LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092922\
Data File : BP011841.D
Acq On : 29 Sep 2022 15:01
Operator : CG/JU
Sample : N4860-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
EB-2022-09-27

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: BP011841.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	5	10	37	rVB	7786768	12424294	51.59%	9.000%
2	5.005	336	343	352	rBV	799177	1203004	5.00%	0.871%
3	5.470	415	422	436	rBV	3687651	5708898	23.70%	4.136%
4	6.093	521	528	537	rBV	206886	316721	1.32%	0.229%
5	7.069	685	694	712	rBV	2311299	3768569	15.65%	2.730%
6	7.905	828	836	844	rBV	1363839	2282407	9.48%	1.653%
7	9.075	1027	1035	1049	rBV	4989904	8633849	35.85%	6.255%
8	10.499	1269	1277	1297	rBV	617822	1377776	5.72%	0.998%
9	10.722	1307	1315	1327	rVB	1921029	3428092	14.23%	2.483%
10	13.181	1725	1733	1748	rBV	12713081	19659941	81.63%	14.242%
11	14.551	1957	1966	1981	rBV	2908362	4501878	18.69%	3.261%
12	16.051	2213	2221	2228	rBV	9386534	14038180	58.29%	10.170%
13	16.292	2257	2262	2266	rVB	243761	345456	1.43%	0.250%
14	17.310	2429	2435	2445	rBV	3651977	5160899	21.43%	3.739%
15	18.198	2580	2586	2609	rBV	3565080	5835512	24.23%	4.227%
16	19.428	2790	2795	2819	rBV	7839136	12106075	50.27%	8.770%
17	19.869	2864	2870	2875	rBV	18335768	24083453	100.00%	17.446%
18	21.392	3124	3129	3144	rVB	4302453	5881333	24.42%	4.261%
19	21.516	3147	3150	3156	rVB	277537	392444	1.63%	0.284%
20	22.586	3328	3332	3341	rVB	1242414	1910726	7.93%	1.384%
21	23.833	3537	3544	3555	rBV2	2435715	4982442	20.69%	3.609%

Sum of corrected areas: 138041949

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092922\
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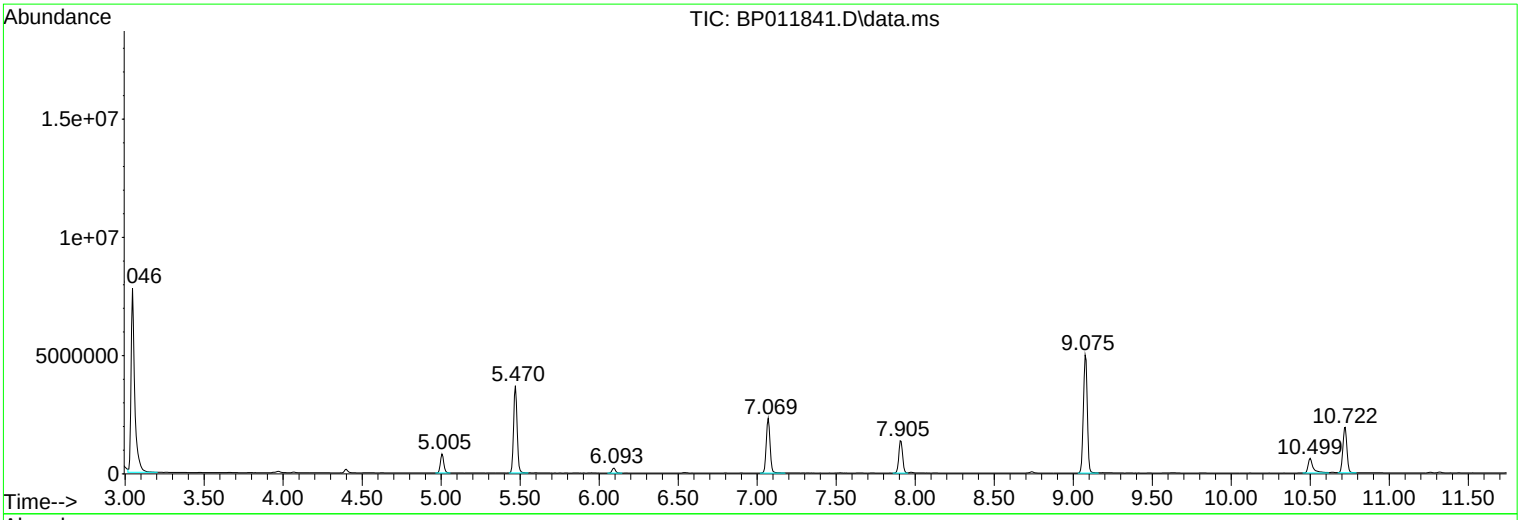
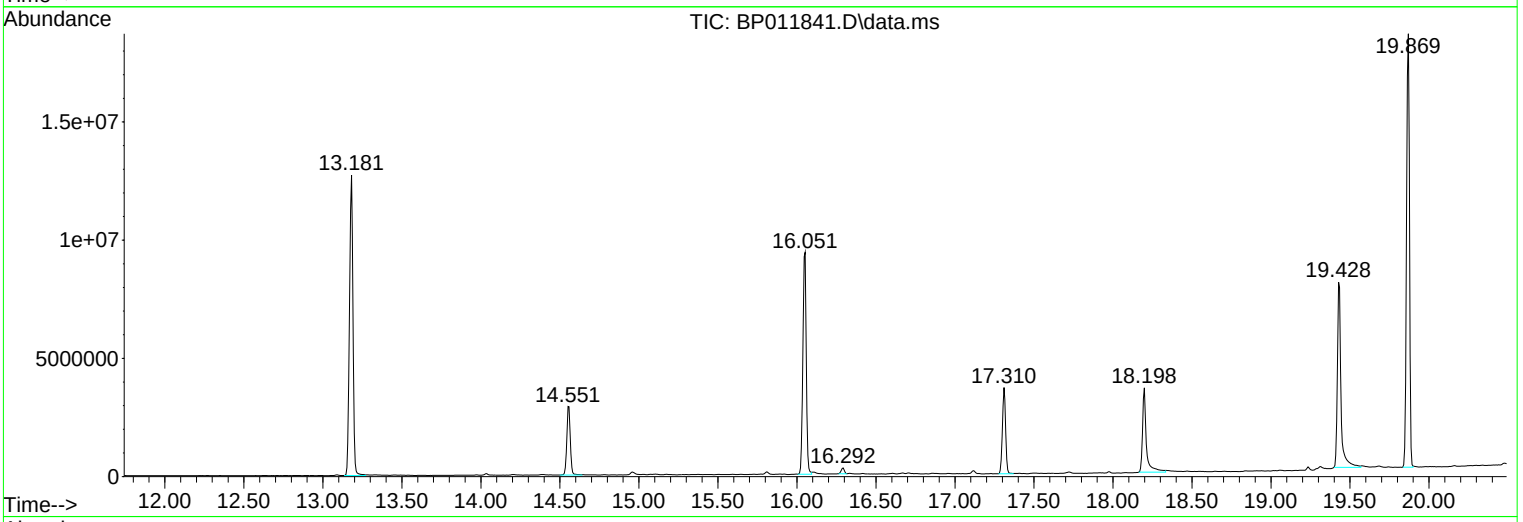
Sample : N4860-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

