LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
Data File : BP006549.D
Acq On : 06 Aug 2021 21:04
Operator : CG/JU
Sample : M3278-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : MW-4

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: BP006549.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.904	305	309	318	rVB	612235	850781	6.44%	1.504%
2	5.357	380	386	393	rBV	2250398	3179440	24.07%	5.622%
3	5.969	485	490	497	rVB	351552	518200	3.92%	0.916%
4	6.934	647	654	665	rVB	1266460	1972700	14.93%	3.488%
5	7.751	787	793	801	rVB	789841	1234664	9.35%	2.183%
6	8.910	983	990	1000	rVB	2984340	4839642	36.63%	8.557%
7	10.328	1224	1231	1241	rBV	494017	783695	5.93%	1.386%
8	10.533	1259	1266	1273	rBV	1019386	1673570	12.67%	2.959%
9	13.010	1679	1687	1699	rBV	6429271	9285714	70.28%	16.418%
10	14.380	1909	1920	1931	rBV	1364648	1987246	15.04%	3.514%
11	15.874	2164	2174	2183	rBV	4648244	6631367	50.19%	11.725%
12	17.133	2381	2388	2399	rBV	1645539	2245258	16.99%	3.970%
13	17.827	2500	2506	2511	rBV	151993	195101	1.48%	0.345%
14	18.039	2537	2542	2551	rBV2	301566	445036	3.37%	0.787%
15	18.962	2695	2699	2703	rVB	465712	529338	4.01%	0.936%
16	19.274	2749	2752	2762	rBV	158321	228790	1.73%	0.405%
17	19.709	2820	2826	2831	rBV	11271458	13211606	100.00%	23.360%
18	20.956	3034	3038	3043	rBV	158063	224865	1.70%	0.398%
19	21.227	3079	3084	3092	rBV	2004875	2589459	19.60%	4.578%
20	22.403	3280	3284	3292	rVB	807301	1121790	8.49%	1.983%
21	23.556	3473	3480	3492	rVB2	1394387	2808917	21.26%	4.967%

