

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071522\
 Data File : BF129242.D
 Acq On : 15 Jul 2022 17:10
 Operator : CG\JU
 Sample : N3649-06
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 A-2-UC

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-BF071522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129242.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.140	482	485	492	rVB	52770	66152	1.08%	0.138%
2	5.522	545	550	553	rBV	5279340	5345746	87.05%	11.180%
3	6.522	714	720	731	rVB	5089684	5484985	89.32%	11.471%
4	6.898	780	784	787	rBV	1589491	1432962	23.33%	2.997%
5	7.457	874	879	882	rBV	3812355	3507253	57.11%	7.335%
6	8.180	997	1002	1005	rBV	2009550	1969395	32.07%	4.119%
7	9.251	1179	1184	1188	rBV	5923283	6141094	100.00%	12.843%
8	9.933	1295	1300	1304	rBV	2435992	2206999	35.94%	4.616%
9	10.727	1430	1435	1438	rBV	3676314	3653530	59.49%	7.641%
10	11.421	1549	1553	1557	rBV	2399008	2197634	35.79%	4.596%
11	11.486	1562	1564	1568	rVB2	89276	73992	1.20%	0.155%
12	11.804	1615	1618	1621	rBV	362754	354476	5.77%	0.741%
13	11.933	1636	1640	1650	rVB2	611339	974024	15.86%	2.037%
14	12.092	1664	1667	1673	rVB2	96060	124255	2.02%	0.260%
15	12.516	1736	1739	1742	rVB	278366	217294	3.54%	0.454%
16	12.598	1749	1753	1755	rBV	100014	125832	2.05%	0.263%
17	12.721	1770	1774	1780	rBV	1258974	1631577	26.57%	3.412%
18	12.774	1781	1783	1795	rVB	233472	454665	7.40%	0.951%
19	13.010	1819	1823	1827	rBV	5889693	5778254	94.09%	12.084%
20	13.486	1899	1904	1910	rVB	223165	354761	5.78%	0.742%
21	13.898	1971	1974	1980	rVB2	54142	72948	1.19%	0.153%
22	14.068	1999	2003	2006	rVB	1914145	1963435	31.97%	4.106%
23	14.157	2014	2018	2022	rVB	202817	199733	3.25%	0.418%
24	14.539	2077	2083	2092	rBV	241869	410234	6.68%	0.858%
25	14.833	2127	2133	2138	rBV3	99423	175957	2.87%	0.368%
26	15.021	2160	2165	2175	rBV	201503	338768	5.52%	0.708%
27	15.180	2188	2192	2196	rVB	83033	101276	1.65%	0.212%
28	15.556	2251	2256	2266	rBV	1135403	1695591	27.61%	3.546%
29	16.009	2329	2333	2338	rBV2	69818	102602	1.67%	0.215%
30	16.215	2364	2368	2377	rVB	96817	202028	3.29%	0.423%
31	16.533	2418	2422	2430	rVB2	62538	108102	1.76%	0.226%
32	16.968	2490	2496	2505	rBV3	66641	181218	2.95%	0.379%
33	17.856	2643	2647	2658	rVB2	69372	170240	2.77%	0.356%

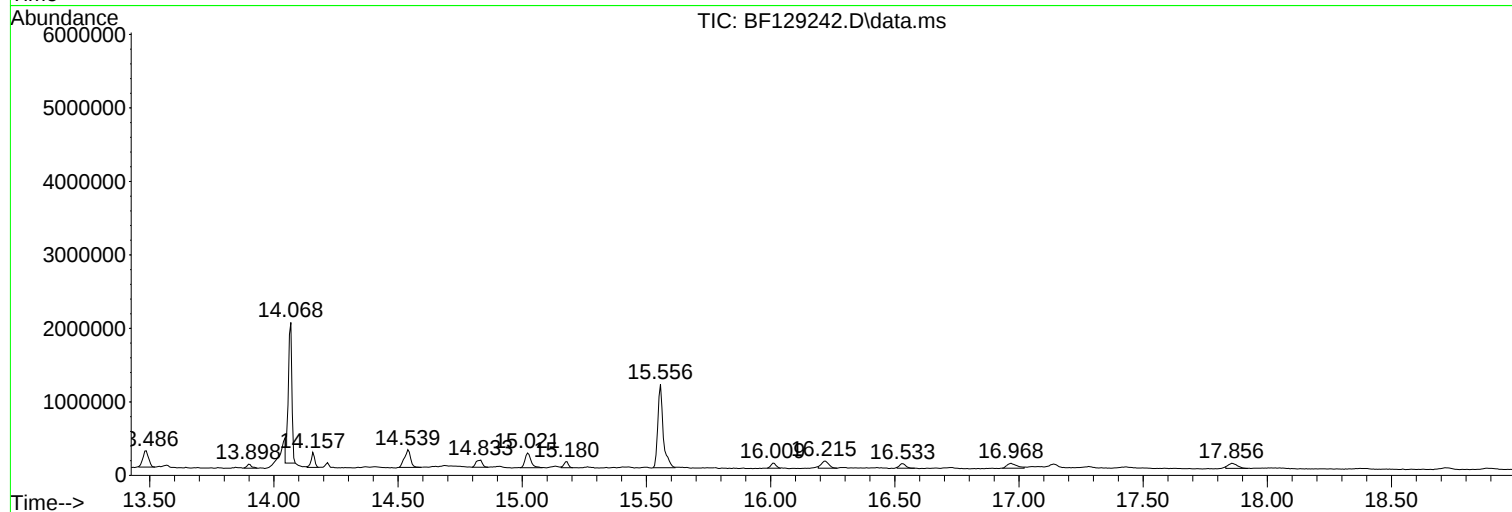
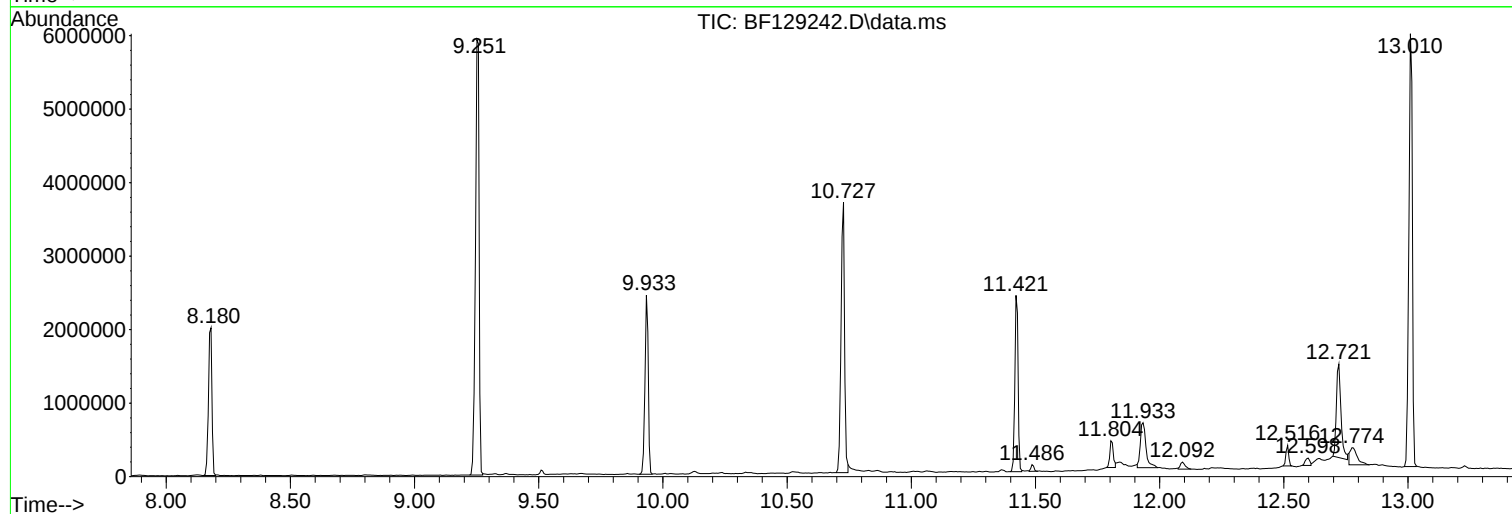
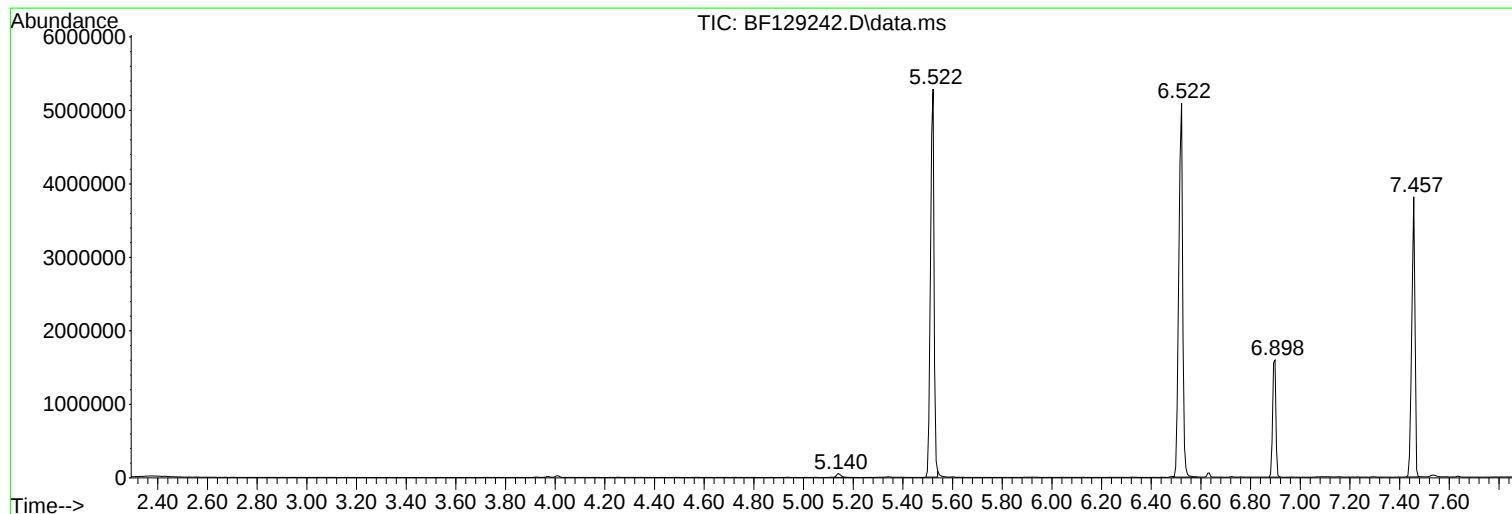
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ClientSampleId :
A-2-UC

