

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040721\
 Data File : BP005217.D
 Acq On : 07 Apr 2021 13:06
 Operator : CG/JU
 Sample : M1933-08
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 BENNETT_BH_04_0-1

Integration Parameters: rteint.p

Integrator: RTE

Smothing : 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-BP032321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005217.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.293	369	375	382	rVB	300539	423169	51.67%	8.214%
2	6.875	638	644	655	rBV	269077	433753	52.97%	8.420%
3	7.693	776	783	790	rVB	77350	121421	14.83%	2.357%
4	8.852	973	980	988	rBV	168205	271137	33.11%	5.263%
5	10.481	1248	1257	1264	rBV	101774	167782	20.49%	3.257%
6	12.963	1672	1679	1689	rBV	376702	562998	68.75%	10.929%
7	13.810	1818	1823	1829	rBV	17183	26031	3.18%	0.505%
8	14.345	1908	1914	1922	rBV	136882	209723	25.61%	4.071%
9	15.845	2160	2169	2177	rBV	272375	406691	49.66%	7.894%
10	17.110	2375	2384	2389	rBV	172606	245054	29.92%	4.757%
11	18.010	2532	2537	2545	rBV2	93747	132770	16.21%	2.577%
12	18.292	2581	2585	2588	rBV6	6210	8997	1.10%	0.175%
13	18.580	2630	2634	2638	rVB4	9413	11521	1.41%	0.224%
14	18.739	2656	2661	2666	rBV	23706	30665	3.74%	0.595%
15	19.133	2720	2728	2734	rBV2	35391	57956	7.08%	1.125%
16	19.245	2743	2747	2756	rBV	38528	62273	7.60%	1.209%
17	19.486	2784	2788	2791	rVB2	9290	11280	1.38%	0.219%
18	19.680	2816	2821	2827	rBV	661219	818906	100.00%	15.896%
19	19.963	2867	2869	2875	rVB7	7428	12180	1.49%	0.236%
20	20.339	2931	2933	2940	rVB3	7916	9941	1.21%	0.193%
21	20.545	2965	2968	2974	rVB	25966	29694	3.63%	0.576%
22	20.874	3022	3024	3028	rVB4	13538	14031	1.71%	0.272%
23	20.922	3028	3032	3041	rBV	115043	172030	21.01%	3.339%
24	21.204	3075	3080	3085	rBV	245380	321132	39.21%	6.234%
25	21.810	3180	3183	3192	rVB	92628	149716	18.28%	2.906%
26	22.780	3345	3348	3353	rBV4	24286	38666	4.72%	0.751%
27	22.833	3354	3357	3365	rVB5	39669	73120	8.93%	1.419%
28	23.486	3462	3468	3476	rVB2	160777	301384	36.80%	5.850%
29	25.815	3862	3864	3866	rBV2	22744	27608	3.37%	0.536%

