

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092221\
 Data File : BP007113.D
 Acq On : 22 Sep 2021 23:43
 Operator : CG/JU
 Sample : M3871-01 5X
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 SS01-BL-(0.0)

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: BP007113.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.469	399	405	414	rBV	596706	892136	3.72%	0.926%
2	7.063	669	676	686	rBV	562651	881306	3.67%	0.914%
3	7.899	811	818	825	rBV	1399946	2184910	9.11%	2.267%
4	9.058	1009	1015	1025	rBV	358377	607293	2.53%	0.630%
5	10.699	1286	1294	1301	rBV	1790685	2958063	12.33%	3.069%
6	13.151	1705	1711	1720	rBV	1105552	1582779	6.60%	1.642%
7	14.528	1937	1945	1950	rBV	2754745	4097738	17.08%	4.252%
8	14.945	2011	2016	2022	rBV	210135	308322	1.29%	0.320%
9	15.845	2165	2169	2176	rBV	408046	604000	2.52%	0.627%
10	16.010	2193	2197	2203	rVB	750706	1047837	4.37%	1.087%
11	16.069	2203	2207	2215	rVB	545519	933978	3.89%	0.969%
12	16.239	2232	2236	2240	rBV2	289747	362928	1.51%	0.377%
13	16.398	2256	2263	2269	rBV6	128328	302928	1.26%	0.314%
14	16.692	2306	2313	2322	rBV	3134889	4903867	20.44%	5.088%
15	16.892	2343	2347	2352	rBV	662259	961541	4.01%	0.998%
16	17.181	2391	2396	2403	rBV2	994334	1676503	6.99%	1.740%
17	17.245	2403	2407	2408	rVV	462533	564105	2.35%	0.585%
18	17.275	2408	2412	2416	rVV	3652183	5085879	21.20%	5.277%
19	17.322	2416	2420	2424	rVV2	2963917	3845732	16.03%	3.990%
20	17.369	2424	2428	2433	rVB2	844265	1280154	5.34%	1.328%
21	17.457	2439	2443	2448	rBV	2226977	2844756	11.86%	2.952%
22	17.504	2448	2451	2454	rVV	536688	722497	3.01%	0.750%
23	17.534	2454	2456	2466	rVB	435942	641334	2.67%	0.665%
24	17.663	2471	2478	2489	rVB3	2572942	4784347	19.95%	4.964%
25	18.069	2539	2547	2553	rBV	6247593	11042467	46.04%	11.458%
26	18.198	2560	2569	2581	rBV	11566325	23986051	100.00%	24.888%
27	18.363	2594	2597	2600	rVB	445150	470202	1.96%	0.488%
28	18.804	2669	2672	2674	rBV2	755417	917885	3.83%	0.952%
29	19.398	2770	2773	2781	rVB	1648502	2146132	8.95%	2.227%
30	19.828	2843	2846	2850	rBV	1895383	2129713	8.88%	2.210%
31	21.357	3102	3106	3111	rVB	4195463	5542661	23.11%	5.751%
32	23.768	3512	3516	3525	rVB2	2911398	6065688	25.29%	6.294%

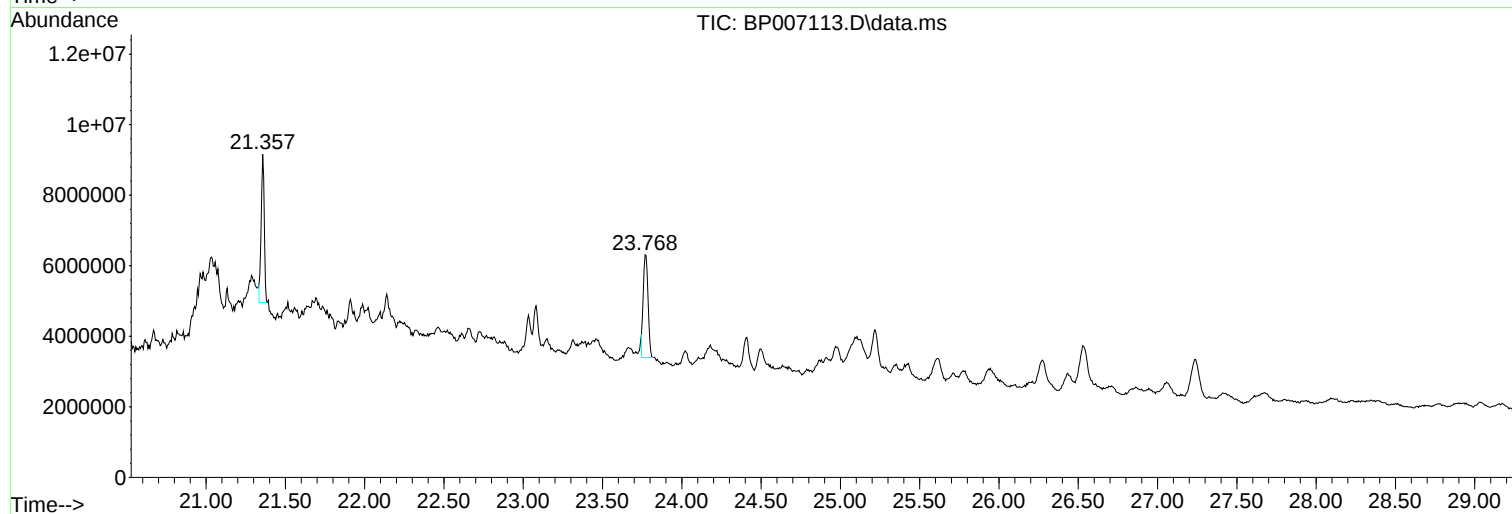
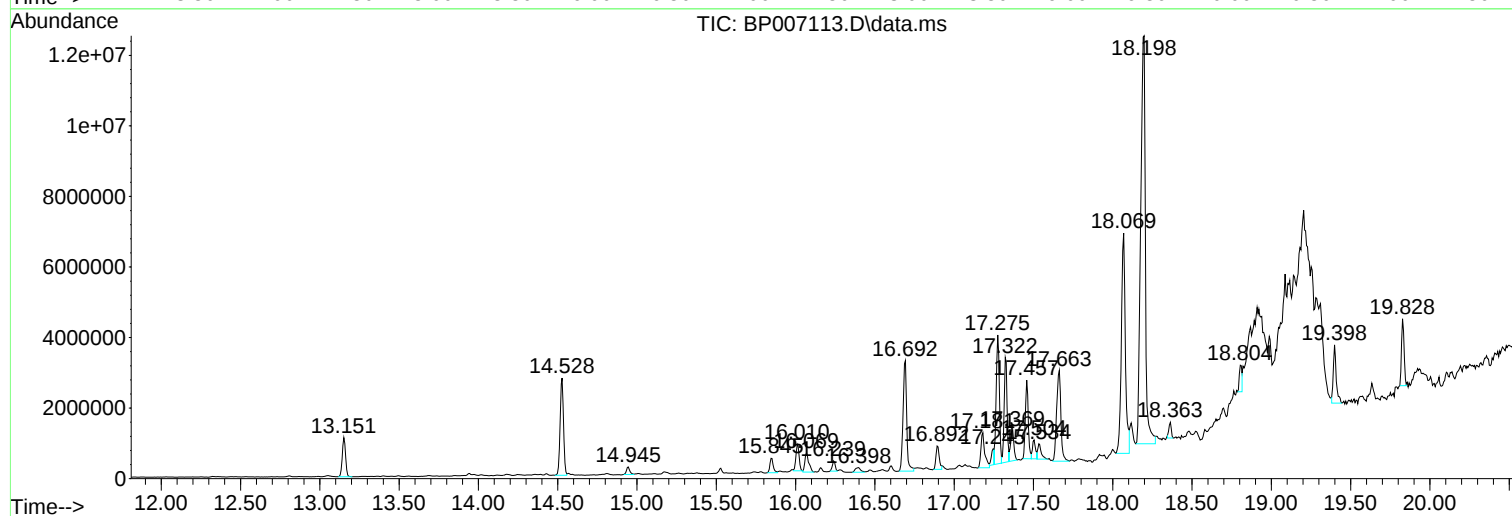
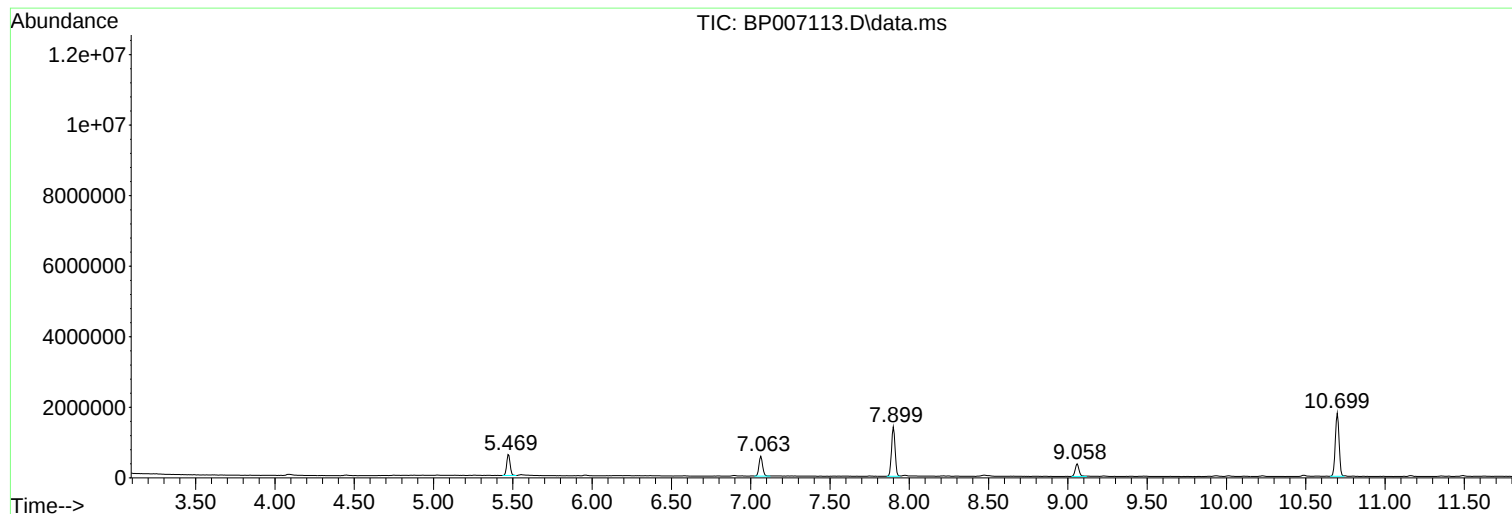
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Instrument :
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ClientSampleId :
SS01-BL-(0.0)