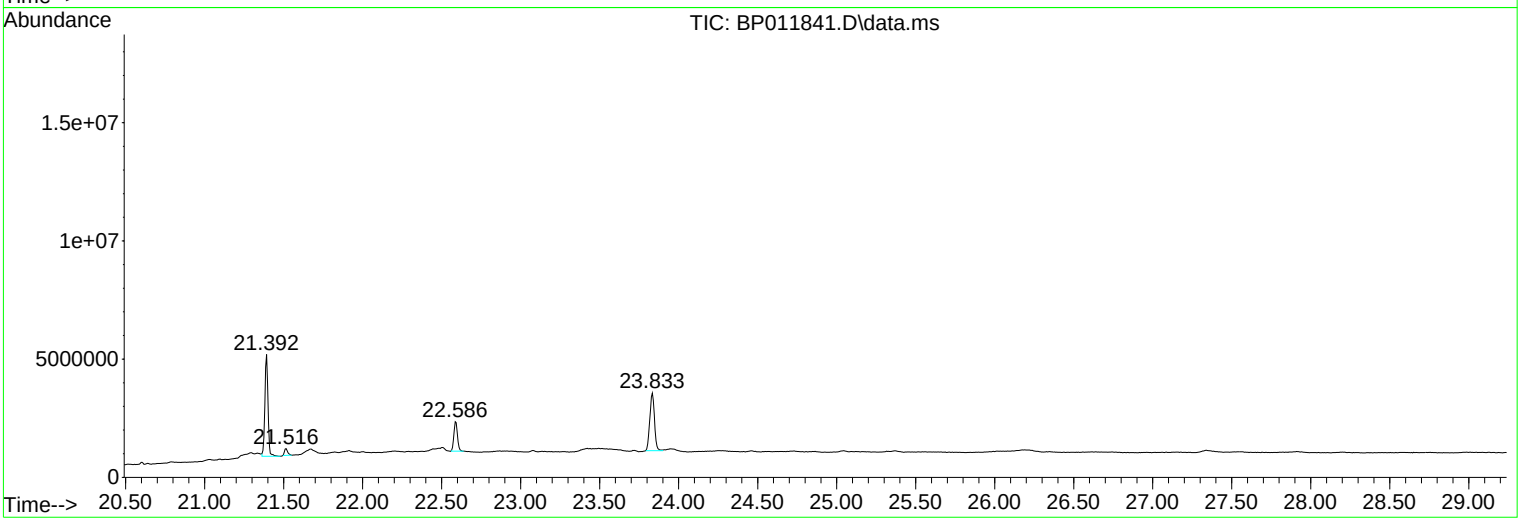
Instrument :
BNA_P
ClientSampleId :
EB-2022-09-27

