

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
 Data File : BP013454.D
 Acq On : 11 Jan 2023 21:03
 Operator : CG/JU
 Sample : 01106-04
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 TP-B

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-BP121322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP013454.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.005	302	309	319	rBV	1807366	2644757	9.06%	1.296%
2	5.475	383	389	402	rVB	7358472	11368332	38.94%	5.570%
3	7.087	655	663	678	rVV	7876820	12529428	42.92%	6.139%
4	7.922	798	805	812	rBV	1780693	2812939	9.64%	1.378%
5	9.093	996	1004	1011	rBV	4509167	7474583	25.60%	3.663%
6	10.734	1272	1283	1291	rBV	2648569	4399459	15.07%	2.156%
7	13.187	1693	1700	1707	rBV	12088988	17726125	60.72%	8.686%
8	14.569	1929	1935	1946	rVB	4372442	6460009	22.13%	3.165%
9	14.957	1996	2001	2011	rBV2	243127	540984	1.85%	0.265%
10	15.928	2161	2166	2171	rVB2	419907	614725	2.11%	0.301%
11	16.063	2183	2189	2203	rBV	13990840	19983625	68.45%	9.792%
12	16.710	2295	2299	2306	rBV2	221367	354905	1.22%	0.174%
13	17.328	2398	2404	2410	rBV	6165906	8659651	29.66%	4.243%
14	18.139	2538	2542	2544	rBV2	481825	734630	2.52%	0.360%
15	18.210	2547	2554	2576	rVB	16287562	29194086	100.00%	14.305%
16	19.322	2735	2743	2757	rBV	8374302	21227370	72.71%	10.401%
17	19.434	2758	2762	2777	rVB	7698261	12018299	41.17%	5.889%
18	19.881	2833	2838	2843	rBV	23036048	27909734	95.60%	13.676%
19	20.398	2923	2926	2935	rBV	3128252	4513339	15.46%	2.212%
20	21.104	3043	3046	3050	rBV	3830659	4383101	15.01%	2.148%
21	21.416	3095	3099	3105	rVB	6610926	8531091	29.22%	4.180%

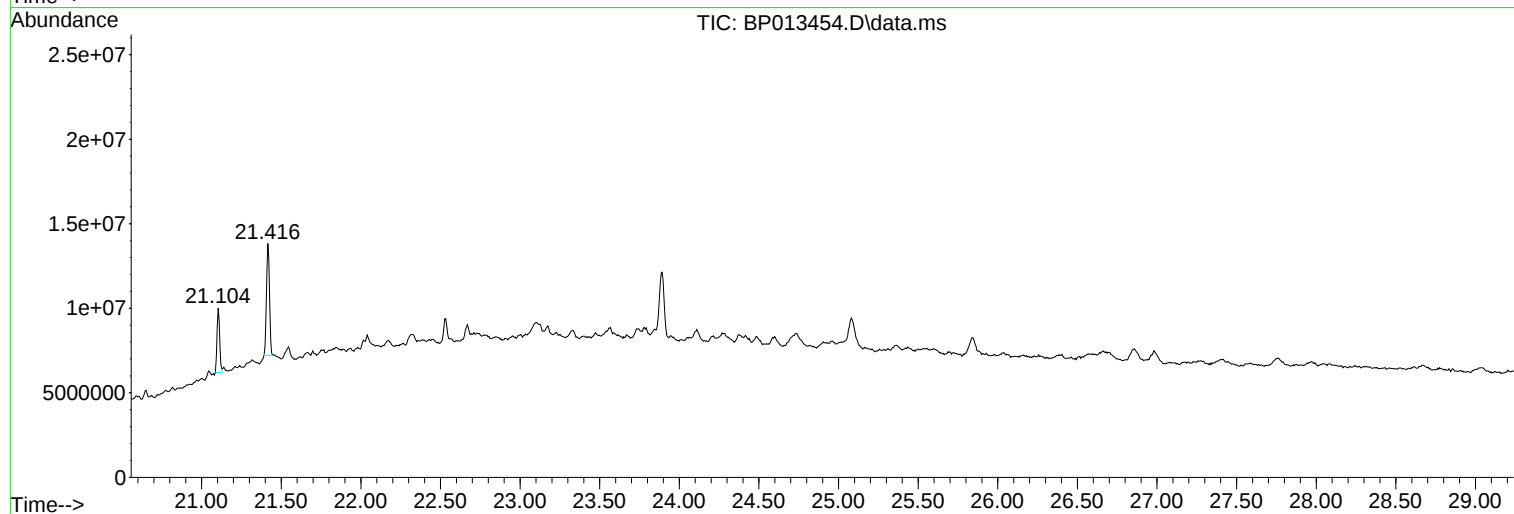
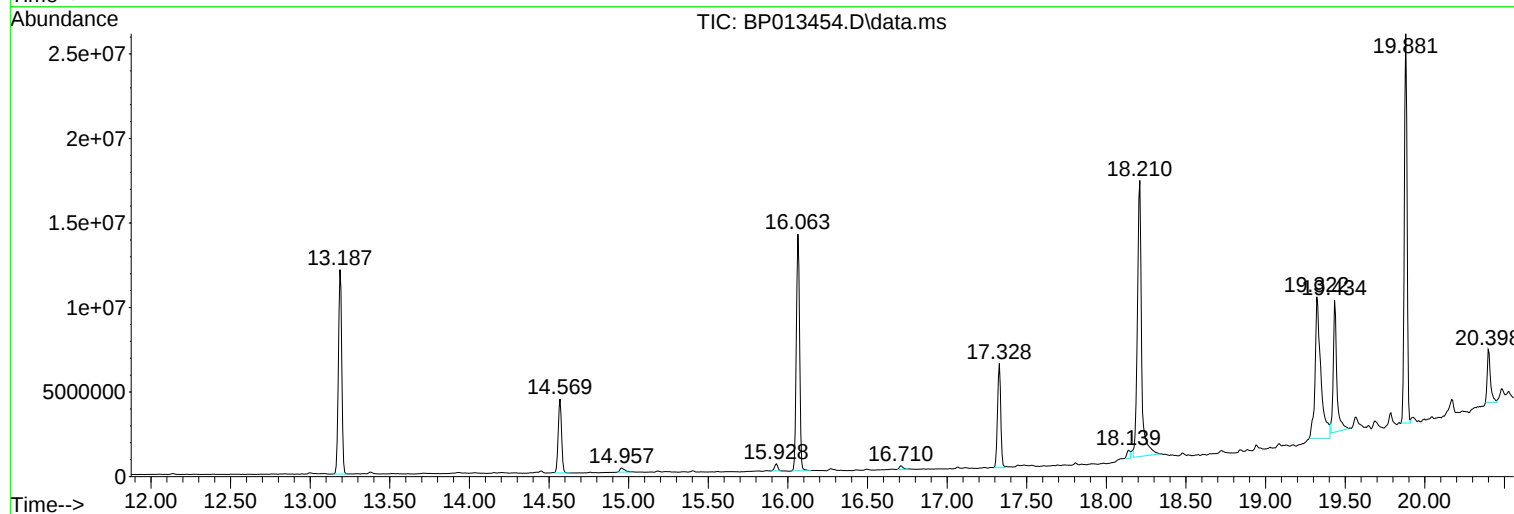
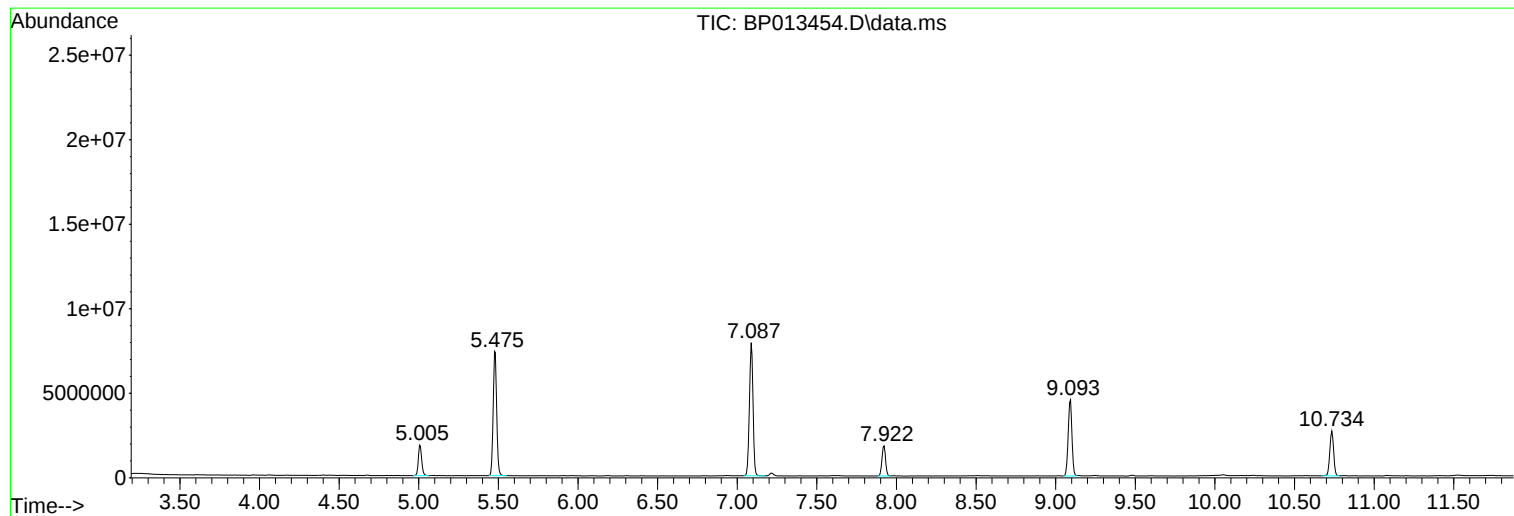
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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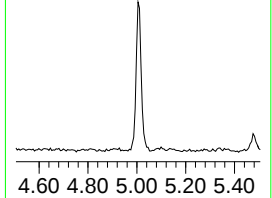