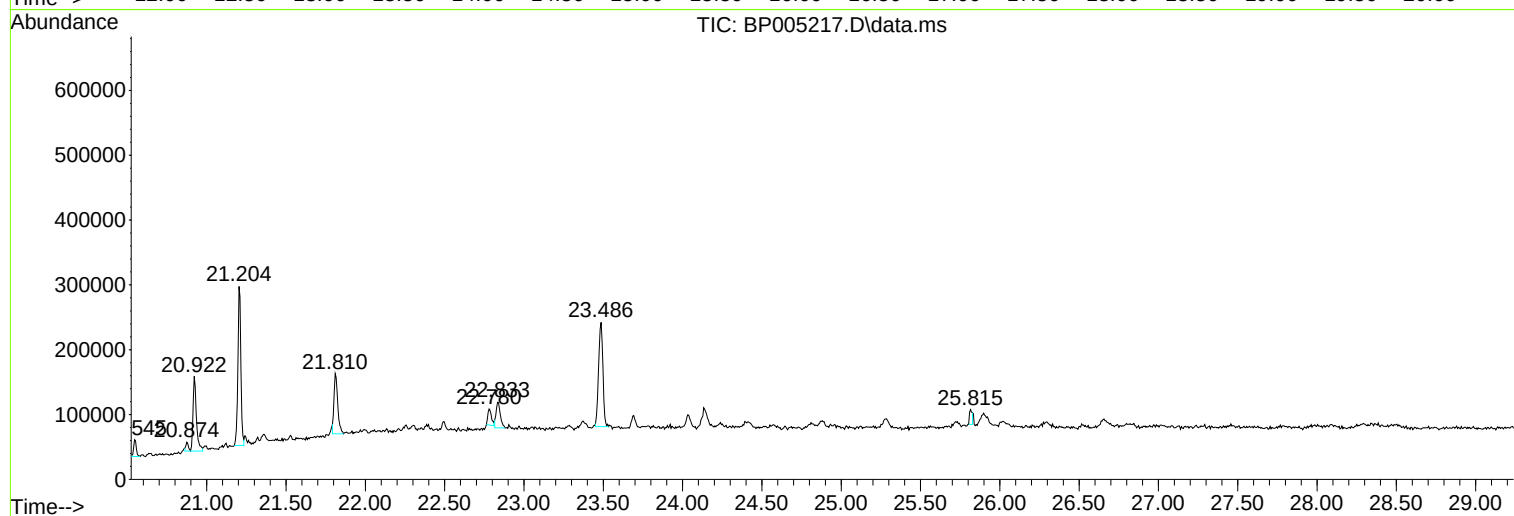
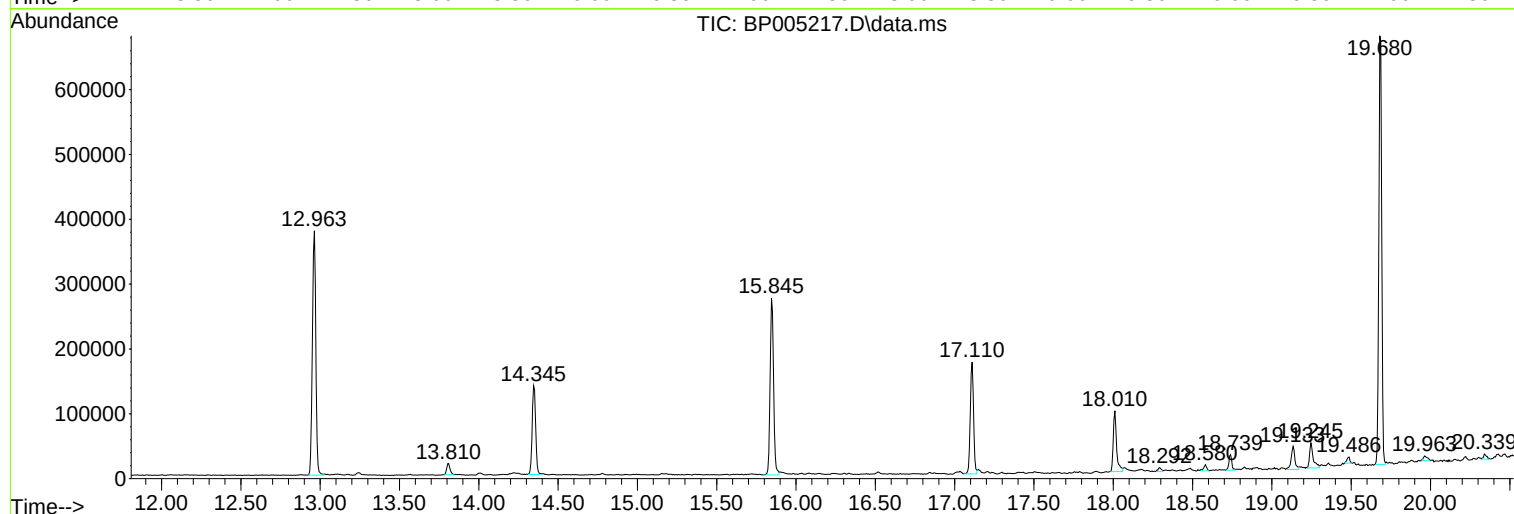
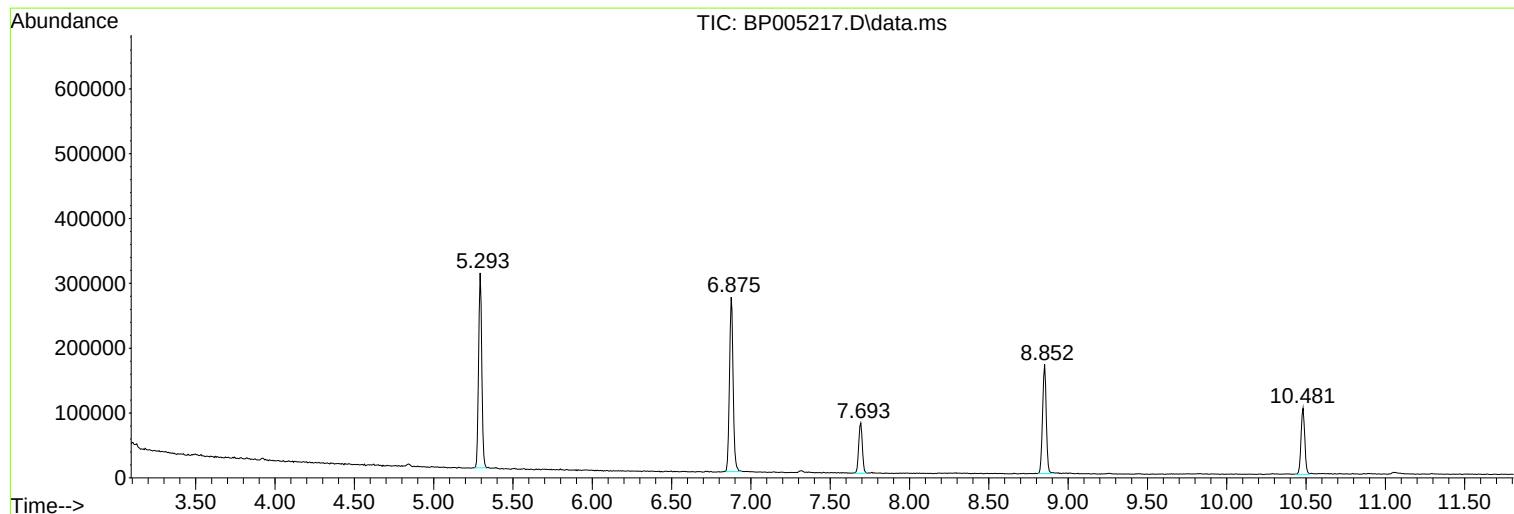
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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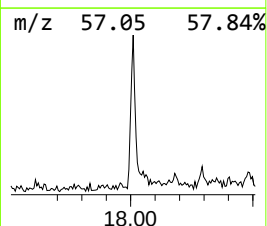
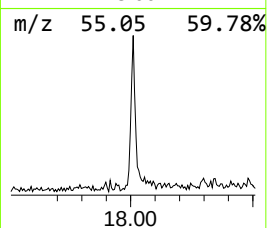
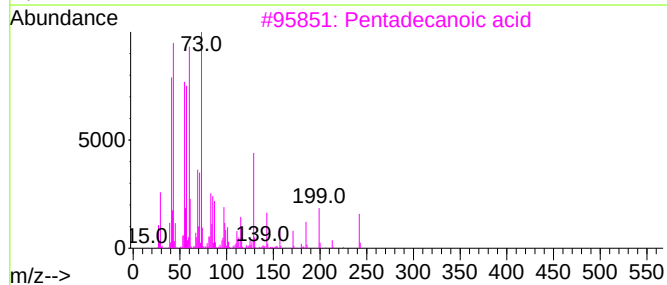
