

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092421\
 Data File : BP007166.D
 Acq On : 24 Sep 2021 19:23
 Operator : CG/JU
 Sample : M3775-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 PE-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-BP092121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP007166.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.999	320	325	333	rBV	305656	422202	4.18%	0.749%
2	5.464	397	404	419	rBV	3081783	4565108	45.16%	8.102%
3	7.058	667	675	696	rBV	2909916	4623015	45.73%	8.204%
4	7.887	807	816	823	rBV	936424	1480973	14.65%	2.628%
5	9.046	1005	1013	1026	rBV	1778562	2978017	29.46%	5.285%
6	10.475	1250	1256	1268	rBV	148251	307772	3.04%	0.546%
7	10.687	1281	1292	1305	rBV	1256095	2108741	20.86%	3.742%
8	13.146	1702	1710	1724	rBV	4830095	7137414	70.60%	12.667%
9	14.369	1911	1918	1935	rBV2	148666	413721	4.09%	0.734%
10	14.516	1937	1943	1953	rVB	1857816	2749756	27.20%	4.880%
11	16.010	2190	2197	2212	rVB	3780215	5576604	55.16%	9.897%
12	17.269	2404	2411	2416	rBV	2222845	3178614	31.44%	5.641%
13	18.157	2557	2562	2583	rBV	971219	1542223	15.25%	2.737%
14	19.275	2748	2752	2760	rVB	153114	194876	1.93%	0.346%
15	19.386	2767	2771	2783	rBV	474205	735885	7.28%	1.306%
16	19.628	2809	2812	2820	rVB	130374	180760	1.79%	0.321%
17	19.828	2840	2846	2851	rBV	8062531	10109728	100.00%	17.941%
18	21.063	3052	3056	3064	rBV	683644	880550	8.71%	1.563%
19	21.351	3100	3105	3110	rBV	2782694	3547779	35.09%	6.296%
20	23.763	3508	3515	3524	rVB2	1782060	3614822	35.76%	6.415%

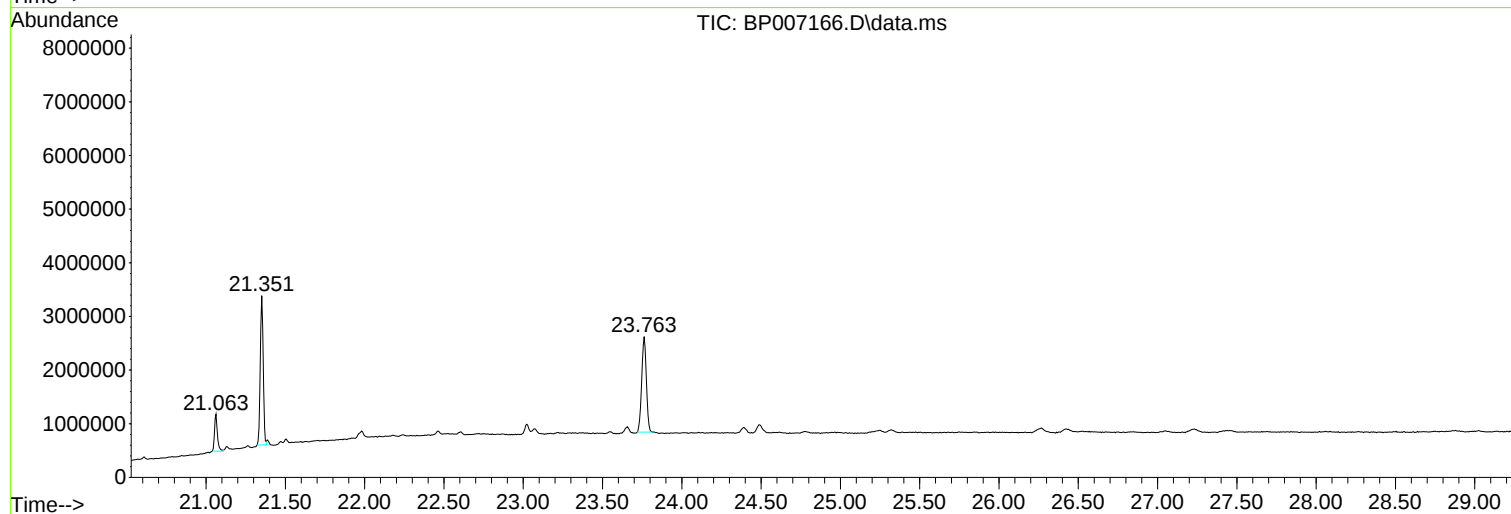
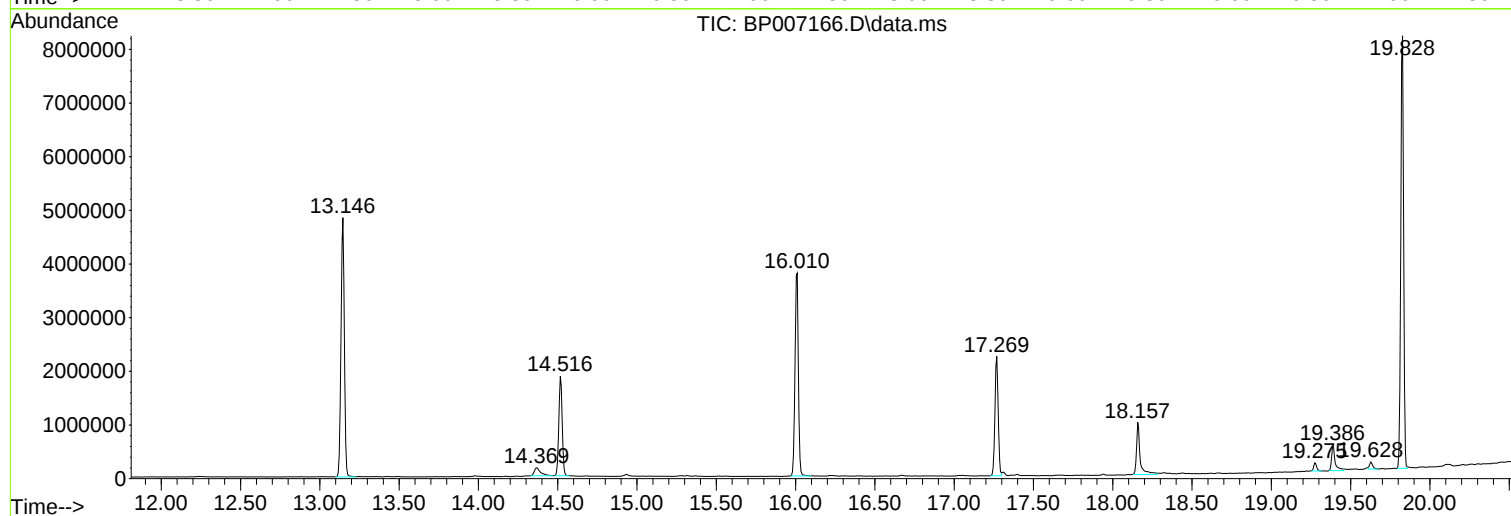
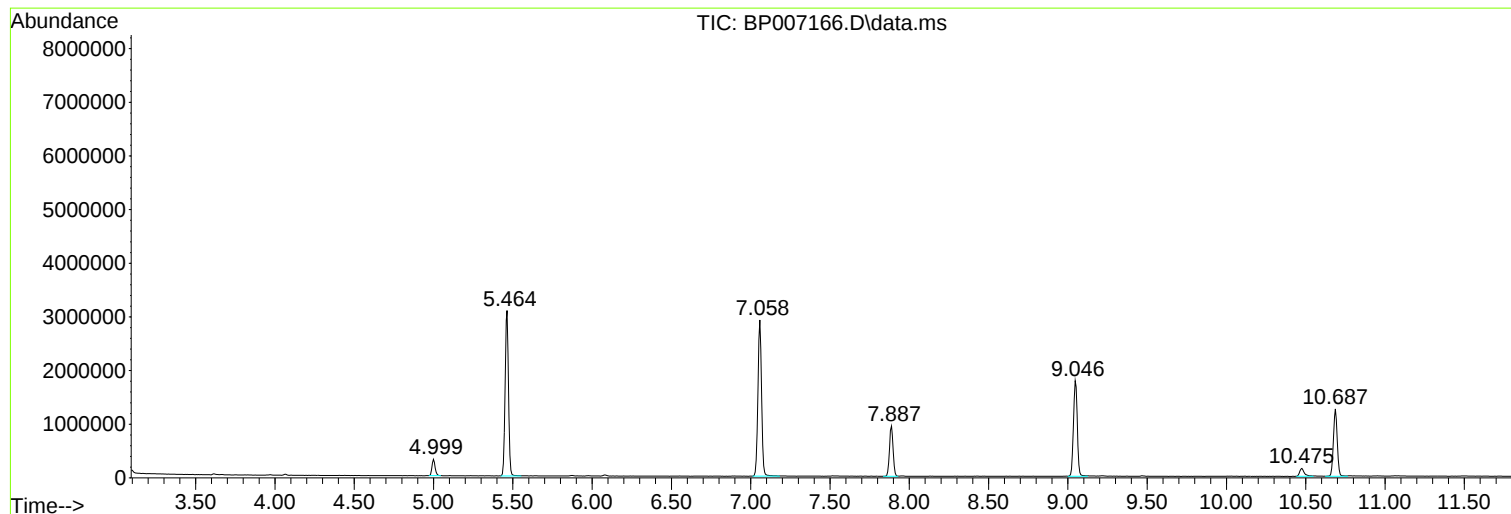