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 : BP011841.D
Acq On : 29 Sep 2022 15:01
Operator : CG/JU
Sample : N4860-10
Misc :
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Instrument :
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ClientSampleId :
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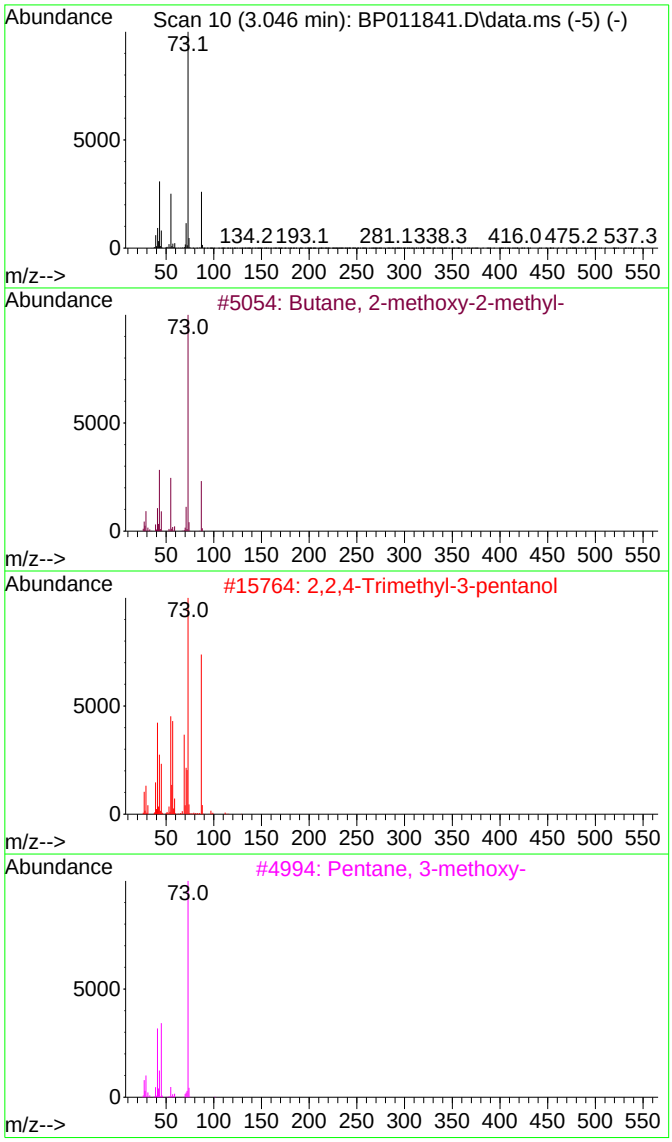
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

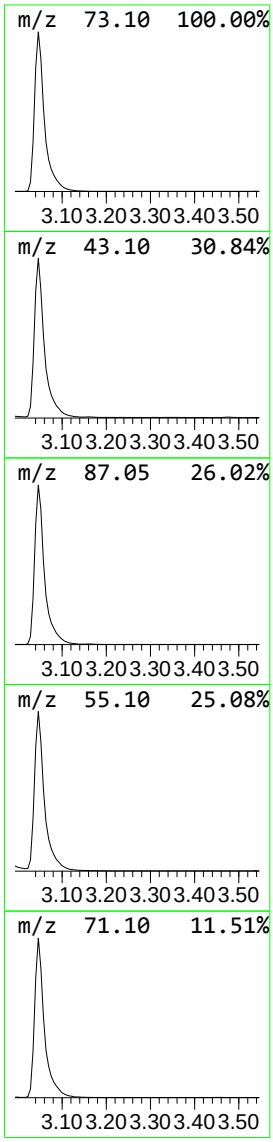
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.046	108.87 ng	12424300	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	43
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9