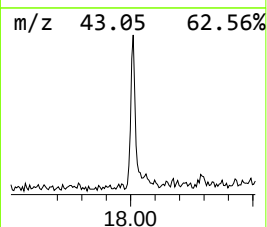
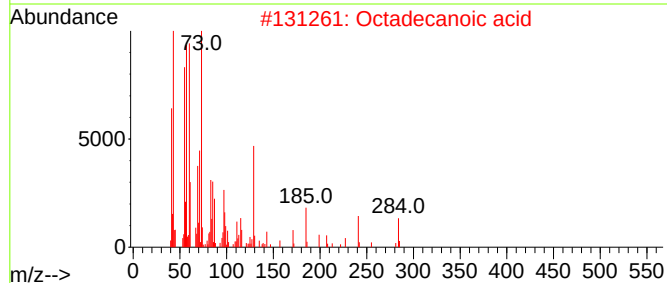
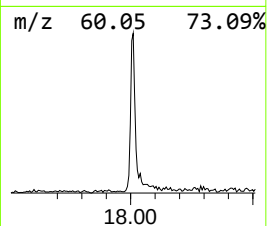
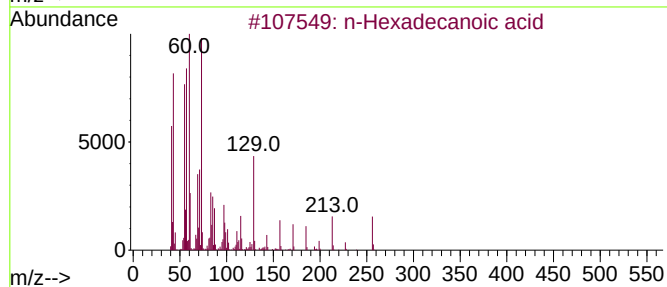
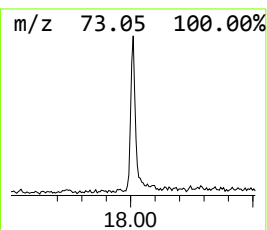
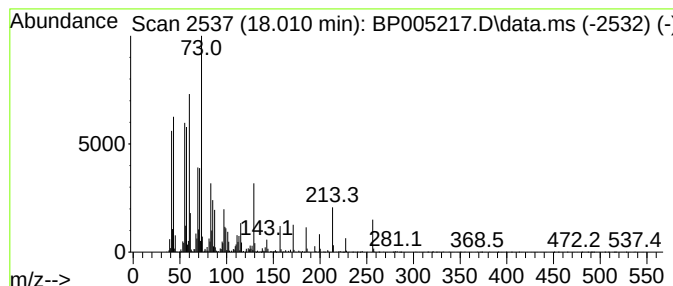
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.010	10.84 ng	132770	Phenanthrene-d10	17.110