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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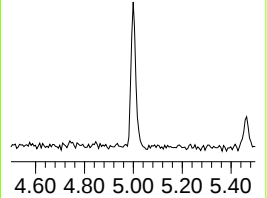
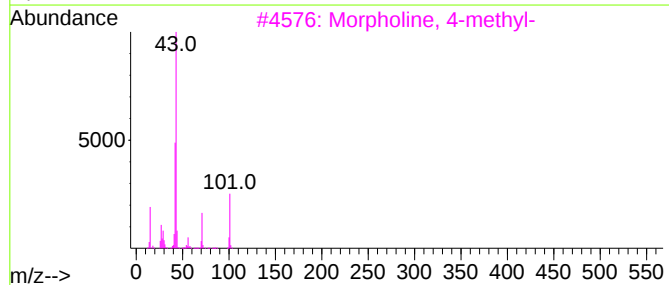
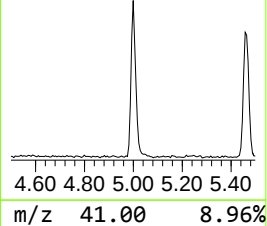
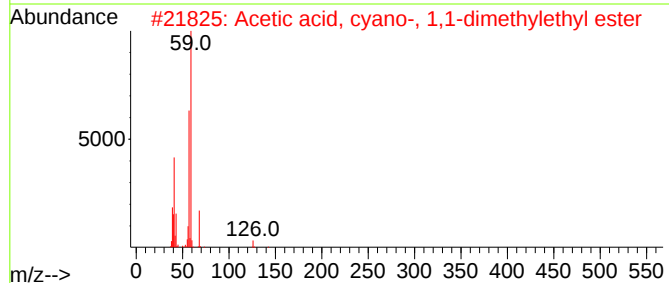
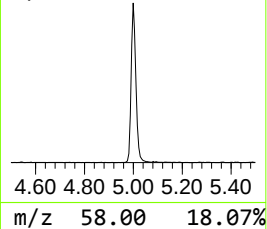
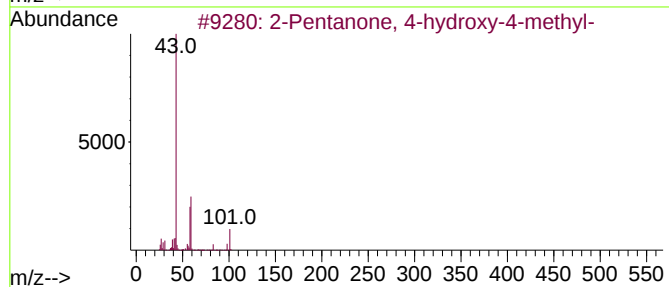
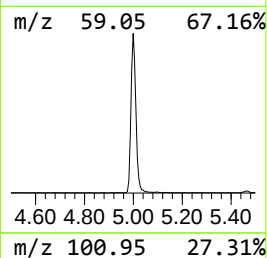
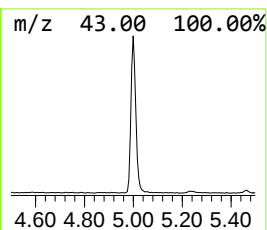
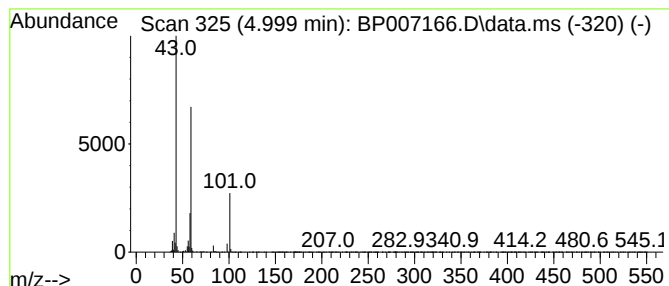
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.999	5.70 ng	422202	1,4-Dichlorobenzene-d4	7.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
4	Guanidine	59	CH5N3	000113-00-8	9		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		



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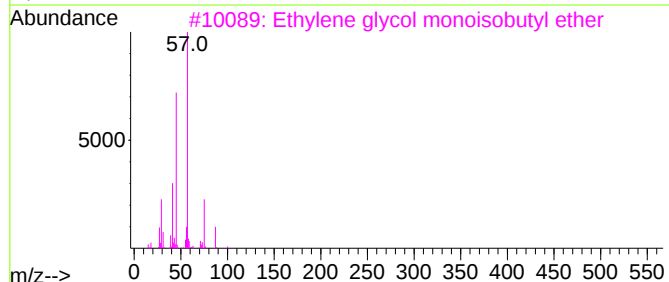
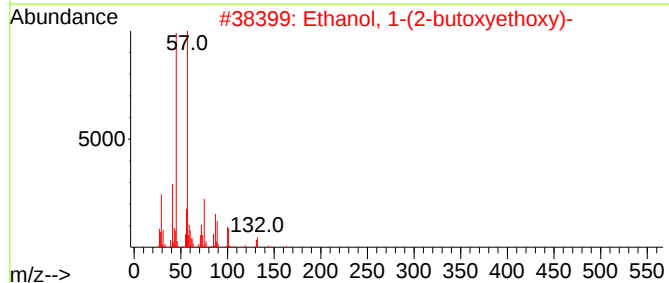