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Acq On : 29 Sep 2022 15:01
Operator : CG/JU
Sample : N4860-10
Misc :
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Instrument :
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ClientSampleId :
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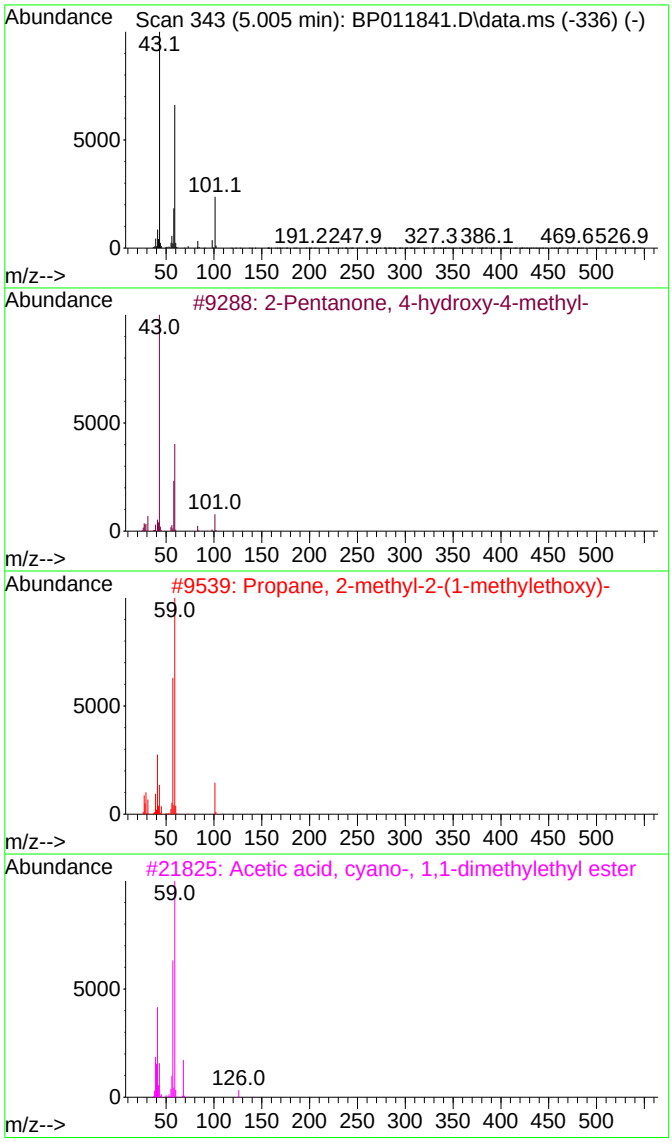
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

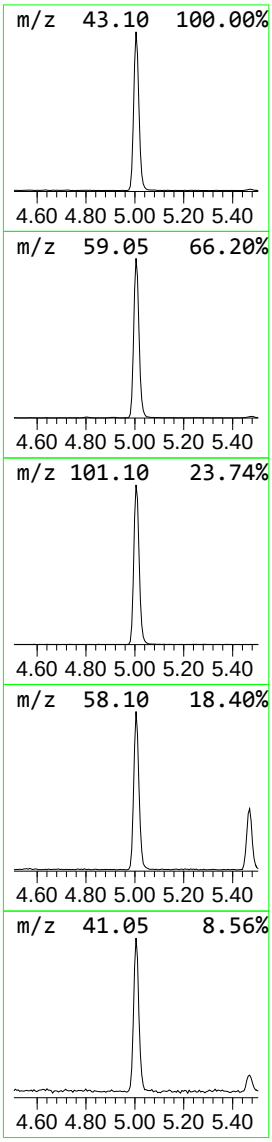
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.005	10.54 ng	1203000	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	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	50
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Guanidine	59	CH5N3	000113-00-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Data File : BP011841.D
Acq On : 29 Sep 2022 15:01
Operator : CG/JU
Sample : N4860-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