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	81
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4			l-(+)-Ascorbic acid 2,6-dihexade...	652	C38H68O8	028474-90-0	72
5			Tridecanoic acid	214	C13H26O2	000638-53-9	62



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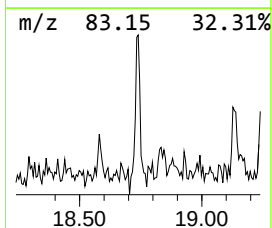
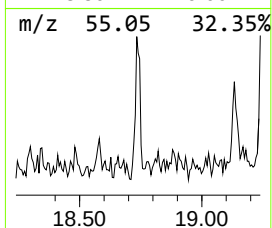
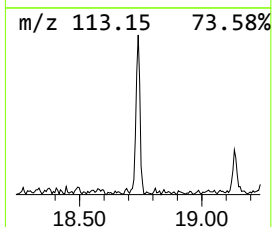
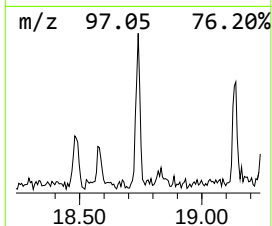
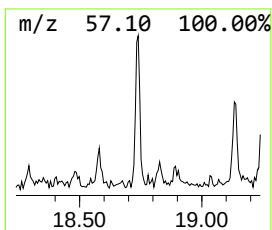
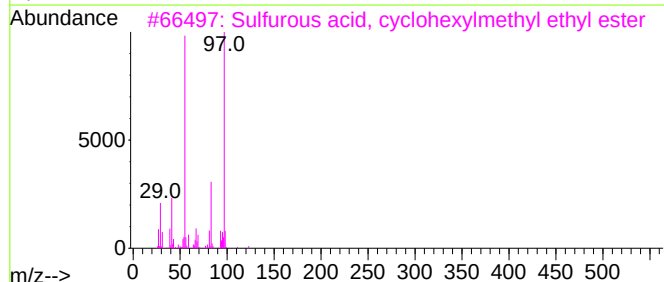
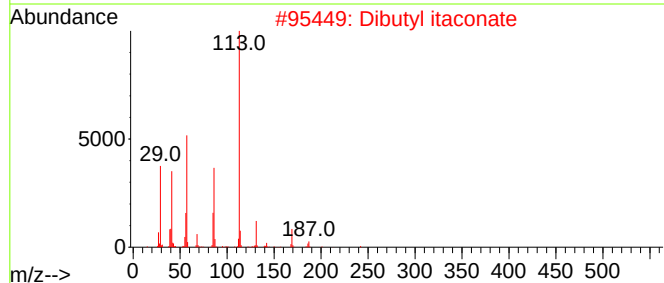
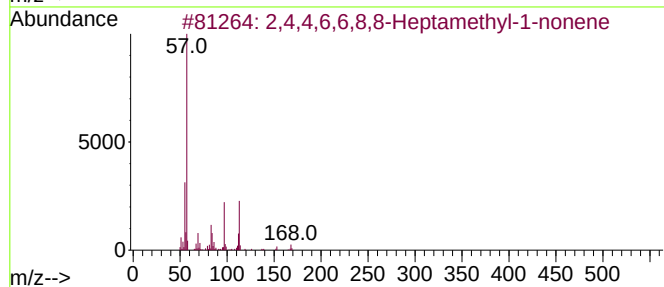
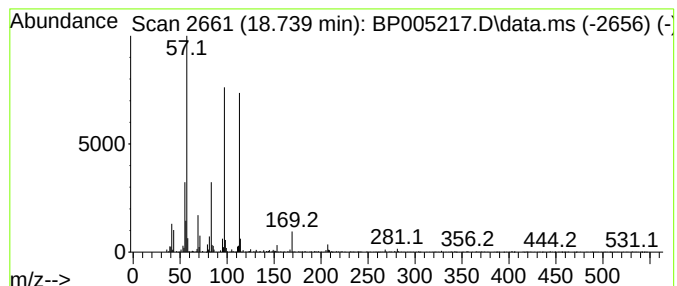
Instrument :
BNA_P
ClientSampleId :
BENNETT_BH_04_0-1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.739	2.50 ng	30665	Phenanthrene-d10	17.110	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	64
2	Dibutyl itaconate	242	C13H22O4	002155-60-4	35
3	Sulfurous acid, cyclohexylmethyl...	206	C9H18O3S	1000309-21-2	35
4	3-Heptadec-8-enyl-2,4,10-trioxa...	378	C24H42O3	1000189-57-5	32
5	Sulfurous acid, cyclohexylmethyl...	430	C25H50O3S	1000309-22-6	25