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071522.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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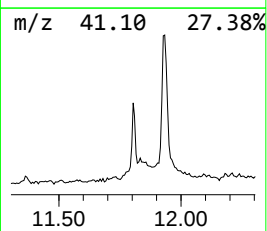
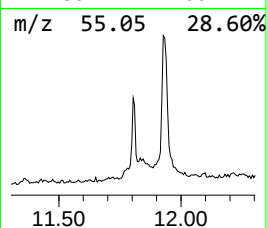
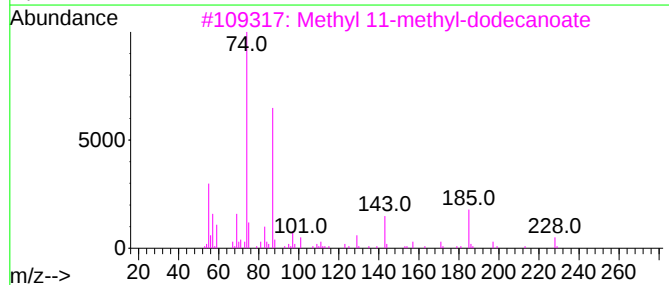
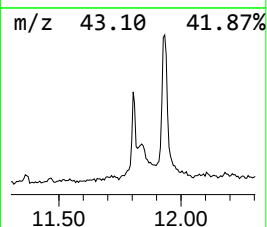
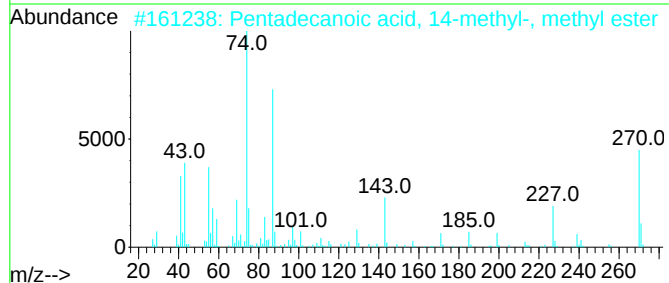
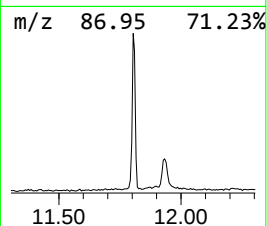
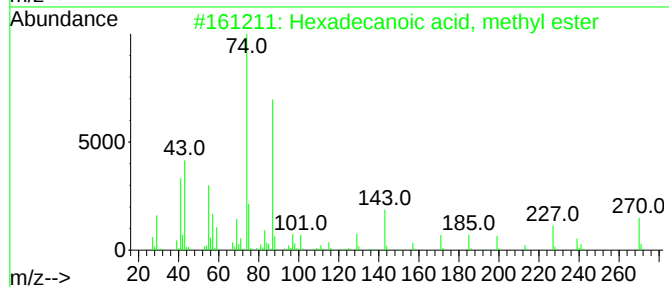
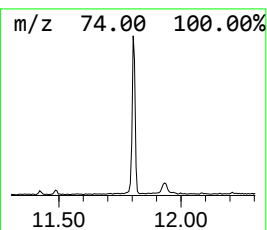
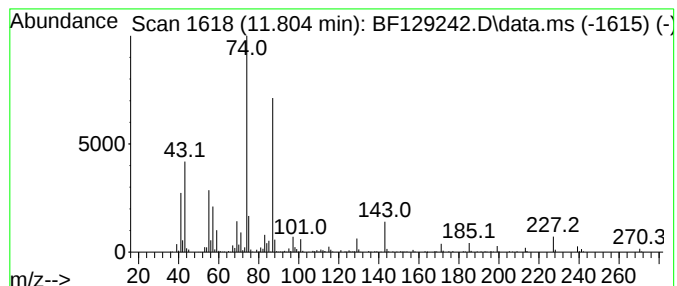
Instrument :
BNA_F
ClientSampleId :
A-2-UC

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071522.M
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 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.804	3.23 ng	354476	Phenanthrene-d10		11.422	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester		270	C17H34O2	000112-39-0	97
2	Pentadecanoic acid, 14-methyl-, ...		270	C17H34O2	005129-60-2	94
3	Methyl 11-methyl-dodecanoate		228	C14H28O2	1000336-45-1	90
4	Tridecanoic acid, methyl ester		228	C14H28O2	001731-88-0	90
5	Pentadecanoic acid, methyl ester		256	C16H32O2	007132-64-1	90