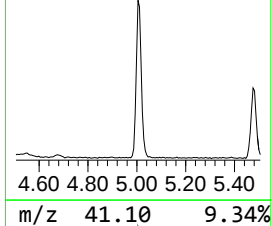
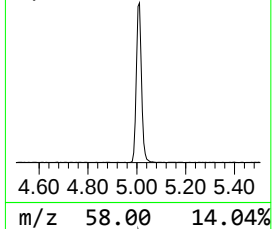
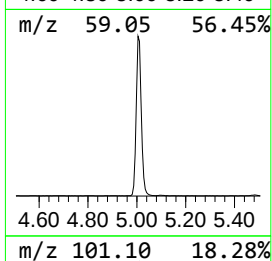
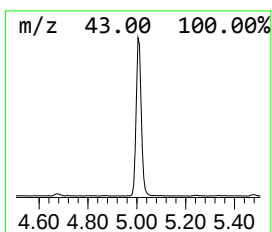
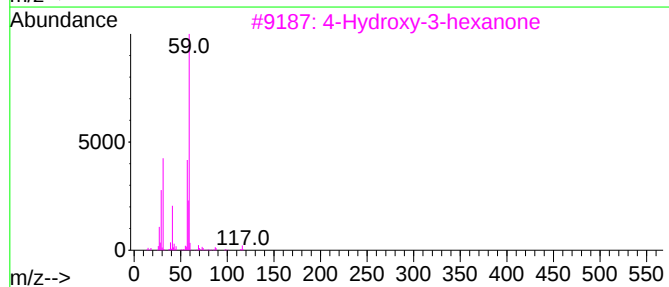
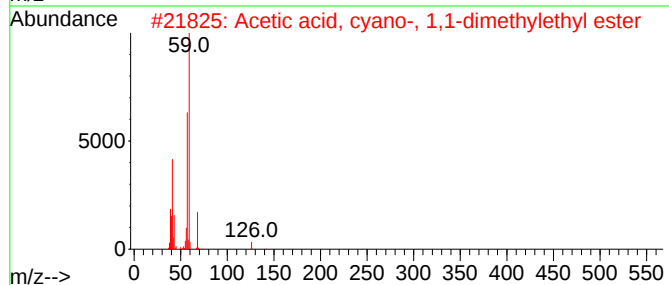
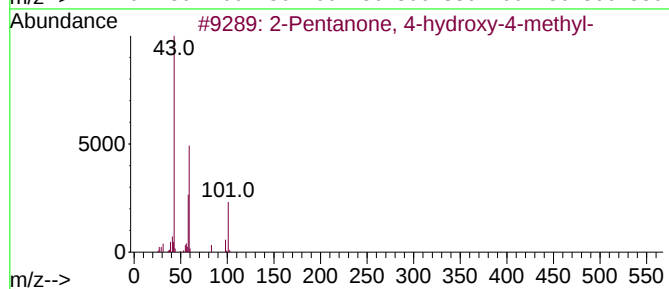
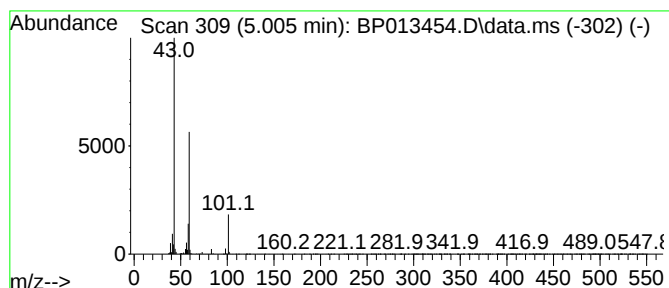
Instrument :
BNA_P
ClientSampleId :
TP-B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121322.M
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 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.005	18.80 ng	2644760	1,4-Dichlorobenzene-d4	7.922	
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	25
3	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	23
4	Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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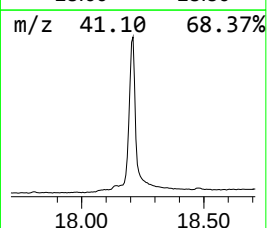
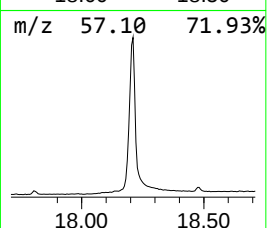
