	11.67 ng	3118860	Phenanthrene-d10	17.310

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	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tridecanoic acid	214	C13H26O2	000638-53-9	89
5	Dodecanoic acid	200	C12H24O2	000143-07-7	53





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Data File : BP011824.D
Acq On : 27 Sep 2022 20:05
Operator : CG/JU
Sample : N4815-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SAND-FILTER-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

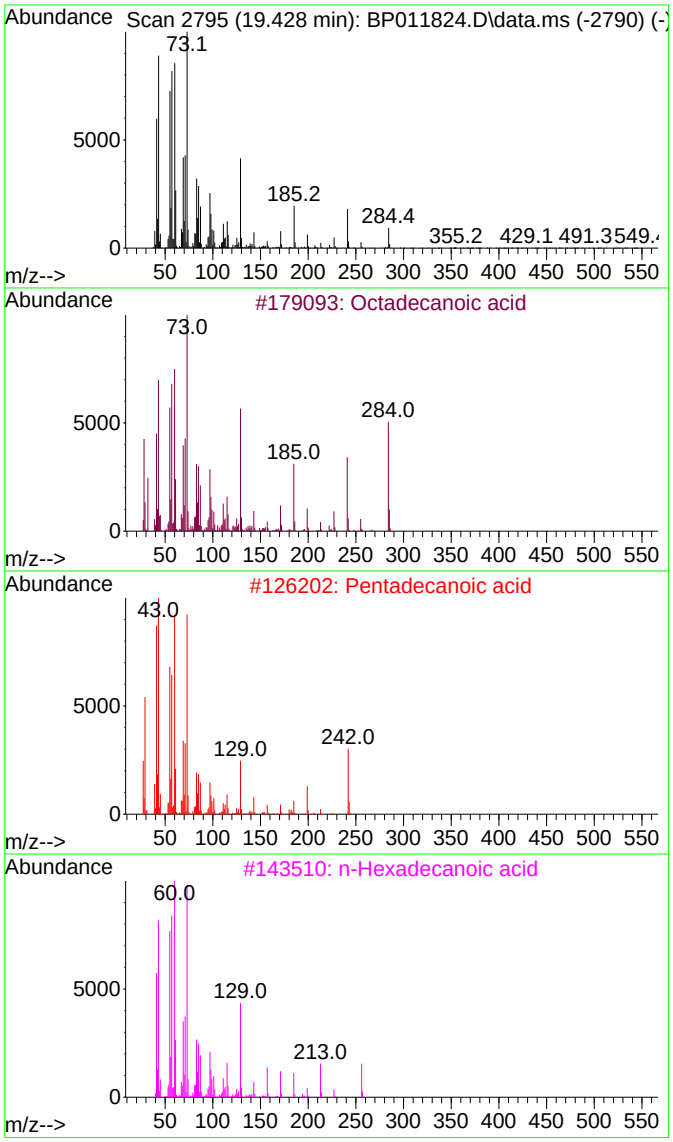
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

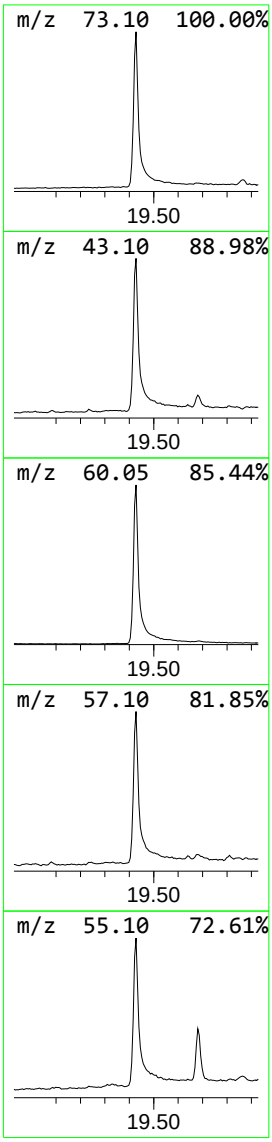
****

Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.428	15.31 ng	4713610	Chrysene-d12	21.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092722\
Data File : BP011824.D
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Operator : CG/JU
Sample : N4815-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SAND-FILTER-1