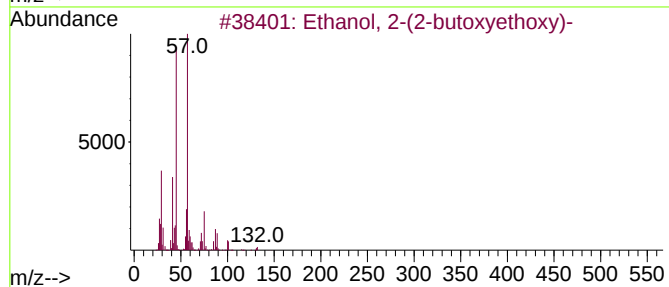
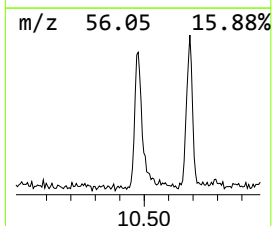
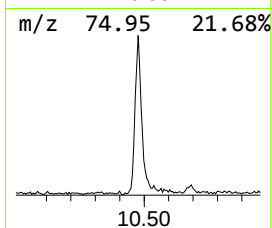
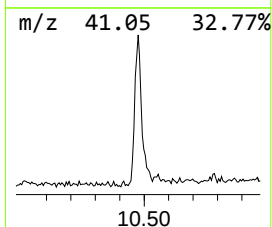
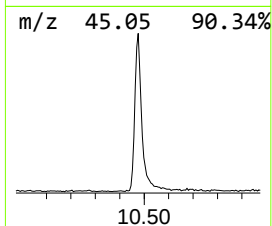
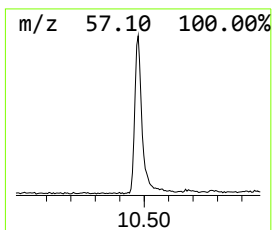
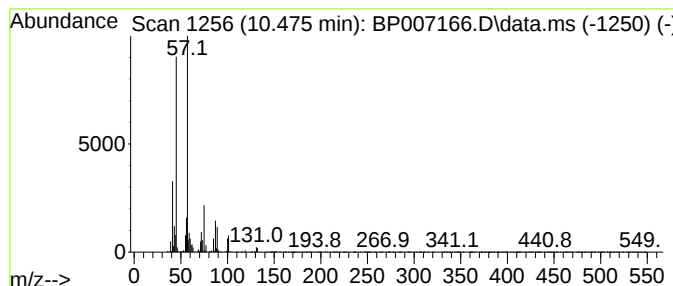
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.475	2.92 ng	307772	Naphthalene-d8	10.687

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	90
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
5			3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	53



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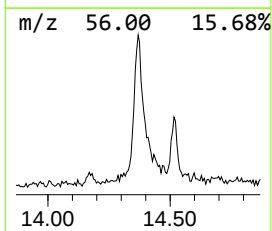
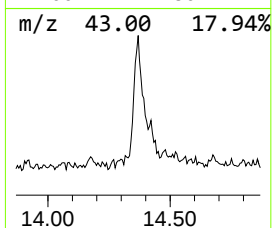
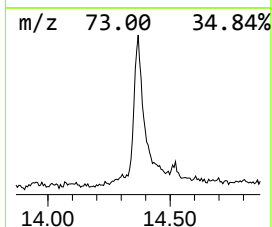
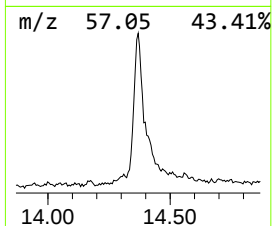
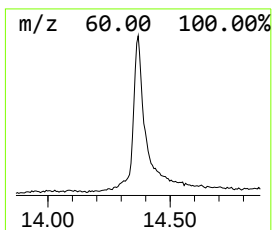
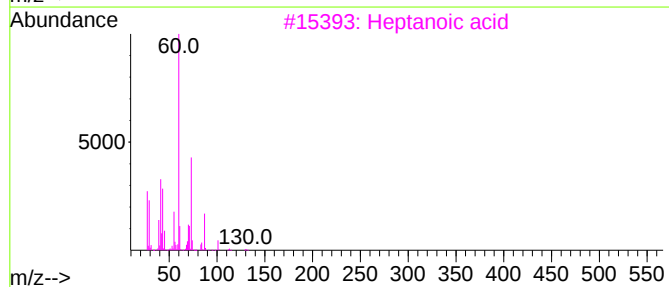