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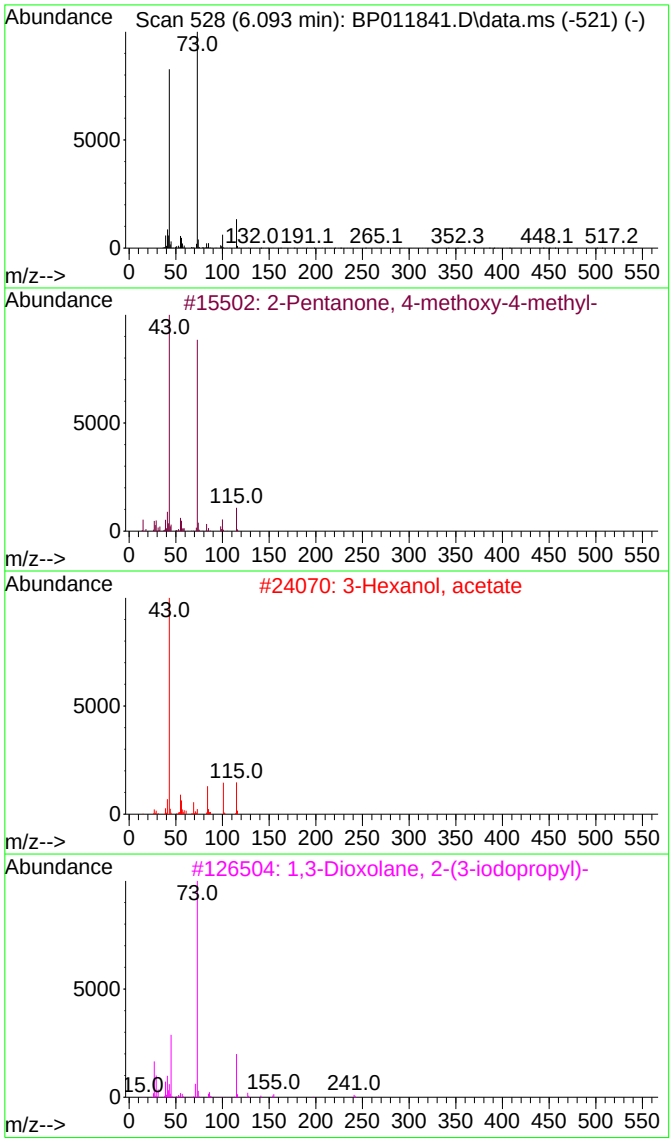
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

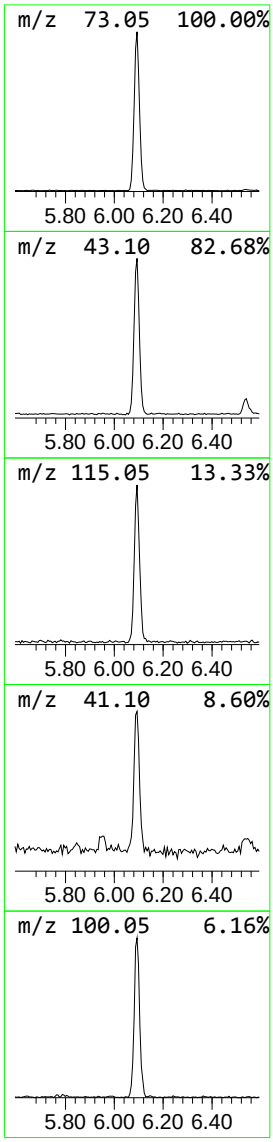
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.093	2.78 ng	316721	1,4-Dichlorobenzene-d4	7.911

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	3-Hexanol, acetate	144	C8H16O2	040780-64-1	37
3	1,3-Dioxolane, 2-(3-iodopropyl)-	242	C6H11IO2	058135-25-4	25
4	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	16
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	16





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Data File : BP011841.D
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Sample : N4860-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
EB-2022-09-27

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
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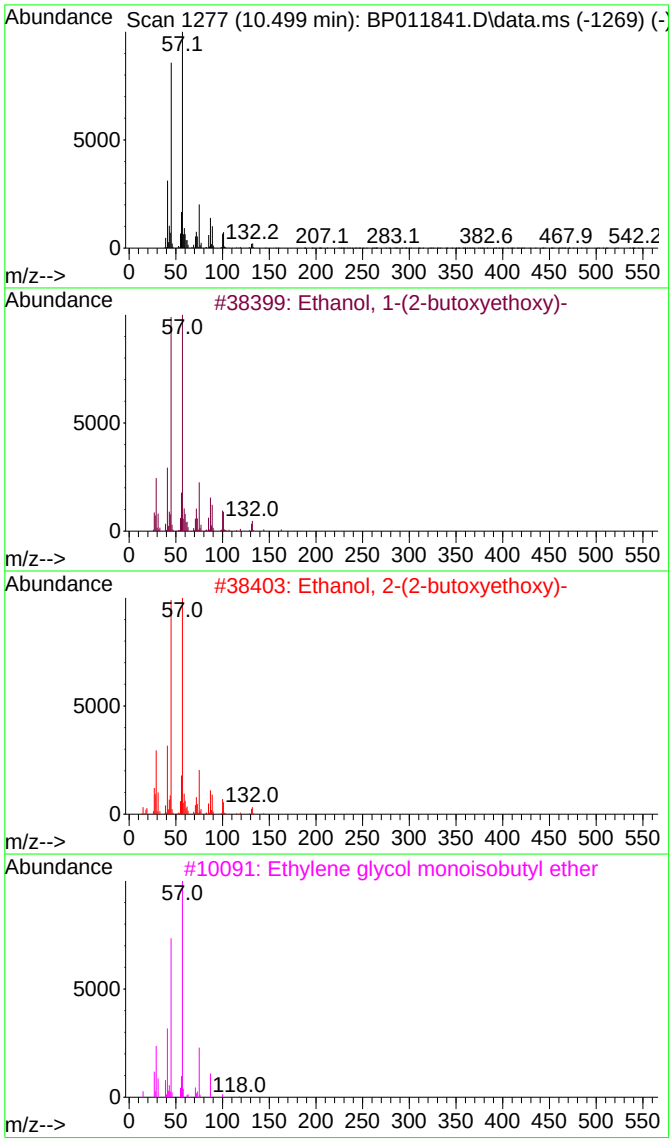
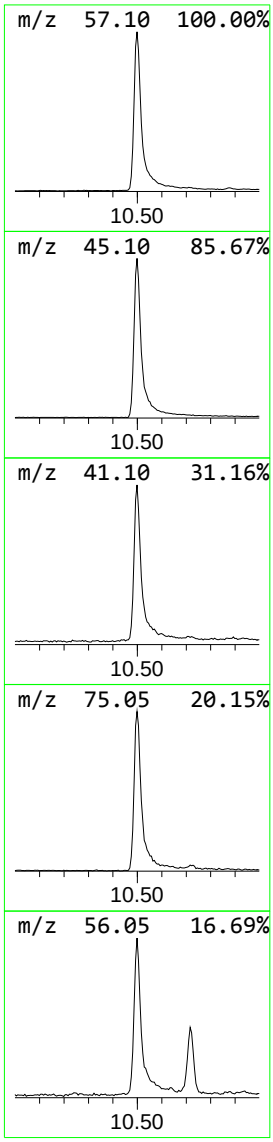
****

