

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061422\
 Data File : BF128815.D
 Acq On : 14 Jun 2022 22:43
 Operator : CG\JU
 Sample : N3328-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BU-02-061022

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_F\Methods\8270-BF060222.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128815.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.422	530	533	549	rBV	1908230	1625002	21.62%	4.591%
2	6.439	702	706	715	rVB	1834958	1571421	20.90%	4.440%
3	6.781	760	764	767	rBV	533449	398466	5.30%	1.126%
4	7.345	855	860	863	rBV	1090692	1007875	13.41%	2.847%
5	8.063	976	982	985	rBV	565566	479740	6.38%	1.355%
6	9.145	1161	1166	1169	rBV	1917048	1745641	23.22%	4.932%
7	9.822	1277	1281	1284	rBV	583471	452916	6.02%	1.280%
8	10.616	1412	1416	1419	rBV	1028393	912876	12.14%	2.579%
9	11.310	1530	1534	1536	rBV	559827	467538	6.22%	1.321%
10	11.333	1536	1538	1541	rVB	231838	169554	2.26%	0.479%
11	11.704	1597	1601	1604	rBV	2133277	1649361	21.94%	4.660%
12	11.880	1621	1631	1634	rBV	2948788	4927714	65.55%	13.922%
13	12.404	1714	1720	1721	rBV	7310500	7517904	100.00%	21.239%
14	12.421	1721	1723	1729	rVB2	5195044	4360260	58.00%	12.318%
15	12.498	1733	1736	1739	rBV	1014724	855321	11.38%	2.416%
16	12.551	1739	1745	1747	rBV2	1055562	1610933	21.43%	4.551%
17	12.645	1757	1761	1771	rVB	1161945	1219872	16.23%	3.446%
18	12.757	1778	1780	1787	rVB	217450	199548	2.65%	0.564%
19	12.904	1801	1805	1808	rVB	2161210	1690308	22.48%	4.775%