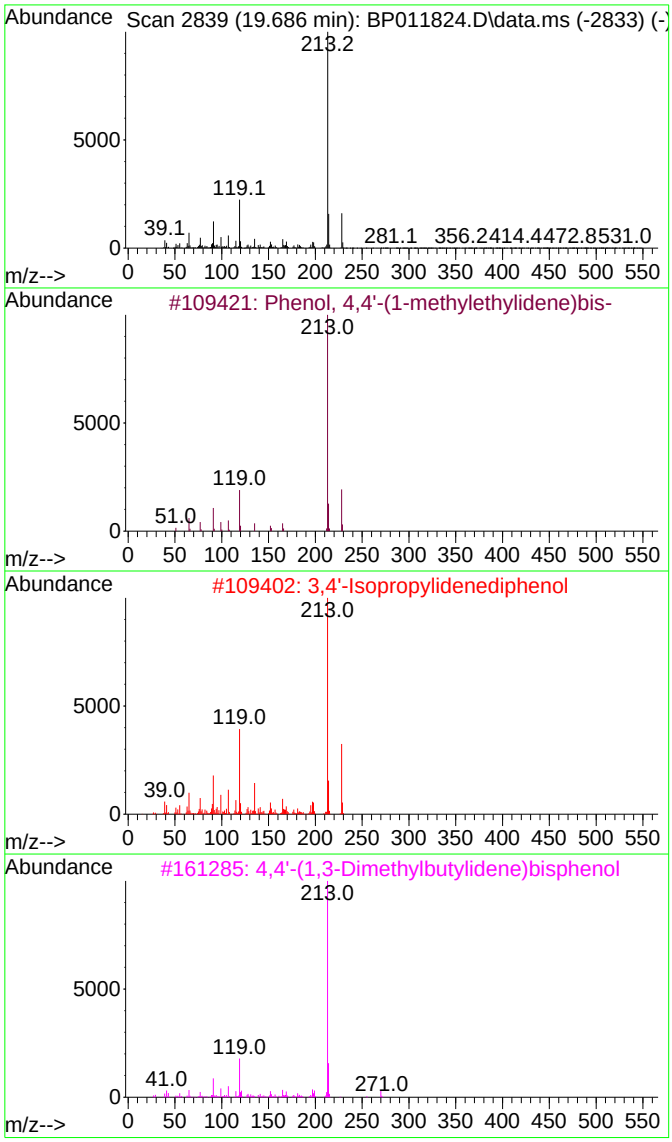
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

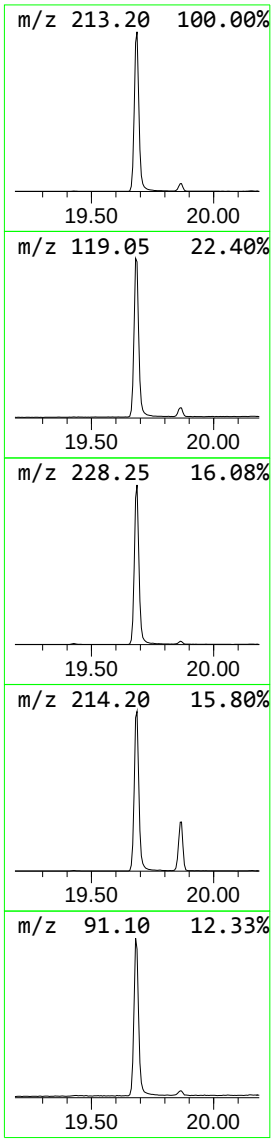
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Phenol, 4,4'-(1-methylethyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.686	30.60 ng	9424190	Chrysene-d12	21.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	98
2	3,4'-Isopropylidenediphenol	228	C15H16O2	046765-25-7	78
3	4,4'-(1,3-Dimethylbutylidene)bis...	270	C18H22O2	006807-17-6	74
4	Diphenolic acid	286	C17H18O4	000126-00-1	64
5	5-Fluoro-2-nitrophenylamine, TMS...	228	C9H13FN2O2Si	1000484-54-5	50





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Instrument :
BNA_P
ClientSampleId :
SAND-FILTER-1