Peak Number 4 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.499	8.04 ng	1377780	Naphthalene-d8	10.722

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
2	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50





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Instrument :
BNA_P
ClientSampleId :
EB-2022-09-27

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

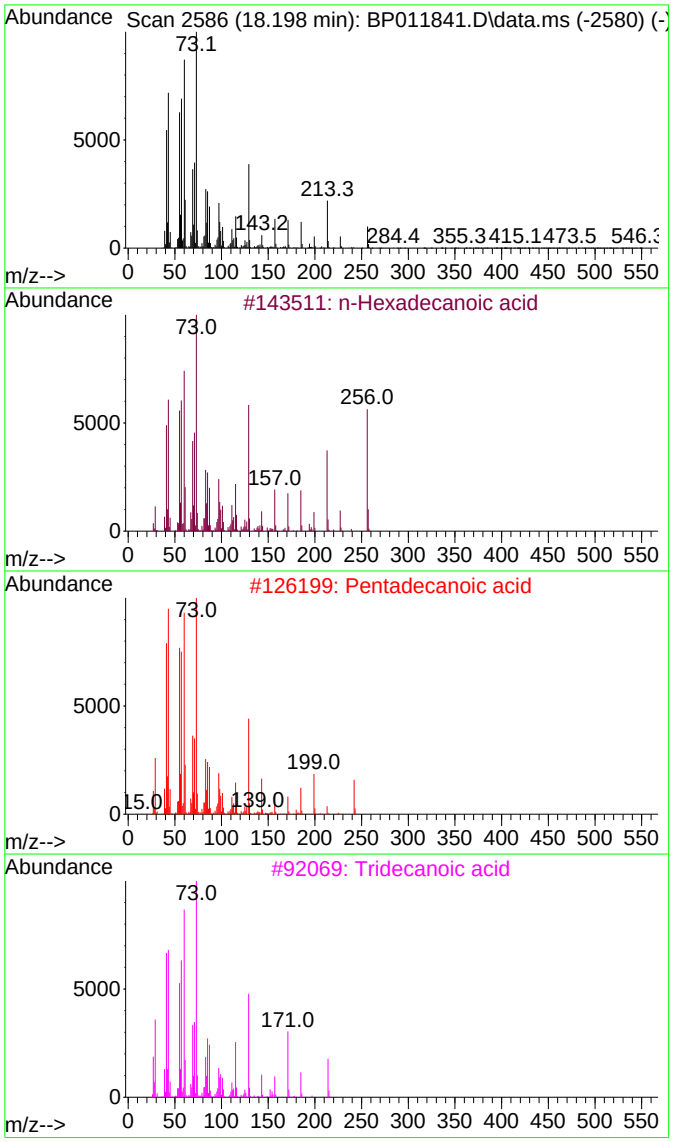
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

