

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040221\
 Data File : BP005166.D
 Acq On : 02 Apr 2021 19:01
 Operator : CG/JU
 Sample : M1887-01 2X
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 TR-03-033121

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-BP032321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005166.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.305	371	377	386	rBV	243041	346053	6.85%	2.278%
2	6.887	638	646	655	rBV	227784	367170	7.27%	2.418%
3	7.705	778	785	800	rVB	136007	211792	4.19%	1.394%
4	8.863	974	982	994	rBV	146935	239662	4.75%	1.578%
5	10.493	1251	1259	1269	rBV	173889	292839	5.80%	1.928%
6	12.975	1673	1681	1688	rBV	356340	506996	10.04%	3.338%
7	14.363	1907	1917	1923	rBV	258154	375198	7.43%	2.470%
8	15.857	2165	2171	2180	rBV	254323	356797	7.07%	2.349%
9	17.122	2380	2386	2391	rBV	310544	417677	8.27%	2.750%
10	17.804	2496	2502	2507	rBV	776416	848642	16.81%	5.588%
11	18.022	2535	2539	2548	rBV	111799	155339	3.08%	1.023%
12	18.916	2685	2691	2694	rBV	4208542	5049830	100.00%	33.249%
13	18.945	2694	2696	2706	rVB2	3011418	3554613	70.39%	23.404%
14	19.069	2713	2717	2722	rBV	411349	471489	9.34%	3.104%
15	19.122	2722	2726	2728	rBV	84911	111610	2.21%	0.735%
16	19.145	2728	2730	2737	rVB2	82938	122935	2.43%	0.809%
17	19.498	2783	2790	2798	rVB2	36706	90970	1.80%	0.599%
18	19.698	2819	2824	2828	rBV	526379	623594	12.35%	4.106%
19	20.139	2895	2899	2902	rBV	44873	56923	1.13%	0.375%
20	20.933	3031	3034	3042	rVB5	91499	125813	2.49%	0.828%
21	21.222	3078	3083	3087	rBV	350145	447048	8.85%	2.943%
22	23.504	3466	3471	3478	rVB2	218226	415010	8.22%	2.732%