20	13.298	1869	1872	1877	rVB	285738	287819	3.83%	0.813%
21	13.357	1880	1882	1886	rVB	174906	159457	2.12%	0.450%
22	13.957	1981	1984	1987	rBV2	487796	455745	6.06%	1.288%
23	13.998	1989	1991	1993	rVB	211357	169742	2.26%	0.480%
24	14.057	1999	2001	2005	rVB	326137	261977	3.48%	0.740%
25	14.145	2013	2016	2020	rVB	396738	343549	4.57%	0.971%
26	15.062	2169	2172	2176	rVB	453744	464463	6.18%	1.312%
27	15.415	2230	2232	2241	rVB2	299069	391187	5.20%	1.105%

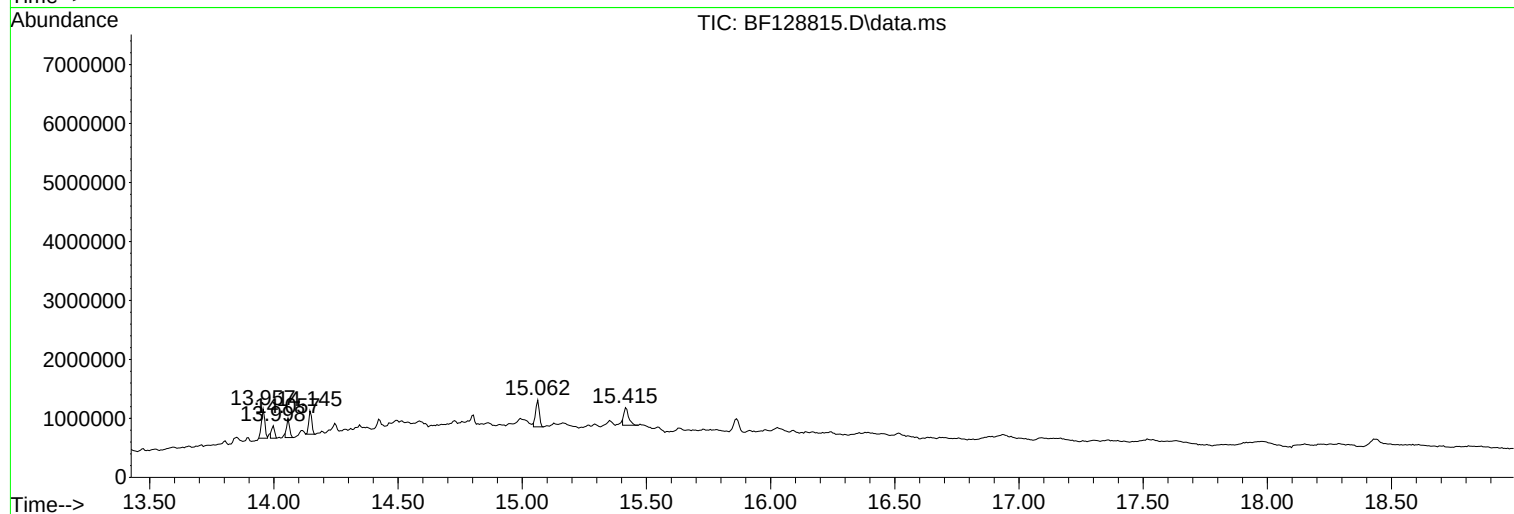
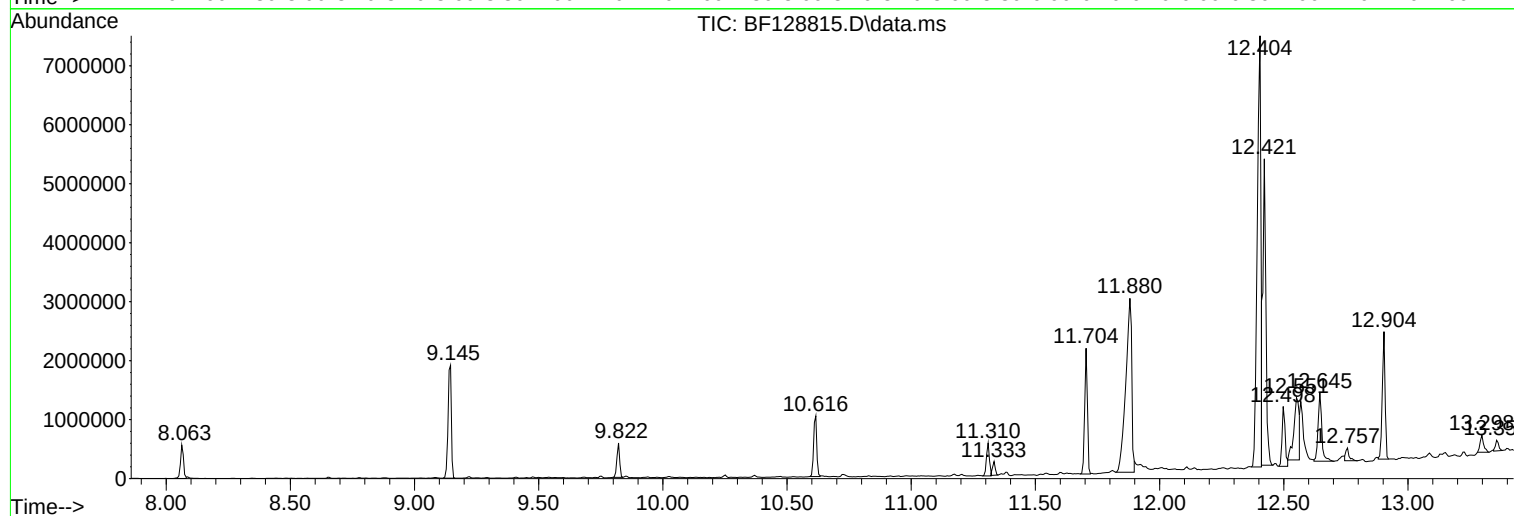
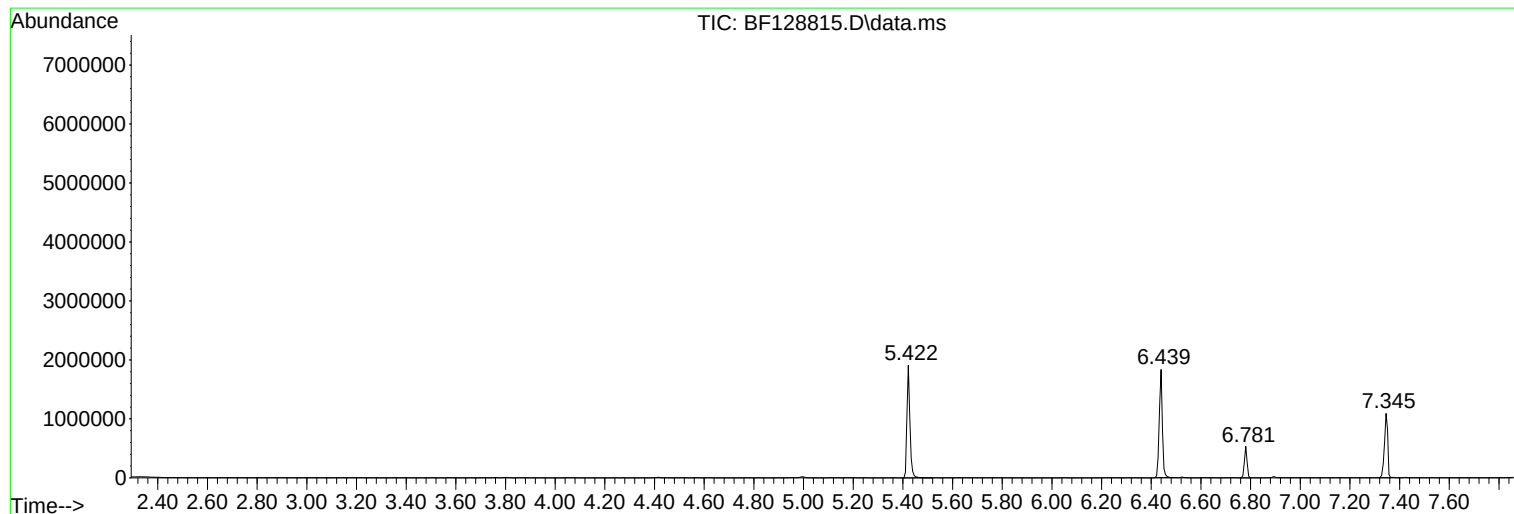
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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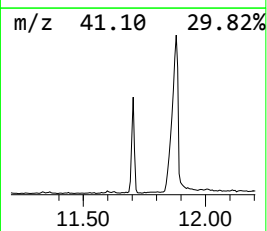
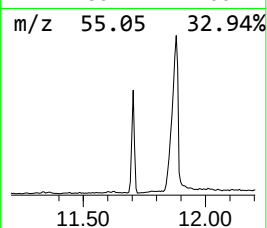
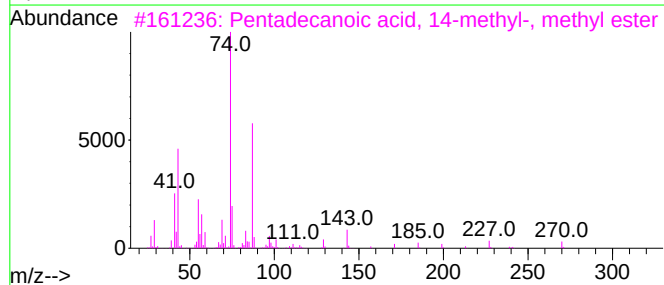
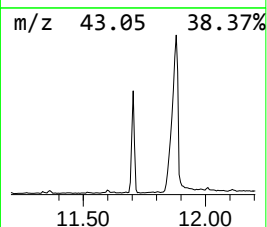
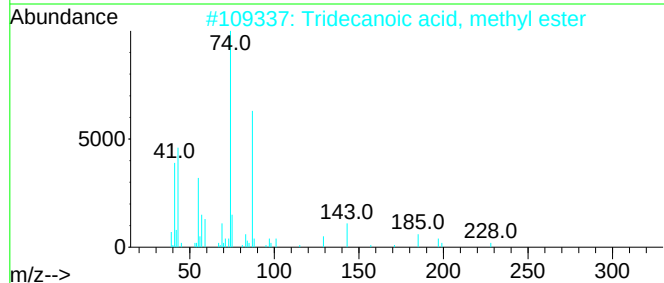
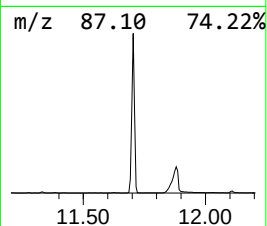
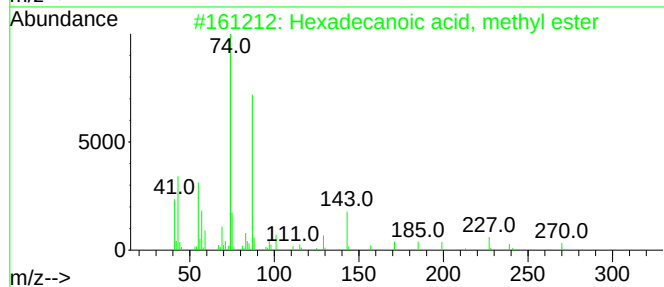
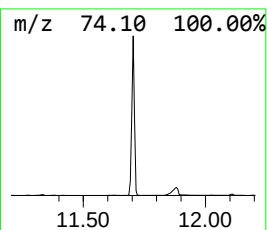
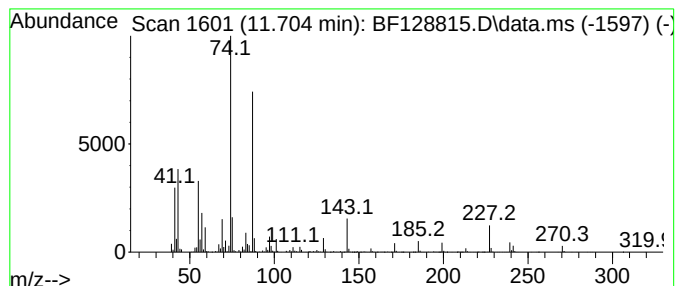
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.704	70.56 ng	1649360	Phenanthrene-d10	11.310

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2		Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	93
3		Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	92
4		Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
5		Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90



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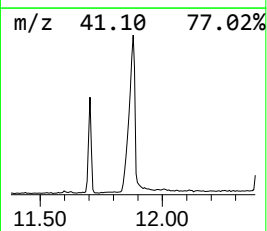