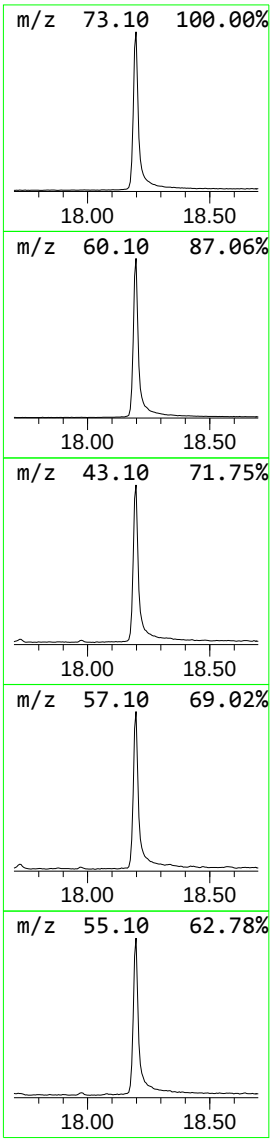
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.198	22.61 ng	5835510	Phenanthrene-d10	17.310

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	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	92
4	n-Decanoic acid	172	C10H20O2	000334-48-5	68
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	68





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Instrument :
BNA_P
ClientSampleId :
EB-2022-09-27

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

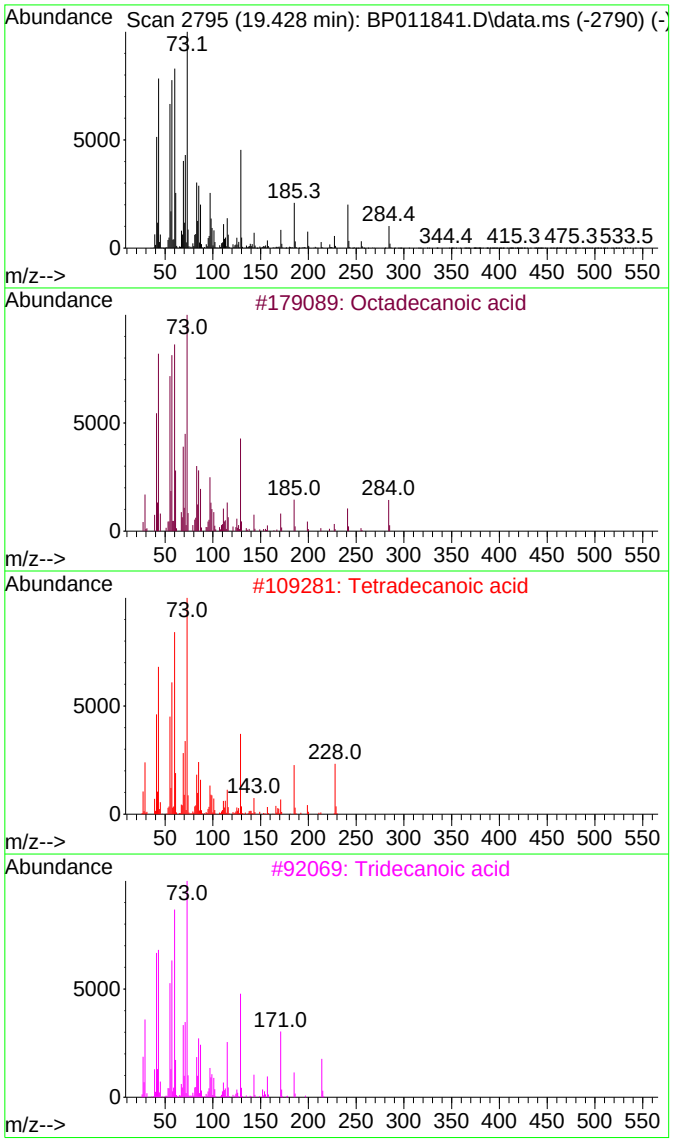
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

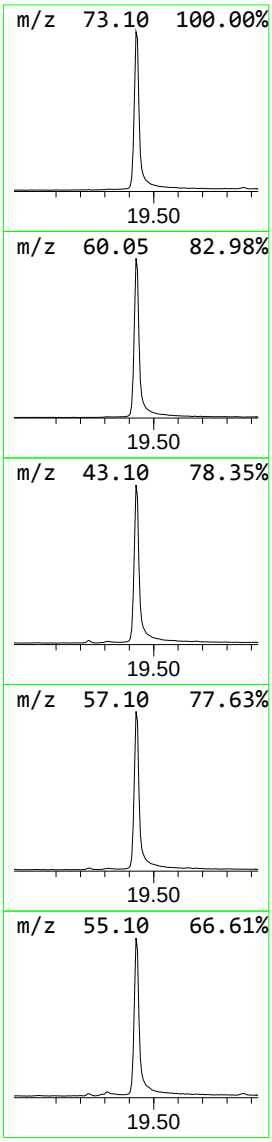
****

Peak Number 6 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.428	41.17 ng	12106100	Chrysene-d12	21.392

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	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	74
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	72