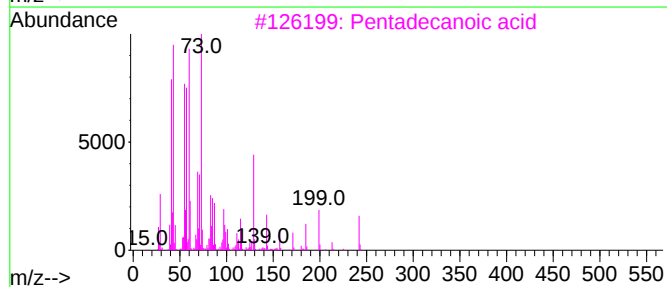
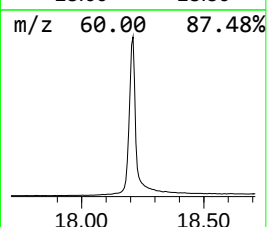
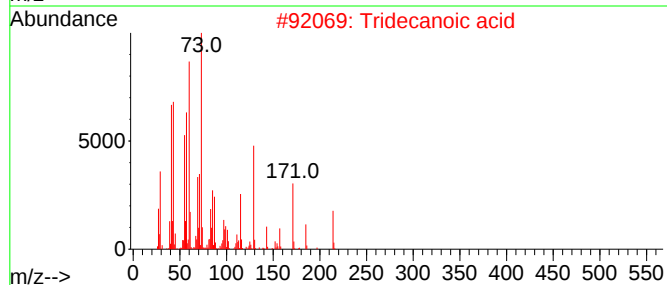
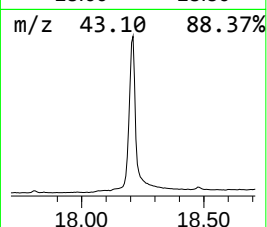
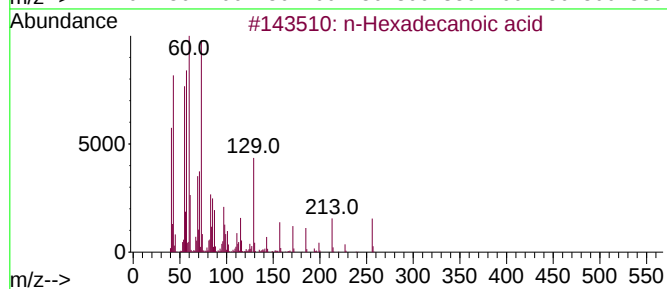
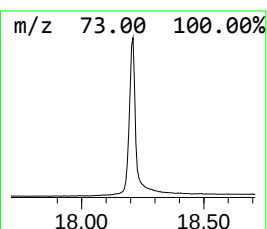
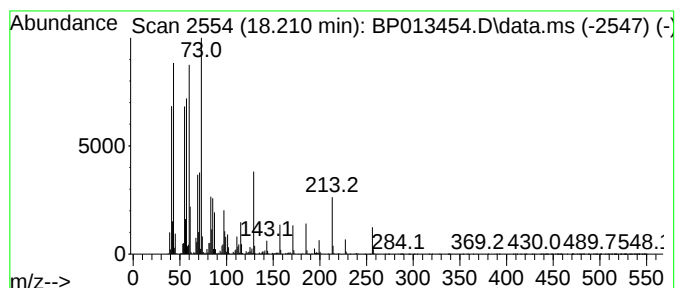
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.210	67.43 ng	29194100	Phenanthrene-d10	17.328

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	91
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5		n-Decanoic acid	172	C10H20O2	000334-48-5	58



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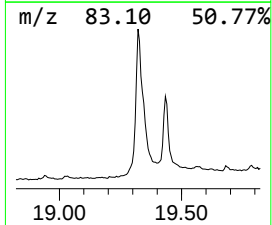
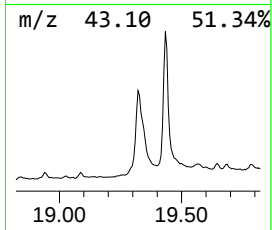
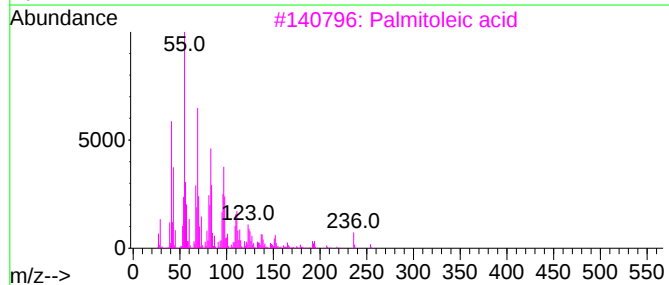
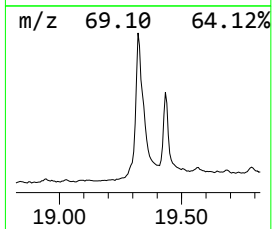
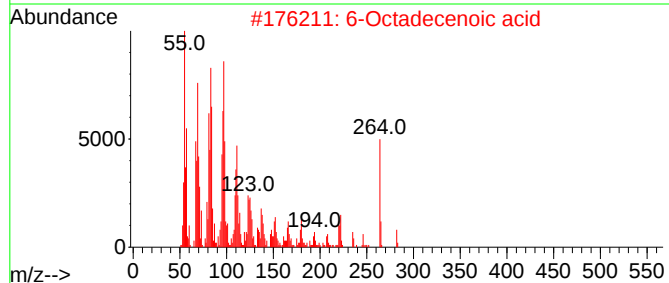
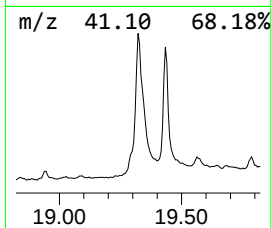
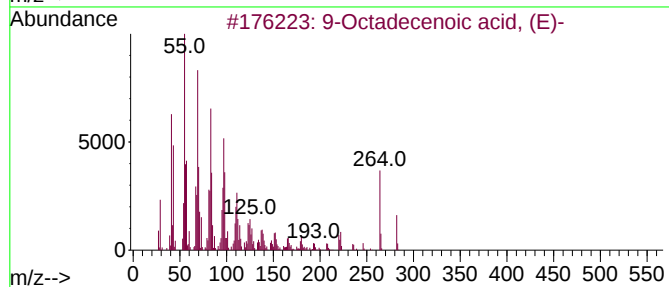
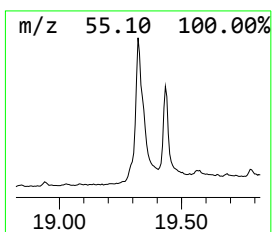