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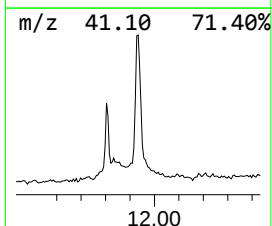
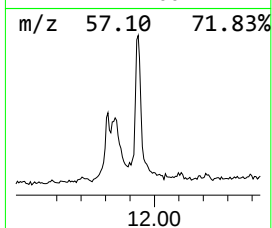
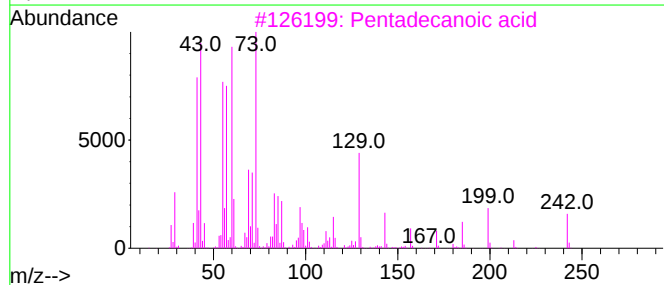
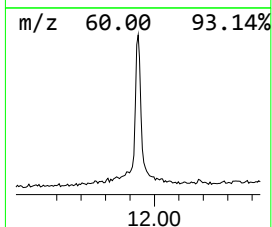
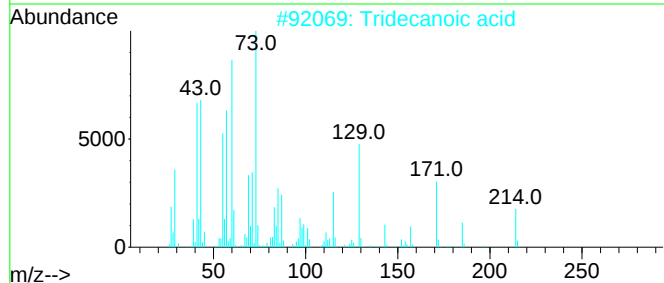
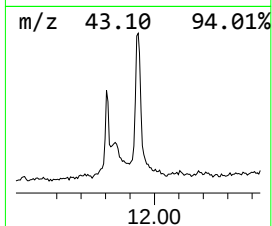
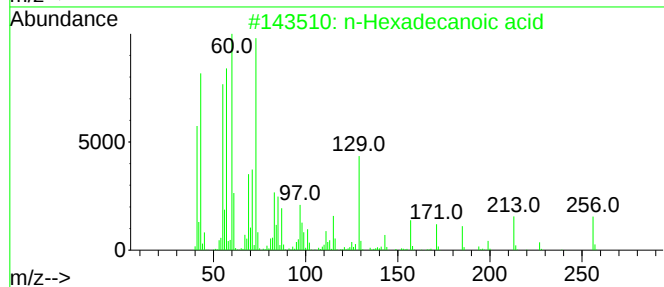
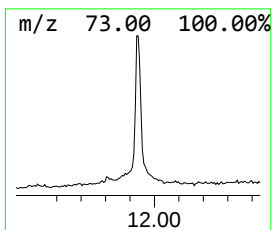
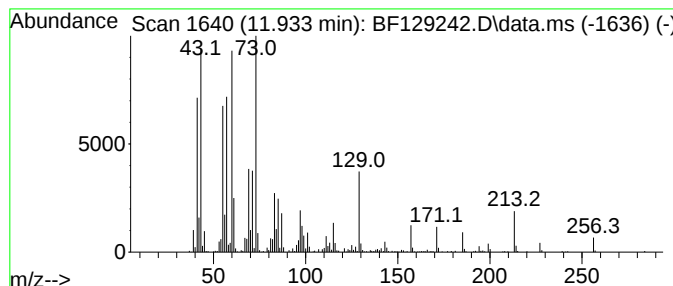
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
11.933	8.86 ng	974024	Phenanthrene-d10	11.422

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	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Octadecanoic acid	284	C18H36O2	000057-11-4	60



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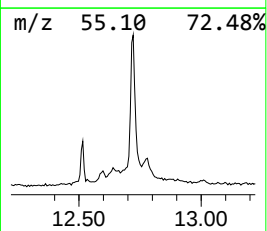
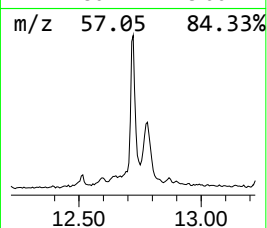
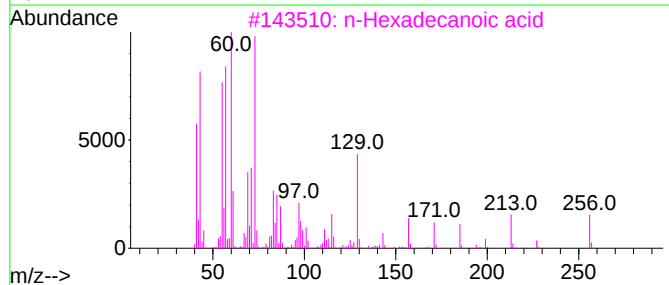
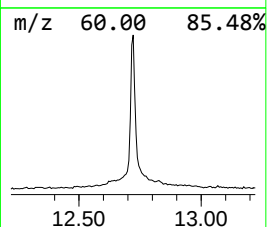
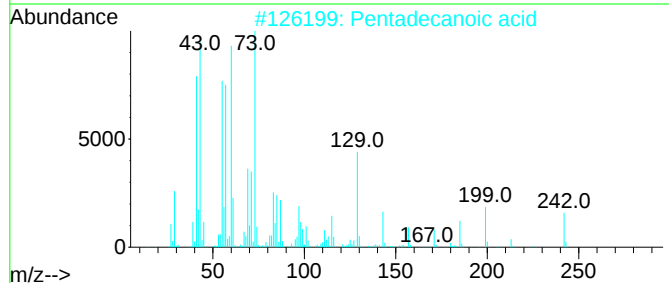
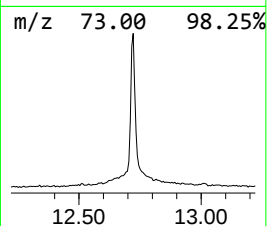
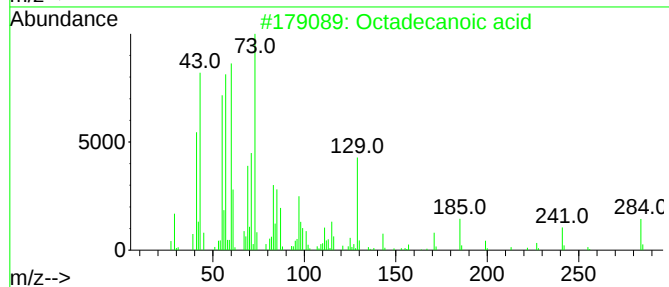
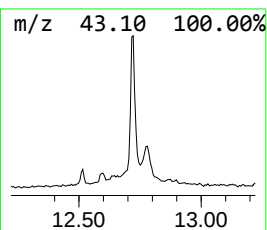
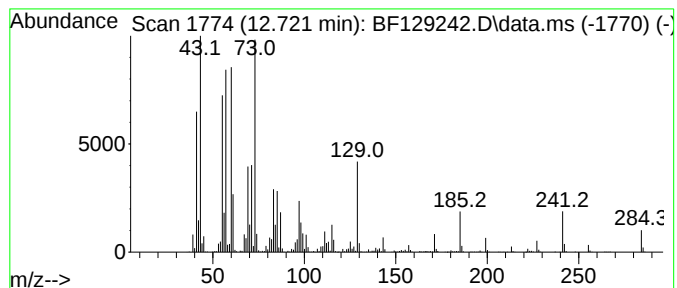
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.721	14.85 ng	1631580	Phenanthrene-d10	11.422

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			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