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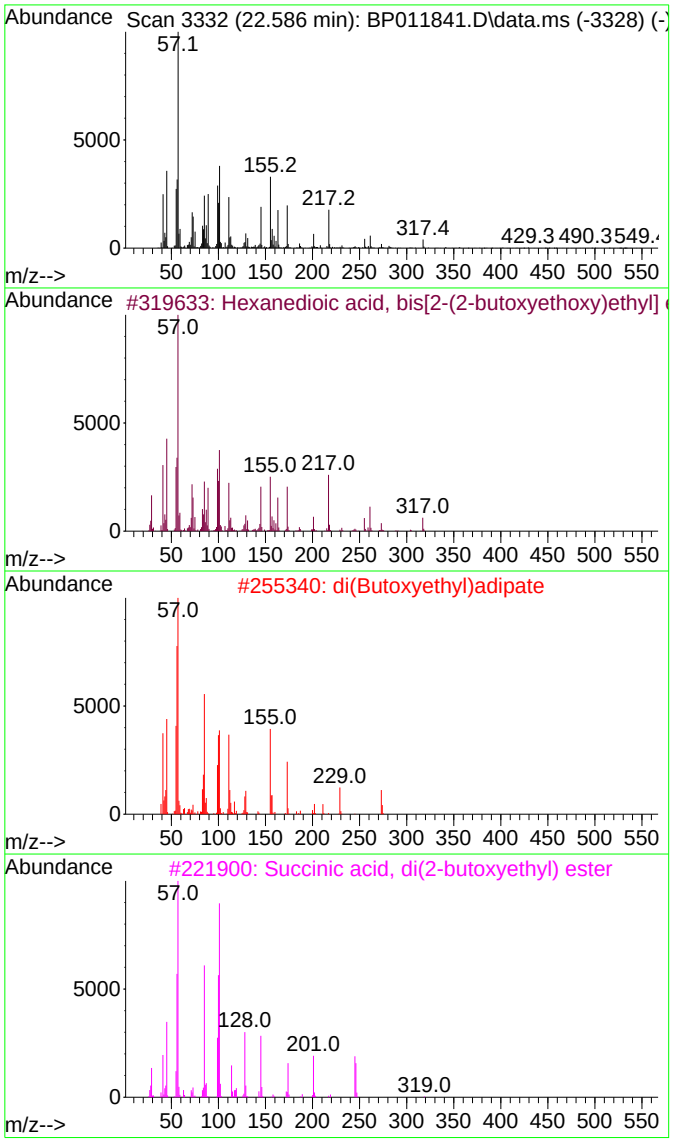
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

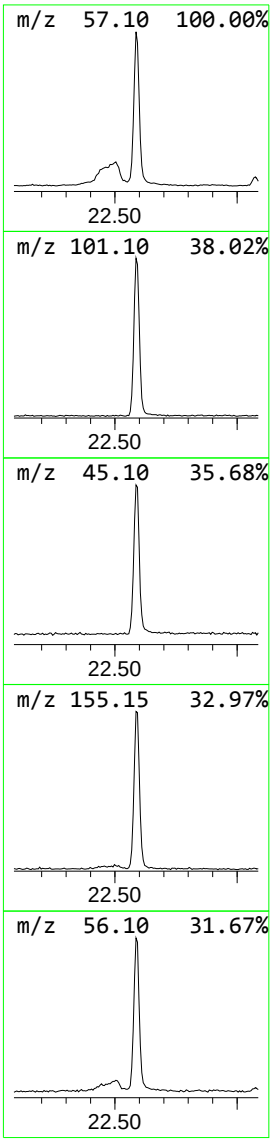
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Hexanedioic acid, bis[2-(2-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.586	6.50 ng	1910730	Chrysene-d12	21.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, bis[2-(2-butox...	434	C22H42O8	000141-17-3	90
2	di(Butoxyethyl)adipate	346	C18H34O6	000141-18-4	12
3	Succinic acid, di(2-butoxyethyl)...	318	C16H30O6	1010325-84-7	12
4	Imidazole, 5-t-buyloxycarbonylam...	201	C8H12FN3O2	330953-79-2	10
5	3,5-Difluorothiophenol, S-trimet...	230	C11H12F2OS	1000470-53-4	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092922\
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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
Butane, 2-metho...	3.046	108.9	ng	12424300	1	7.911	2282410	20.0
2-Pentanone, 4-...	5.005	10.5	ng	1203000	1	7.911	2282410	20.0
2-Pentanone, 4-...	6.093	2.8	ng	316721	1	7.911	2282410	20.0
Ethanol, 1-(2-b...	10.499	8.0	ng	1377780	2	10.722	3428090	20.0
n-Hexadecanoic ...	18.198	22.6	ng	5835510	4	17.310	5160900	20.0
Octadecanoic acid	19.428	41.2	ng	12106100	5	21.392	5881330	20.0
Hexanedioic aci...	22.586	6.5	ng	1910730	5	21.392	5881330	20.0