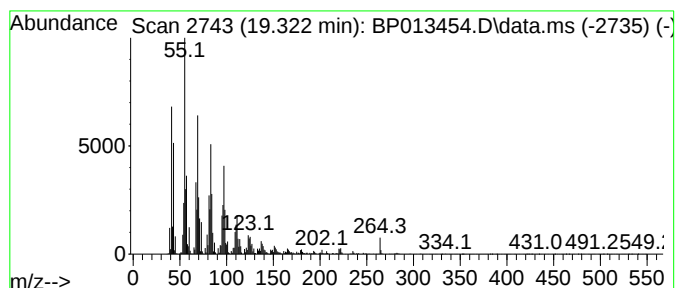
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BNA_P
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TIC Integration Parameters: LSCINT.P

Peak Number 3 9-Octadecenoic acid, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.322	49.03 ng	21227400	Phenanthrene-d10	17.328	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	99
2	6-Octadecenoic acid	282	C18H34O2	1000336-66-8	95
3	Palmitoleic acid	254	C16H30O2	000373-49-9	95
4	cis-Vaccenic acid	282	C18H34O2	000506-17-2	94
5	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	91



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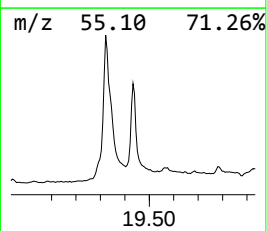
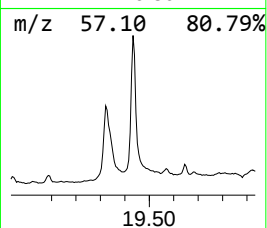
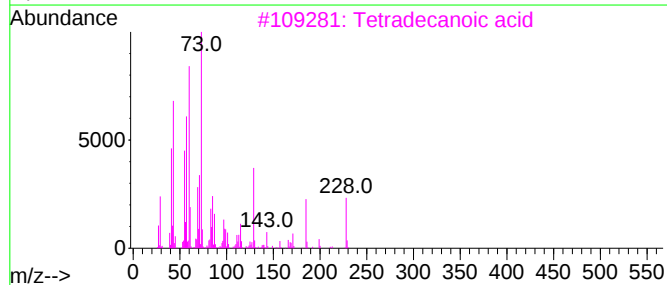
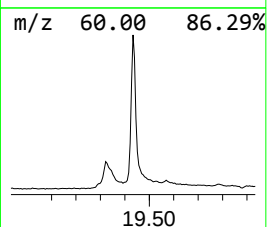
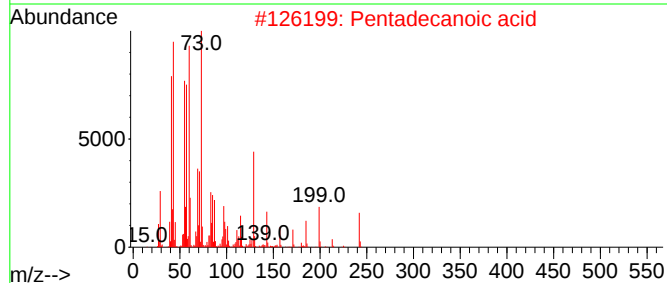
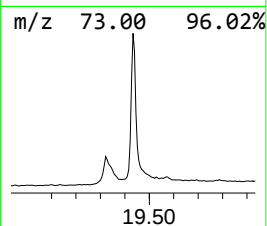
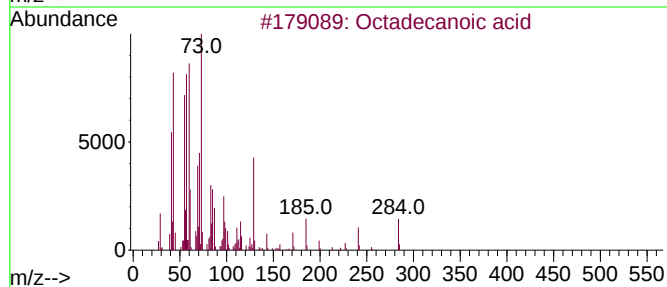