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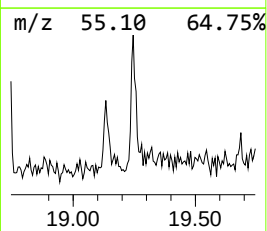
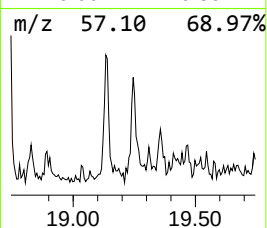
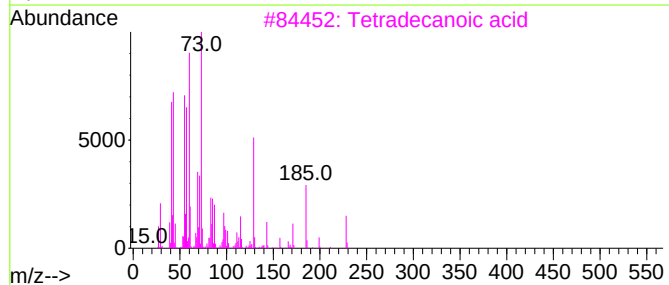
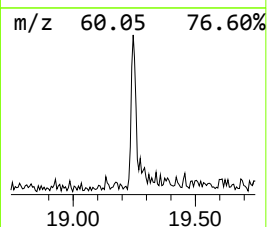
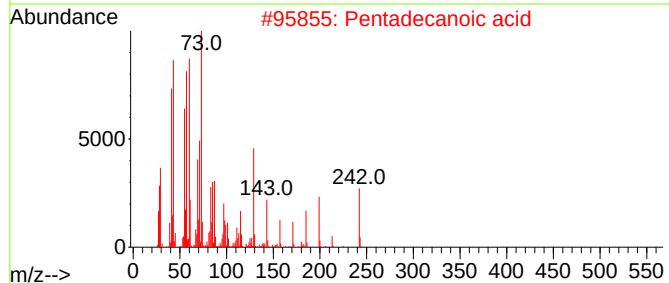
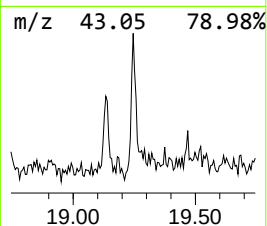
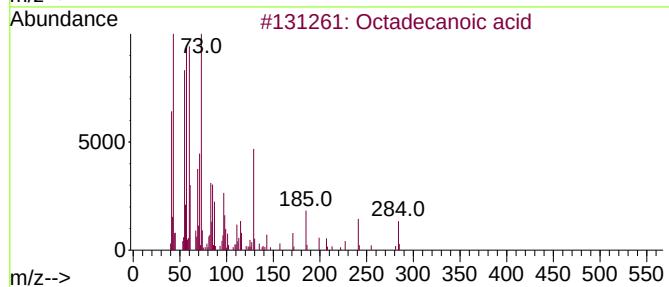
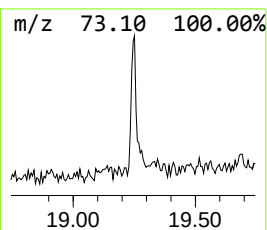
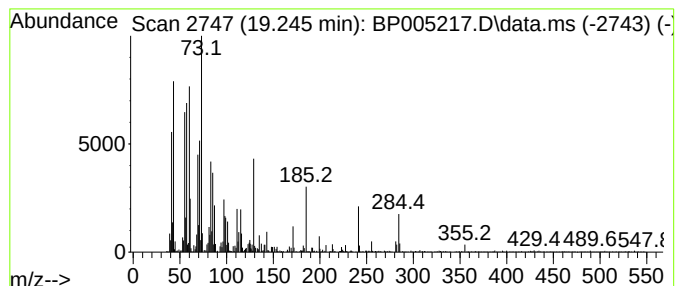
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.245	3.88 ng	62273	Chrysene-d12	21.204

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	96
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	53
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	52
4			Dodecanoic acid	200	C12H24O2	000143-07-7	47
5			n-Decanoic acid	172	C10H20O2	000334-48-5	45



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Instrument :
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ClientSampleId :
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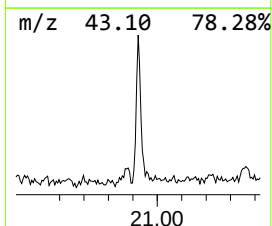
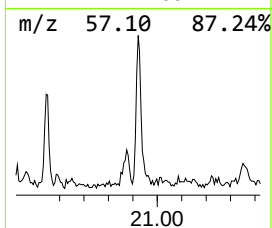
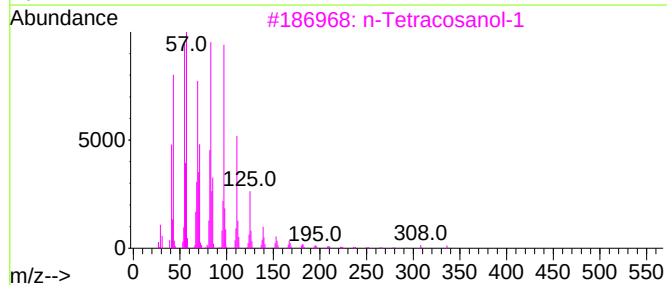
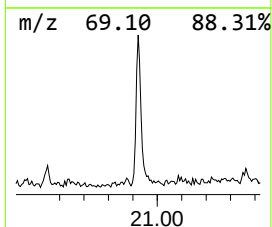
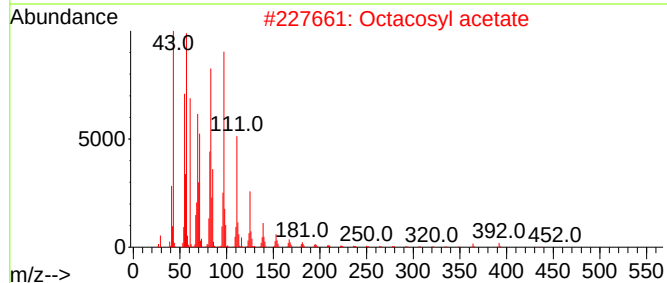
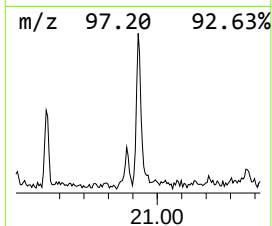
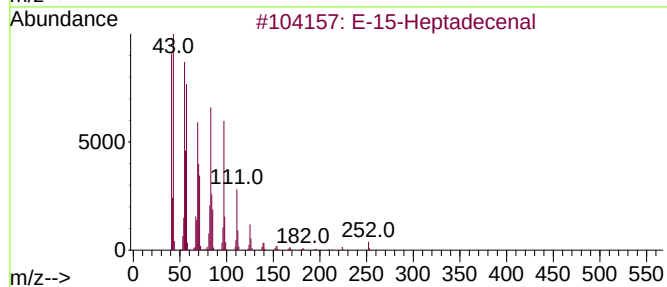
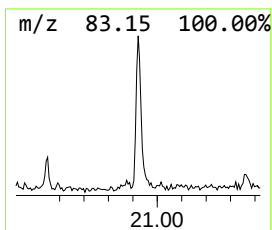
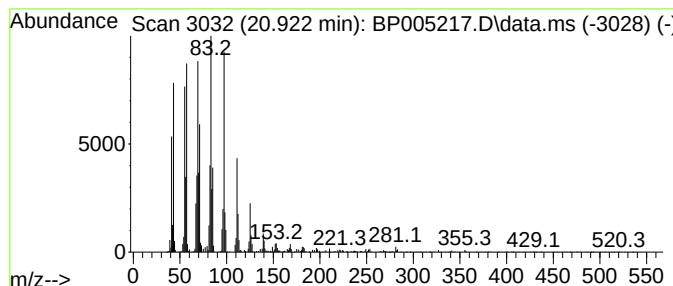
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 E-15-Heptadecenal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.922	10.71 ng	172030	Chrysene-d12	21.204