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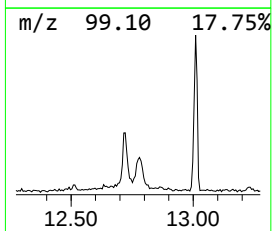
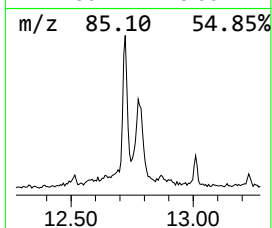
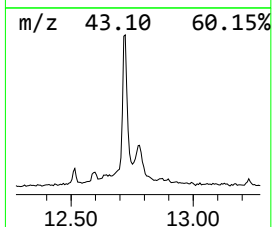
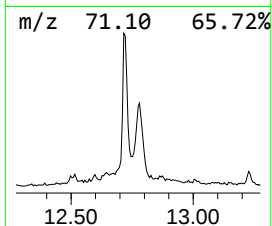
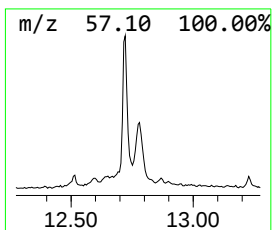
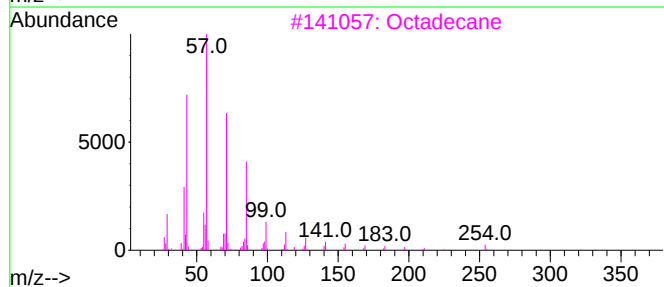
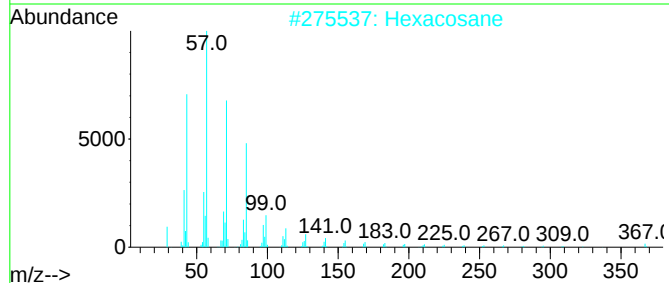
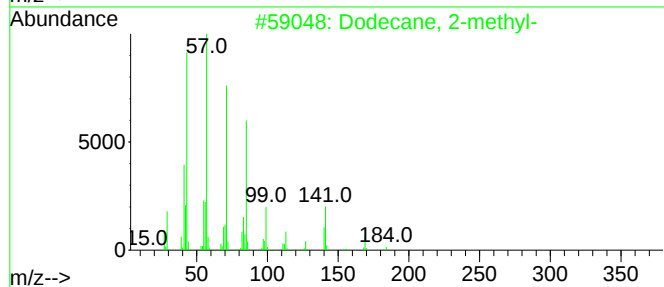
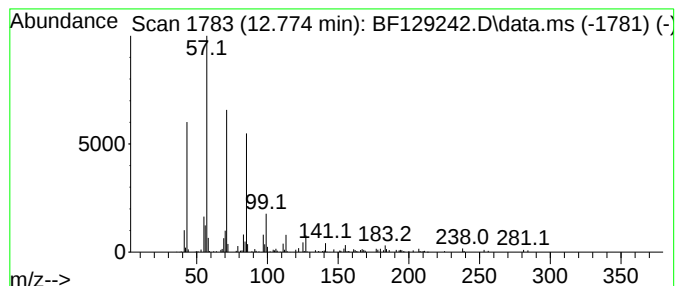
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Dodecane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.774	4.63 ng	454665	Chrysene-d12	14.068

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2-methyl-	184	C13H28	001560-97-0	87
2			Hexacosane	366	C26H54	000630-01-3	86
3			Octadecane	254	C18H38	000593-45-3	86
4			Tridecane, 3-methyl-	198	C14H30	006418-41-3	80
5			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	78



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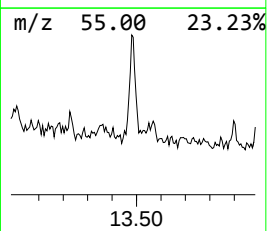
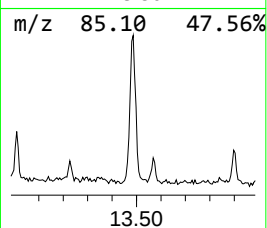
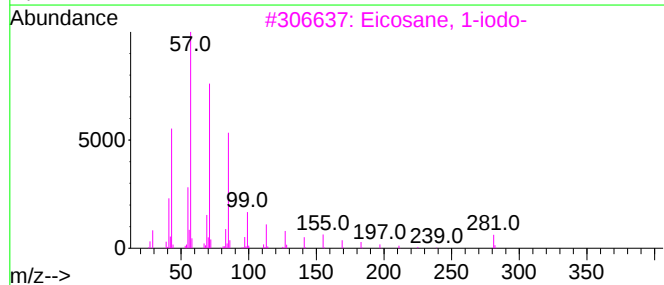
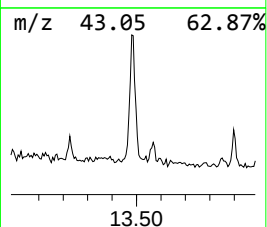
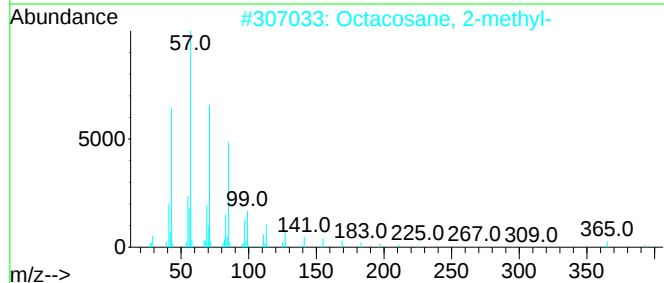
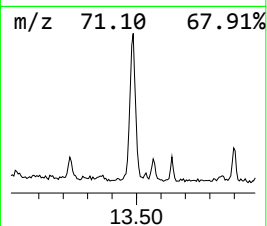
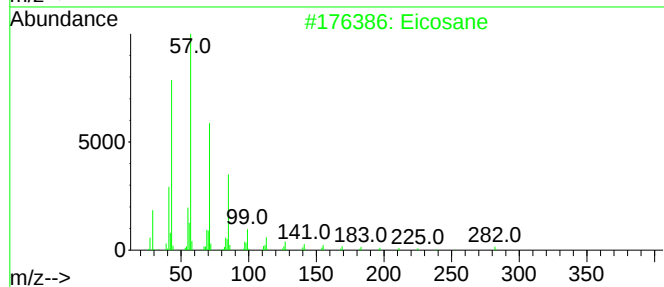
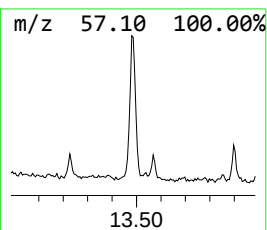
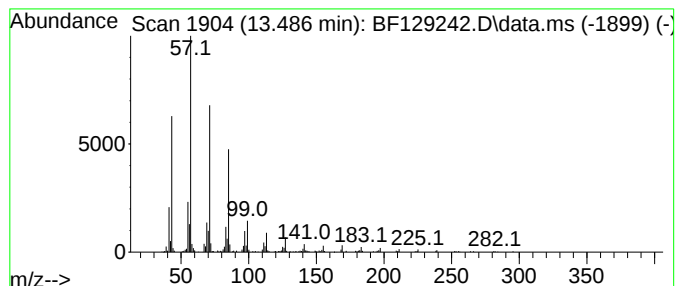
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.486	3.61 ng	354761	Chrysene-d12	14.068