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



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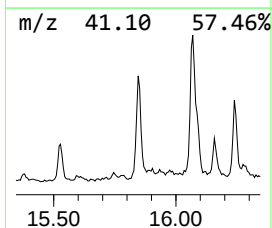
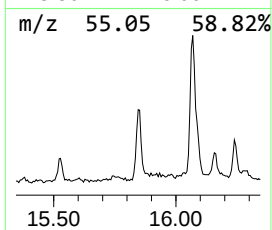
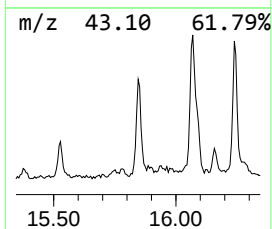
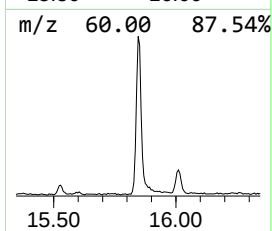
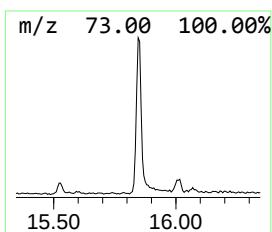
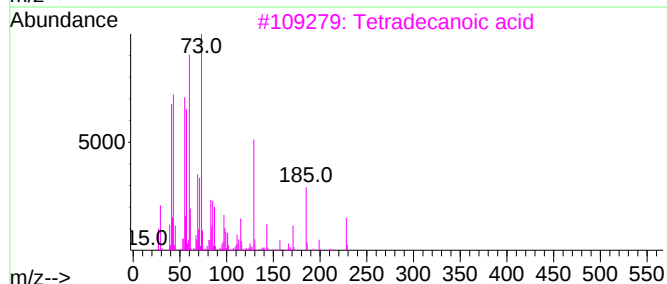
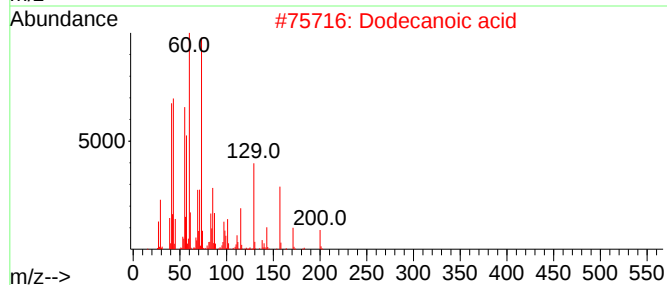
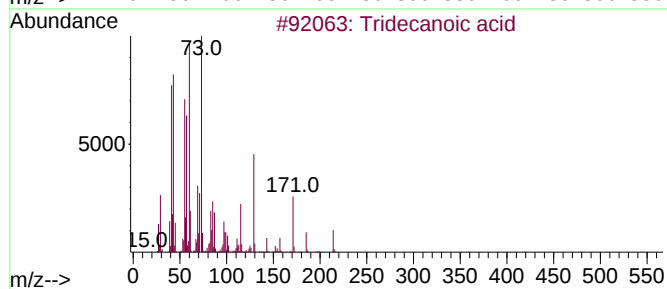
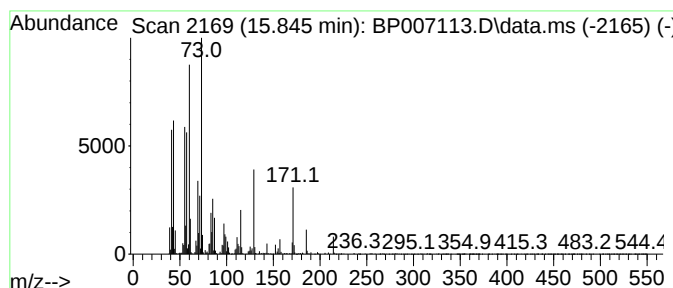
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Tridecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.845	2.95 ng	604000	Acenaphthene-d10	14.528

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	99
2			Dodecanoic acid	200	C12H24O2	000143-07-7	72
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	59
4			n-Decanoic acid	172	C10H20O2	000334-48-5	58
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	47



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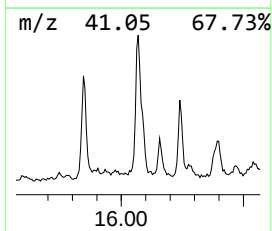
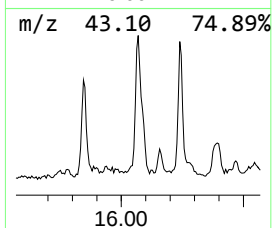
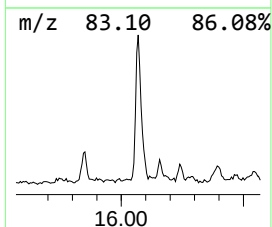
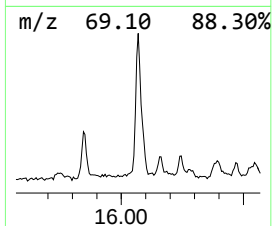
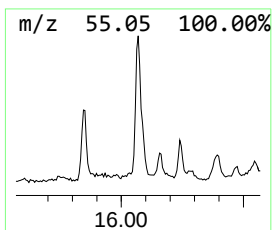
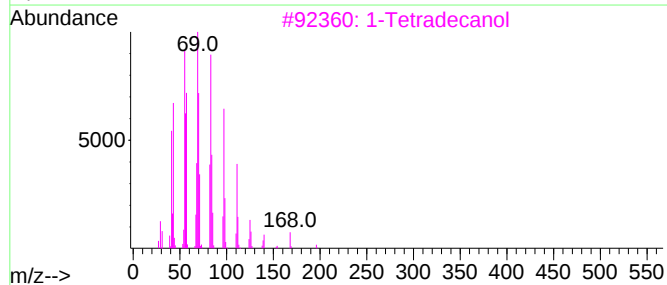
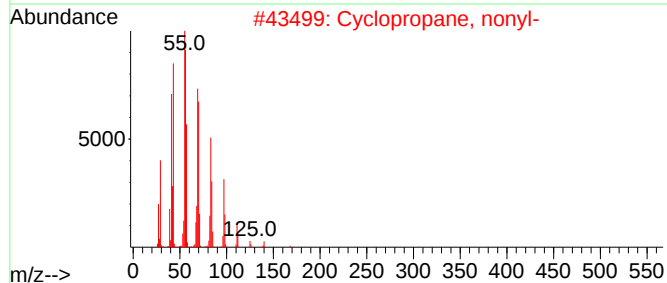
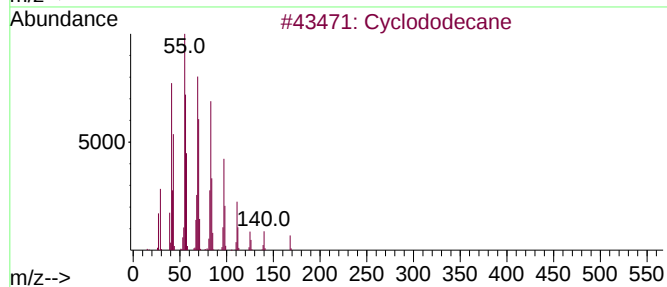
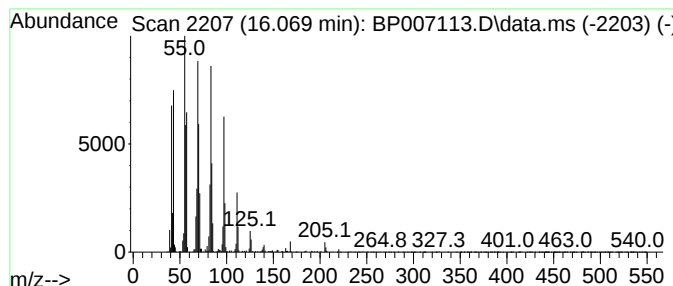
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Cyclohexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.069	3.67 ng	933978	Phenanthrene-d10	17.275