Sum of corrected areas: 56557179

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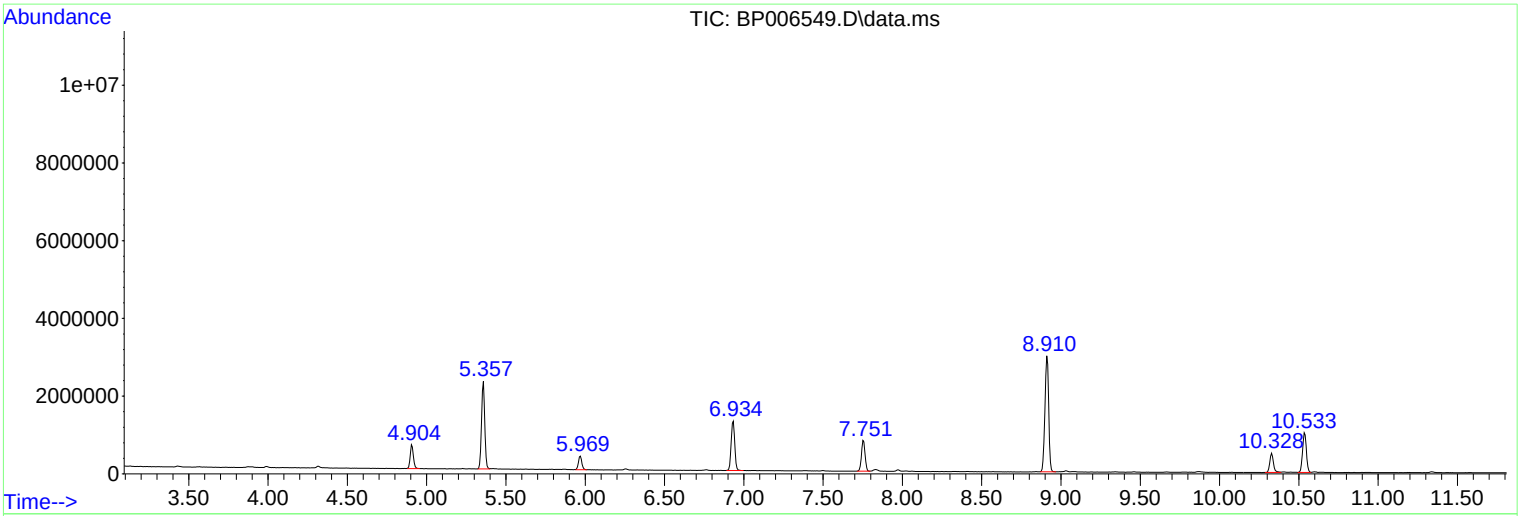
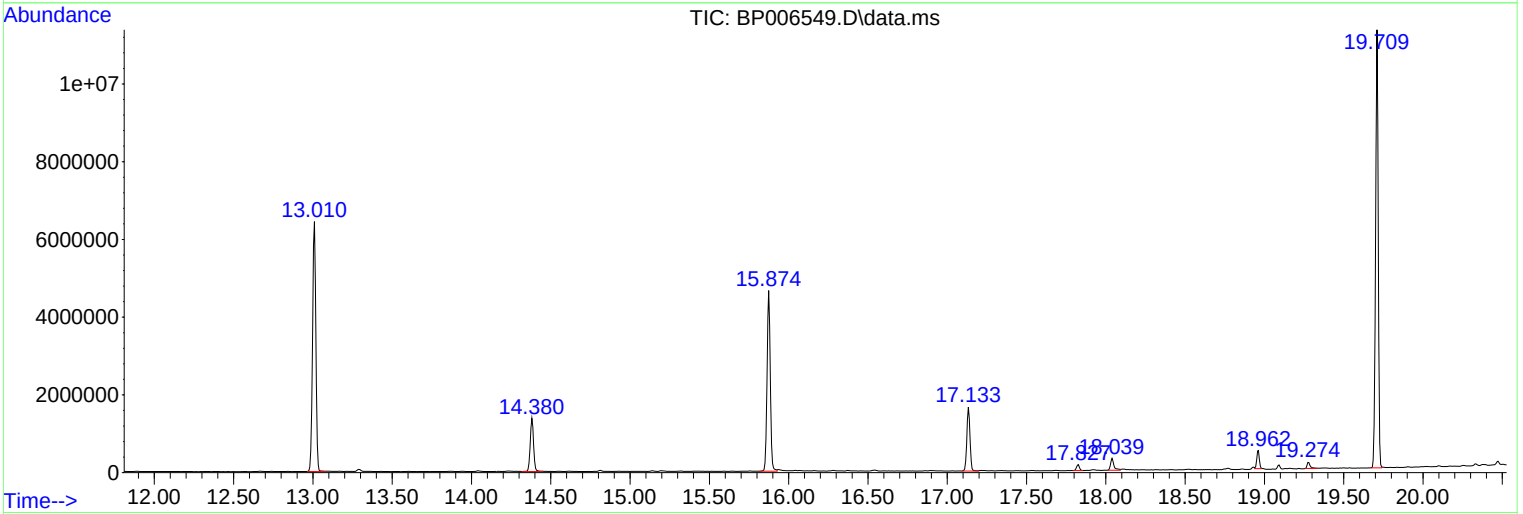
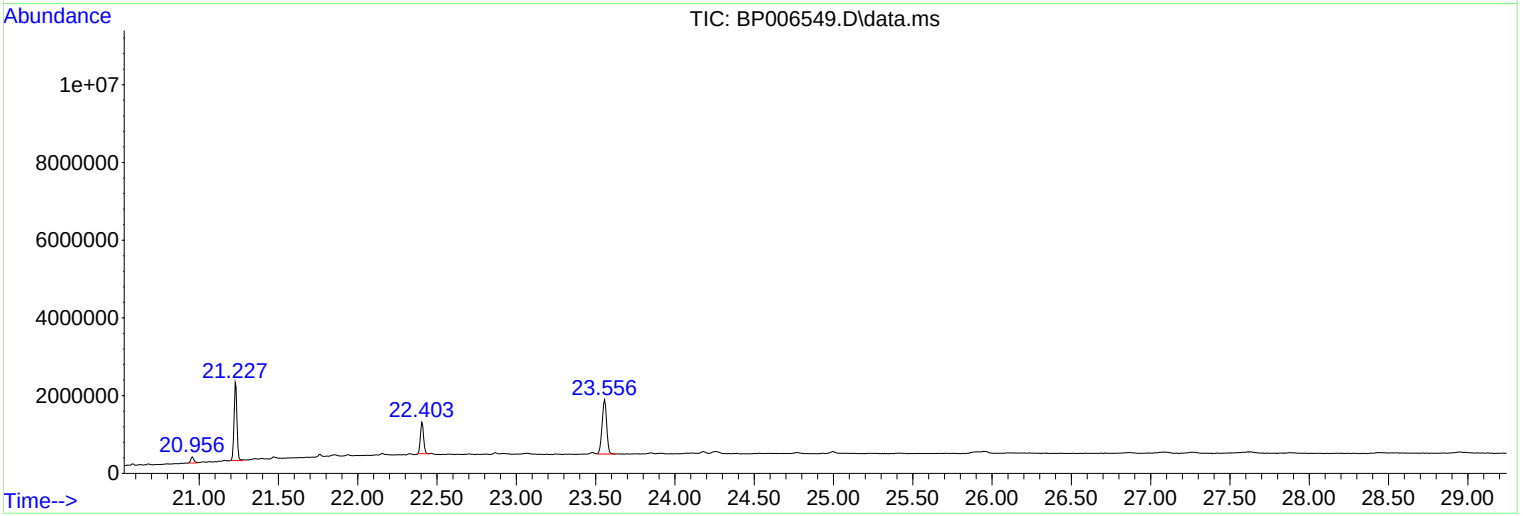
Instrument :
BNA_P
ClientSampleId :
MW-4