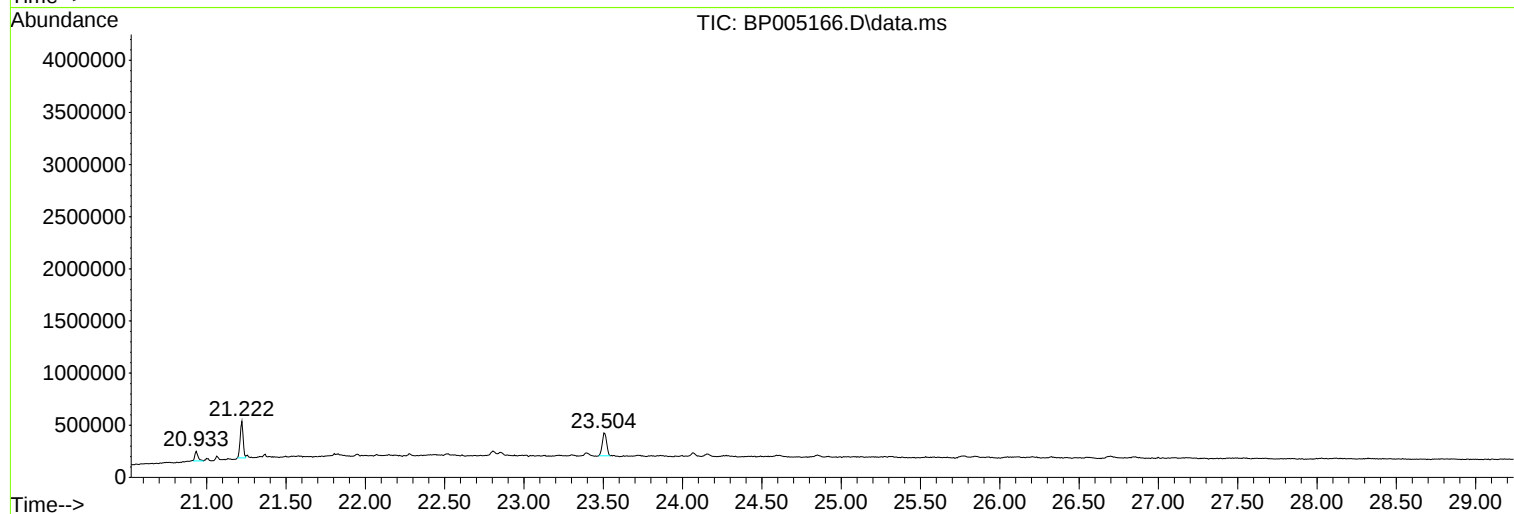
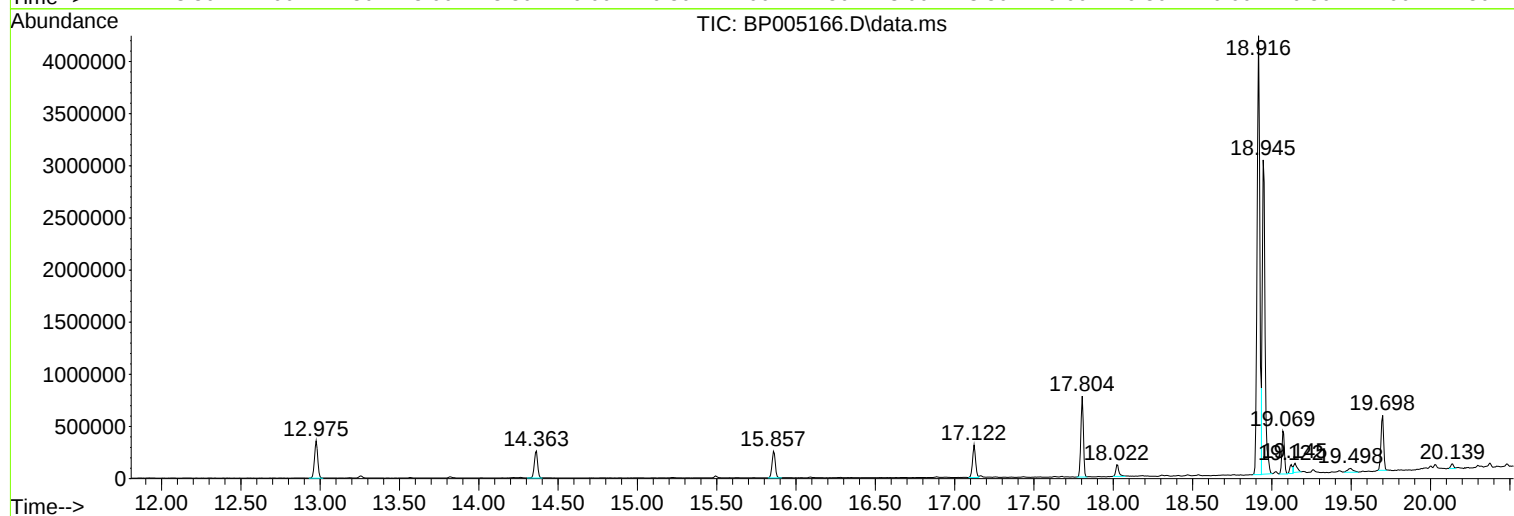
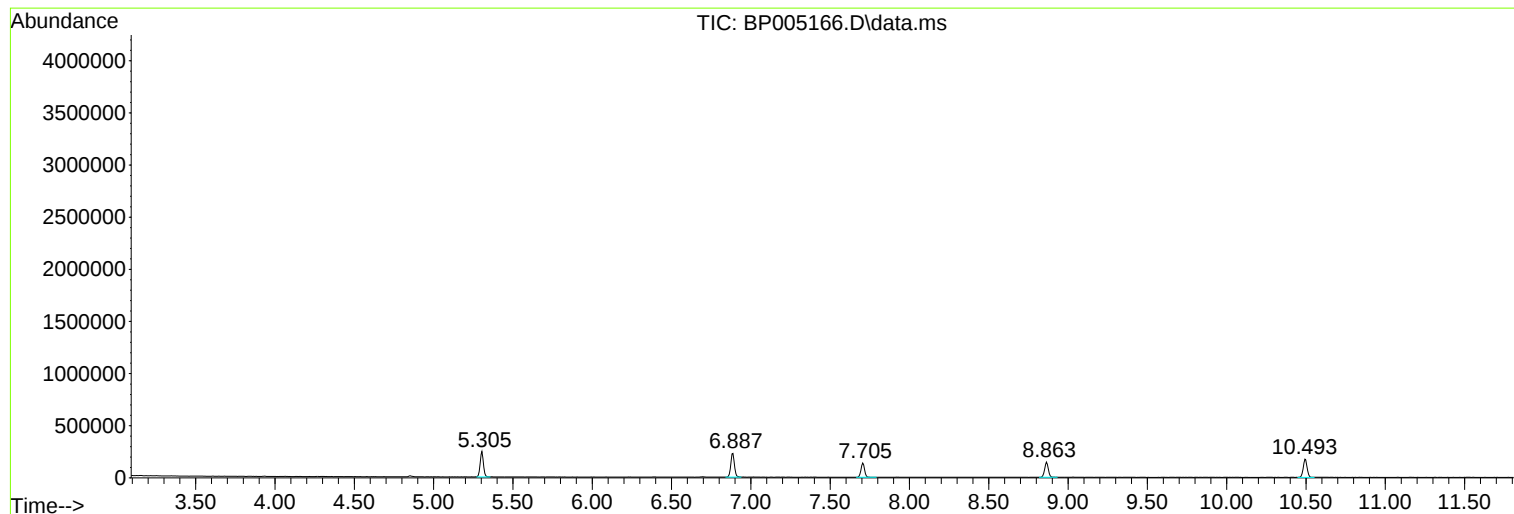
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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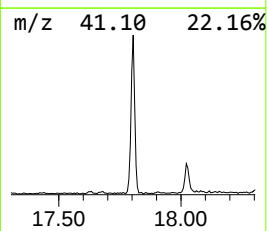
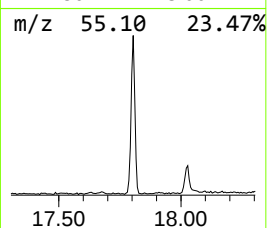
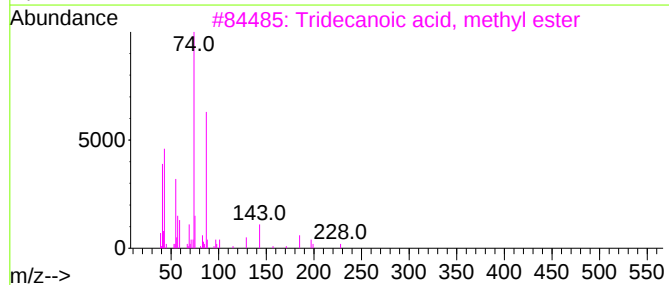
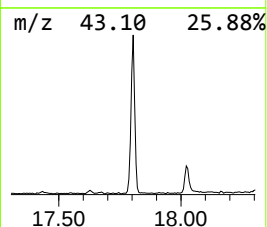
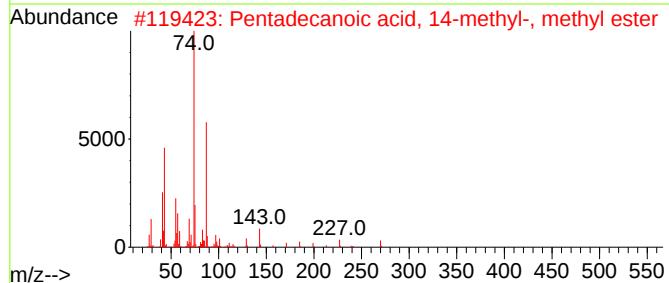
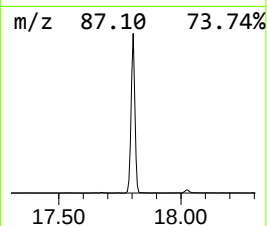
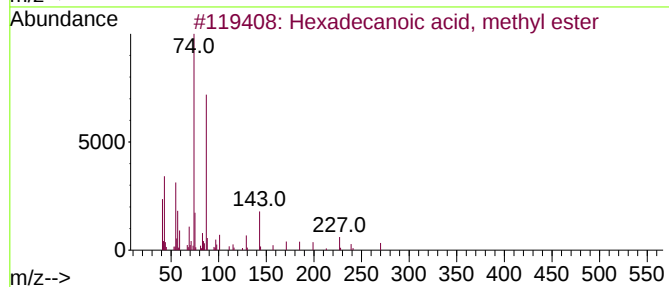
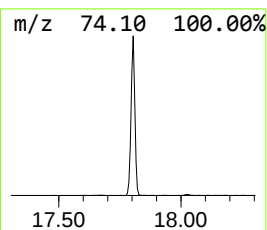
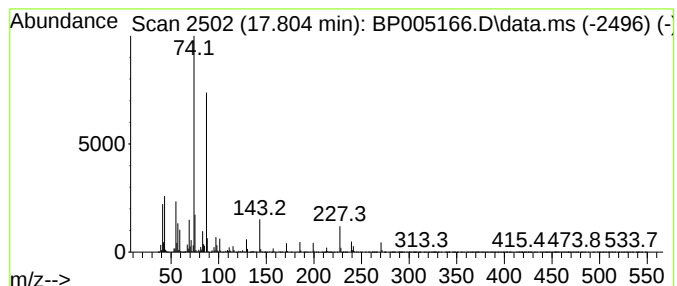
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.804	40.64 ng	848642	Phenanthrene-d10	17.122