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			E-15-Heptadecenal	252	C17H32O	1000130-97-9	96
2			Octacosyl acetate	452	C30H60O2	018206-97-8	95
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4			1-Triacontanol	438	C30H62O	000593-50-0	93
5			Behenic alcohol	326	C22H46O	000661-19-8	91



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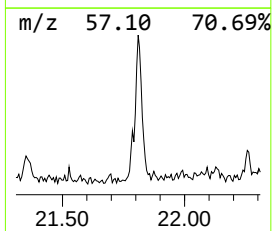
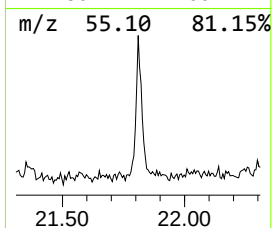
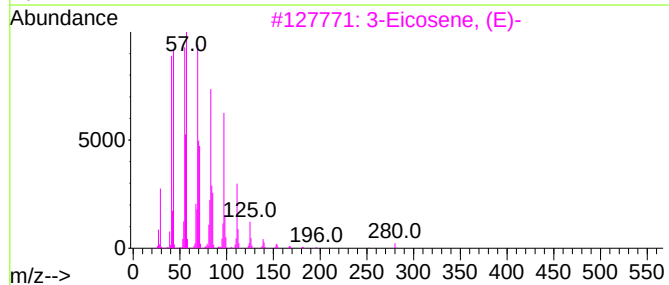
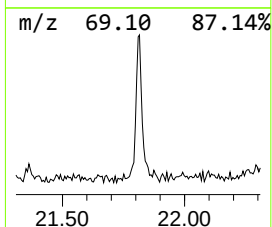
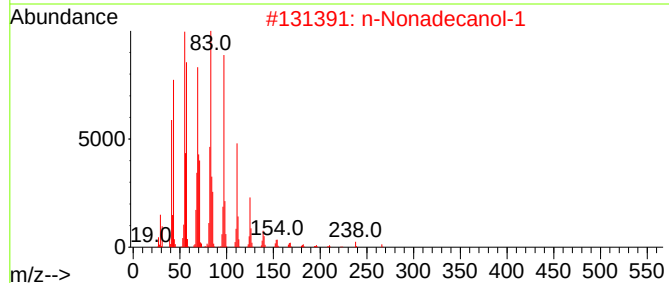
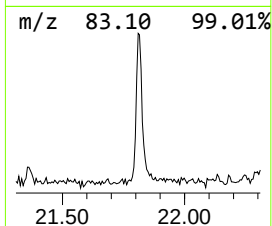
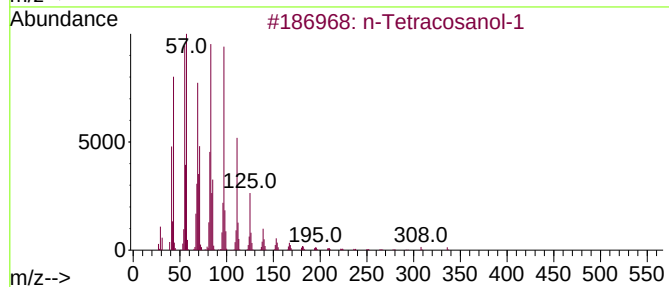
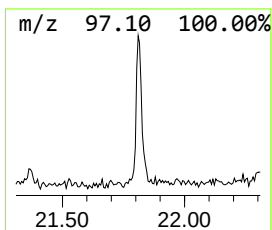
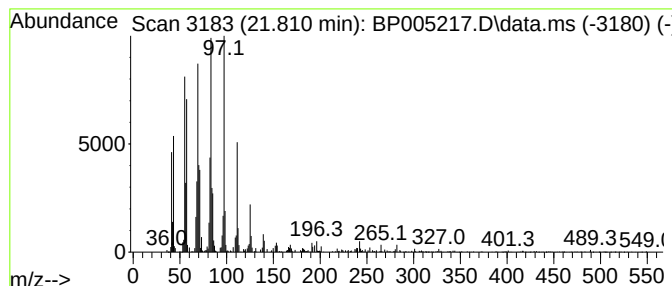
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Tetracosanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.810	9.32 ng	149716	Chrysene-d12	21.204