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclododecane	168	C12H24	000294-62-2	97
2			Cyclopropane, nonyl-	168	C12H24	074663-85-7	95
3			1-Tetradecanol	214	C14H30O	000112-72-1	91
4			n-Tridecan-1-ol	200	C13H28O	000112-70-9	91
5			n-Pentadecanol	228	C15H32O	000629-76-5	91



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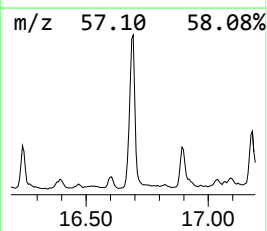
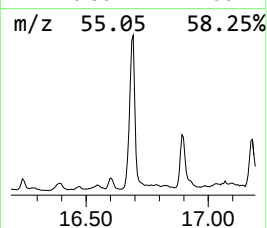
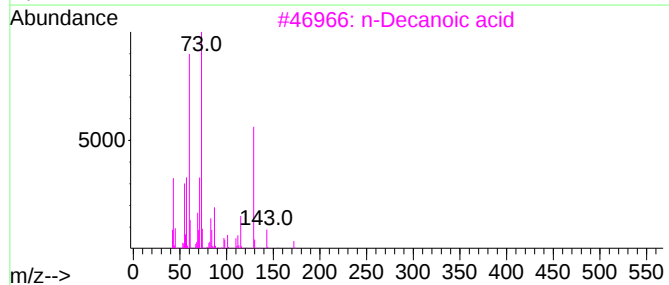
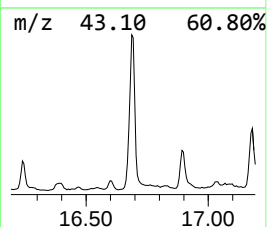
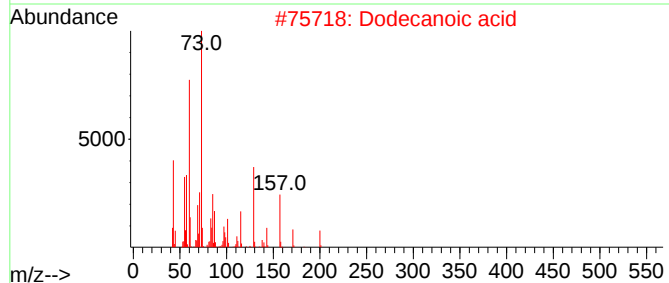
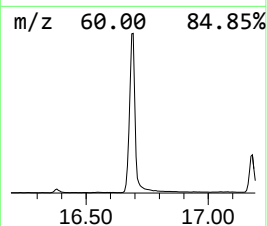
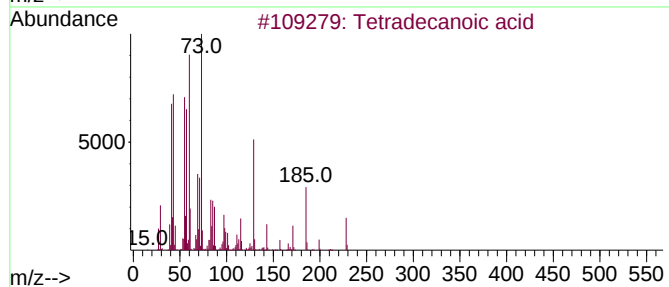
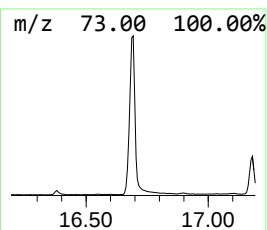
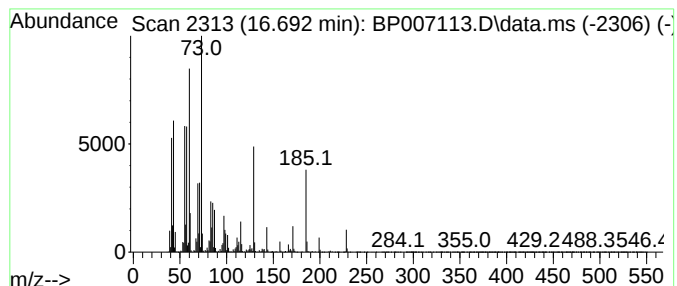
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Tetradecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.692	19.28 ng	4903870	Phenanthrene-d10	17.275

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	99
2			Dodecanoic acid	200	C12H24O2	000143-07-7	64
3			n-Decanoic acid	172	C10H20O2	000334-48-5	64
4			Undecanoic acid	186	C11H22O2	000112-37-8	58
5			Tridecanoic acid	214	C13H26O2	000638-53-9	53



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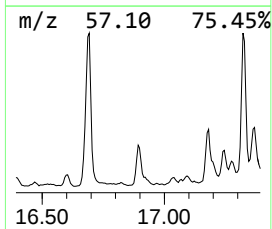
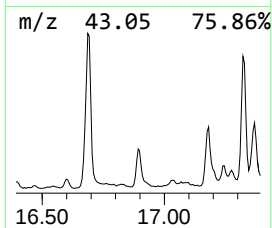
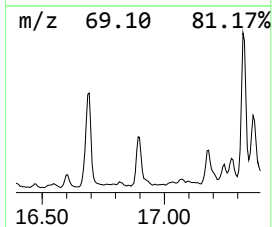
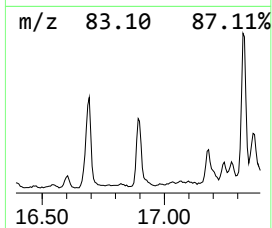
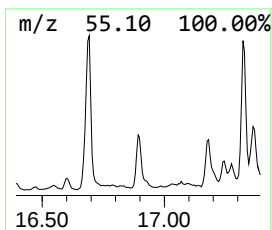
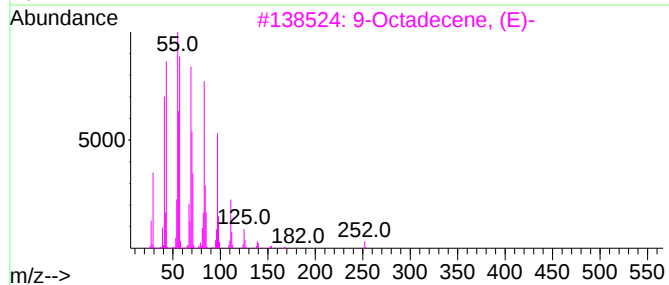
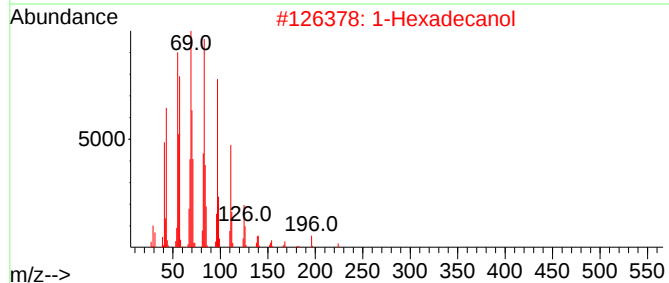
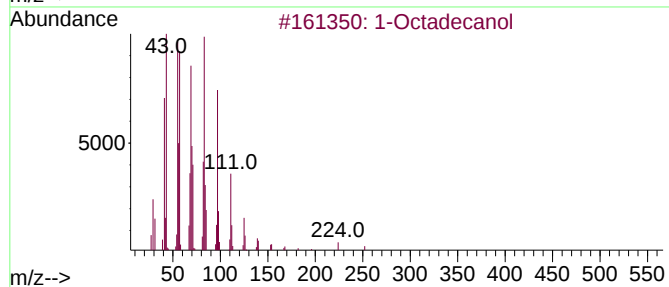
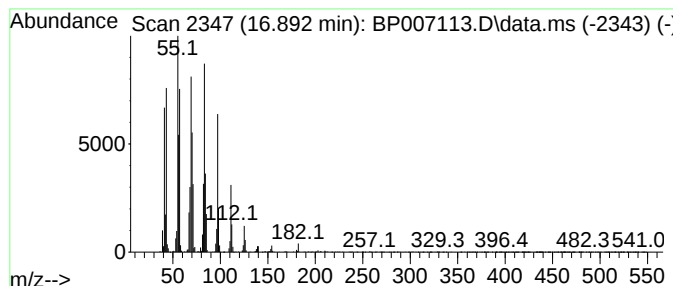
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1-Octadecanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.892	3.78 ng	961541	Phenanthrene-d10	17.275