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	95
3			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	93
4			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
5			Hexadecanoic acid, 2-methyl-	270	C17H34O2	027147-71-3	86



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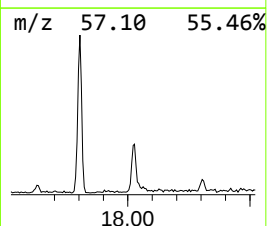
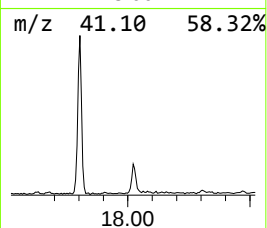
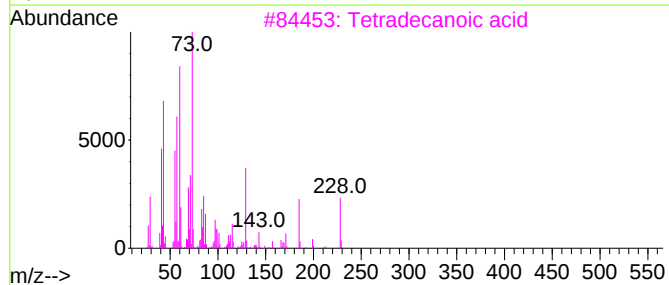
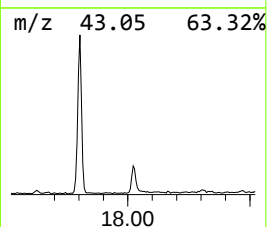
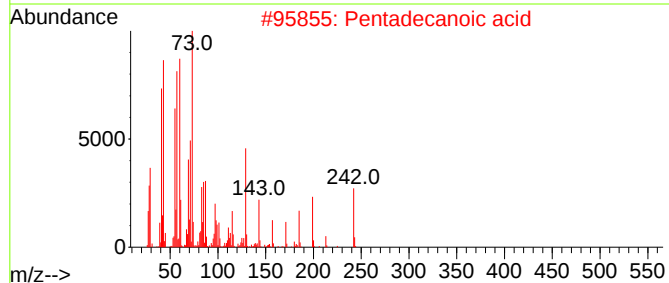
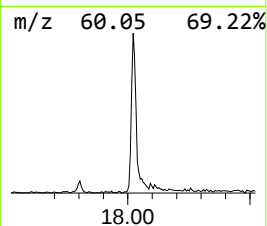
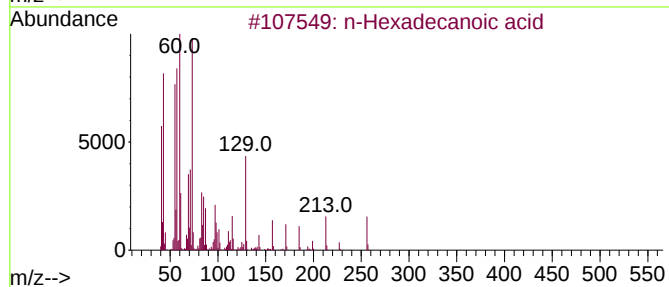
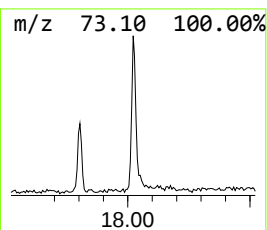
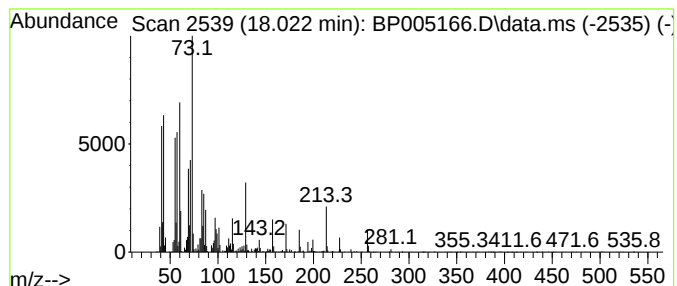
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.022	7.44 ng	155339	Phenanthrene-d10	17.122

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4			Tetradecane	198	C14H30	000629-59-4	56
5			Octadecanoic acid	284	C18H36O2	000057-11-4	53