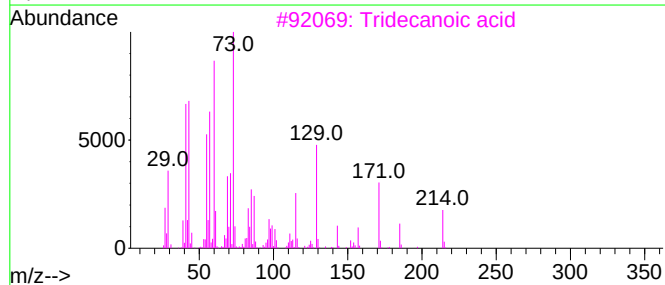
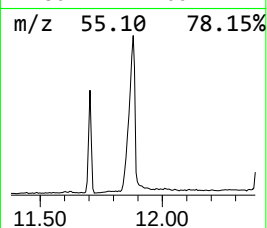
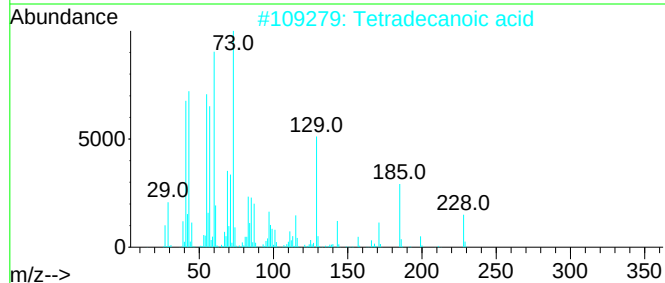
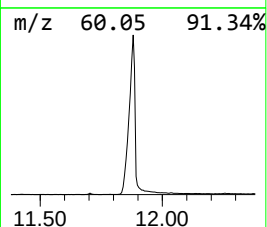
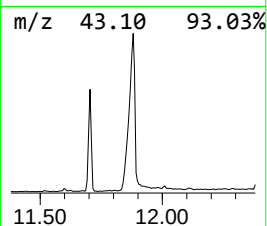
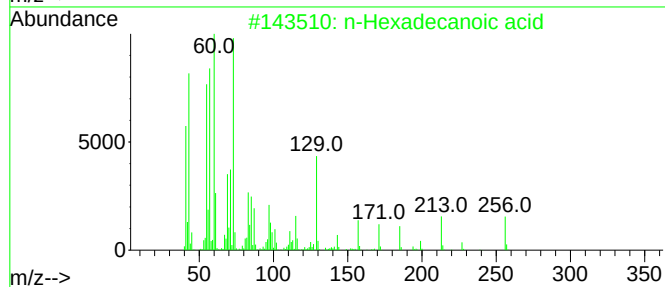
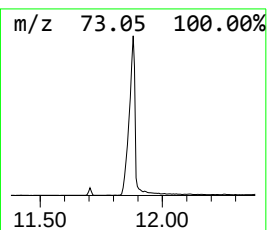
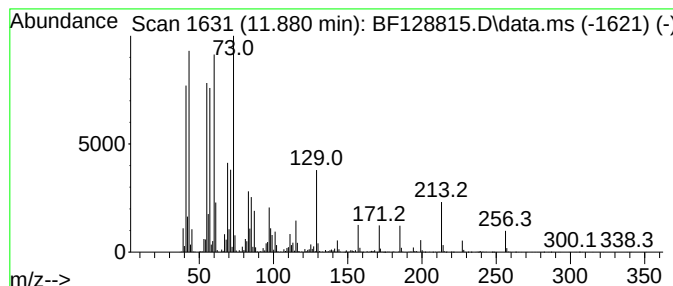
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.880	210.79 ng	4927710	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Tridecanoic acid	214	C13H26O2	000638-53-9	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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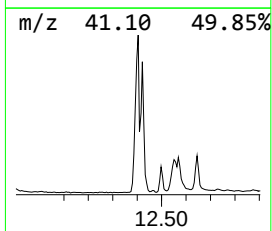
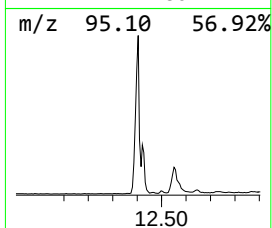
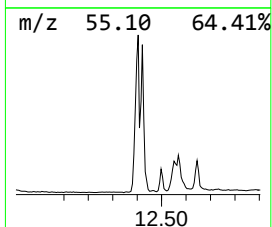
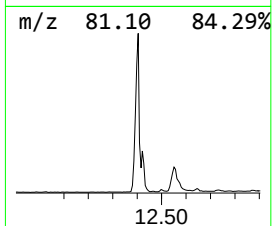
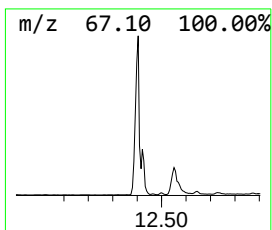
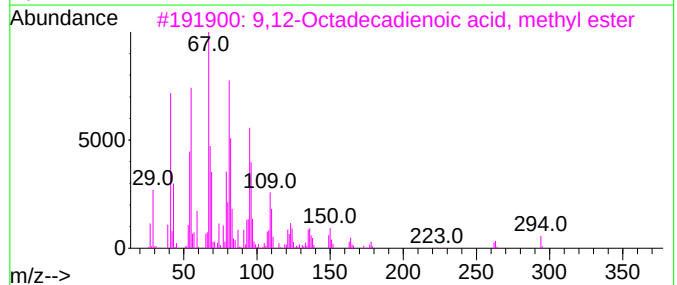
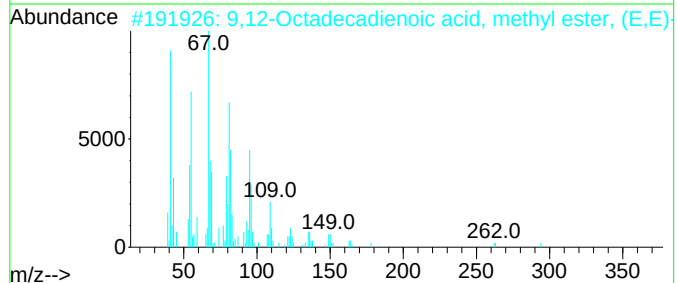
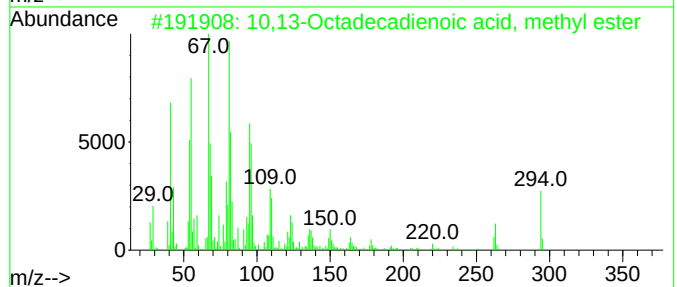
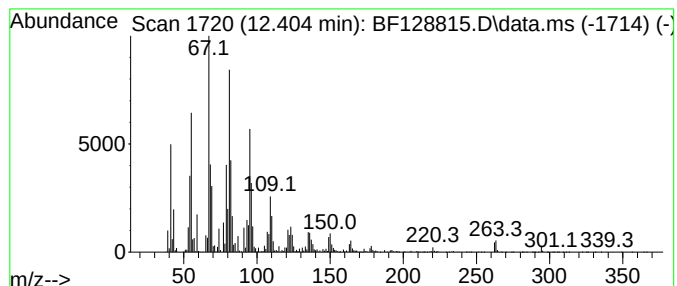
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 10,13-Octadecadienoic acid,... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.404	321.60 ng	7517900	Phenanthrene-d10	11.310
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1	10,13-Octadecadienoic acid, meth...	294 C19H34O2	056554-62-2	99
2	9,12-Octadecadienoic acid, methy...	294 C19H34O2	002566-97-4	99
3	9,12-Octadecadienoic acid, methy...	294 C19H34O2	002462-85-3	99
4	9,15-Octadecadienoic acid, methy...	294 C19H34O2	017309-05-6	99