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







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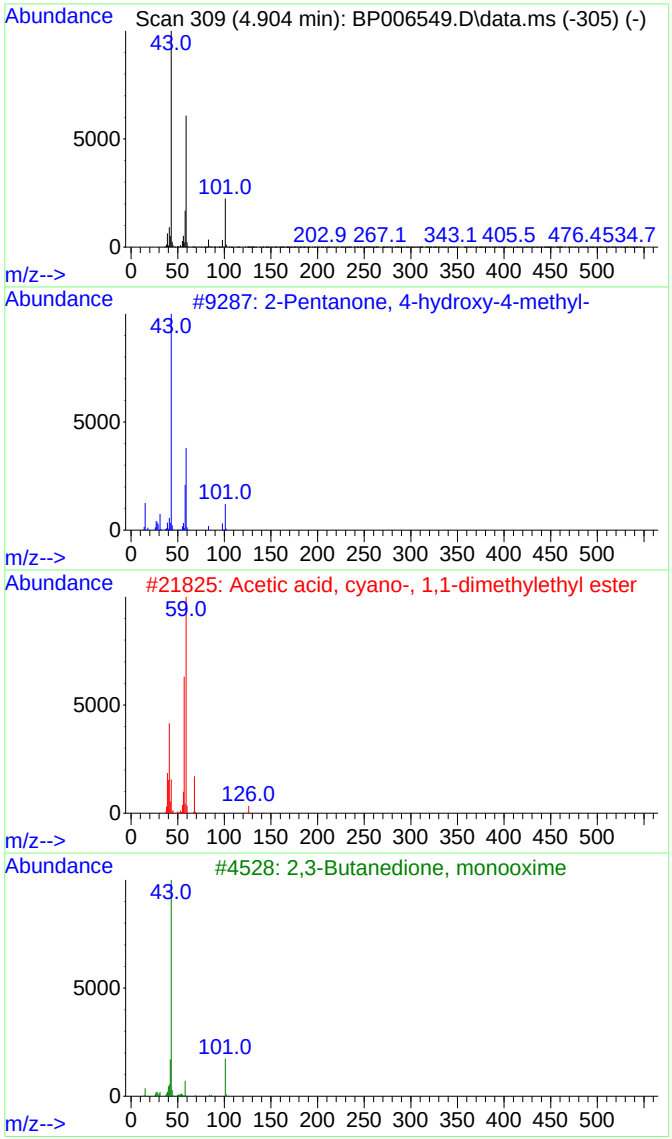
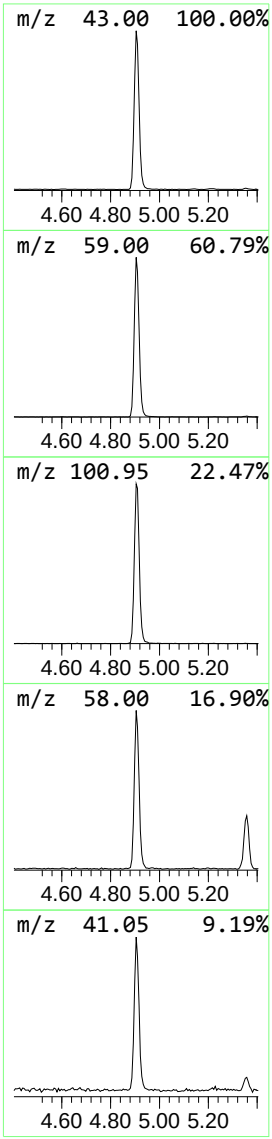
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.904	13.78 ng	850781	1,4-Dichlorobenzene-d4	7.751