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	93
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	91
4			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	91
5			Tetracosane	338	C24H50	000646-31-1	90



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A-2-UC

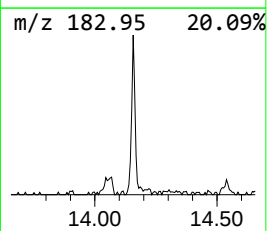
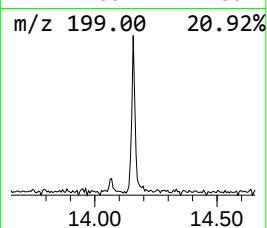
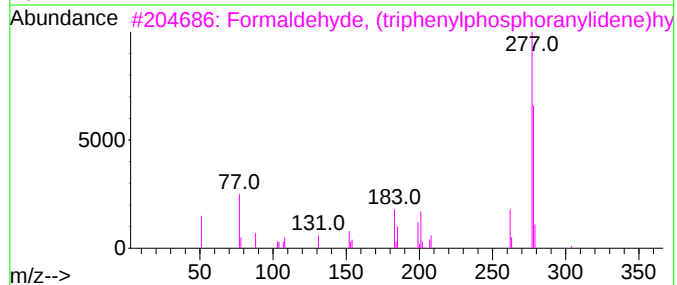
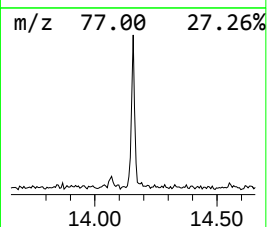
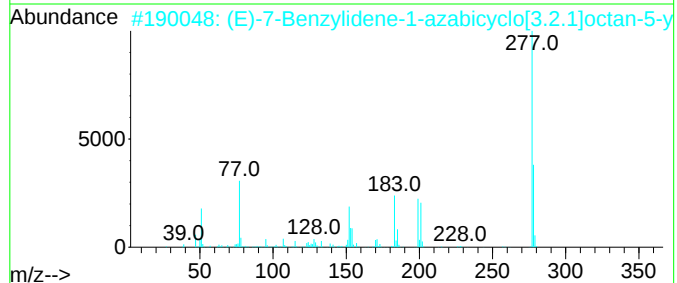
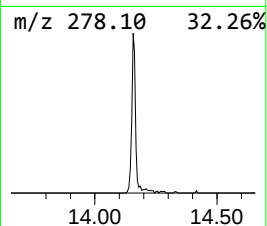
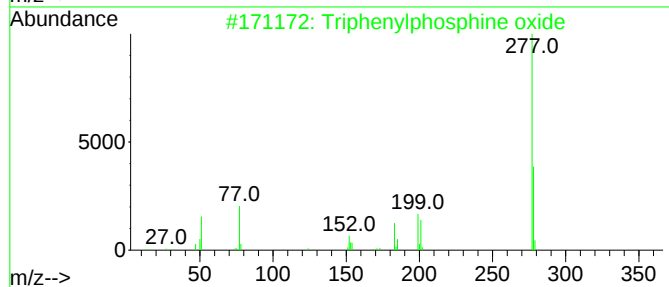
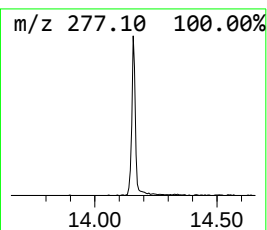
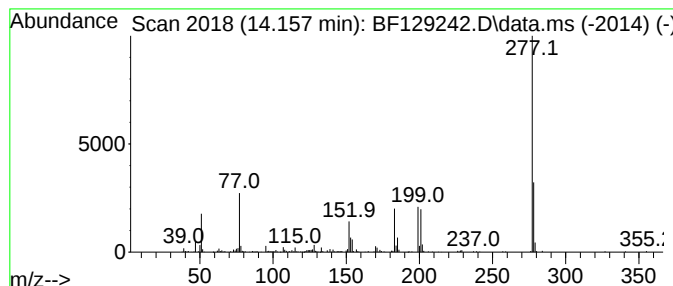
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triphenylphosphine oxide Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.157	2.03 ng	199733	Chrysene-d12	14.068

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	94
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	53
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	50
4			4-Nitro-4'-methyldiphenylsulfone	277	C13H11NO4S	004094-37-5	43
5			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	36



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071522\
Data File : BF129242.D
Acq On : 15 Jul 2022 17:10
Operator : CG\JU
Sample : N3649-06
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A-2-UC

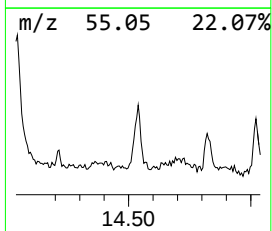
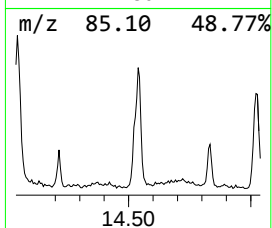
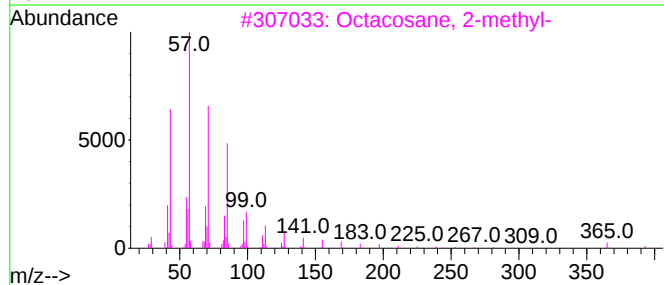
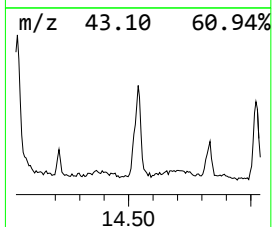
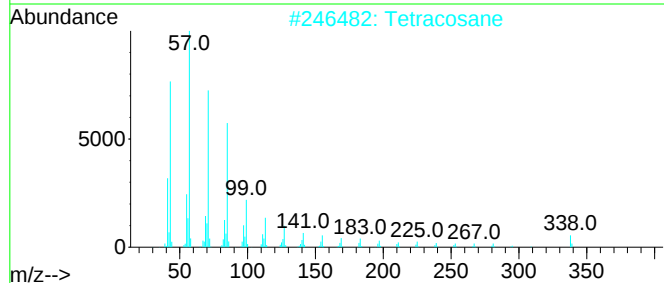
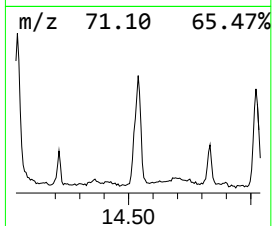
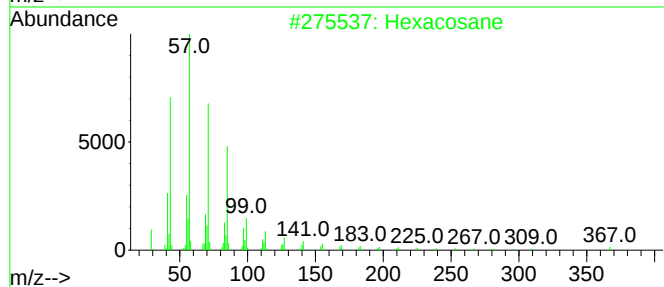
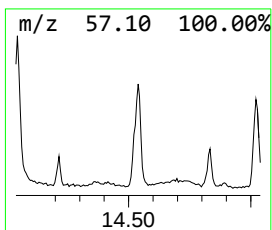
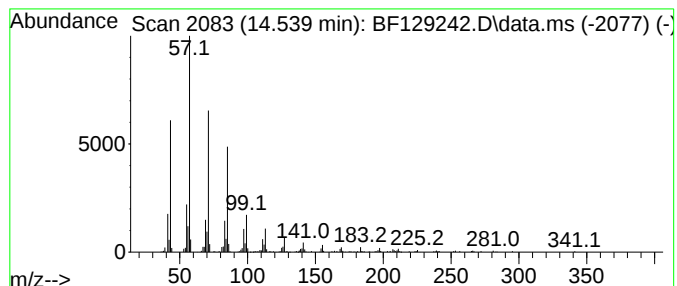
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.539	4.18 ng	410234	Chrysene-d12	14.068