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2		n-Nonadecanol-1	284	C19H40O	001454-84-8	93
3		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4		1-Heneicosanol	312	C21H44O	015594-90-8	91
5		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	87



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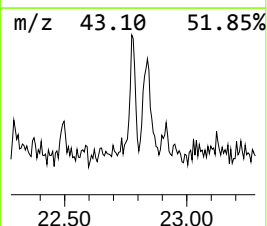
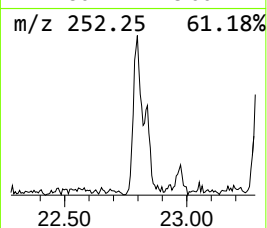
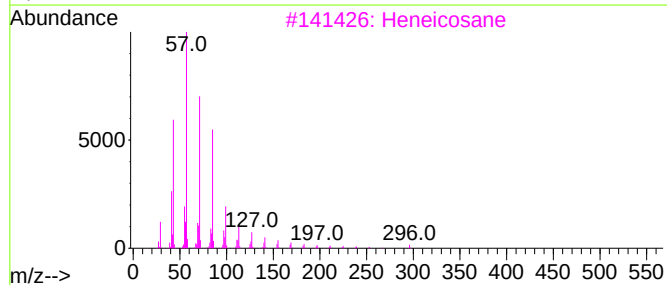
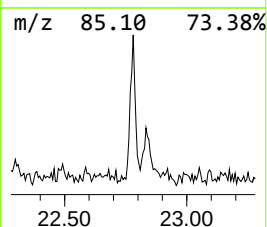
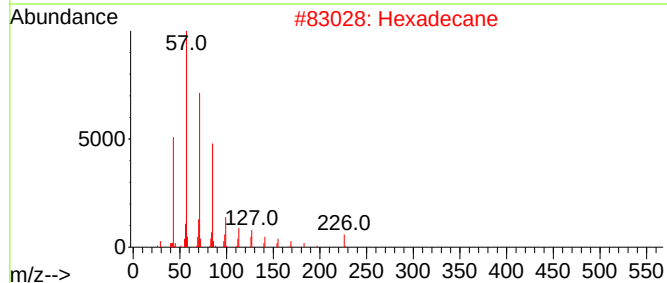
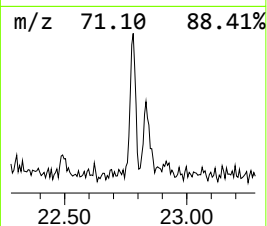
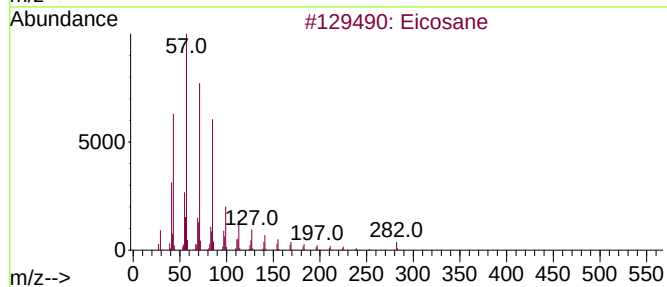
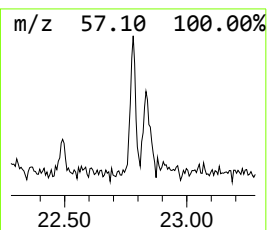
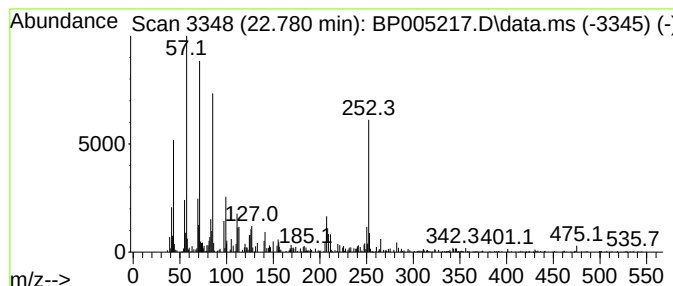
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.780	2.57 ng	38666	Perylene-d12	23.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	93
2			Hexadecane	226	C16H34	000544-76-3	93
3			Heneicosane	296	C21H44	000629-94-7	89
4			3,5-Dimethyldodecane	198	C14H30	107770-99-0	76
5			Pentadecane	212	C15H32	000629-62-9	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040721\
Data File : BP005217.D
Acq On : 07 Apr 2021 13:06
Operator : CG/JU
Sample : M1933-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BENNETT_BH_04_0-1