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Octadecanol	270	C18H38O	000112-92-5	95
2		1-Hexadecanol	242	C16H34O	036653-82-4	94
3		9-Octadecene, (E)-	252	C18H36	007206-25-9	91
4		n-Pentadecanol	228	C15H32O	000629-76-5	91
5		5-Octadecene, (E)-	252	C18H36	007206-21-5	91



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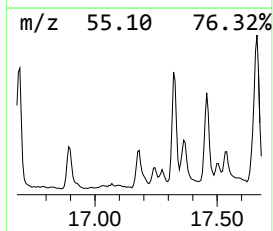
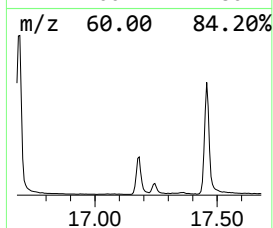
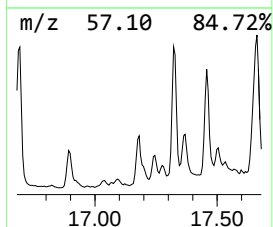
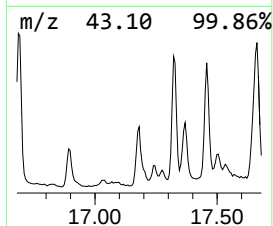
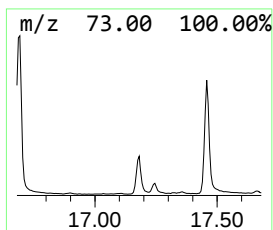
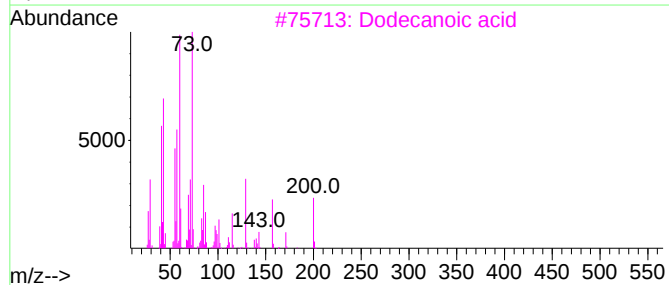
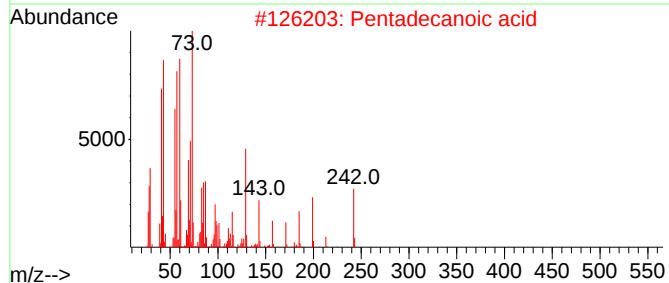
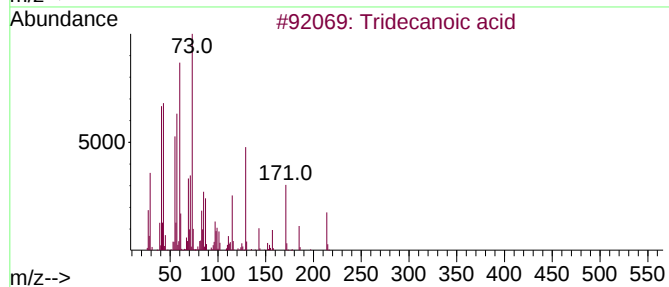
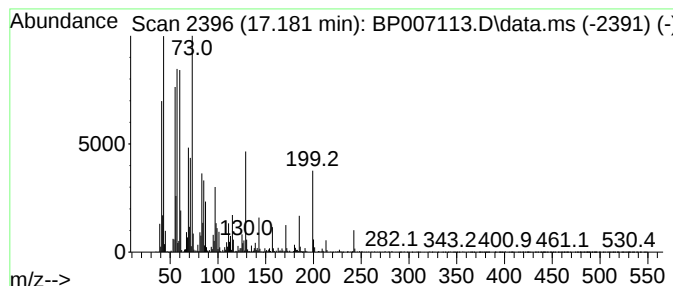
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Peak Number 5 Pentadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.181	6.59 ng	1676500	Phenanthrene-d10	17.275

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	91
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Dodecanoic acid	200	C12H24O2	000143-07-7	87
4			Octadecanoic acid	284	C18H36O2	000057-11-4	87
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	80



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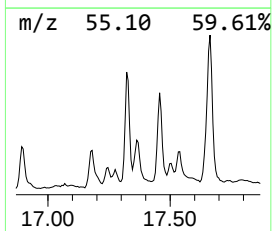
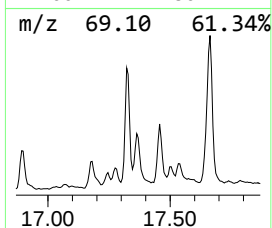
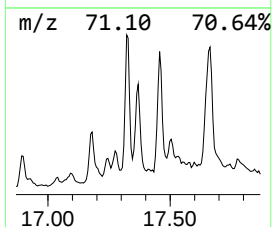
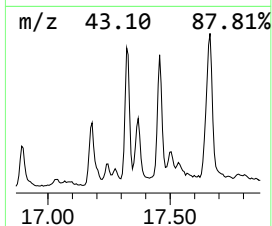
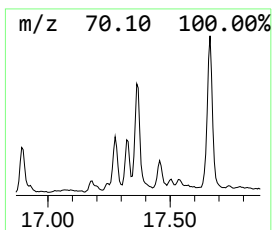
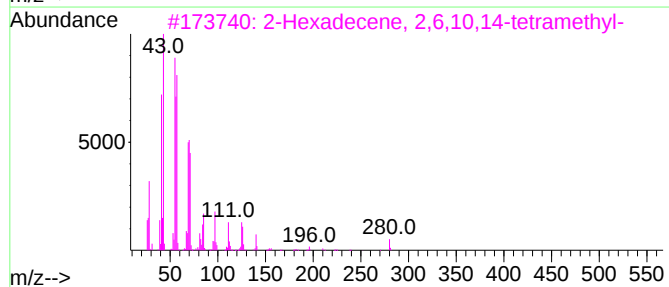
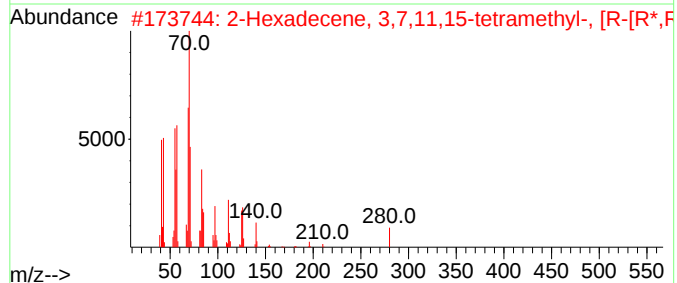
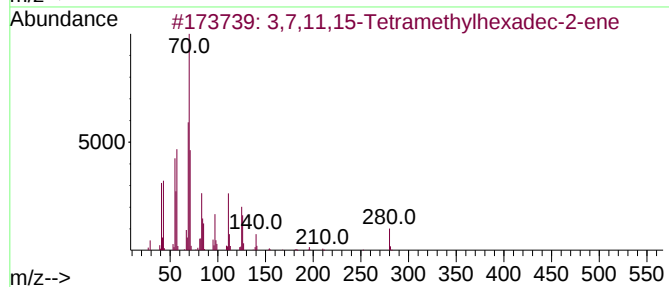
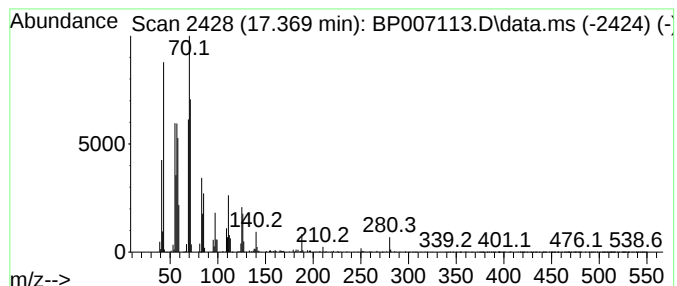
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 3,7,11,15-Tetramethylhexade... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.369	5.03 ng	1280150	Phenanthrene-d10	17.275