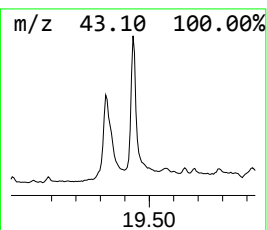
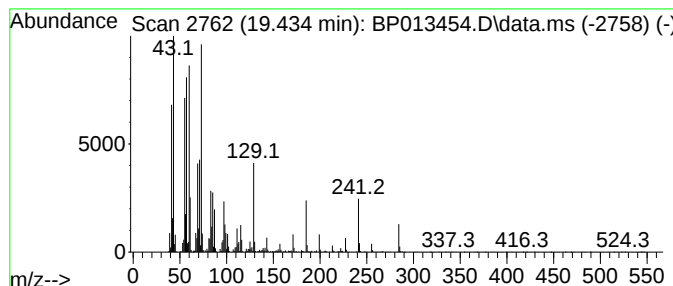
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.433	28.18 ng	12018300	Chrysene-d12	21.416

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	87
5			Tridecanoic acid	214	C13H26O2	000638-53-9	76



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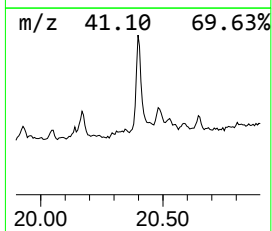
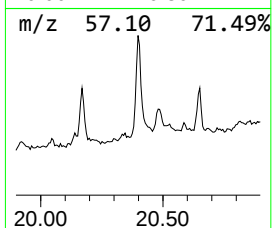
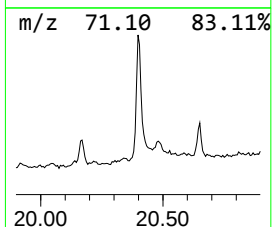
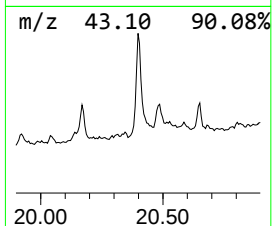
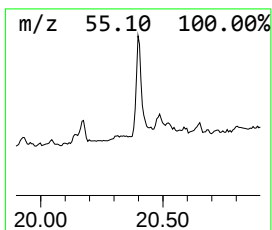
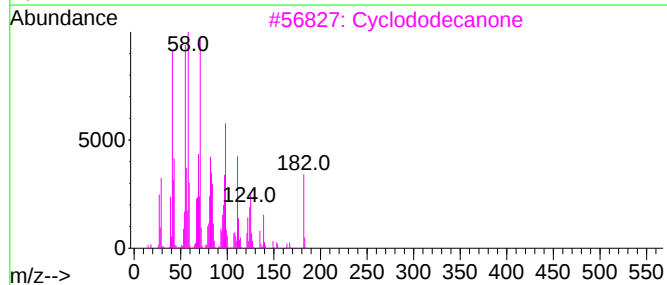
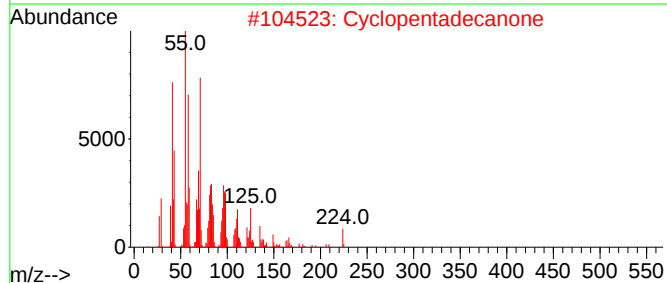
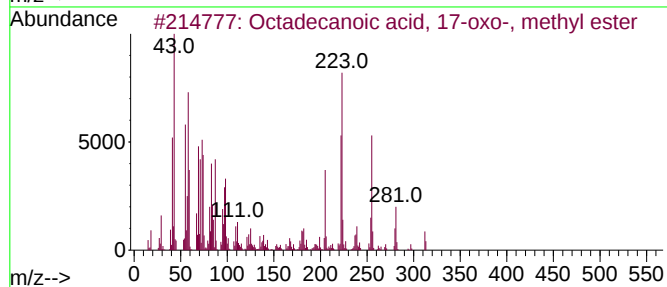
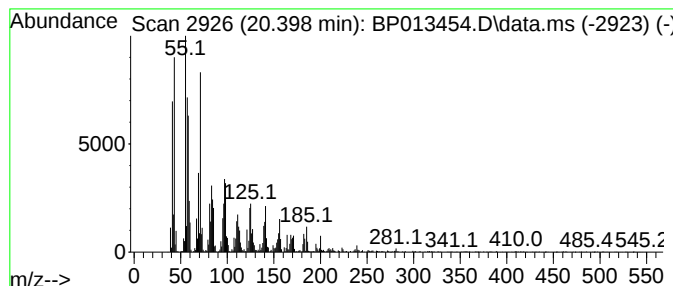
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid, 17-oxo-,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.398	10.58 ng	4513340	Chrysene-d12	21.416	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, 17-oxo-, meth...	312	C19H36O3	002380-32-7	90