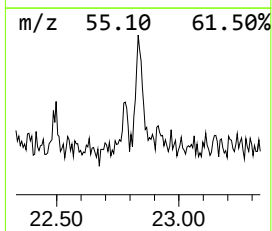
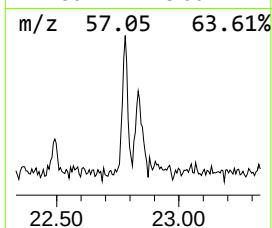
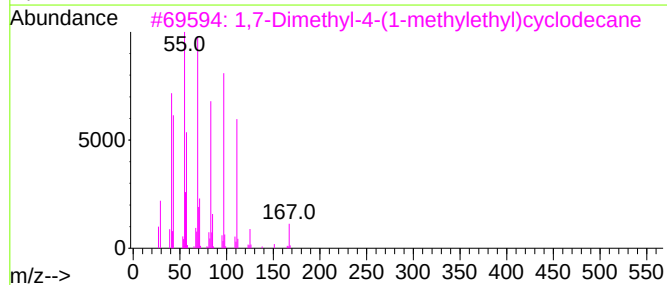
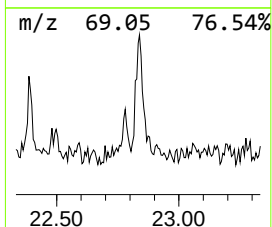
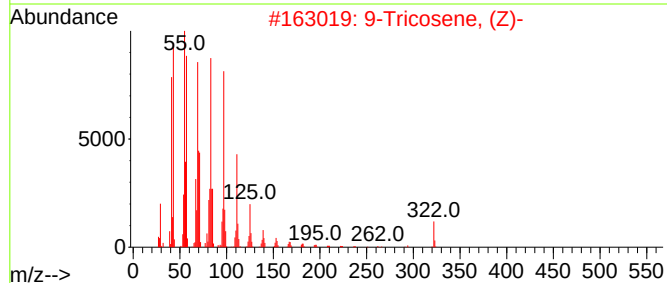
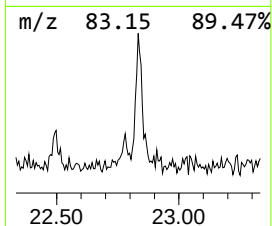
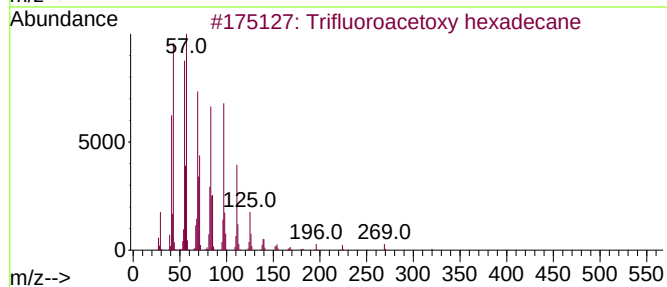
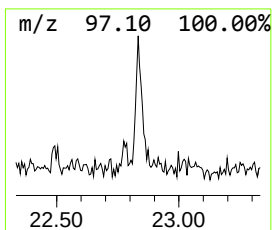
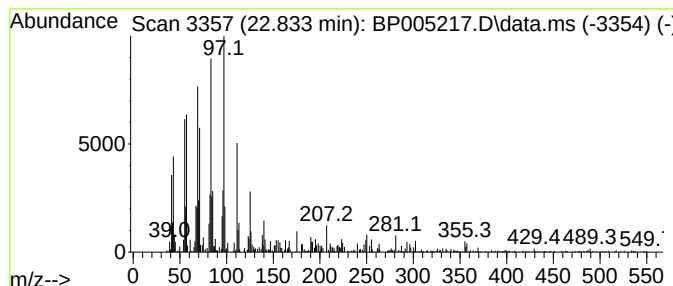
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.833	4.85 ng	73120	Perylene-d12	23.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90
2			9-Tricosene, (Z)-	322	C23H46	027519-02-4	90
3			1,7-Dimethyl-4-(1-methylethyl)cy...	210	C15H30	000645-10-3	59
4			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	43
5			Cyclohexadecane	224	C16H32	000295-65-8	41



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040721\
Data File : BP005217.D
Acq On : 07 Apr 2021 13:06
Operator : CG/JU
Sample : M1933-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BENNETT_BH_04_0-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	18.010	10.8	ng	132770	4	17.110	245054	20.0
2,4,4,6,6,8,8-H...	18.739	2.5	ng	30665	4	17.110	245054	20.0
Octadecanoic acid	19.245	3.9	ng	62273	5	21.204	321132	20.0
E-15-Heptadecenal	20.922	10.7	ng	172030	5	21.204	321132	20.0
n-Tetracosanol-1	21.810	9.3	ng	149716	5	21.204	321132	20.0
Eicosane	22.780	2.6	ng	38666	6	23.486	301384	20.0
Trifluoroacetox...	22.833	4.8	ng	73120	6	23.486	301384	20.0