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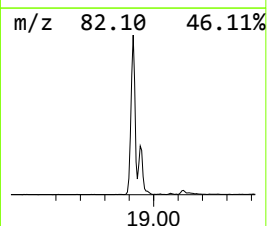
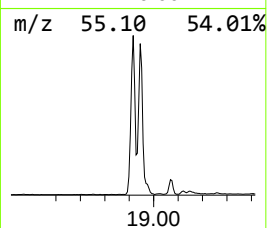
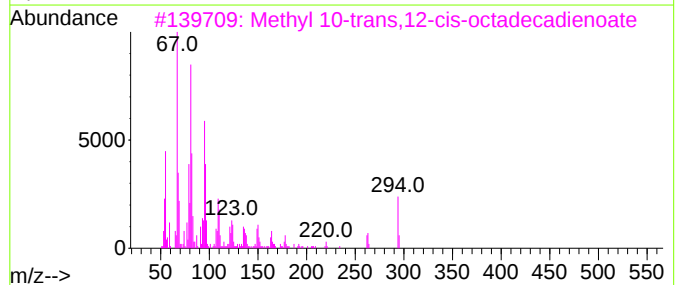
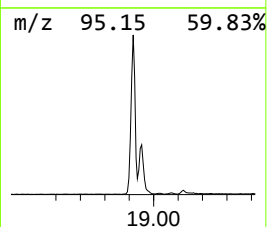
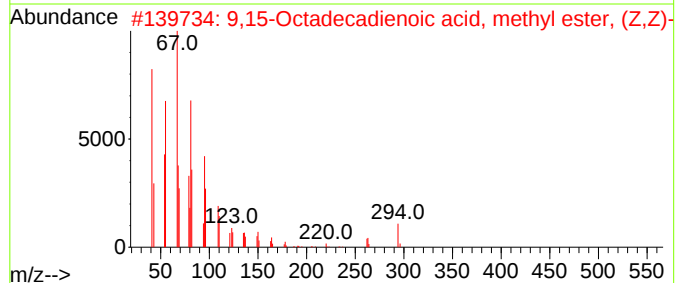
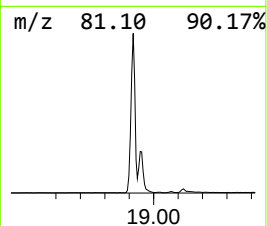
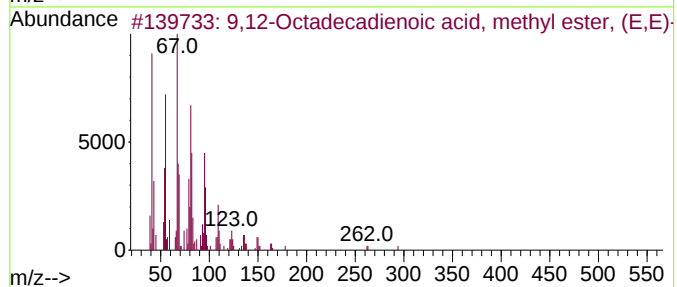
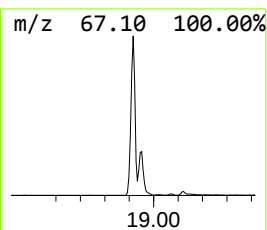
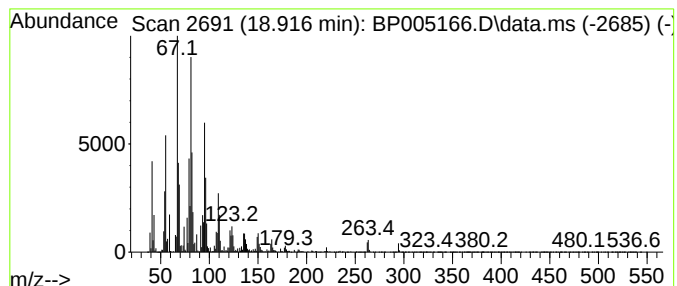
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Peak Number 3 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.916	241.81 ng	5049830	Phenanthrene-d10	17.122	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	98
2	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	98
3	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	97
4	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	97
5	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	95



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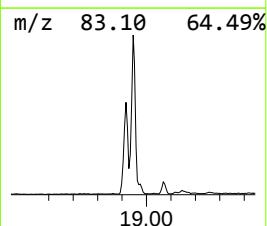
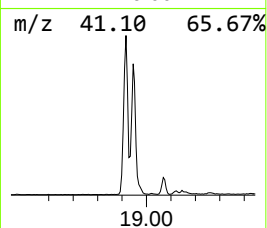
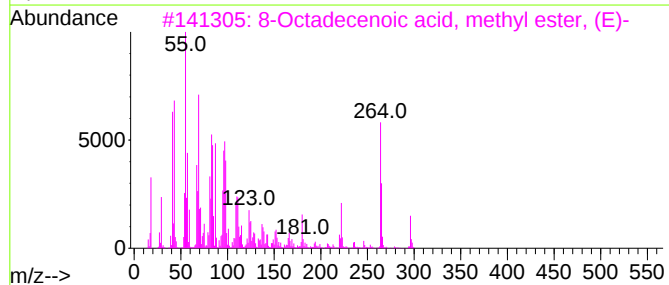
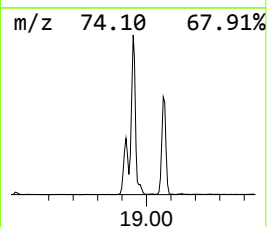
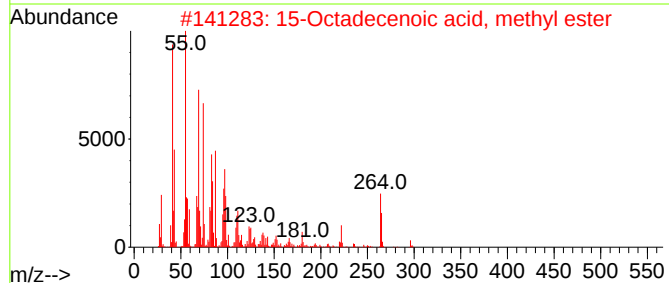
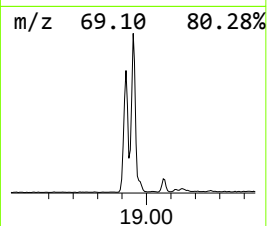
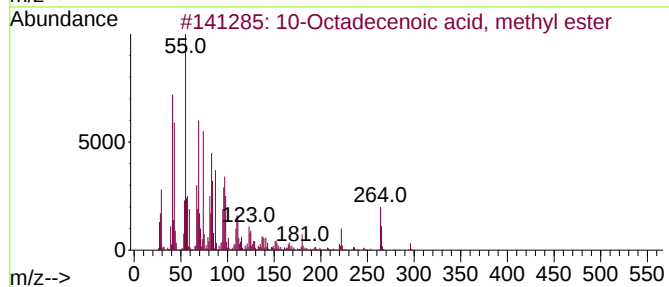
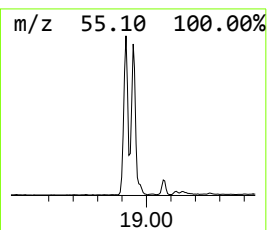
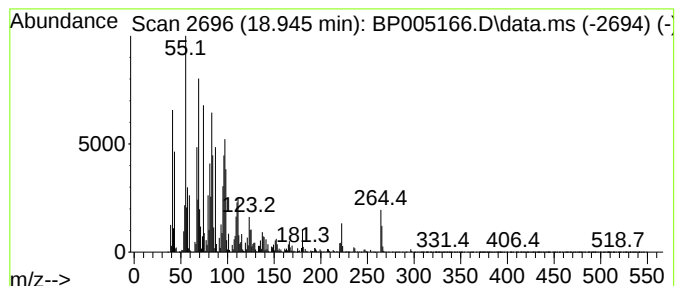
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TIC Integration Parameters: LSCINT.P