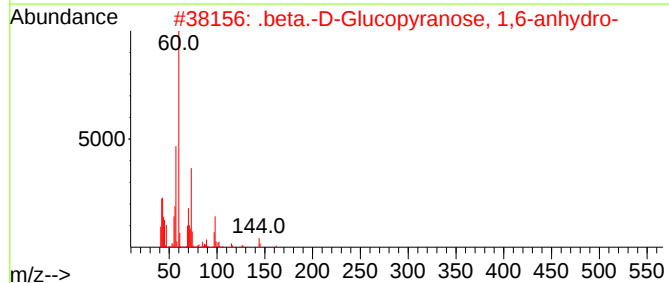
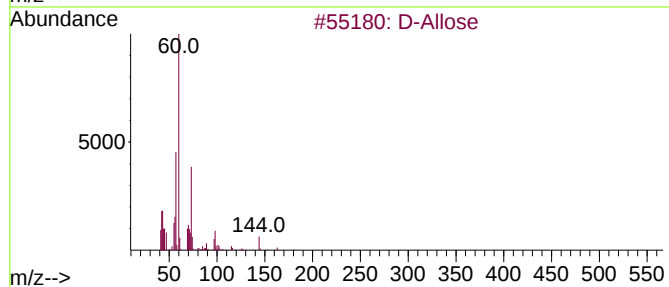
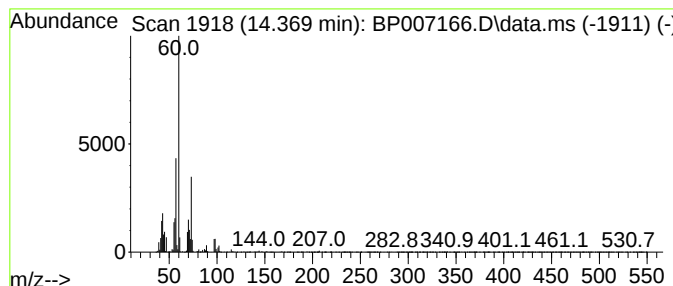
Instrument :
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Peak Number 3 D-Allose Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.369	3.01 ng	413721	Acenaphthene-d10		14.516	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	D-Allose		180	C6H12O6	002595-97-3	90
2	.beta.-D-Glucopyranose, 1,6-anhy...		162	C6H10O5	000498-07-7	83
3	Heptanoic acid		130	C7H14O2	000111-14-8	64
4	3,4-Altrosan		162	C6H10O5	1000129-76-4	58
5	Pentanoic acid		102	C5H10O2	000109-52-4	50



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BNA_P
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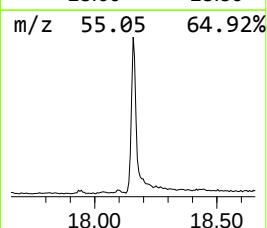
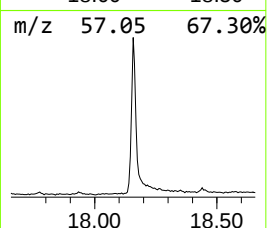
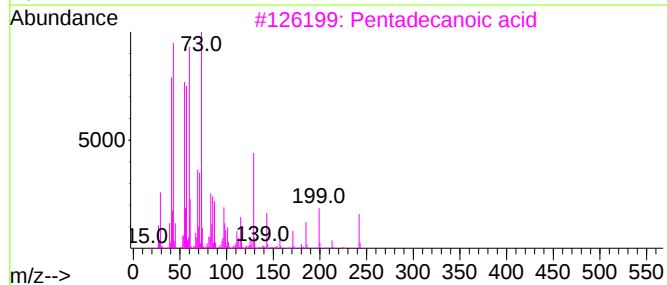