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	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
4	Acetone	58	C3H6O	000067-64-1	10
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





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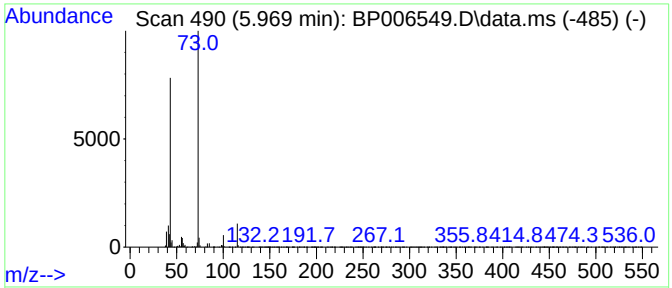
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

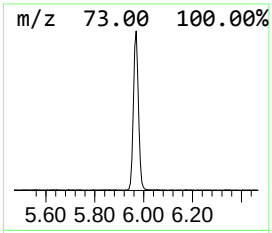
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

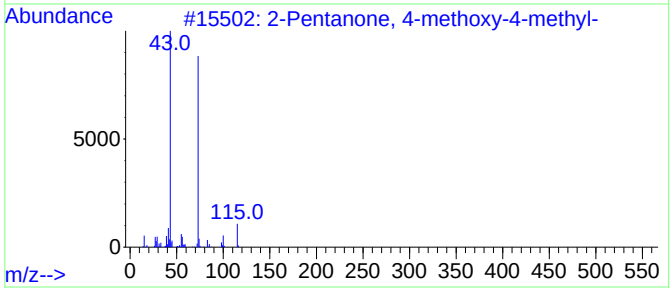
****
Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 3

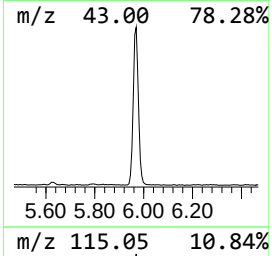
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.969	8.39 ng	518200	1,4-Dichlorobenzene-d4	7.751

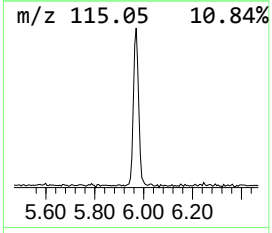
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	3-Hexanol, acetate	144	C8H16O2	040780-64-1	38
3	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	33
4	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	12
5	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10