2	Cyclopentadecanone	224	C15H28O	000502-72-7	83
3	Cyclododecanone	182	C12H22O	000830-13-7	53
4	Cyclohexanol, 1-methyl-4-(1-meth...	156	C10H20O	003901-93-7	50
5	11-Dodecen-2-one	182	C12H22O	005009-33-6	49



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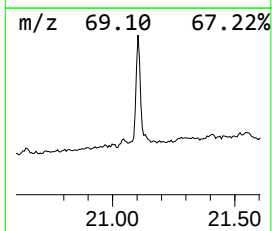
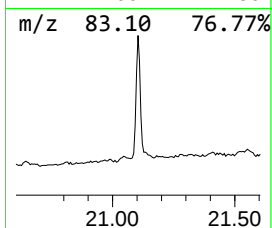
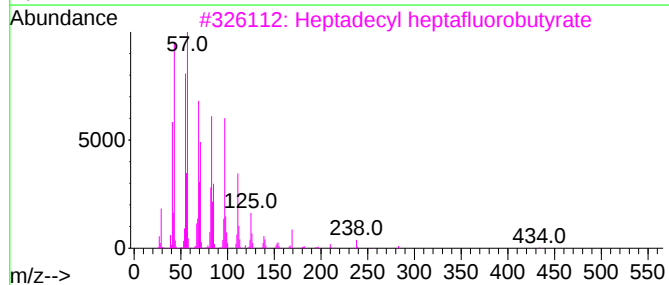
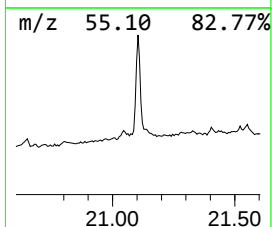
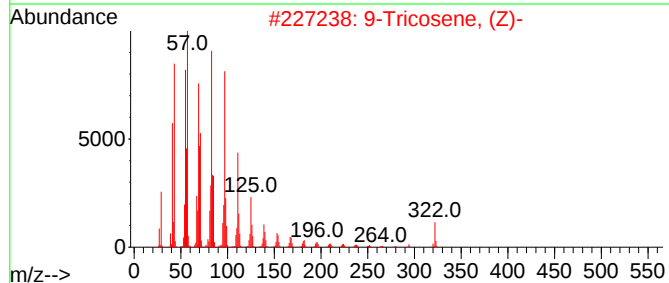
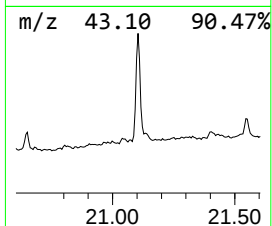
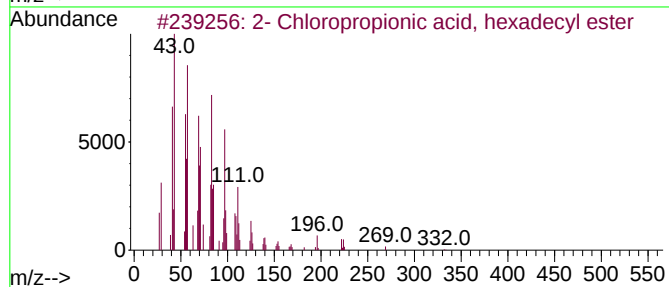
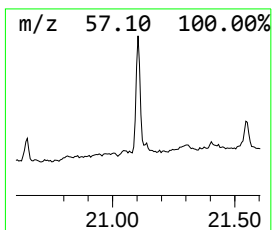
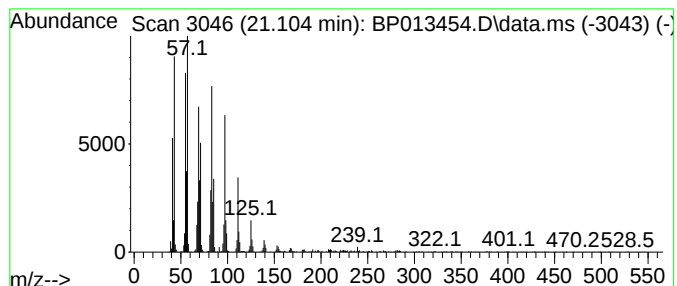
Instrument :
BNA_P
ClientSampleId :
TP-B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2- Chloropropionic acid, he... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.104	10.28 ng	4383100	Chrysene-d12		21.416	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, hexadec...		332	C19H37ClO2	086711-81-1	95
2	9-Tricosene, (Z)-		322	C23H46	027519-02-4	95
3	Heptadecyl heptafluorobutyrate		452	C21H35F7O2	959085-66-6	94
4	1-Hexacosene		364	C26H52	018835-33-1	94
5	Trichloroacetic acid, hexadecyl ...		386	C18H33Cl3O2	074339-54-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
Data File : BP013454.D
Acq On : 11 Jan 2023 21:03
Operator : CG/JU
Sample : 01106-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121322.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-...	5.005	18.8	ng	2644760	1	7.922	2812940	20.0
n-Hexadecanoic ...	18.210	67.4	ng	29194100	4	17.328	8659650	20.0
9-Octadecenoic ...	19.322	49.0	ng	21227400	4	17.328	8659650	20.0
Octadecanoic acid	19.433	28.2	ng	12018300	5	21.416	8531090	20.0
Octadecanoic ac...	20.398	10.6	ng	4513340	5	21.416	8531090	20.0
2-Chloropropio...	21.104	10.3	ng	4383100	5	21.416	8531090	20.0