5	9,12-Octadecadienoic acid (Z,Z)-...	294 C19H34O2	000112-63-0	99



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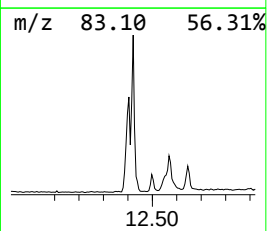
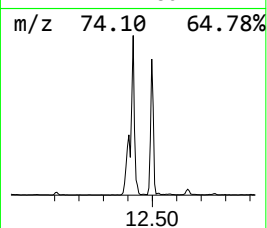
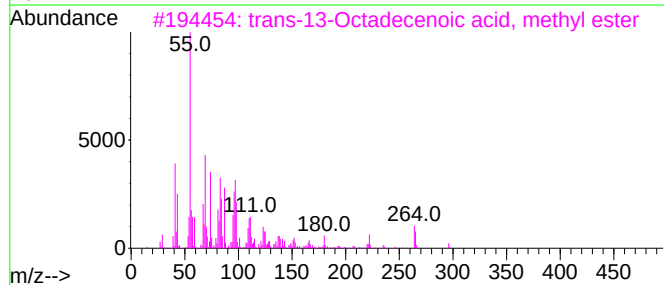
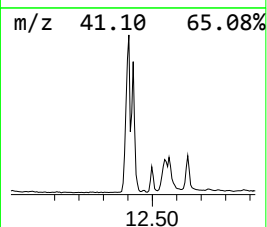
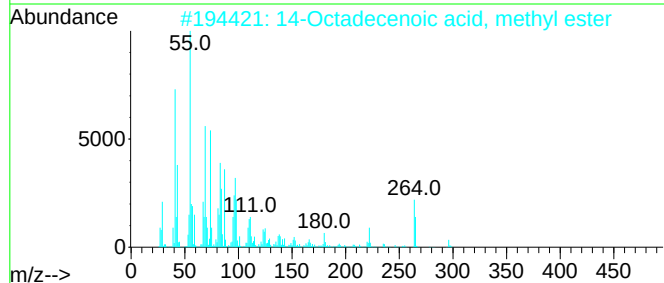
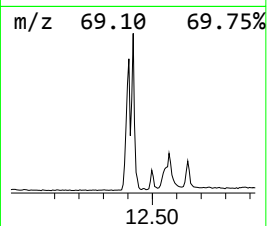
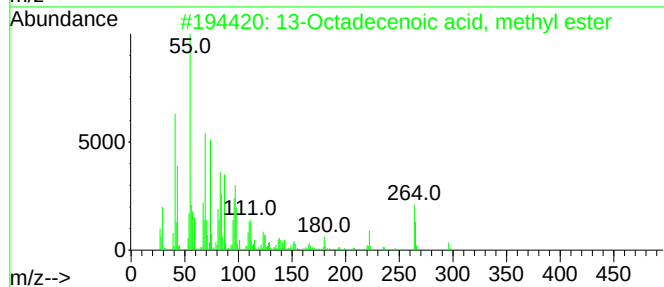
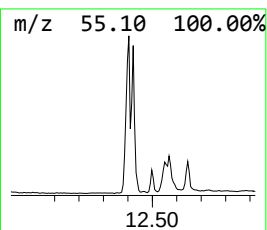
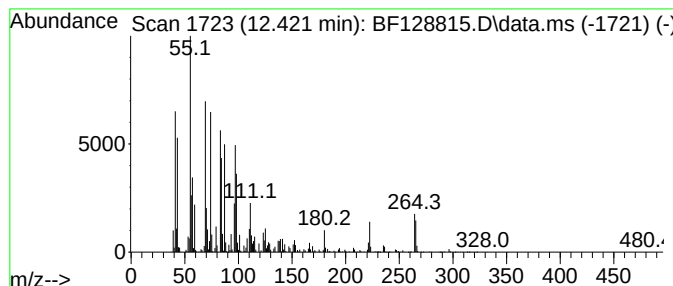
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 13-Octadecenoic acid, methyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.421	186.52 ng	4360260	Phenanthrene-d10	11.310

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	93
2		14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	93
3		trans-13-Octadecenoic acid, methyl ester	296	C19H36O2	1000333-61-3	87
4		11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	87
5		8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	86



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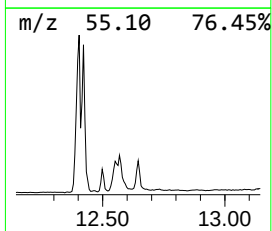
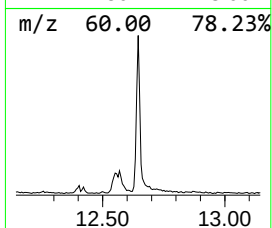
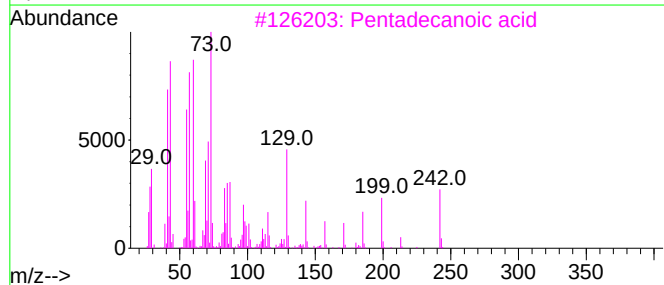
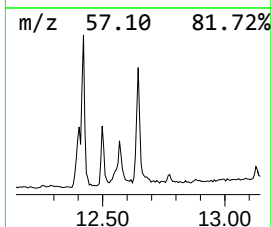
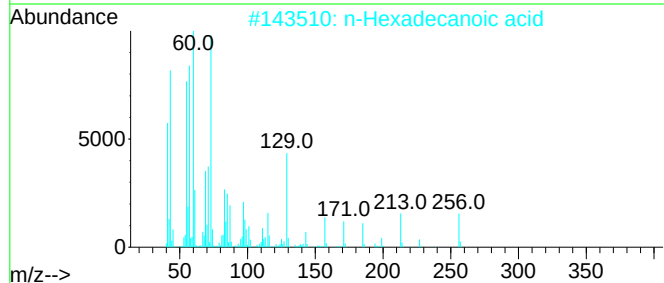
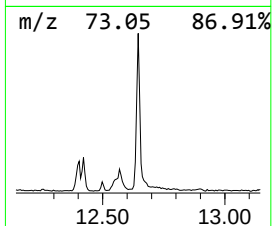
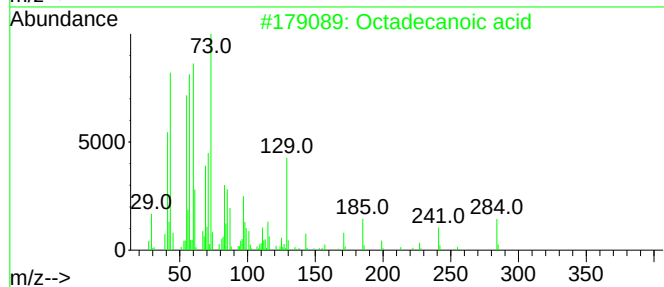
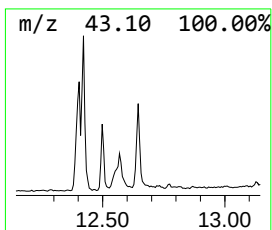
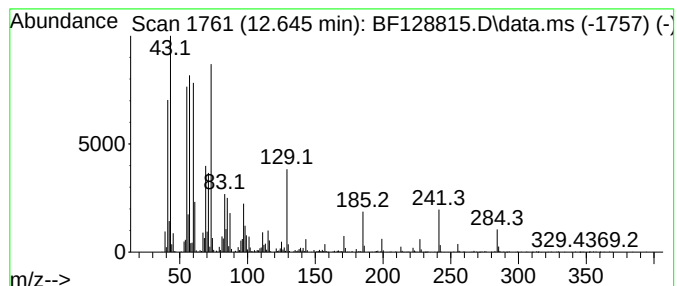
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.645	53.53 ng	1219870	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4			Tridecanoic acid	214	C13H26O2	000638-53-9	70