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	94
2			Tetracosane	338	C24H50	000646-31-1	91
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4			Heneicosane	296	C21H44	000629-94-7	91
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071522\
Data File : BF129242.D
Acq On : 15 Jul 2022 17:10
Operator : CG\JU
Sample : N3649-06
Misc :
ALS Vial : 4 Sample Multiplier: 1

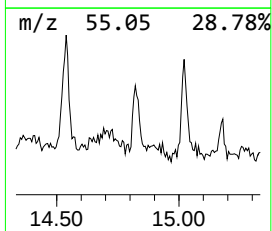
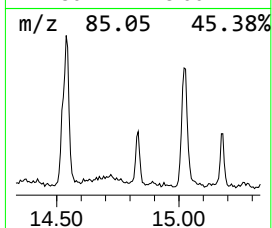
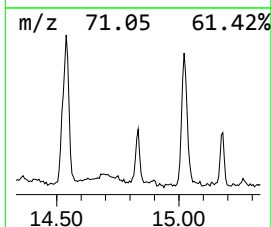
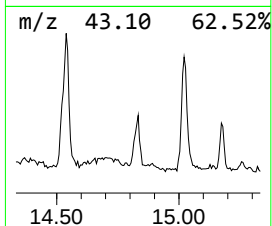
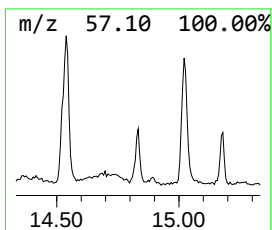
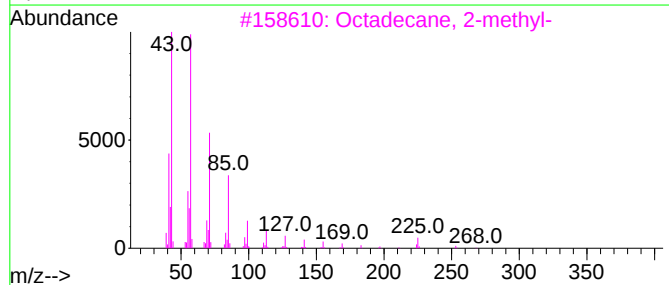
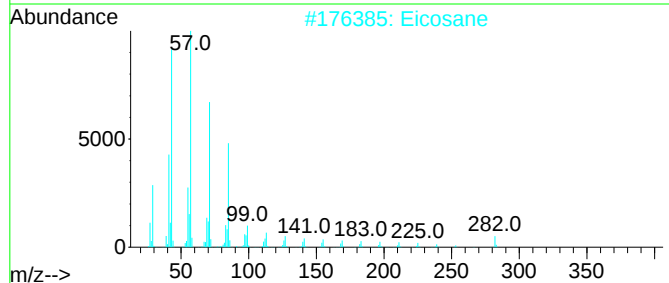
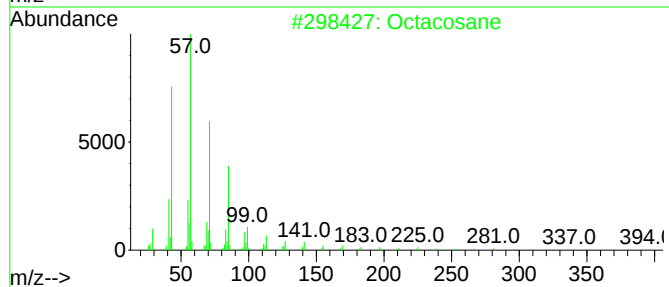
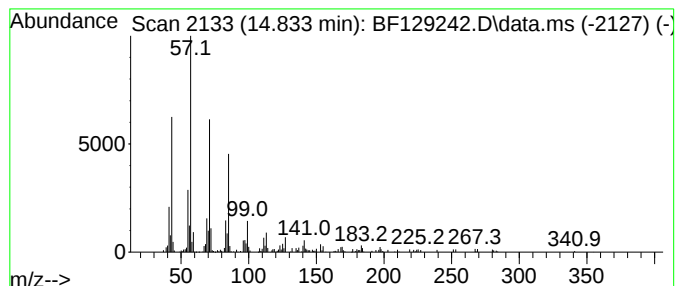
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ClientSampleId :
A-2-UC

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.833	2.08 ng	175957	Perylene-d12	15.557	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	81
2	Eicosane	282	C20H42	000112-95-8	81
3	Octadecane, 2-methyl-	268	C19H40	001560-88-9	76
4	Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	74
5	Tetracosane	338	C24H50	000646-31-1	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071522\
Data File : BF129242.D
Acq On : 15 Jul 2022 17:10
Operator : CG\JU
Sample : N3649-06
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A-2-UC

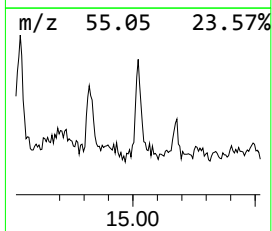
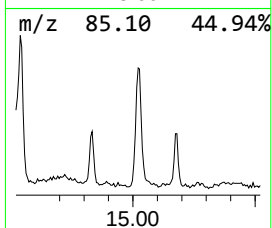
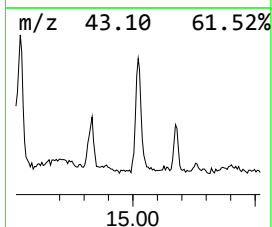
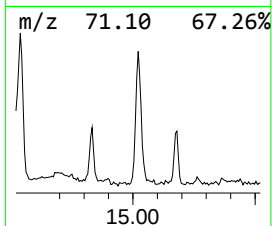
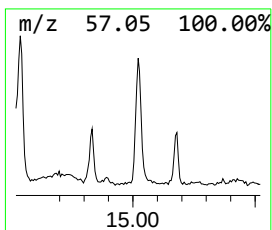
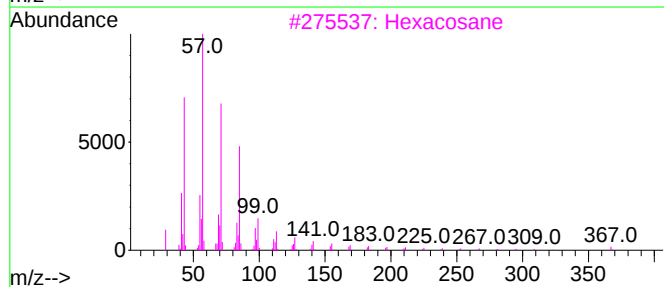
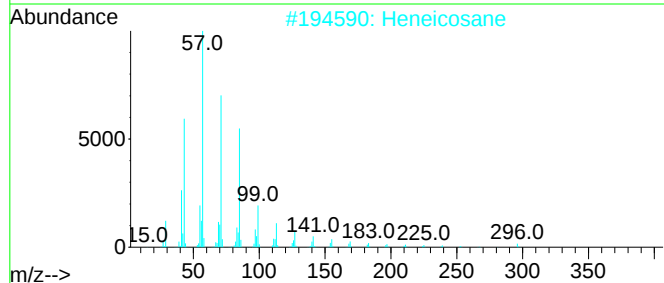
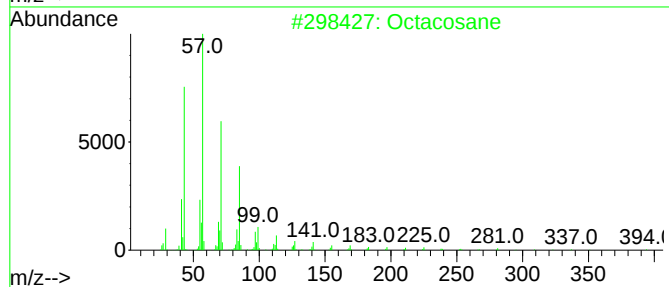
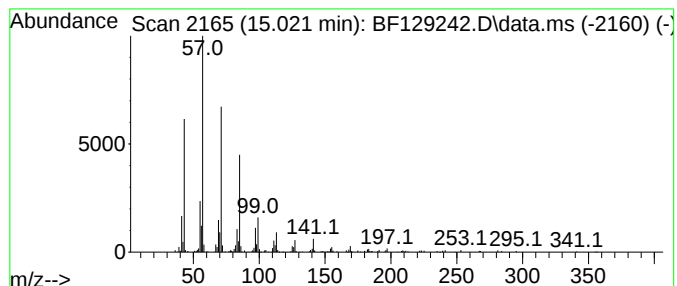
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.021	4.00 ng	338768	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Heneicosane	296	C21H44	000629-94-7	91
3			Hexacosane	366	C26H54	000630-01-3	91
4			Hexatriacontane	507	C36H74	000630-06-8	91
5			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071522\
Data File : BF129242.D
Acq On : 15 Jul 2022 17:10
Operator : CG\JU
Sample : N3649-06
Misc :
ALS Vial : 4 Sample Multiplier: 1