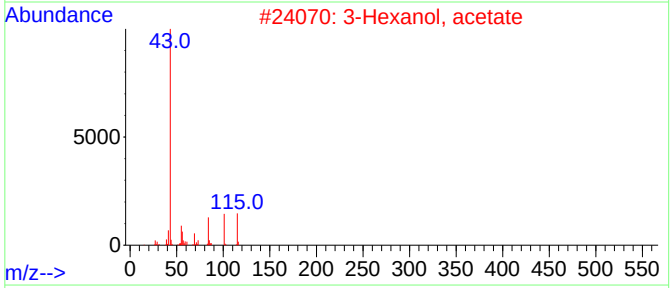


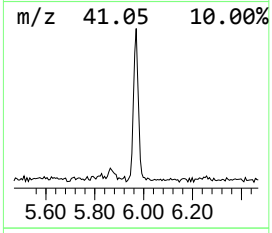


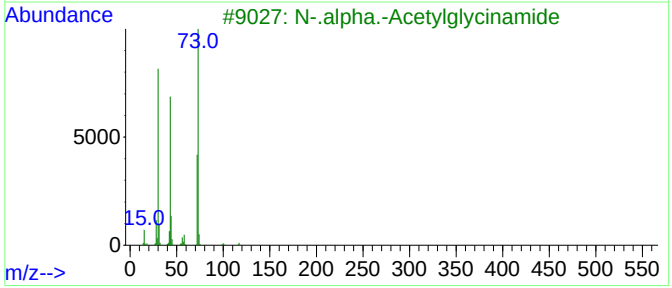


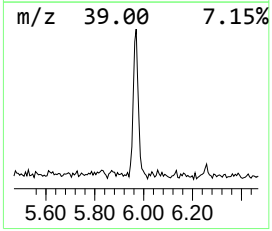












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Acq On : 06 Aug 2021 21:04
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Sample : M3278-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-4

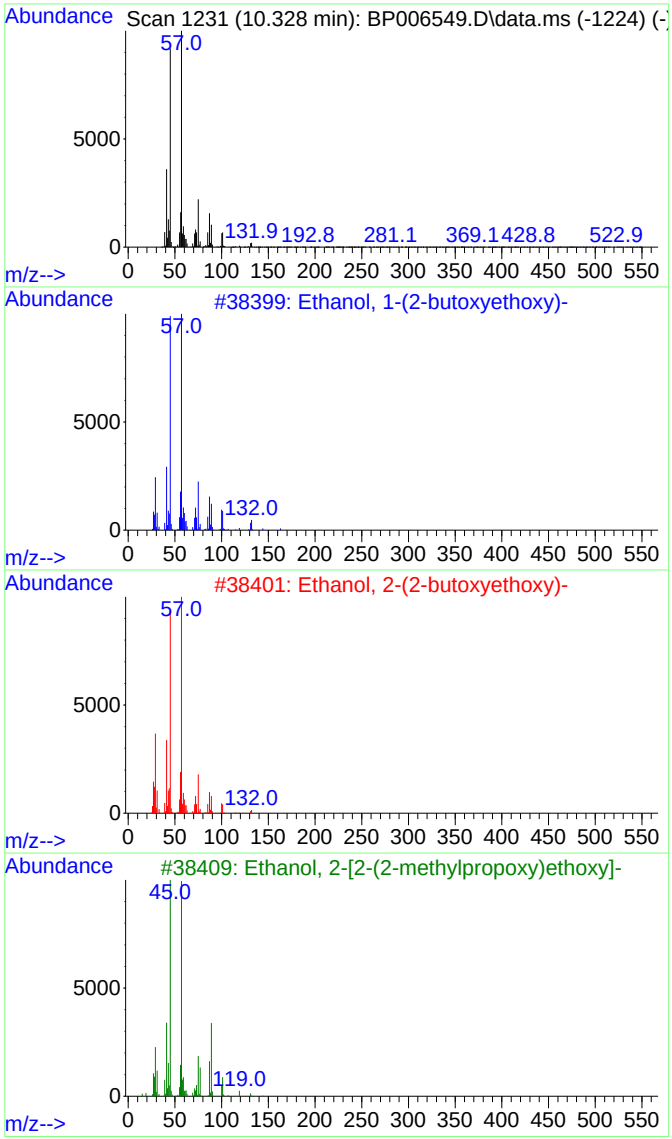
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

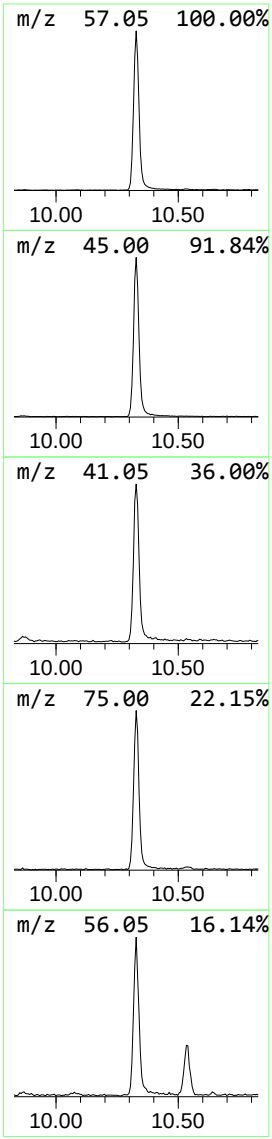
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.328	9.37 ng	783695	Naphthalene-d8	10.534