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	68



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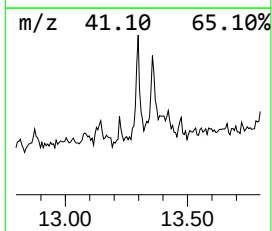
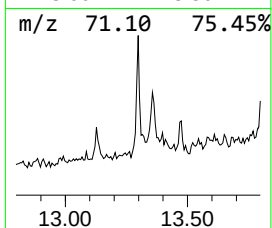
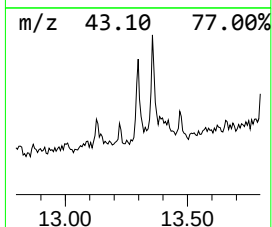
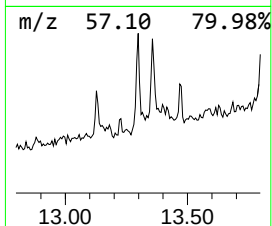
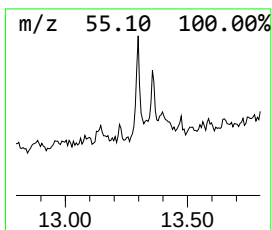
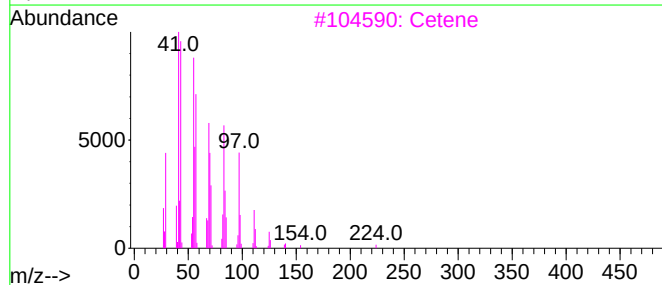
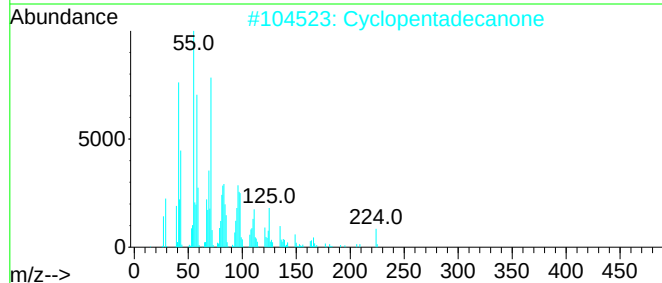
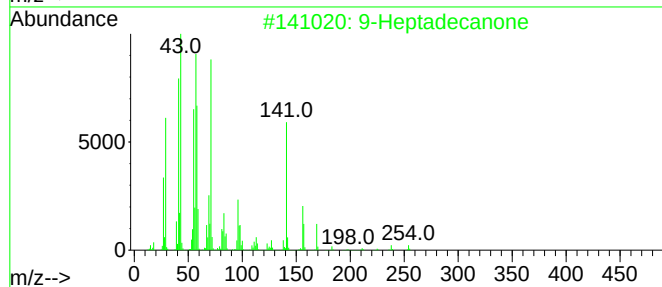
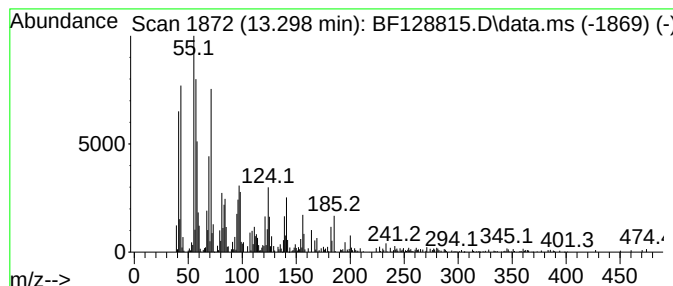
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ClientSampleId :
BU-02-061022

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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 9-Heptadecanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.298	12.63 ng	287819	Chrysene-d12		13.957	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	9-Heptadecanone		254	C17H34O	000540-08-9	60
2	Cyclopentadecanone		224	C15H28O	000502-72-7	58
3	Cetene		224	C16H32	000629-73-2	44
4	Cyclopentanol, 1-methyl-		100	C6H12O	001462-03-9	38
5	Oxacycloheptadecan-2-one		254	C16H30O2	000109-29-5	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061422\
Data File : BF128815.D
Acq On : 14 Jun 2022 22:43
Operator : CG\JU
Sample : N3328-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-02-061022

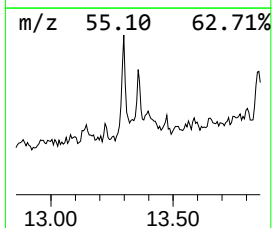
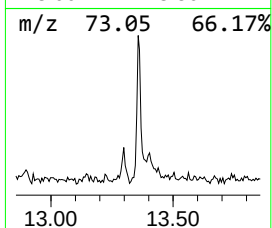
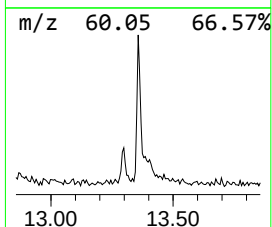
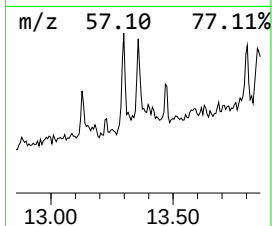