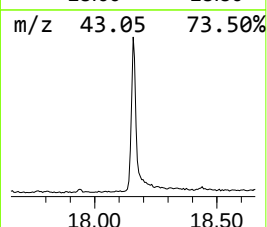
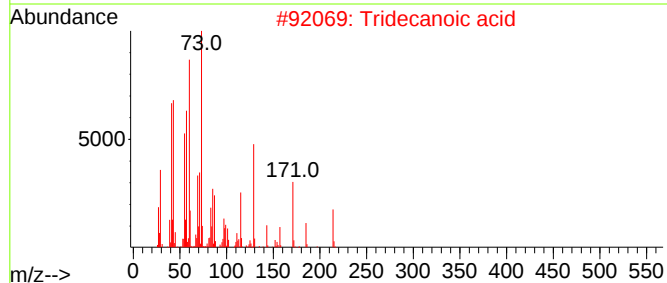
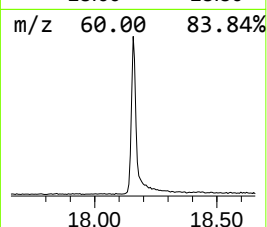
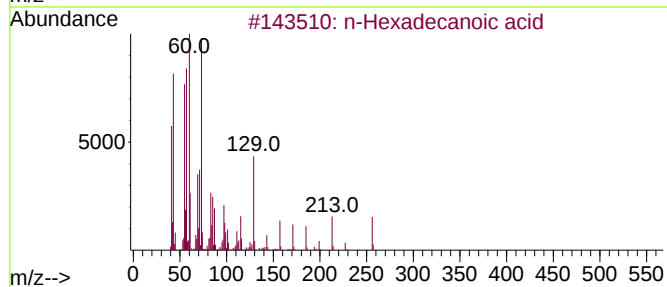
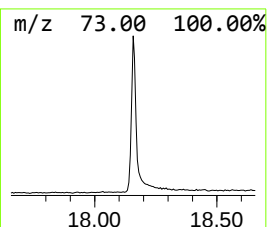
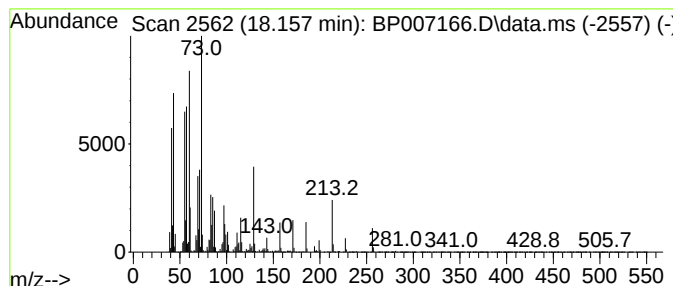
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.157	9.70 ng	1542220	Phenanthrene-d10	17.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
5			n-Decanoic acid	172	C10H20O2	000334-48-5	76



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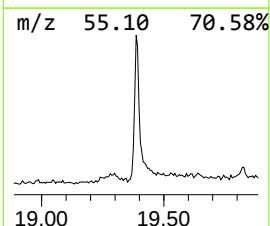
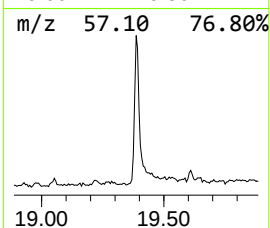
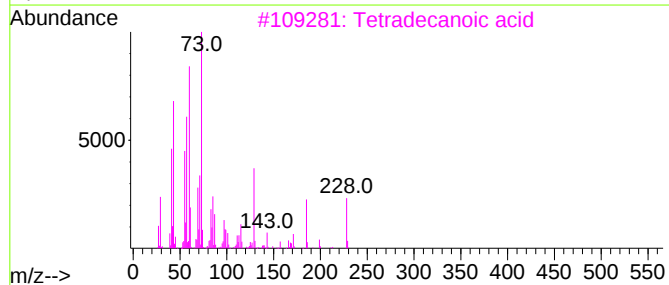
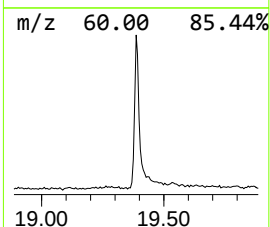
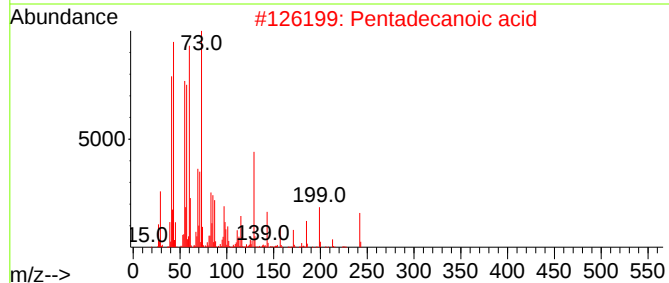
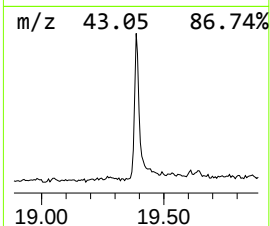
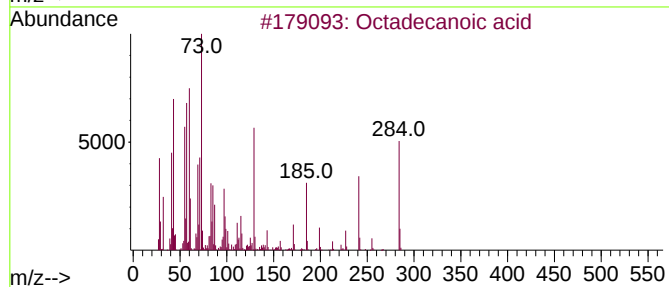
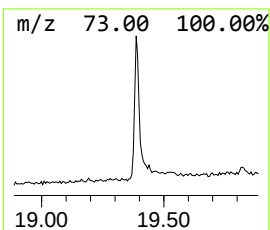