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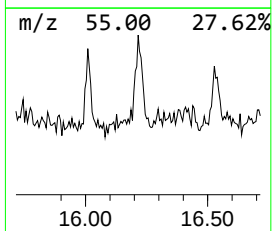
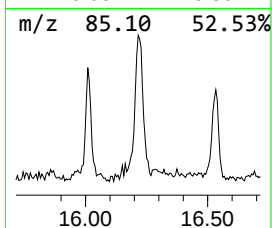
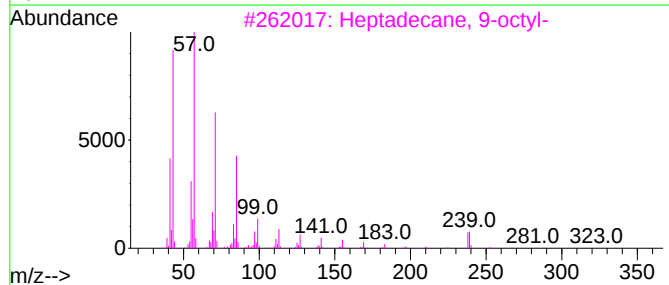
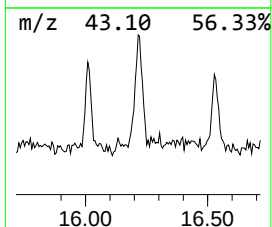
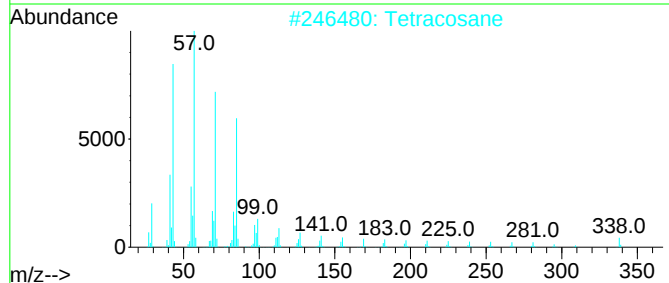
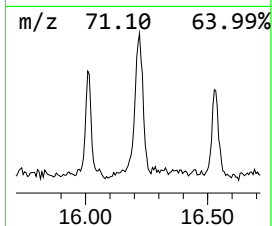
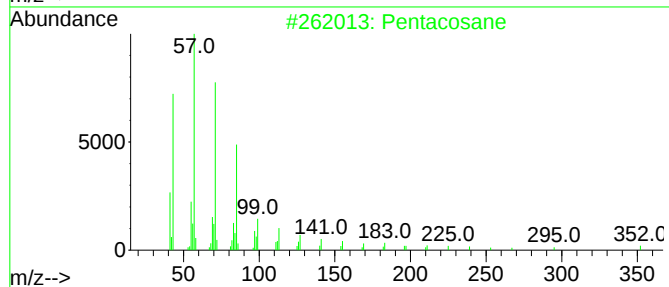
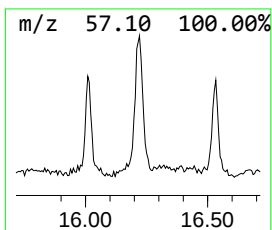
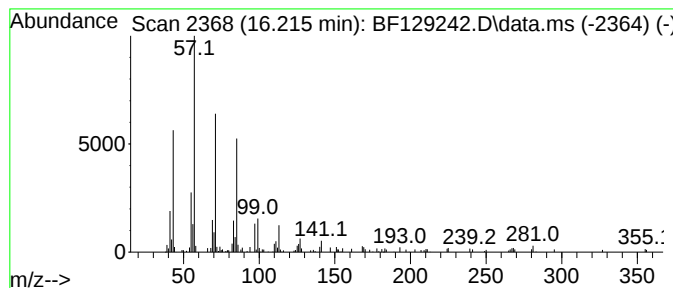
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Pentacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.215	2.38 ng	202028	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	90
2			Tetracosane	338	C24H50	000646-31-1	90
3			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
4			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87
5			Heptadecane	240	C17H36	000629-78-7	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071522\
Data File : BF129242.D
Acq On : 15 Jul 2022 17:10
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Sample : N3649-06
Misc :
ALS Vial : 4 Sample Multiplier: 1