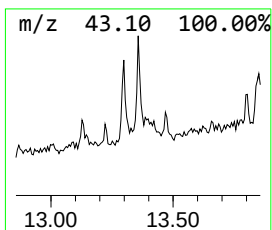
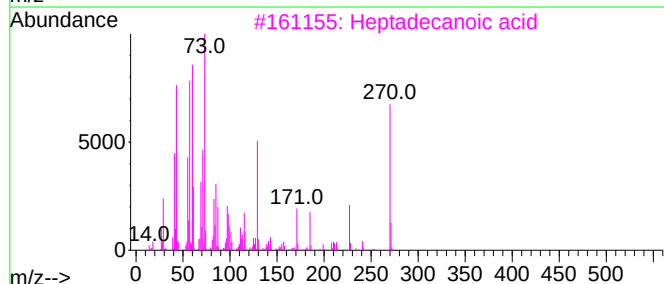
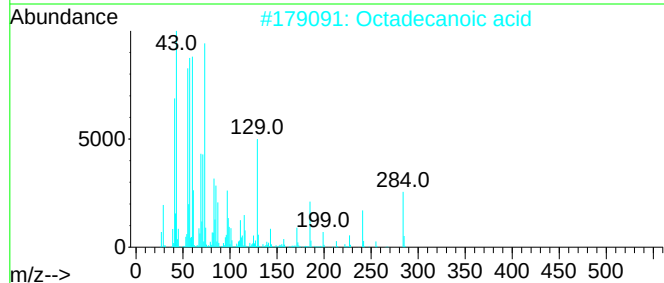
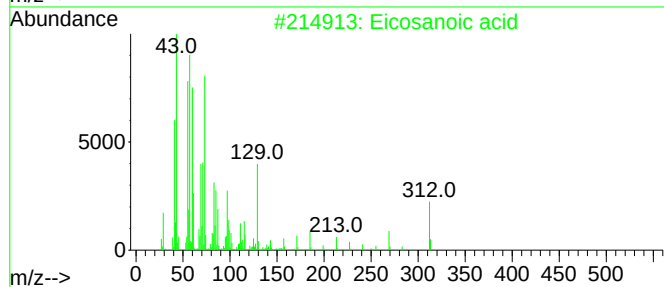
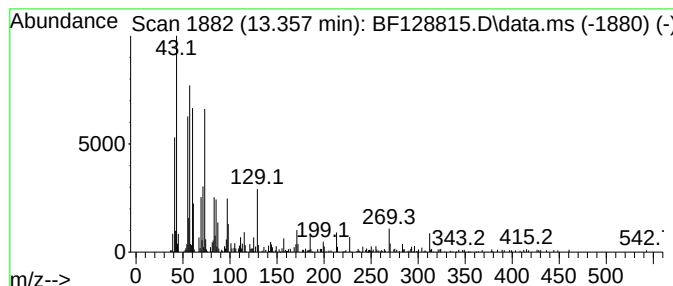
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.357	7.00 ng	159457	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosanoic acid	312	C20H40O2	000506-30-9	97
2			Octadecanoic acid	284	C18H36O2	000057-11-4	97
3			Heptadecanoic acid	270	C17H34O2	000506-12-7	97
4			Tetracosanoic acid	368	C24H48O2	000557-59-5	83
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061422\
Data File : BF128815.D
Acq On : 14 Jun 2022 22:43
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Misc :
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ClientSampleId :
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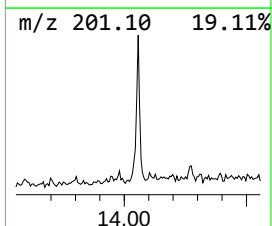
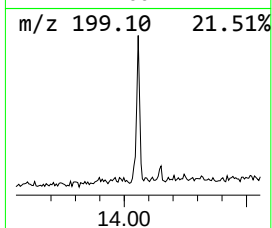
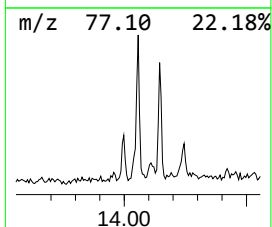
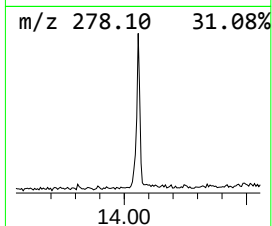
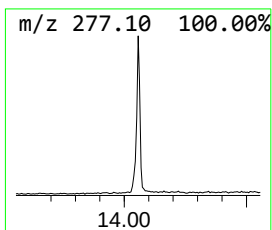
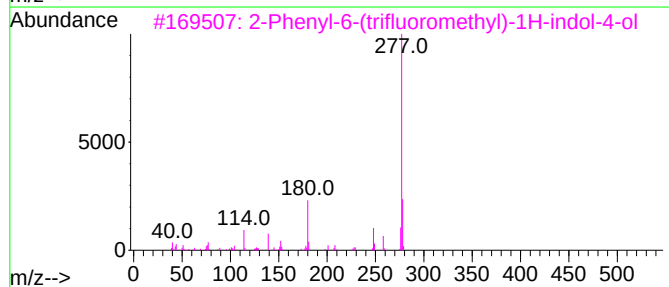
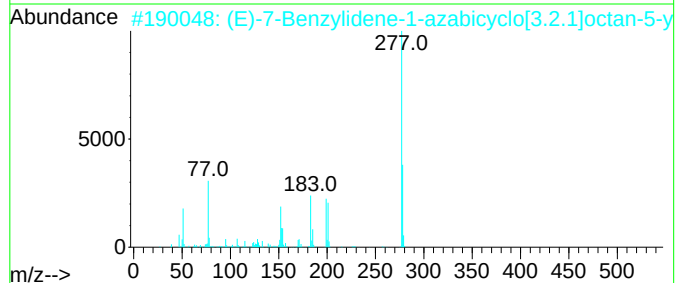
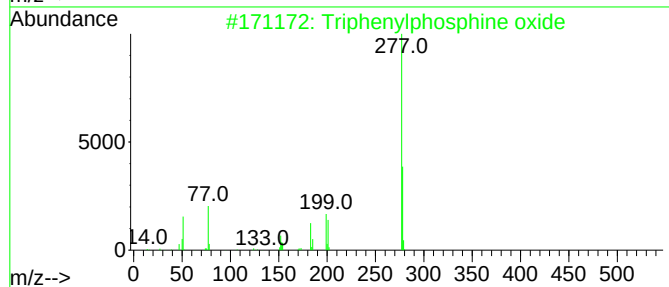
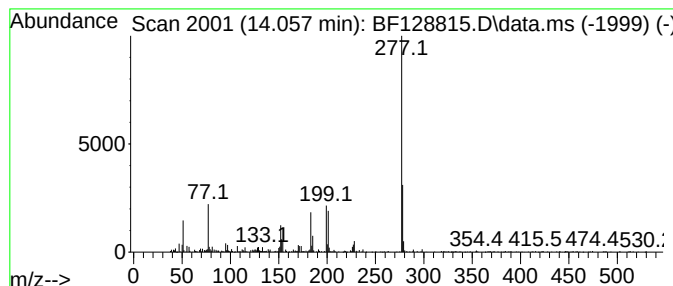
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Triphenylphosphine oxide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.057	11.50 ng	261977	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	74
3			2-Phenyl-6-(trifluoromethyl)-1H...	277	C15H10F3NO	1000387-59-3	40