Peak Number 4 10-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.945	170.21 ng	3554610	Phenanthrene-d10	17.122	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
2	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99
3	8-Octadecenoic acid, methyl este...	296	C19H36O2	026528-50-7	99
4	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99
5	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99



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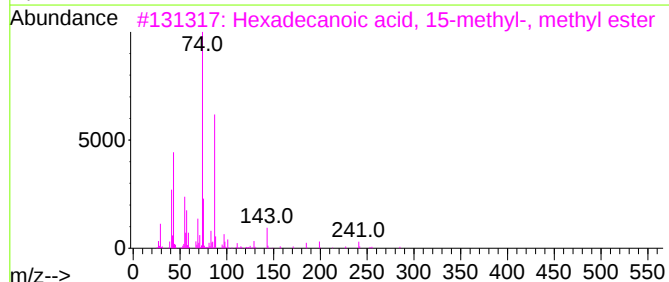
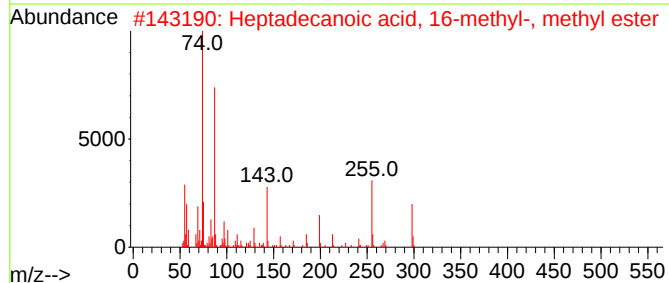
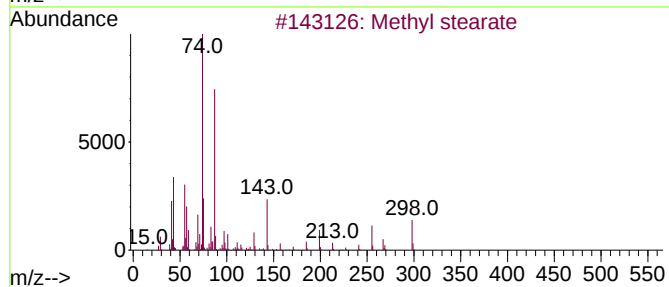
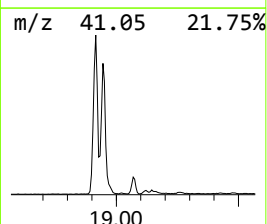
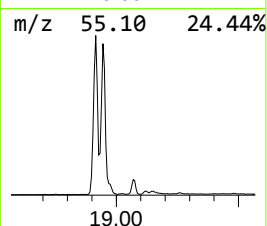
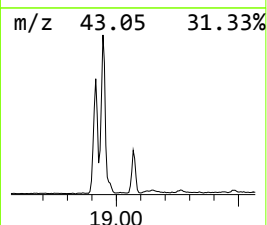
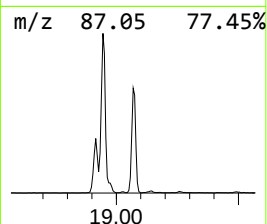
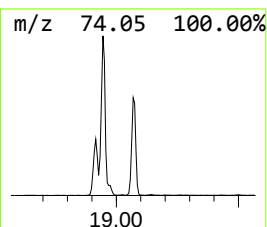
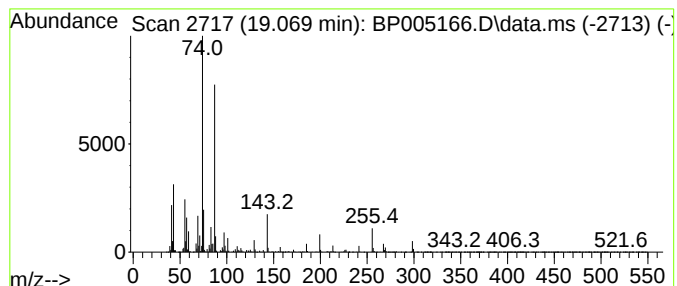
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Peak Number 5 Methyl stearate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.069	22.58 ng	471489	Phenanthrene-d10	17.122

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	98
2			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	93
3			Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	90
4			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	87
5			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	87