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3,7,11,15-Tetramethylhexadec-2-ene	280	C20H40	002437-93-6	93
2		2-Hexadecene, 3,7,11,15-tetramet...	280	C20H40	014237-73-1	90
3		2-Hexadecene, 2,6,10,14-tetramet...	280	C20H40	056554-34-8	55
4		Cyclohexane, (1,1-dimethylpropyl)-	154	C11H22	031797-64-5	38
5		2-Octene, 3,7-dimethyl-, (Z)-	140	C10H20	006874-32-4	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092221\
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Acq On : 22 Sep 2021 23:43
Operator : CG/JU
Sample : M3871-01 5X
Misc :
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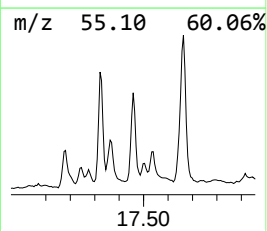
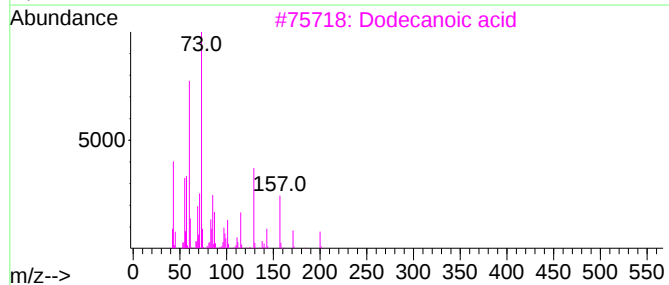
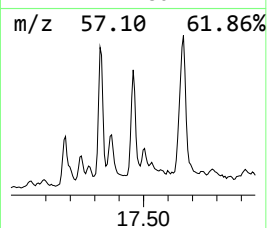
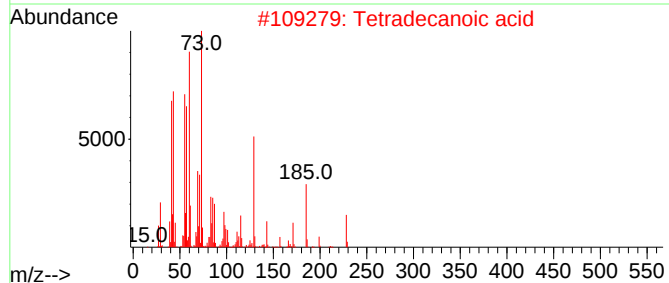
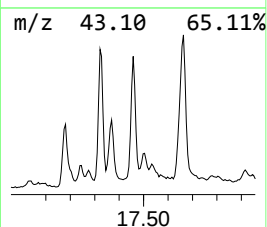
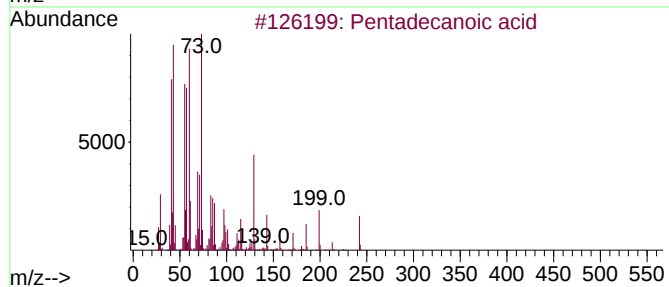
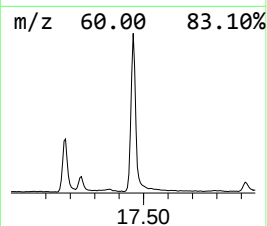
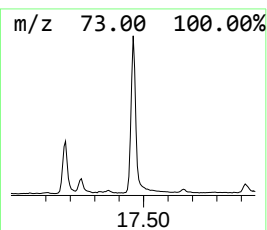
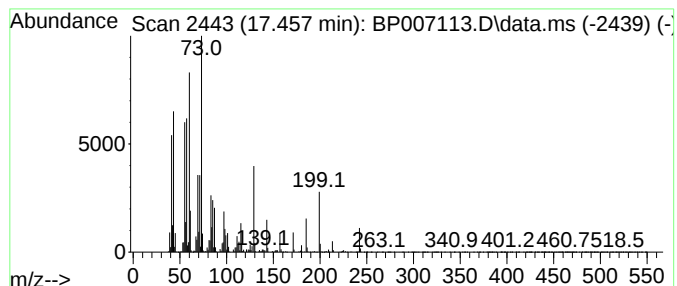
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Dodecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.457	11.19 ng	2844760	Phenanthrene-d10	17.275	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	96
3	Dodecanoic acid	200	C12H24O2	000143-07-7	81
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092221\
Data File : BP007113.D
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Operator : CG/JU
Sample : M3871-01 5X
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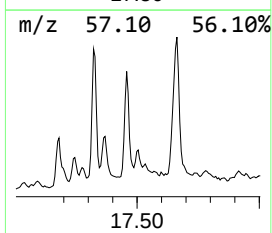
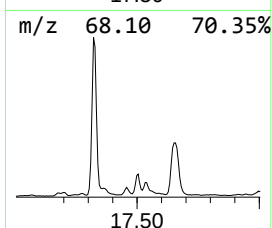
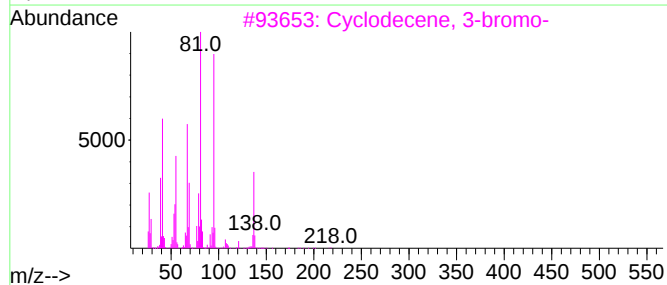
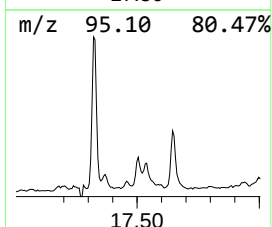
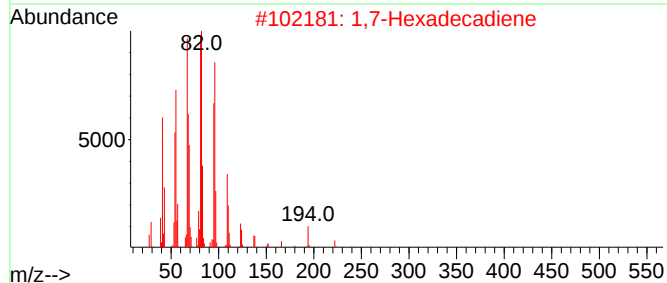
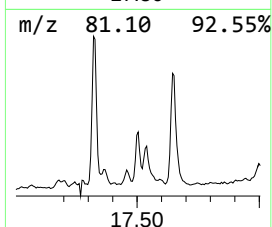
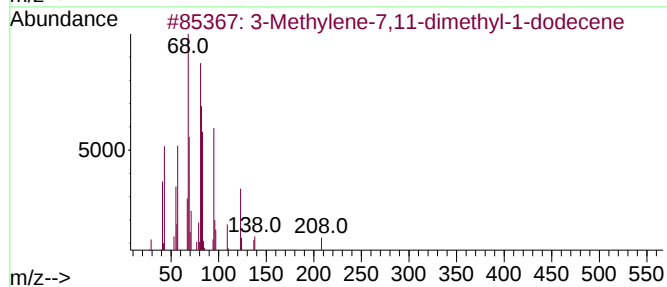
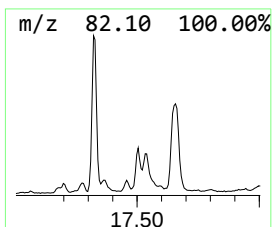
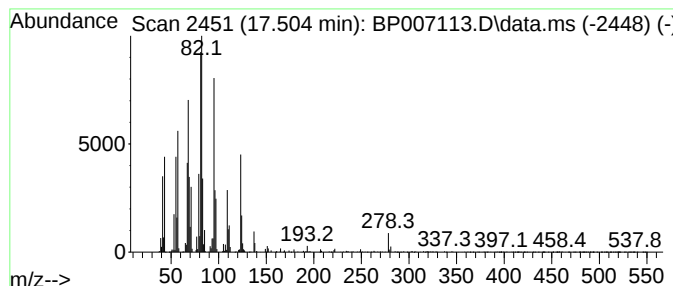
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 3-Methylene-7,11-dimethyl-1... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.504	2.84 ng	722497	Phenanthrene-d10	17.275