4			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	36
5			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061422\
Data File : BF128815.D
Acq On : 14 Jun 2022 22:43
Operator : CG\JU
Sample : N3328-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

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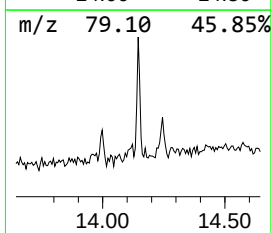
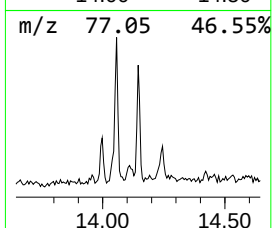
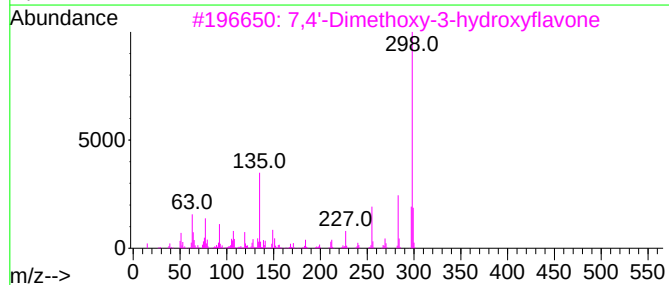
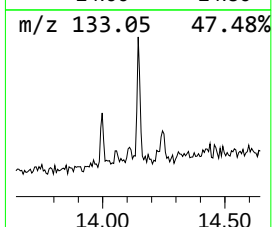
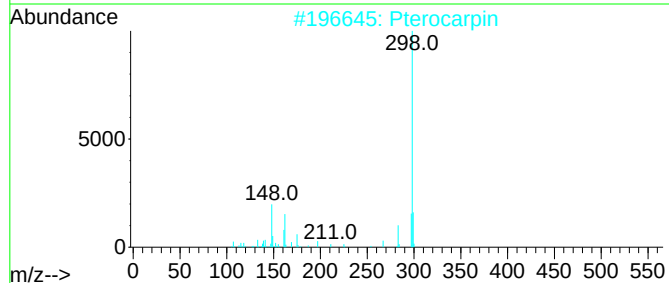
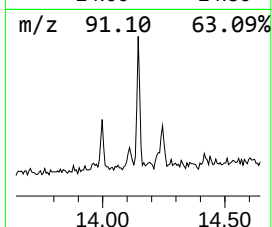
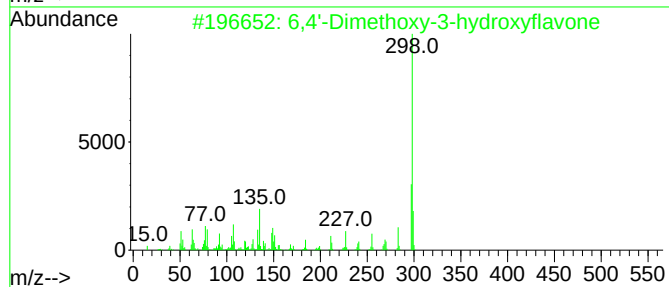
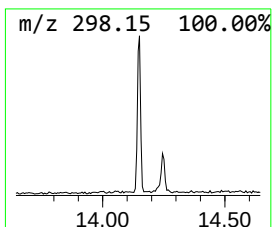
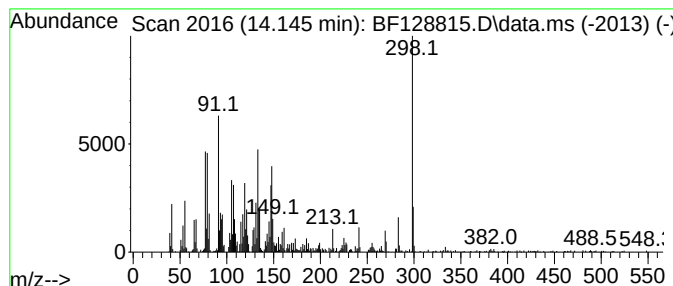
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown14.145 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.145	15.08 ng	343549	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			6,4'-Dimethoxy-3-hydroxyflavone	298	C17H14O5	093176-02-4	41
2			Pterocarpin	298	C17H14O5	000524-97-0	38
3			7,4'-Dimethoxy-3-hydroxyflavone	298	C17H14O5	013198-99-7	38
4			4H-1-Benzopyran-4-one, 5-hydroxy...	298	C17H14O5	034086-51-6	38
5			4H-1-Benzopyran-4-one, 2-(3,4-di...	298	C17H14O5	033513-36-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061422\
Data File : BF128815.D
Acq On : 14 Jun 2022 22:43
Operator : CG\JU
Sample : N3328-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

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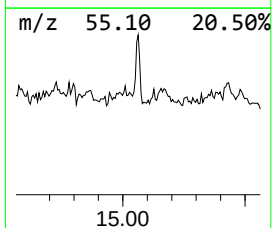
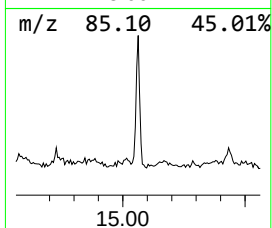