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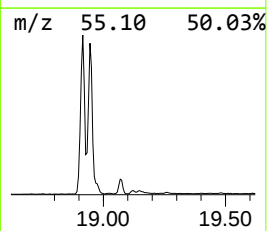
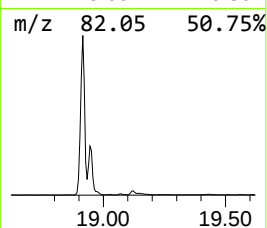
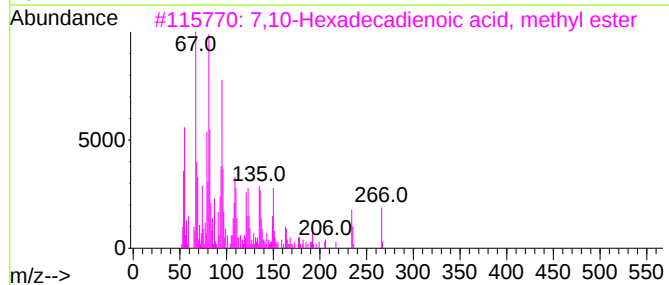
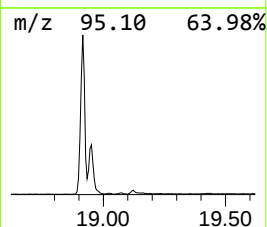
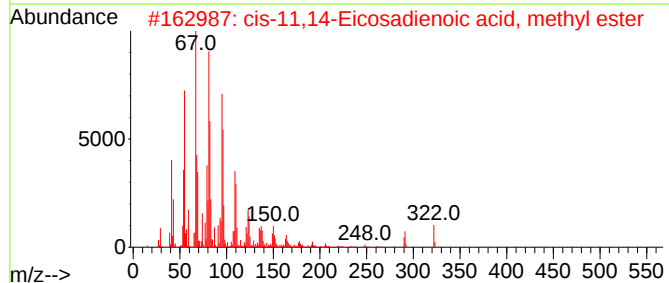
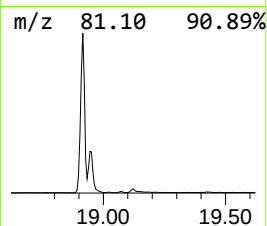
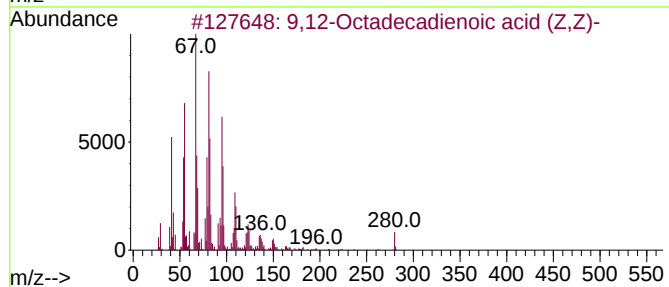
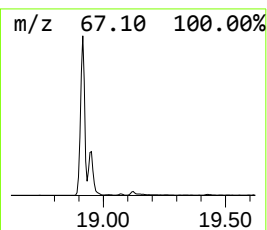
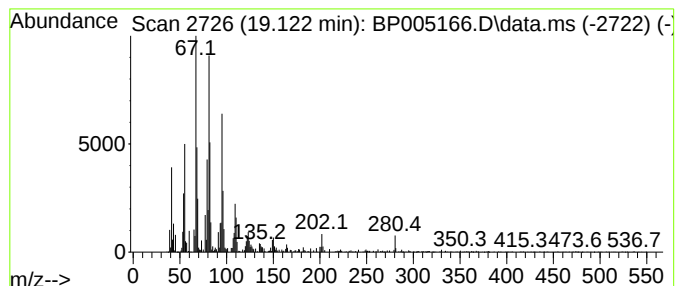
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9,12-Octadecadienoic acid (... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.122	5.34 ng	111610	Phenanthrene-d10	17.122

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	95
2			cis-11,14-Eicosadienoic acid, me...	322	C21H38O2	1000333-61-8	91
3			7,10-Hexadecadienoic acid, methy...	266	C17H30O2	016106-03-9	90
4			5-Hexadecyne	222	C16H30	071899-37-1	74
5			9-Octadecyne	250	C18H34	035365-59-4	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040221\
Data File : BP005166.D
Acq On : 02 Apr 2021 19:01
Operator : CG/JU
Sample : M1887-01 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TR-03-033121