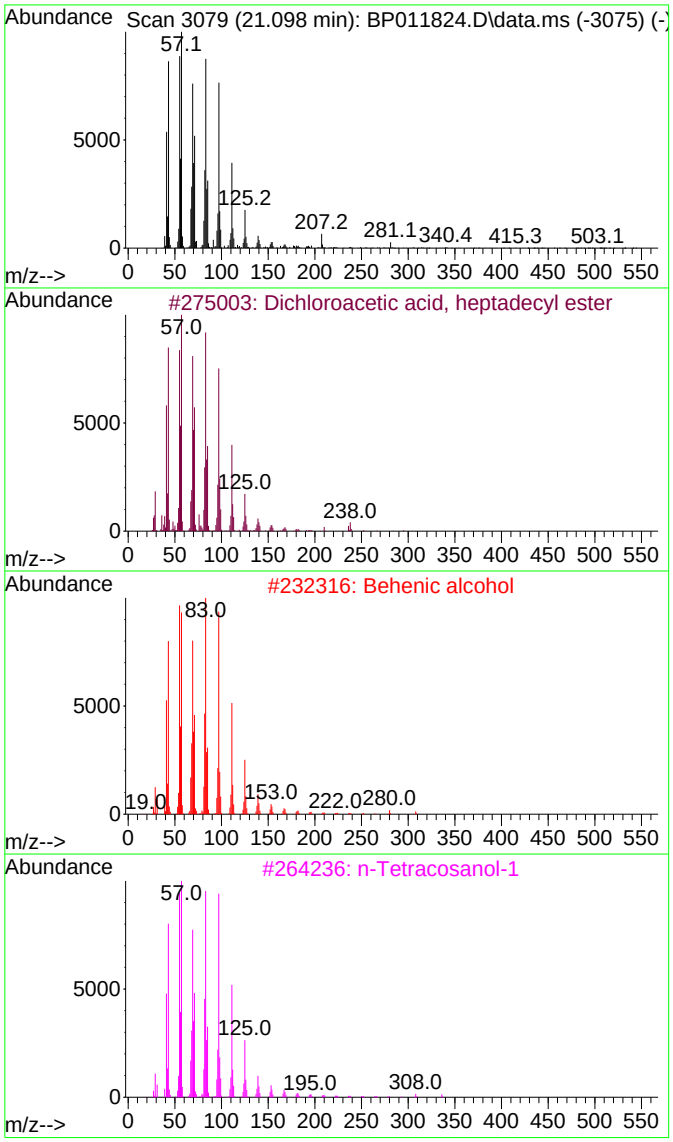
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

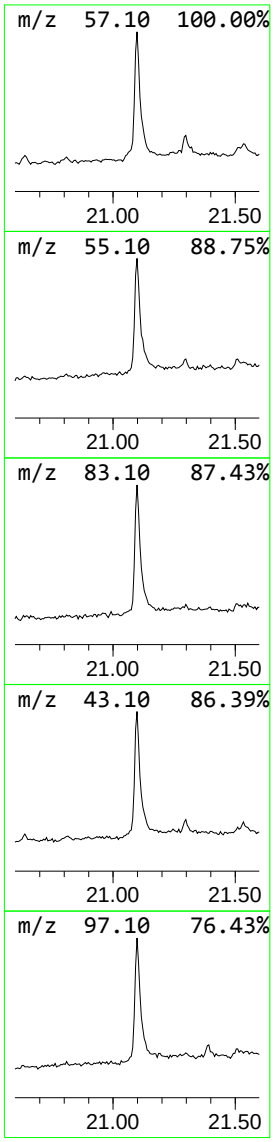
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Dichloroacetic acid, heptad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.098	5.31 ng	1635300	Chrysene-d12	21.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
2	Behenic alcohol	326	C22H46O	000661-19-8	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91





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Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