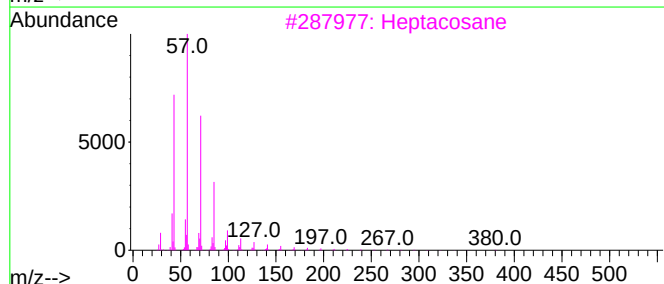
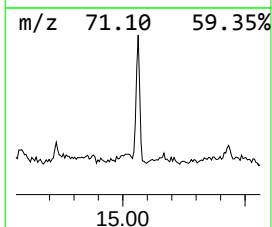
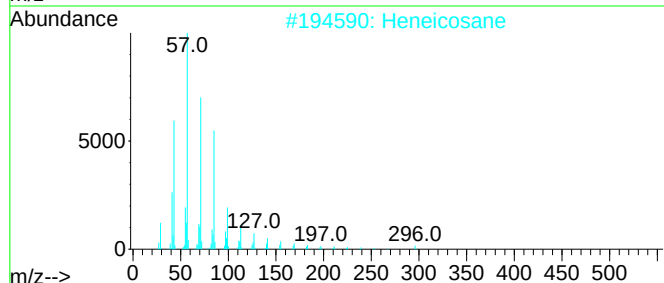
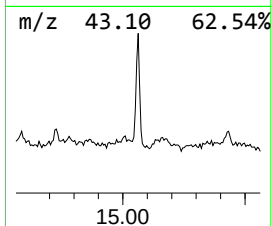
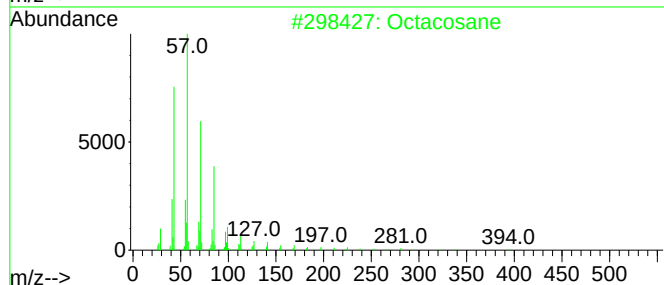
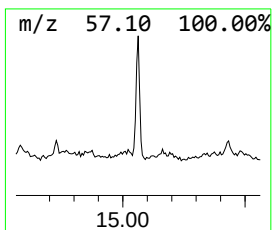
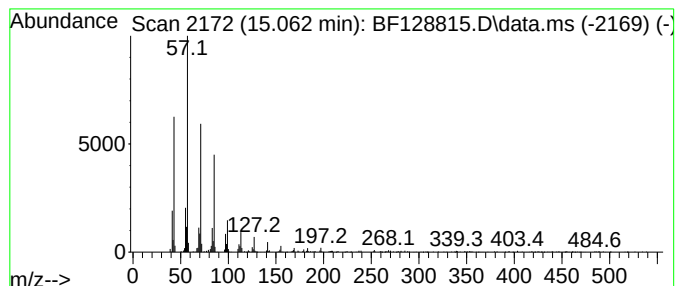
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.062	23.75 ng	464463	Perylene-d12	15.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	99
2			Heneicosane	296	C21H44	000629-94-7	90
3			Heptacosane	380	C27H56	000593-49-7	90
4			Tetracosane	338	C24H50	000646-31-1	87
5			Octadecane	254	C18H38	000593-45-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061422\
Data File : BF128815.D
Acq On : 14 Jun 2022 22:43
Operator : CG\JU
Sample : N3328-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-02-061022

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.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
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n-Hexadecanoic ...	11.880	210.8	ng	4927710	4	11.310	467538	20.0
10,13-Octadecad...	12.404	321.6	ng	7517900	4	11.310	467538	20.0
13-Octadecenoic...	12.421	186.5	ng	4360260	4	11.310	467538	20.0
Octadecanoic acid	12.645	53.5	ng	1219870	5	13.957	455745	20.0
9-Heptadecanone	13.298	12.6	ng	287819	5	13.957	455745	20.0
Eicosanoic acid	13.357	7.0	ng	159457	5	13.957	455745	20.0
Triphenylphosph...	14.057	11.5	ng	261977	5	13.957	455745	20.0
unknown14.145	14.145	15.1	ng	343549	5	13.957	455745	20.0
Octacosane	15.062	23.8	ng	464463	6	15.415	391187	20.0