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Methylene-7,11-dimethyl-1-dodec...	208	C15H28	1000432-21-6	86
2		1,7-Hexadecadiene	222	C16H30	125110-62-5	59
3		Cyclodecene, 3-bromo-	216	C10H17Br	056325-56-5	50
4		Neophytadiene	278	C20H38	000504-96-1	49
5		Cyclohexanol, 1-ethynyl-	124	C8H12O	000078-27-3	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092221\
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Sample : M3871-01 5X
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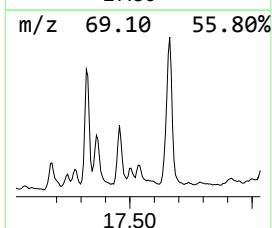
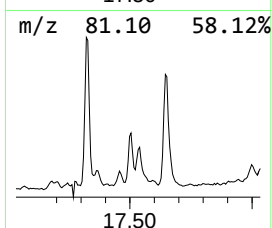
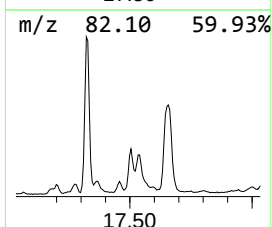
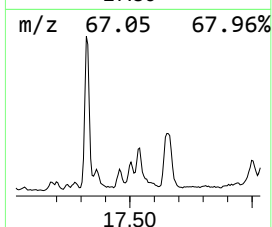
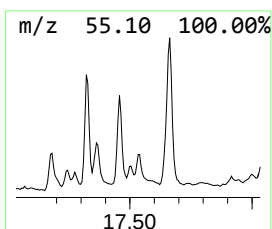
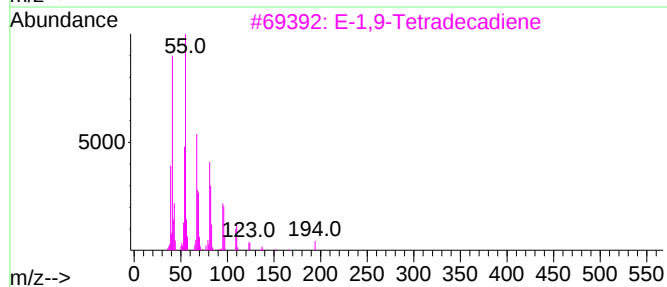
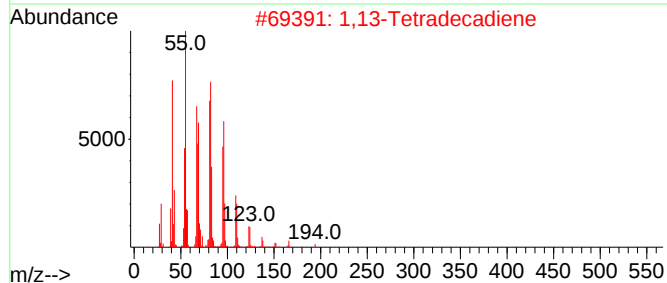
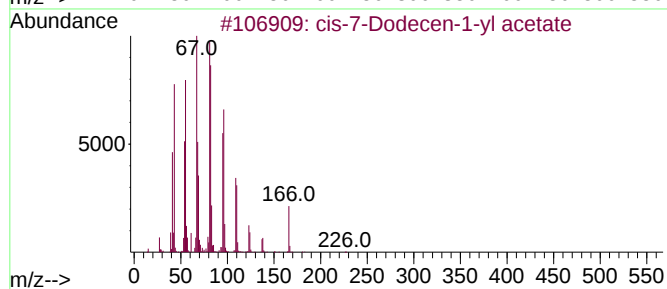
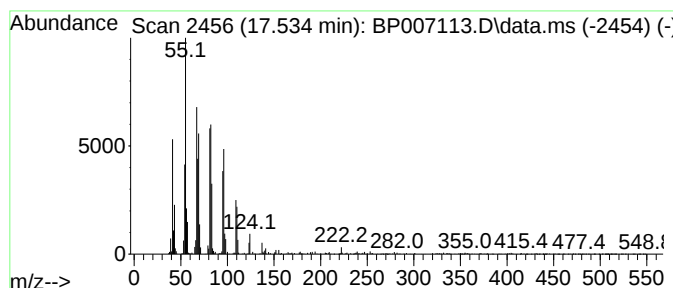
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 cis-7-Dodecen-1-yl acetate Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.534	2.52 ng	641334	Phenanthrene-d10	17.275	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-7-Dodecen-1-yl acetate	226	C14H26O2	014959-86-5	94
2	1,13-Tetradecadiene	194	C14H26	021964-49-8	94
3	E-1,9-Tetradecadiene	194	C14H26	1000245-70-7	94
4	9-Octadecen-1-ol, (E)-	268	C18H36O	000506-42-3	93
5	11-Eicosenol	296	C20H40O	1010424-20-3	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092221\
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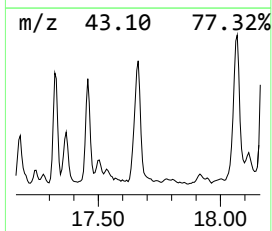
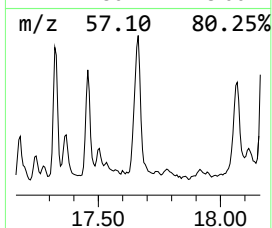
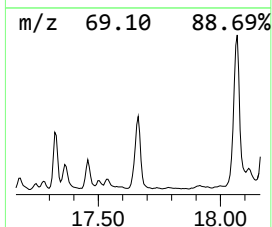
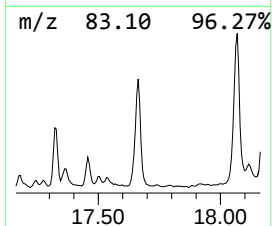
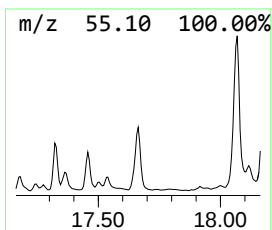
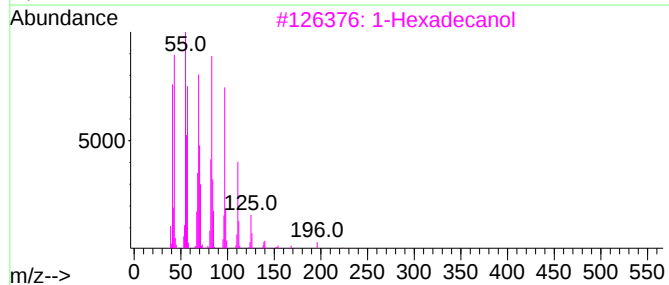
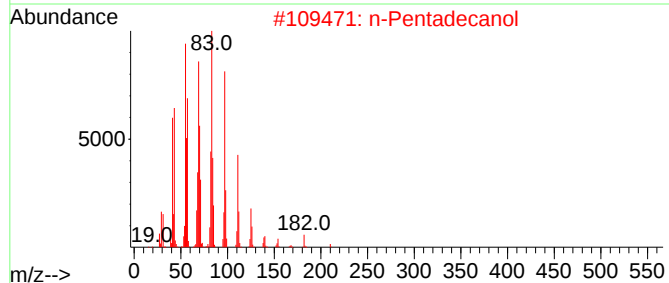
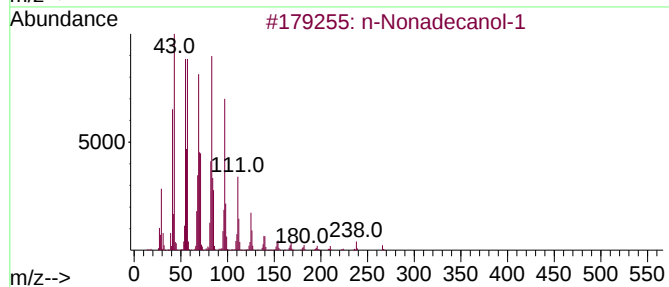
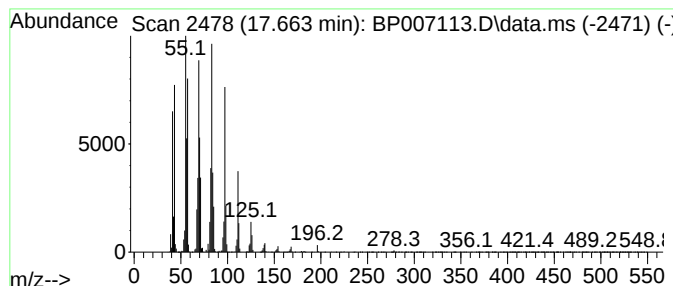
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 n-Nonadecanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.663	18.81 ng	4784350	Phenanthrene-d10	17.275

