

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081122\
 Data File : BF129710.D
 Acq On : 11 Aug 2022 11:06
 Operator : CG\JU
 Sample : PB146625BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB146625BL

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-BF072522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129710.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.487	539	544	547	rBV	5610236	5340845	68.93%	11.781%
2	6.492	710	715	718	rBV	4692124	5533659	71.41%	12.207%
3	6.834	769	773	777	rBV	1498646	1178674	15.21%	2.600%
4	7.404	864	870	873	rBV	3381052	3794737	48.97%	8.371%
5	8.116	986	991	995	rBV	1818631	1670944	21.56%	3.686%
6	9.198	1168	1175	1178	rBV	6891330	7219704	93.17%	15.926%
7	9.875	1284	1290	1293	rBV	2312871	1982275	25.58%	4.373%
8	10.675	1419	1426	1429	rBV	4730701	4459967	57.56%	9.838%
9	11.369	1539	1544	1547	rBV	2141702	2003211	25.85%	4.419%
10	12.757	1777	1780	1783	rBV	312999	238011	3.07%	0.525%
11	12.957	1808	1814	1817	rBV	7516534	7748670	100.00%	17.093%
12	13.463	1896	1900	1903	rBV	212180	170285	2.20%	0.376%
13	14.015	1989	1994	1997	rBV	1609921	1534826	19.81%	3.386%
14	14.098	2002	2008	2013	rBV	304241	344792	4.45%	0.761%
15	14.757	2117	2120	2124	rBV	87026	86056	1.11%	0.190%
16	15.092	2173	2177	2188	rVB	113553	150337	1.94%	0.332%
17	15.486	2237	2244	2251	rVB	983288	1309058	16.89%	2.888%
18	15.898	2310	2314	2320	rVB	94609	132019	1.70%	0.291%
19	16.398	2394	2399	2407	rVB	80517	142600	1.84%	0.315%
20	16.986	2494	2499	2515	rVB6	69477	204450	2.64%	0.451%
21	17.680	2613	2617	2625	rVB3	39822	87710	1.13%	0.193%

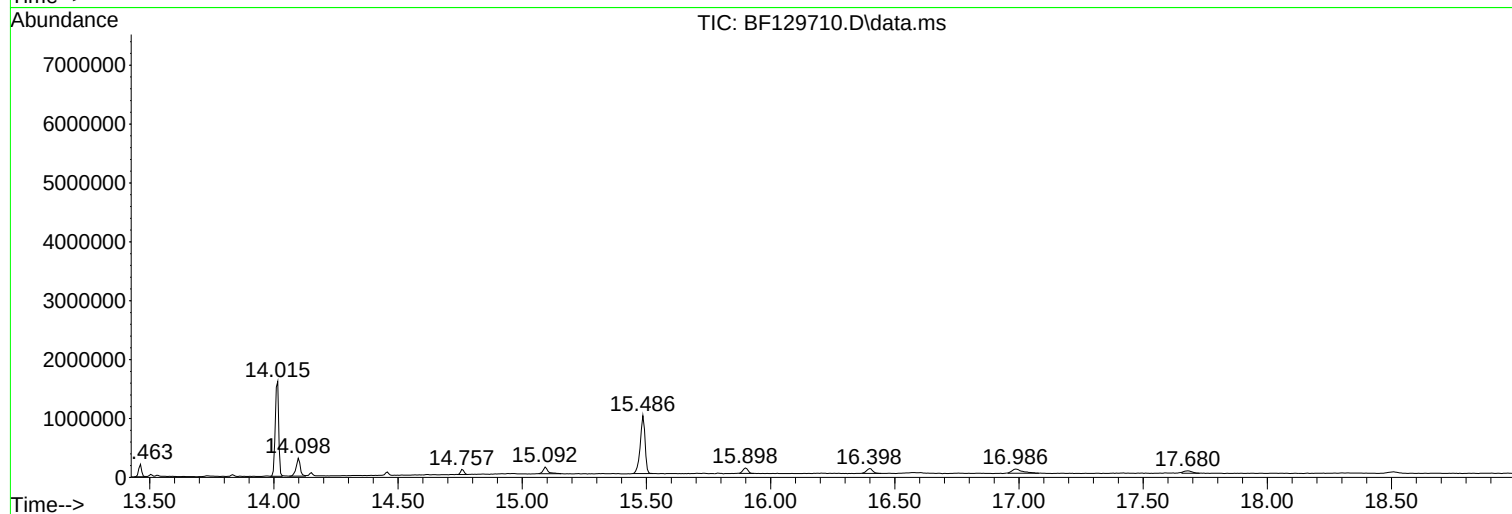