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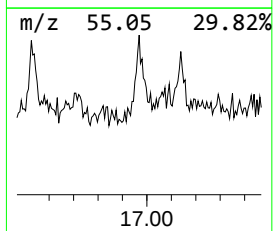
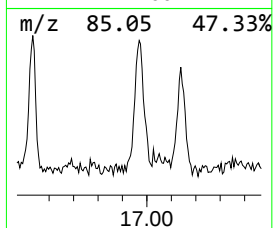
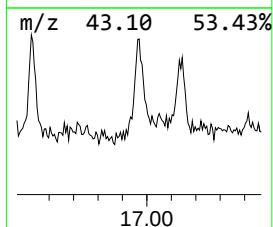
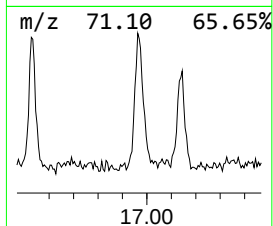
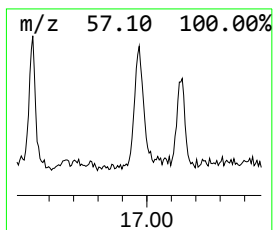
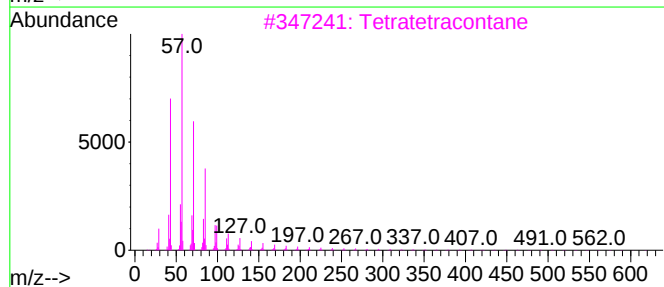
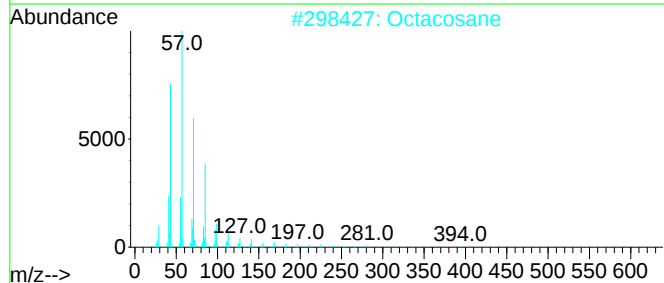
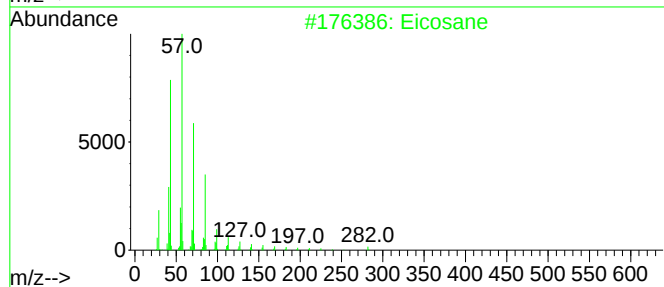
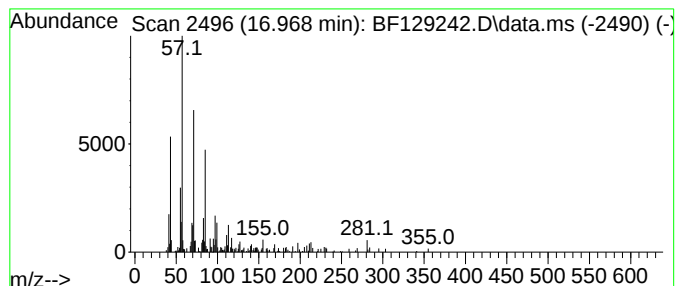
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Tetratetracontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.968	2.14 ng	181218	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	95
2			Octacosane	394	C28H58	000630-02-4	90
3			Tetratetracontane	619	C44H90	007098-22-8	90
4			Hentriacontane	437	C31H64	000630-04-6	87
5			Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071522\
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Sample : N3649-06
Misc :
ALS Vial : 4 Sample Multiplier: 1

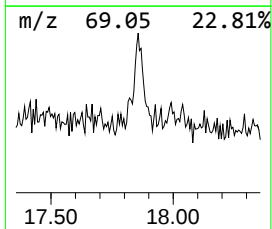
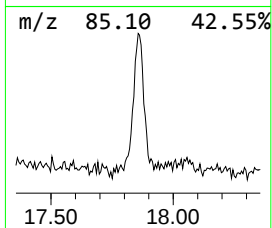
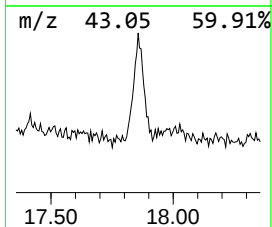
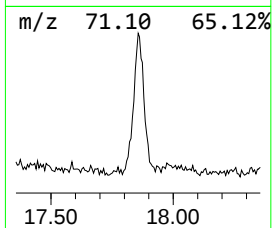
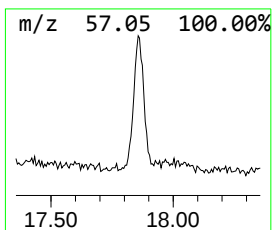
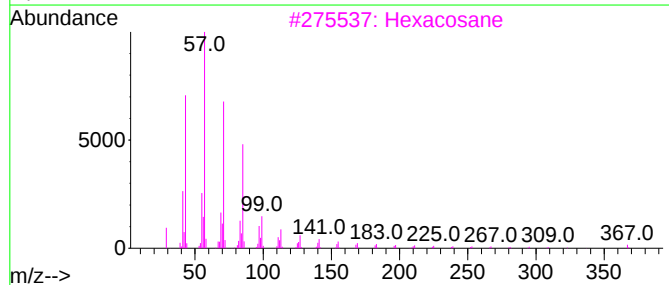
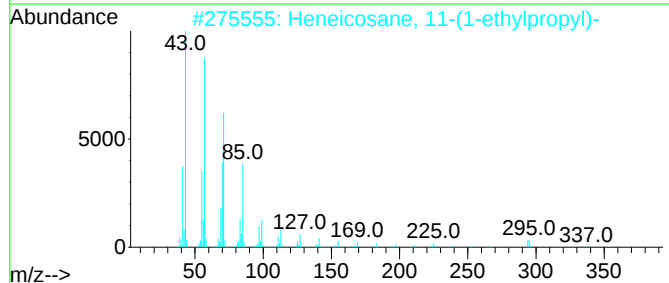
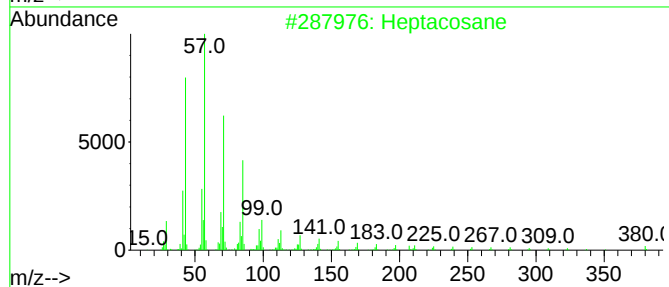
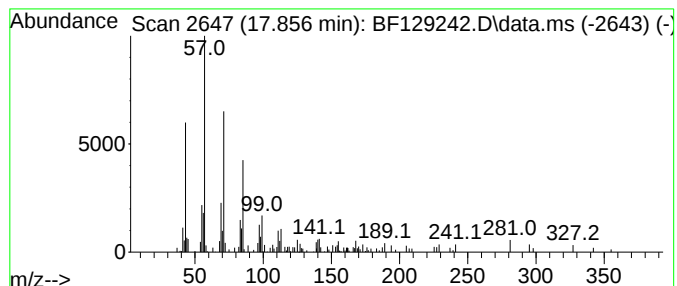
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A-2-UC

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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 Heptacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.	
17.856	2.01 ng	170240	Perylene-d12		15.557	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	91
2	Heneicosane, 11-(1-ethylpropyl)-		366	C26H54	055282-11-6	90
3	Hexacosane		366	C26H54	000630-01-3	87
4	Tetratetracontane		619	C44H90	007098-22-8	87
5	Heneicosane, 11-decyl-		437	C31H64	055320-06-4	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071522\
 Data File : BF129242.D
 Acq On : 15 Jul 2022 17:10
 Operator : CG\JU
 Sample : N3649-06
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 A-2-UC

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071522.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
Hexadecanoic ac...	11.804	3.2	ng	354476	4	11.422	2197630	20.0
n-Hexadecanoic ...	11.933	8.9	ng	974024	4	11.422	2197630	20.0
Octadecanoic acid	12.721	14.9	ng	1631580	4	11.422	2197630	20.0
Dodecane, 2-met...	12.774	4.6	ng	454665	5	14.068	1963440	20.0
Eicosane	13.486	3.6	ng	354761	5	14.068	1963440	20.0
Triphenylphosph...	14.157	2.0	ng	199733	5	14.068	1963440	20.0
Hexacosane	14.539	4.2	ng	410234	5	14.068	1963440	20.0
Octacosane	14.833	2.1	ng	175957	6	15.557	1695590	20.0
Heneicosane	15.021	4.0	ng	338768	6	15.557	1695590	20.0
Pentacosane	16.215	2.4	ng	202028	6	15.557	1695590	20.0
Tetratetracontane	16.968	2.1	ng	181218	6	15.557	1695590	20.0
Heptacosane	17.856	2.0	ng	170240	6	15.557	1695590	20.0