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	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	52





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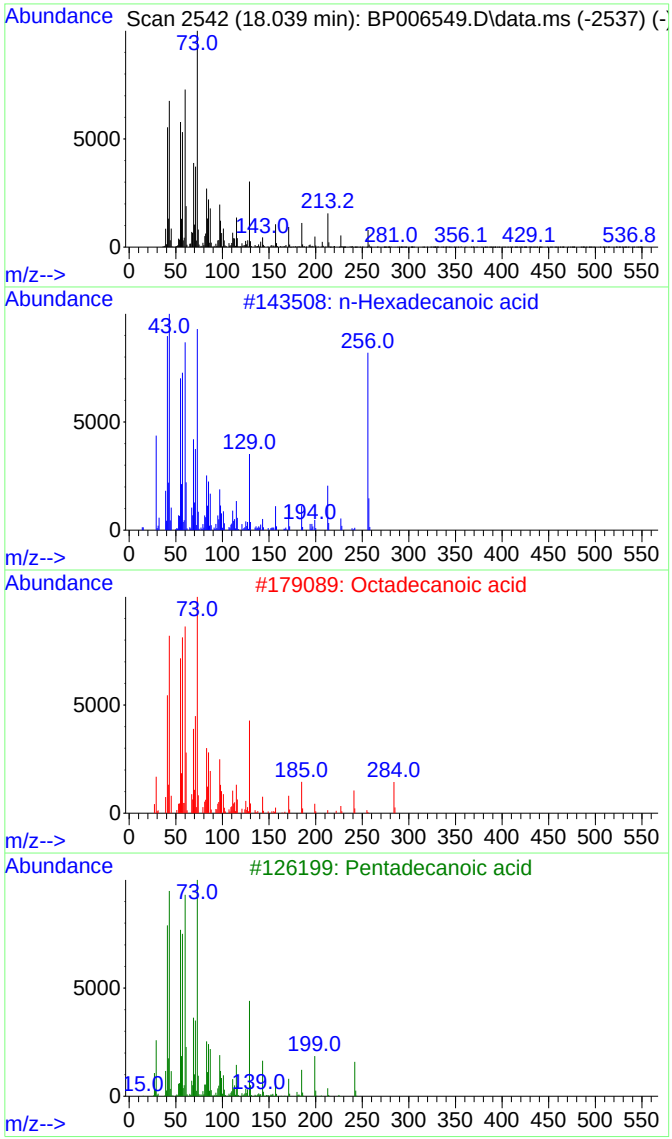
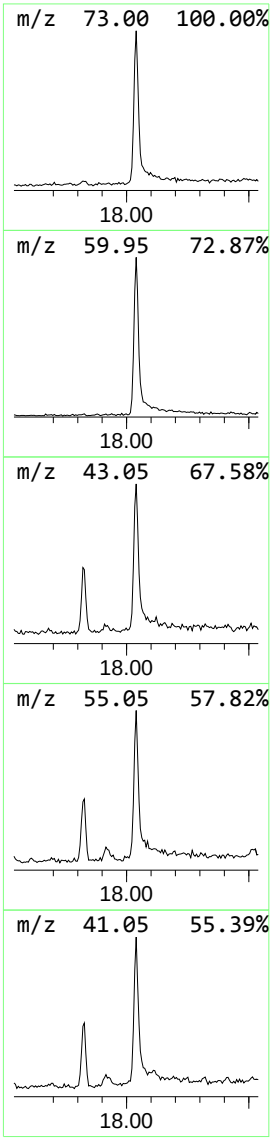
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.039	3.96 ng	445036	Phenanthrene-d10	17.133

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	76
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Nonanoic acid	158	C9H18O2	000112-05-0	38
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	38





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Sample : M3278-02
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ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : MW-4