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
2		n-Pentadecanol	228	C15H32O	000629-76-5	95
3		1-Hexadecanol	242	C16H34O	036653-82-4	95
4		Cyclotetradecane	196	C14H28	000295-17-0	95
5		1-Octadecanol	270	C18H38O	000112-92-5	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092221\
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Sample : M3871-01 5X
Misc :
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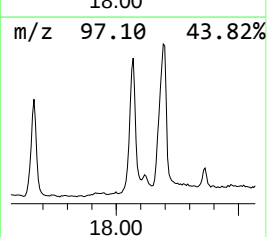
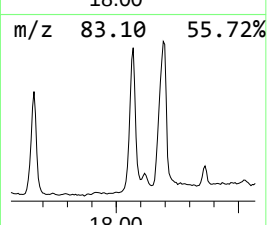
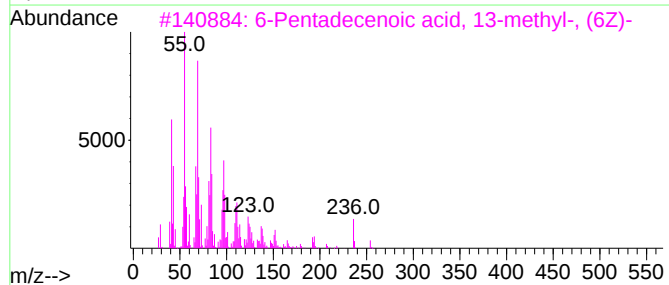
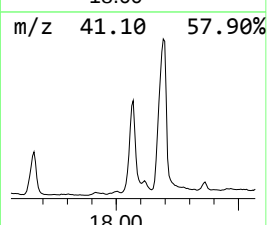
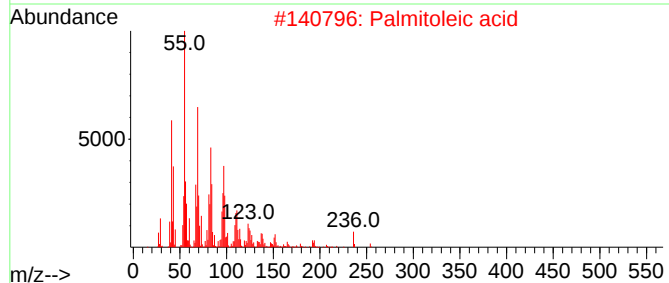
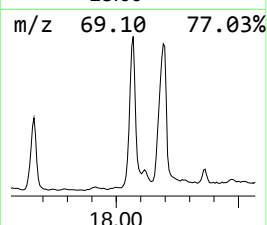
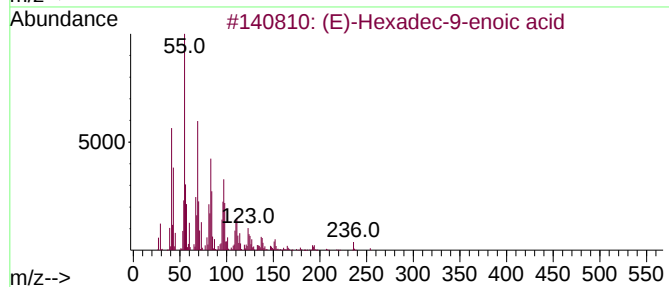
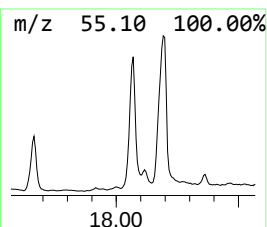
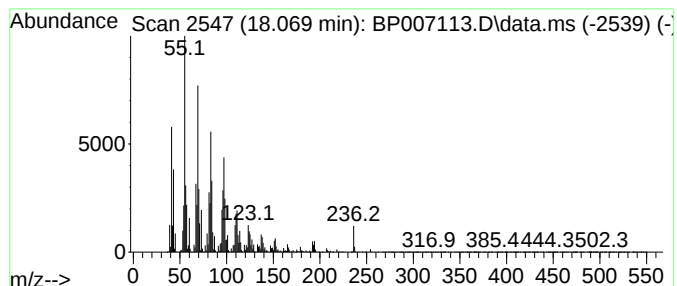
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 (E)-Hexadec-9-enoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.069	43.42 ng	11042500	Phenanthrene-d10	17.275	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	99
2	Palmitoleic acid	254	C16H30O2	000373-49-9	99
3	6-Pentadecenoic acid, 13-methyl-...	254	C16H30O2	682751-34-4	93
4	cis-7-Hexadecenoic acid	254	C16H30O2	002416-19-5	83
5	9-Hexadecenoic acid	254	C16H30O2	002091-29-4	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092221\
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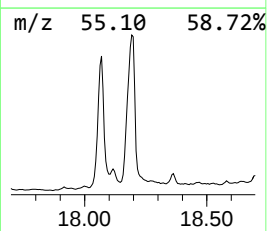
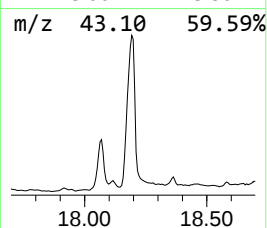
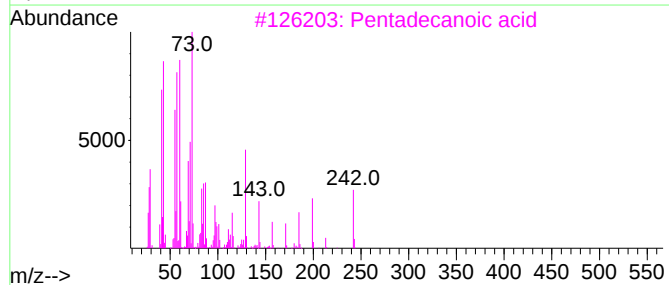
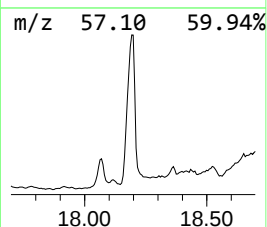
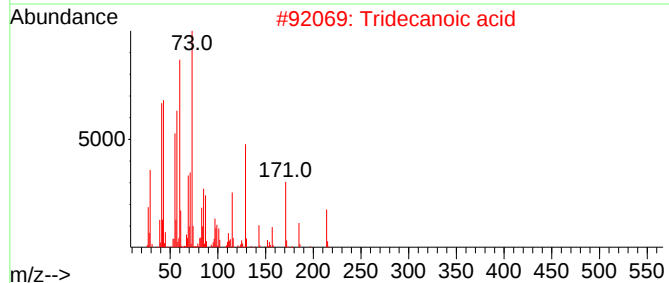
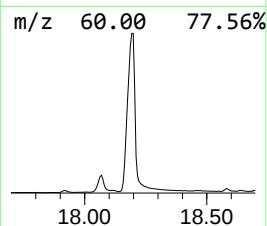
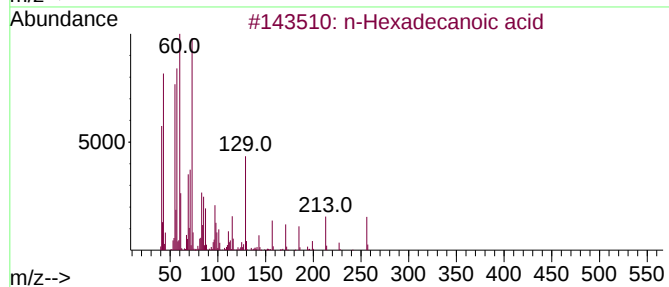
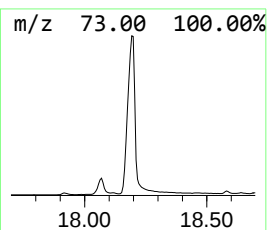
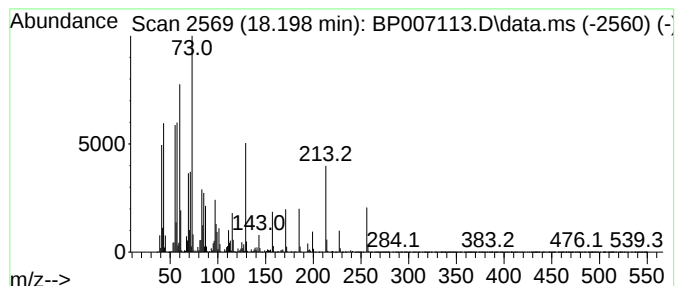
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.198	94.32 ng	23986100	Phenanthrene-d10	17.275

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	83
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4			n-Decanoic acid	172	C10H20O2	000334-48-5	55
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092221\
Data File : BP007113.D
Acq On : 22 Sep 2021 23:43
Operator : CG/JU
Sample : M3871-01 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SS01-BL-(0.0)