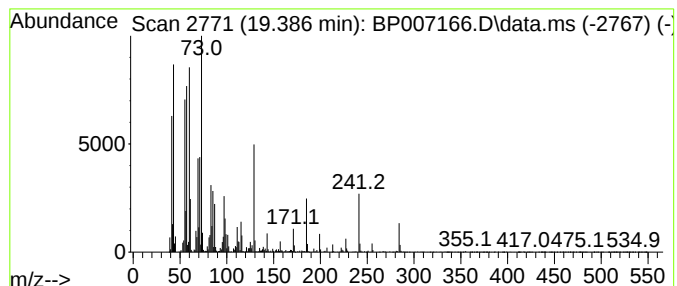
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Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.386	4.15 ng	735885	Chrysene-d12	21.351

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			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
5			n-Decanoic acid	172	C10H20O2	000334-48-5	78



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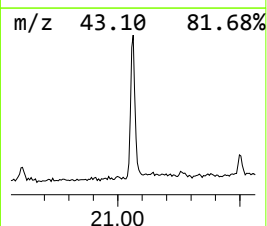
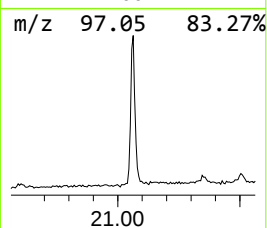
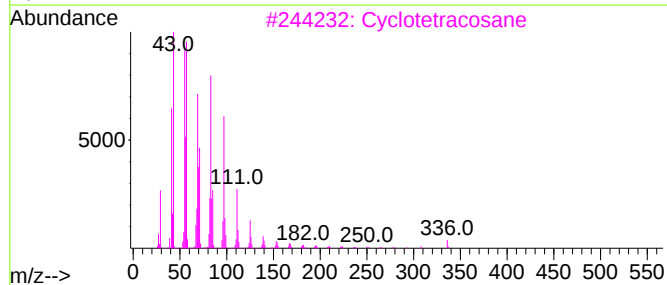
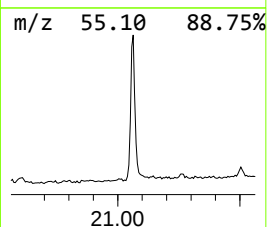
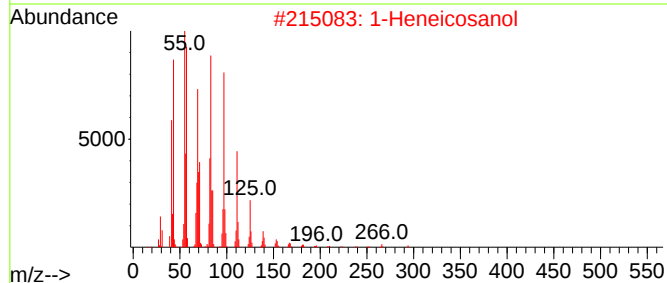
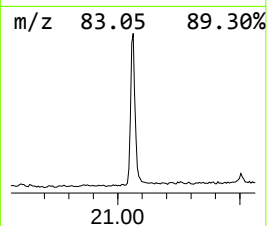
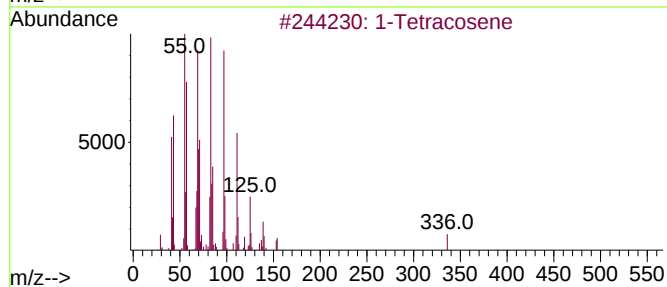
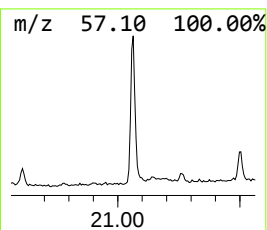
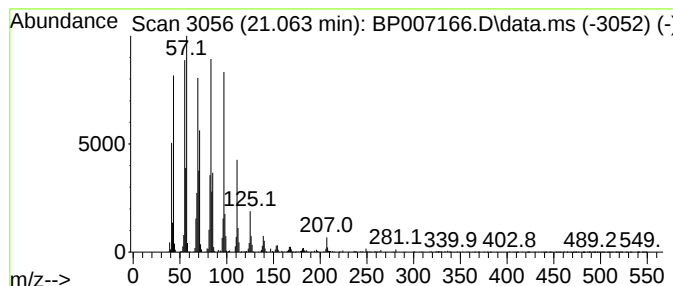
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Tetracosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.063	4.96 ng	880550	Chrysene-d12	21.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Tetracosene	336	C24H48	010192-32-2	99
2			1-Heneicosanol	312	C21H44O	015594-90-8	95
3			Cyclotetracosane	336	C24H48	000297-03-0	95
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092421\
Data File : BP007166.D
Acq On : 24 Sep 2021 19:23
Operator : CG/JU
Sample : M3775-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PE-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.999	5.7	ng	422202	1	7.887	1480970	20.0
Ethanol, 2-(2-b...	10.475	2.9	ng	307772	2	10.687	2108740	20.0
D-Allose	14.369	3.0	ng	413721	3	14.516	2749760	20.0
n-Hexadecanoic ...	18.157	9.7	ng	1542220	4	17.269	3178610	20.0
Octadecanoic acid	19.386	4.2	ng	735885	5	21.351	3547780	20.0
1-Tetracosene	21.063	5.0	ng	880550	5	21.351	3547780	20.0