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
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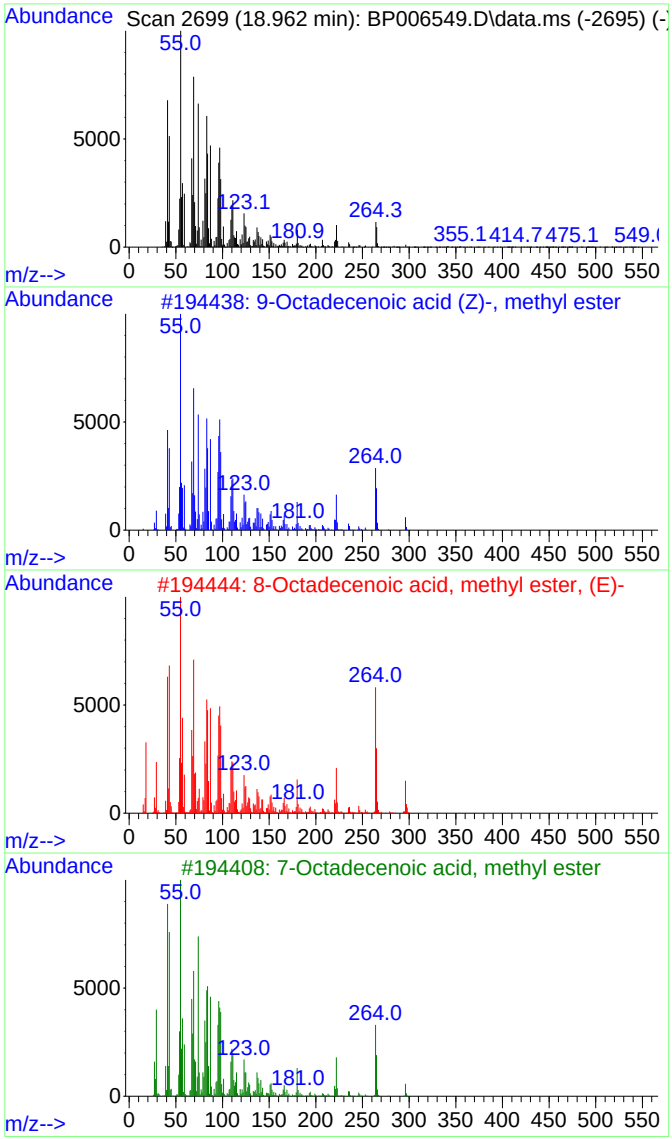
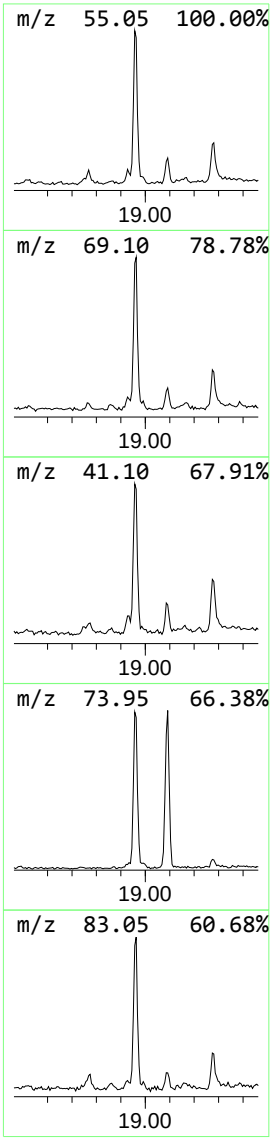
****
Peak Number 5 9-Octadecenoic acid (Z)-, m... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.962	4.72 ng	529338	Phenanthrene-d10	17.133

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	8-Octadecenoic acid, methyl este...	296	C19H36O2	026528-50-7	99
3	7-Octadecenoic acid, methyl ester	296	C19H36O2	057396-98-2	99
4	8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	99
5	6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	98