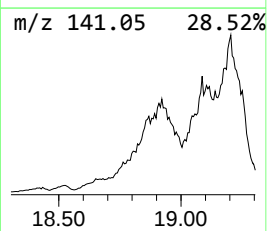
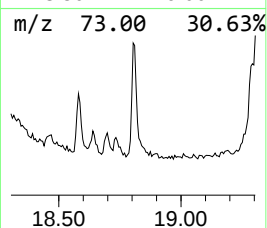
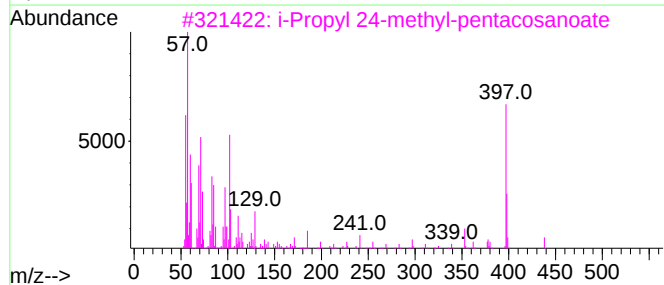
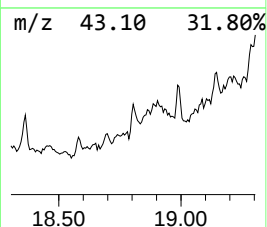
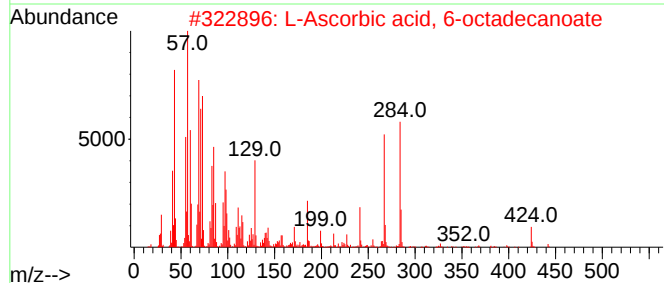
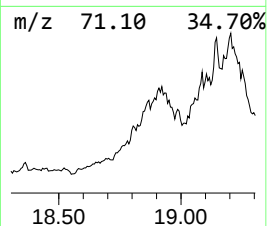
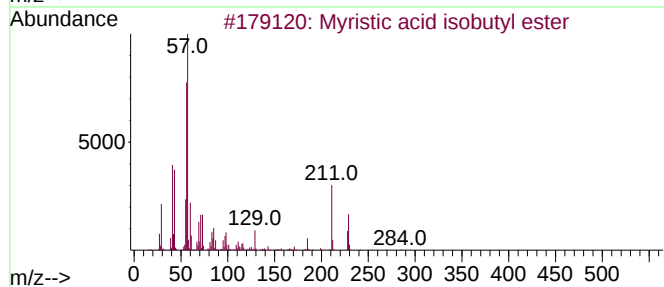
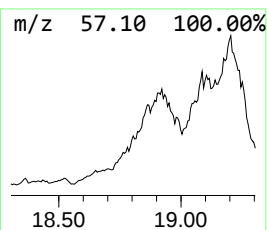
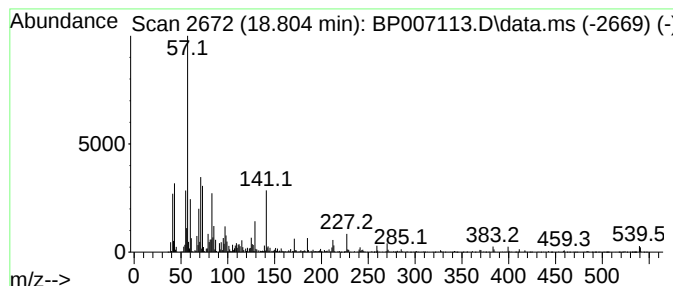
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown18.804 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.804	3.61 ng	917885	Phenanthrene-d10	17.275

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Myristic acid isobutyl ester	284	C18H36O2	025263-97-2	37
2			L-Ascorbic acid, 6-octadecanoate	442	C24H42O7	010605-09-1	35
3			i-Propyl 24-methyl-pentacosanoate	438	C29H58O2	1000336-57-0	32
4			Tricosanoic acid, isobutyl ester	410	C27H54O2	1000405-17-2	25
5			.beta.-D-Glucopyranoside, methyl...	292	C14H28O6	1010157-04-9	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092221\
Data File : BP007113.D
Acq On : 22 Sep 2021 23:43
Operator : CG/JU
Sample : M3871-01 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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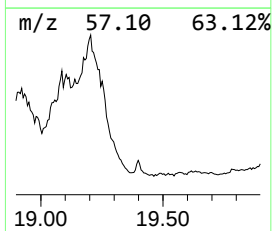
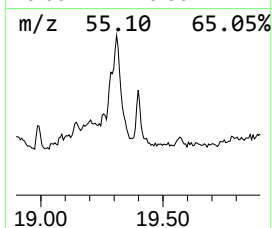
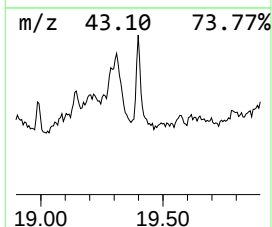
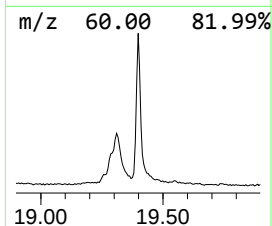
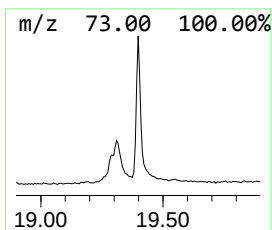
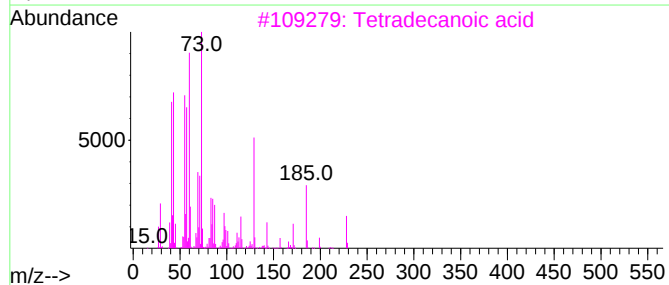
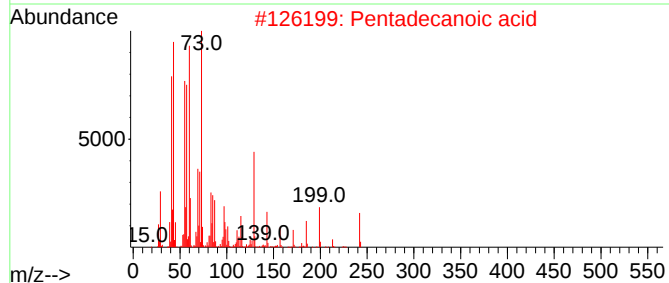
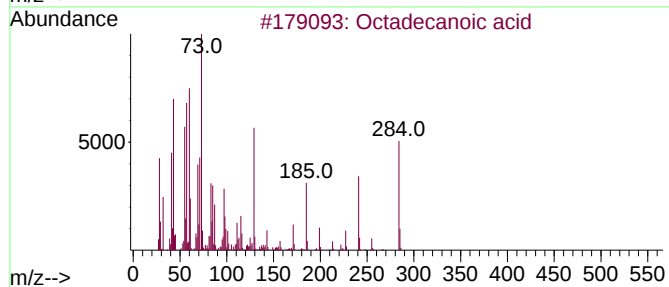
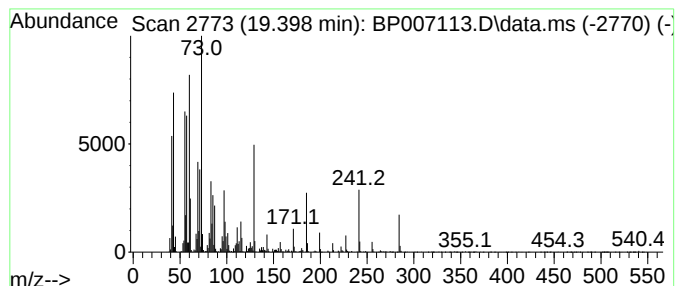
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.398	7.74 ng	2146130	Chrysene-d12	21.357

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	90
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4		Tridecanoic acid	214	C13H26O2	000638-53-9	72
5		Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092221\
Data File : BP007113.D
Acq On : 22 Sep 2021 23:43
Operator : CG/JU
Sample : M3871-01 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SS01-BL-(0.0)

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Tridecanoic acid	15.845	3.0	ng	604000	3	14.528	4097740	20.0
Cyclododecane	16.069	3.7	ng	933978	4	17.275	5085880	20.0
Tetradecanoic acid	16.692	19.3	ng	4903870	4	17.275	5085880	20.0
1-Octadecanol	16.892	3.8	ng	961541	4	17.275	5085880	20.0
Pentadecanoic acid	17.181	6.6	ng	1676500	4	17.275	5085880	20.0
3,7,11,15-Tetra...	17.369	5.0	ng	1280150	4	17.275	5085880	20.0
Dodecanoic acid	17.457	11.2	ng	2844760	4	17.275	5085880	20.0
3-Methylene-7,1...	17.504	2.8	ng	722497	4	17.275	5085880	20.0
cis-7-Dodecen-1...	17.534	2.5	ng	641334	4	17.275	5085880	20.0
n-Nonadecanol-1	17.663	18.8	ng	4784350	4	17.275	5085880	20.0
(E)-Hexadec-9-e...	18.069	43.4	ng	11042500	4	17.275	5085880	20.0
n-Hexadecanoic ...	18.198	94.3	ng	23986100	4	17.275	5085880	20.0
unknown18.804	18.804	3.6	ng	917885	4	17.275	5085880	20.0
Octadecanoic acid	19.398	7.7	ng	2146130	5	21.357	5542660	20.0