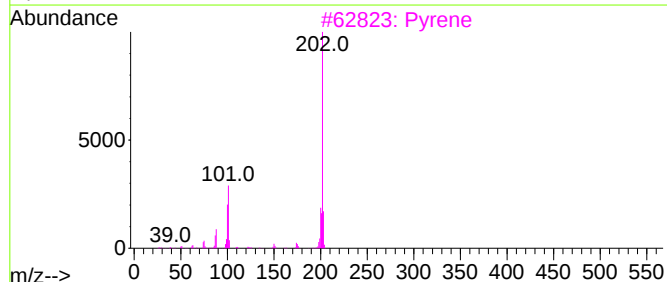
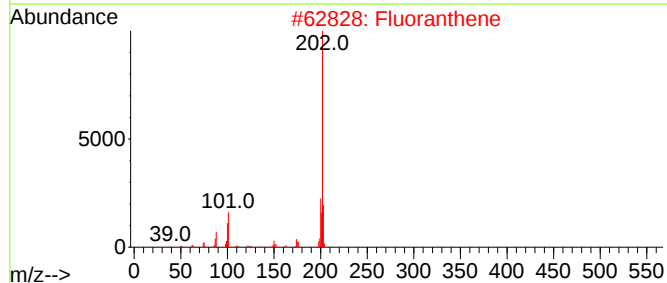
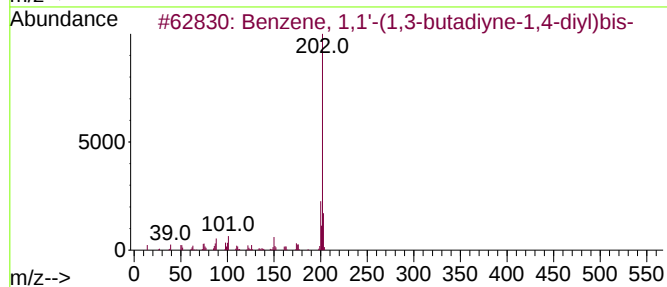
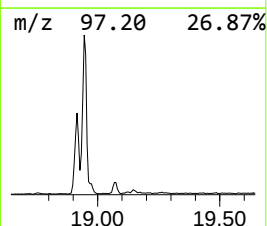
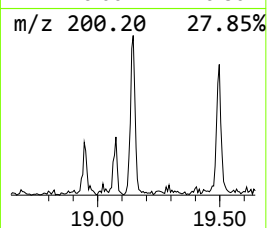
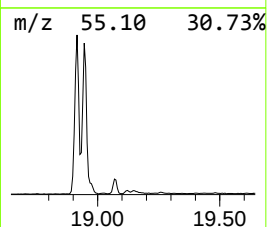
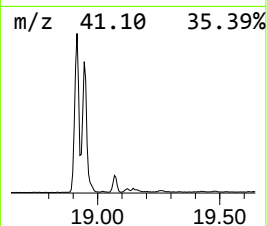
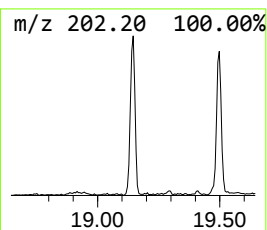
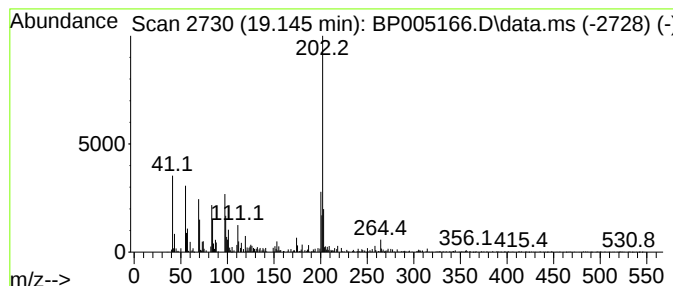
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.145	5.89 ng	122935	Phenanthrene-d10	17.122

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	53
2			Fluoranthene	202	C16H10	000206-44-0	53
3			Pyrene	202	C16H10	000129-00-0	49
4			Pyrimidine, 4-methoxy-6-(2-hydro...	202	C11H10N2O2	097630-79-0	43
5			1,4-Pentadiyn-3-one, 1,5-diphenyl-	230	C17H10O	015814-30-9	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040221\
Data File : BP005166.D
Acq On : 02 Apr 2021 19:01
Operator : CG/JU
Sample : M1887-01 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TR-03-033121

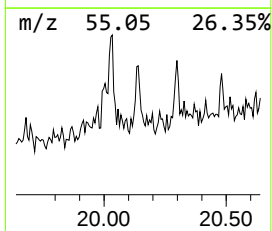
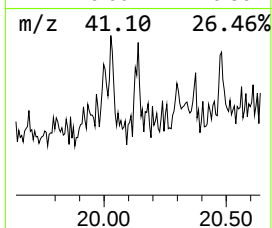
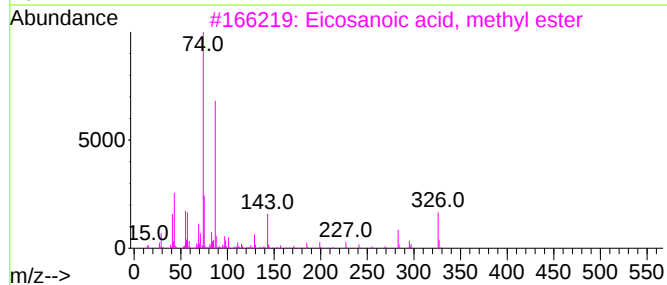
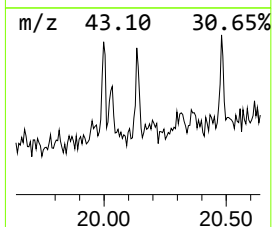
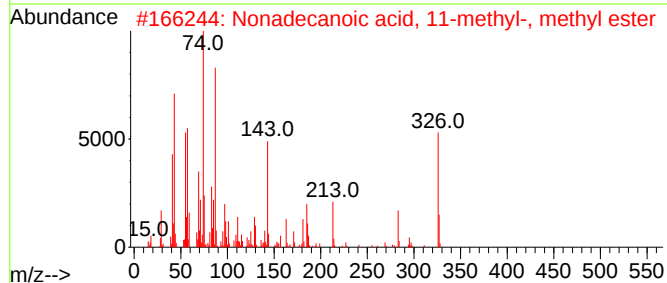
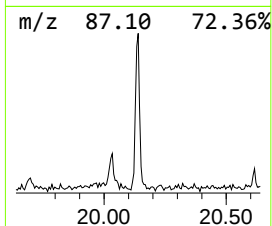
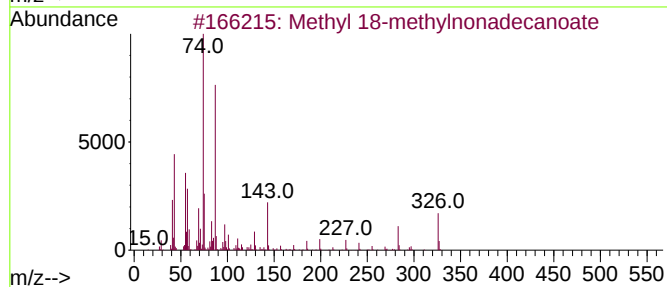
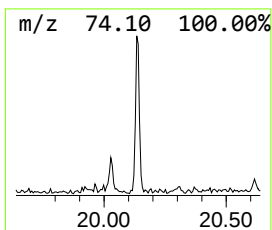
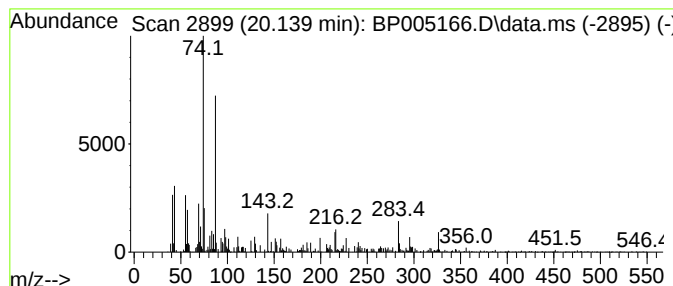
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Methyl 18-methylnonadecanoate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.139	2.55 ng	56923	Chrysene-d12	21.222