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TIC Library : C:\Database\NIST20.L
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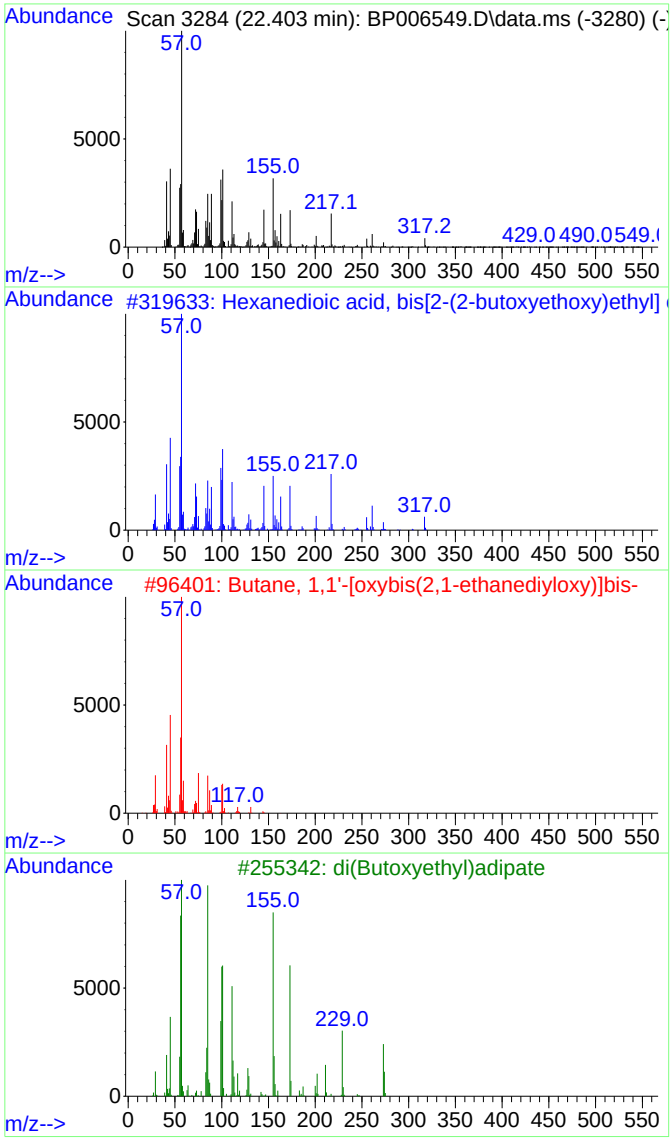
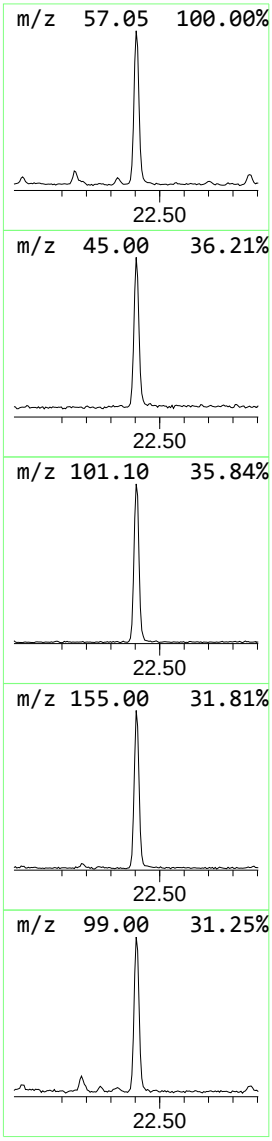
****
Peak Number 6 Hexanedioic acid, bis[2-(2-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.403	7.99 ng	1121790	Perylene-d12	23.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, bis[2-(2-butox...	434	C22H42O8	000141-17-3	90
2	Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	27
3	di(Butoxyethyl)adipate	346	C18H34O6	000141-18-4	23
4	5,8,12,15-Tetraoxanonadecane, 10...	304	C17H36O4	1000159-84-9	12
5	3,5-Difluorothiophenol, S-trimet...	230	C11H12F2OS	1000470-53-4	11





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	4.904	13.8	ng	850781	1	7.751	1234660	20.0
2-Pentanone, 4-...	5.969	8.4	ng	518200	1	7.751	1234660	20.0
Ethanol, 1-(2-b...	10.328	9.4	ng	783695	2	10.534	1673570	20.0
n-Hexadecanoic ...	18.039	4.0	ng	445036	4	17.133	2245260	20.0
9-Octadecenoic ...	18.962	4.7	ng	529338	4	17.133	2245260	20.0
Hexanedioic aci...	22.403	8.0	ng	1121790	6	23.556	2808920	20.0