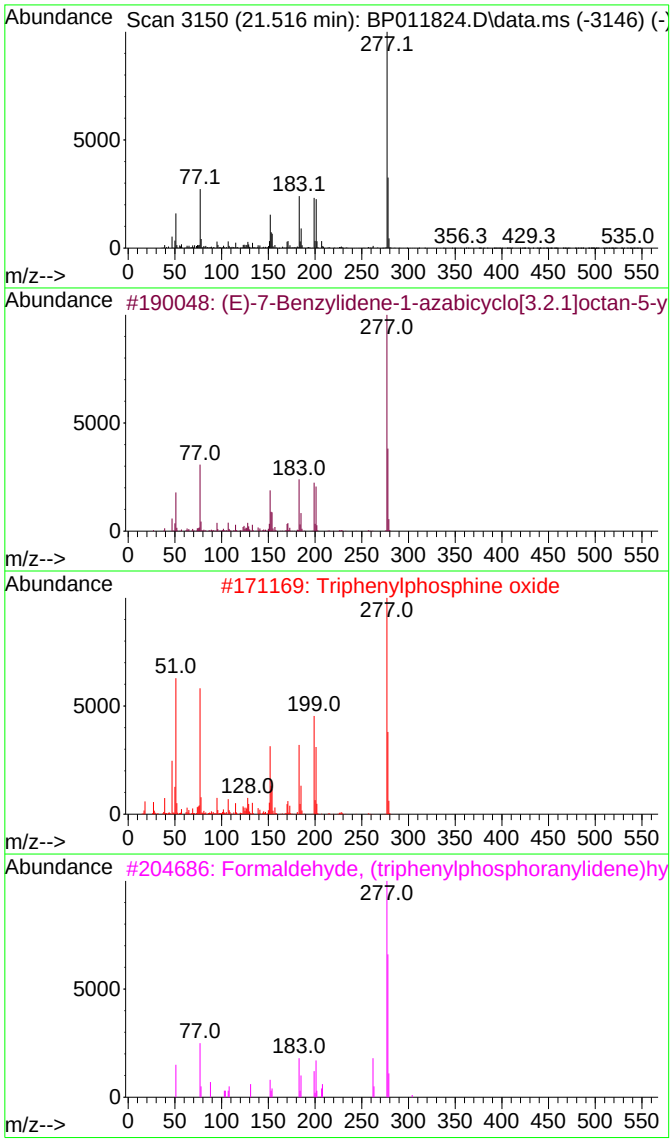
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

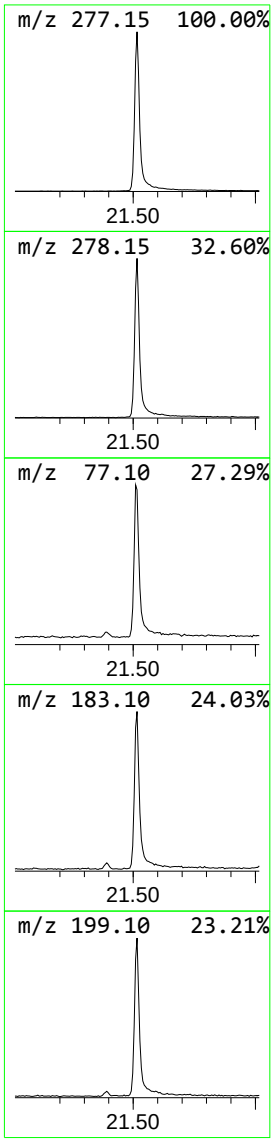
****

Peak Number 7 (E)-7-Benzylidene-1-azabicy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.516	6.08 ng	1872050	Chrysene-d12	21.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	95
2	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	81
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45
4	4-Nitro-4'-methyldiphenylsulfone	277	C13H11NO4S	004094-37-5	43
5	Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	32





Tentatively Identified Compound (LSC) summary

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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...	3.046	28.4	ng	3133520	1	7.911	2209180	20.0
2-Pentanone, 4-...	5.011	5.5	ng	613513	1	7.911	2209180	20.0
n-Hexadecanoic ...	18.192	11.7	ng	3118860	4	17.310	5343680	20.0
Octadecanoic acid	19.428	15.3	ng	4713610	5	21.392	6159220	20.0
Phenol, 4,4'-(1...	19.686	30.6	ng	9424190	5	21.392	6159220	20.0
Dichloroacetic ...	21.098	5.3	ng	1635300	5	21.392	6159220	20.0
(E)-7-Benzylide...	21.516	6.1	ng	1872050	5	21.392	6159220	20.0