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl 18-methylnonadecanoate	326	C21H42O2	1000352-20-6	90
2			Nonadecanoic acid, 11-methyl-, m...	326	C21H42O2	055334-33-3	81
3			Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	81
4			Hexadecanoic acid, 14-methyl-, m...	284	C18H36O2	002490-49-5	76
5			Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040221\
Data File : BP005166.D
Acq On : 02 Apr 2021 19:01
Operator : CG/JU
Sample : M1887-01 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TR-03-033121

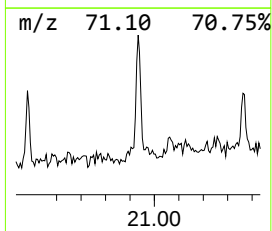
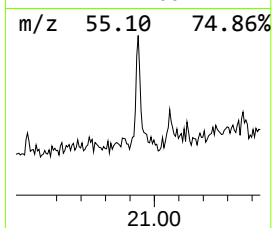
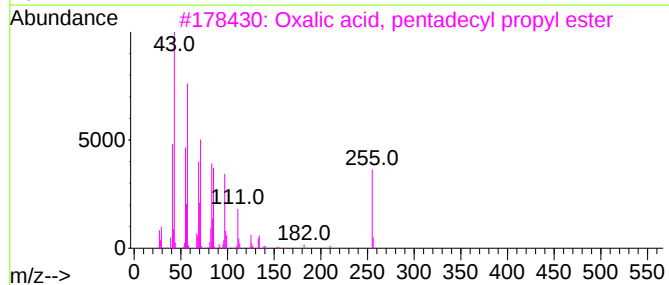
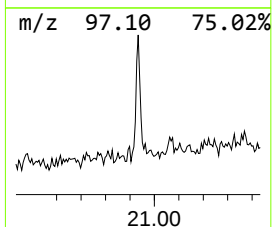
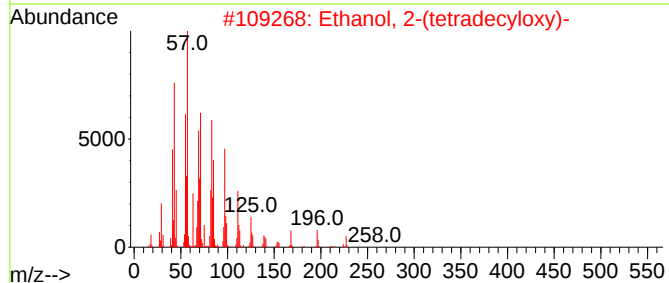
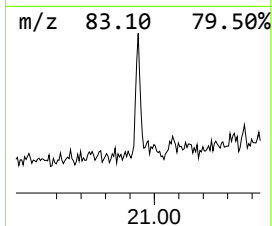
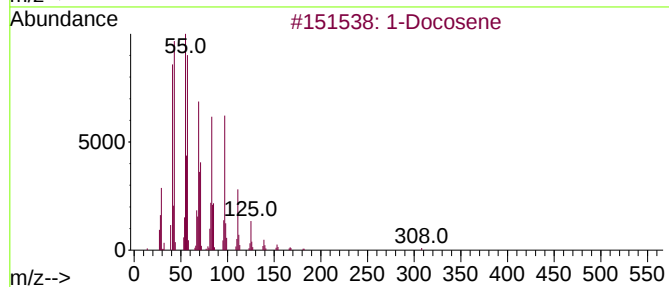
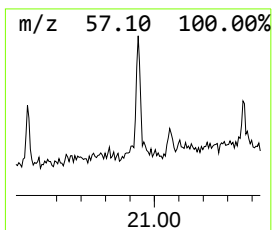
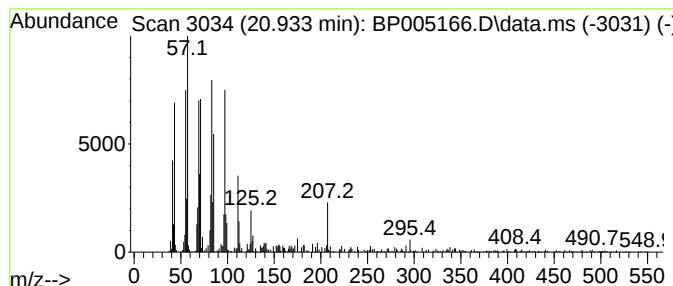
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Docosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.933	5.63 ng	125813	Chrysene-d12	21.222

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Docosene	308	C22H44	001599-67-3	91
2			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90
3			Oxalic acid, pentadecyl propyl e...	342	C20H38O4	1000309-26-8	87
4			1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	83
5			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040221\
Data File : BP005166.D
Acq On : 02 Apr 2021 19:01
Operator : CG/JU
Sample : M1887-01 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TR-03-033121

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
Hexadecanoic ac...	17.804	40.6	ng	848642	4	17.122	417677	20.0
n-Hexadecanoic ...	18.022	7.4	ng	155339	4	17.122	417677	20.0
9,12-Octadecadi...	18.916	241.8	ng	5049830	4	17.122	417677	20.0
10-Octadecenoic...	18.945	170.2	ng	3554610	4	17.122	417677	20.0
Methyl stearate	19.069	22.6	ng	471489	4	17.122	417677	20.0
9,12-Octadecadi...	19.122	5.3	ng	111610	4	17.122	417677	20.0
Benzene, 1,1'-(...	19.145	5.9	ng	122935	4	17.122	417677	20.0
Methyl 18-methy...	20.139	2.5	ng	56923	5	21.222	447048	20.0
1-Docosene	20.933	5.6	ng	125813	5	21.222	447048	20.0