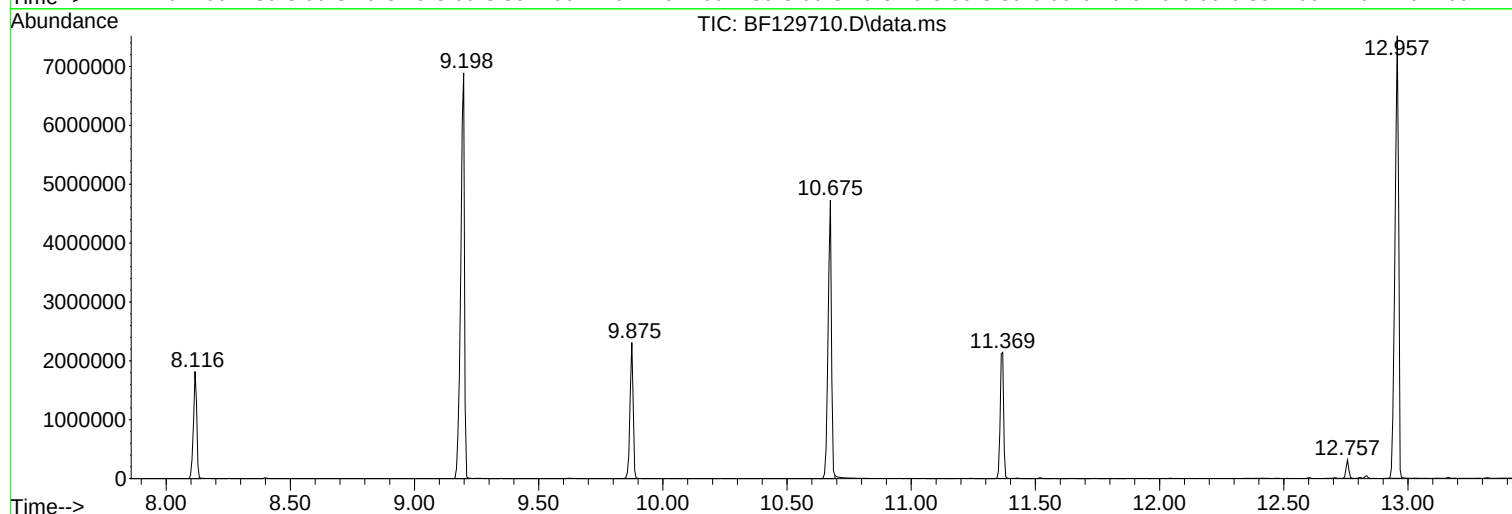
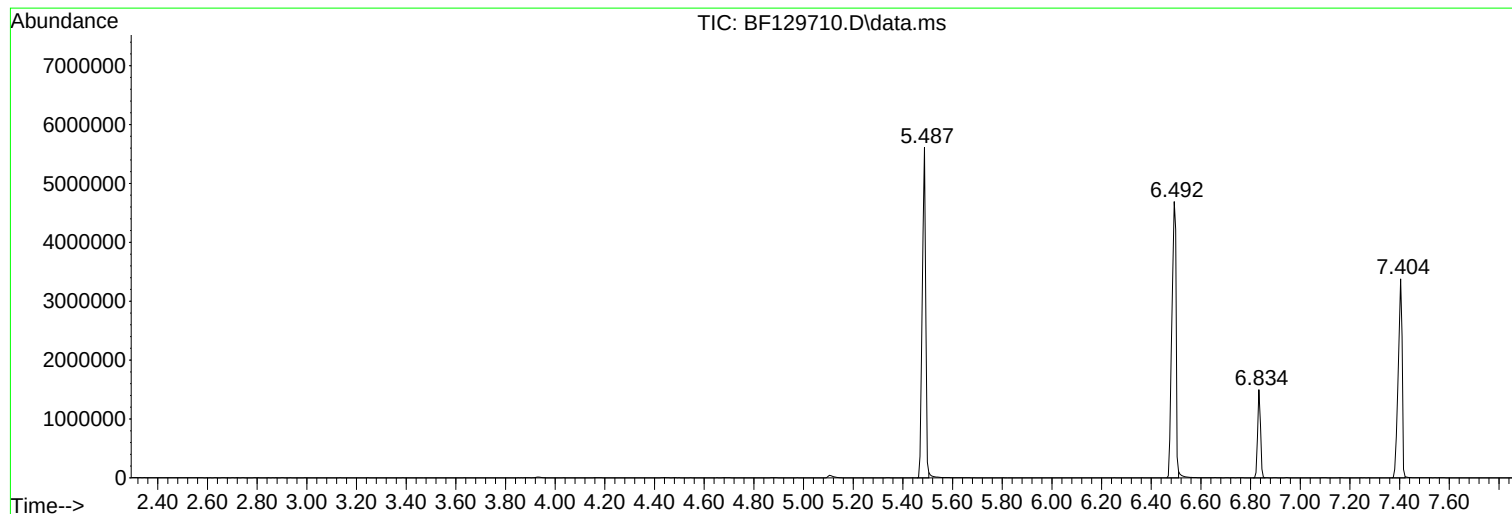
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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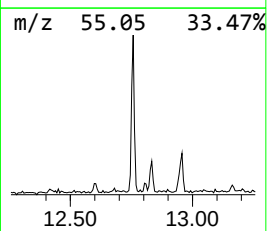
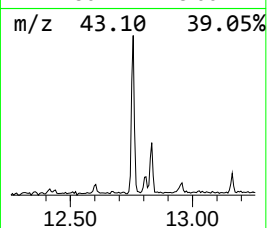
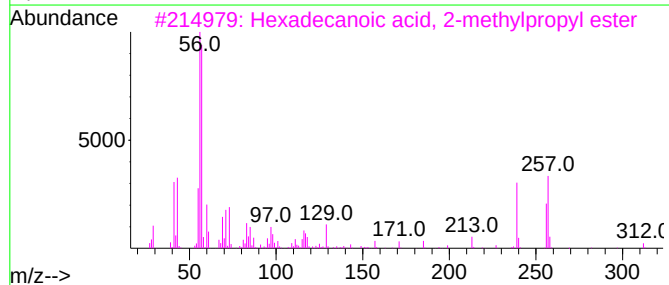
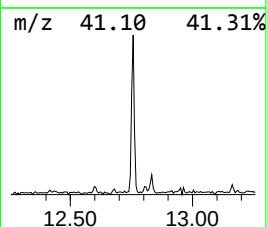
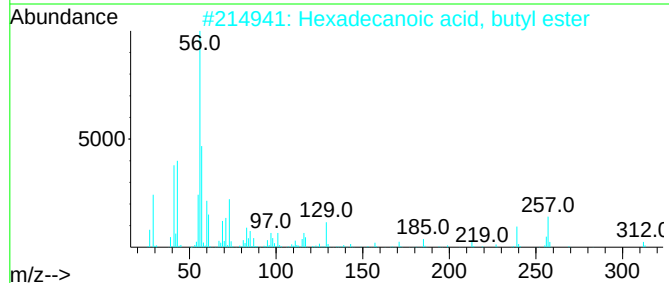
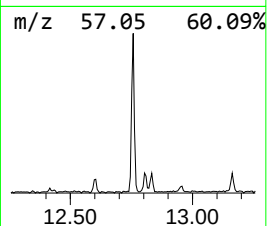
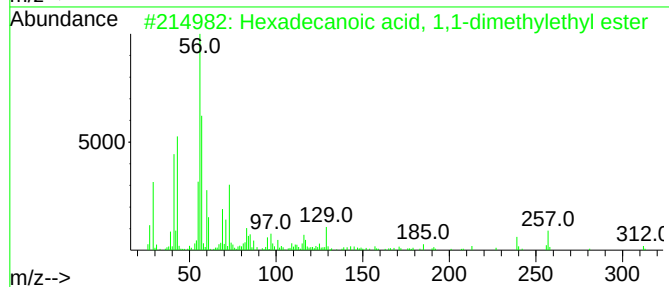
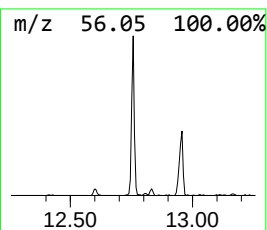
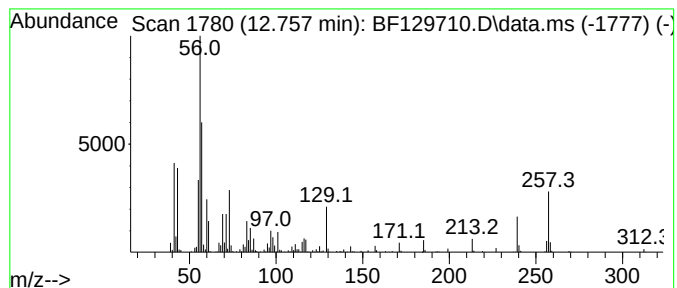
Instrument :
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ClientSampleId :
PB146625BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.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, 1,1-dime... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.757	3.10 ng	238011	Chrysene-d12		14.015	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...		312	C20H40O2	031158-91-5	95
2	Hexadecanoic acid, butyl ester		312	C20H40O2	000111-06-8	94
3	Hexadecanoic acid, 2-methylpropy...		312	C20H40O2	000110-34-9	64
4	Piperidin-4-carboxylic acid		129	C6H11NO2	000498-94-2	38
5	1,3-Hexanediol, 2-ethyl- (isomer 1)		146	C8H18O2	1000484-18-2	32



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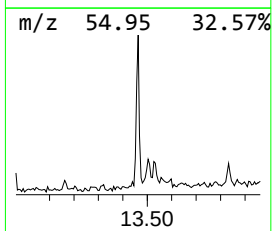
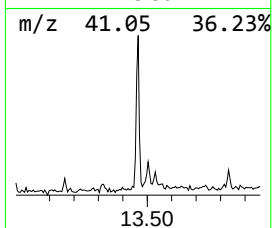
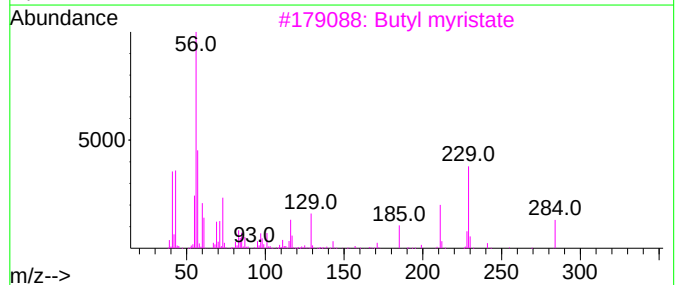
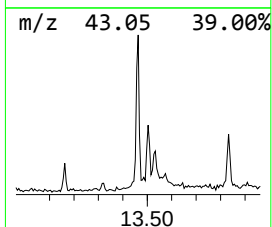
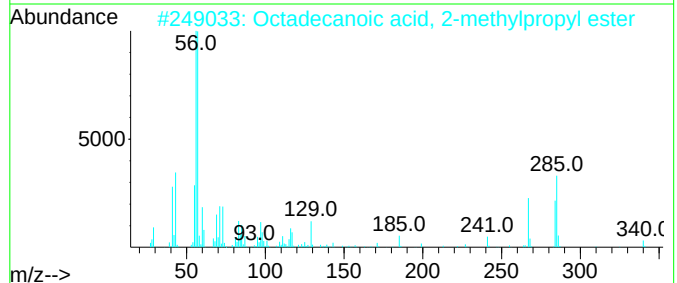
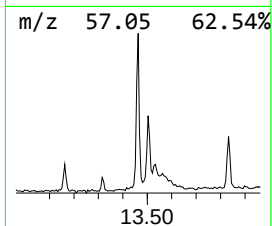
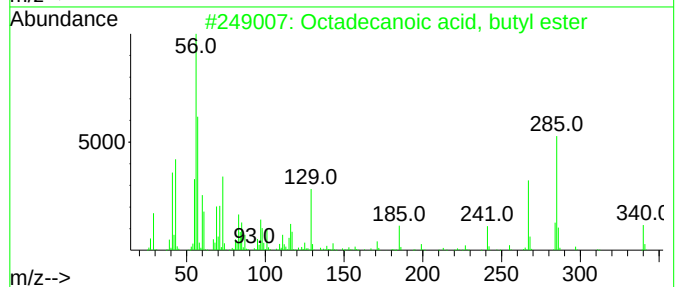
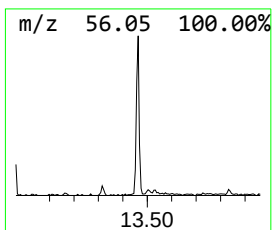
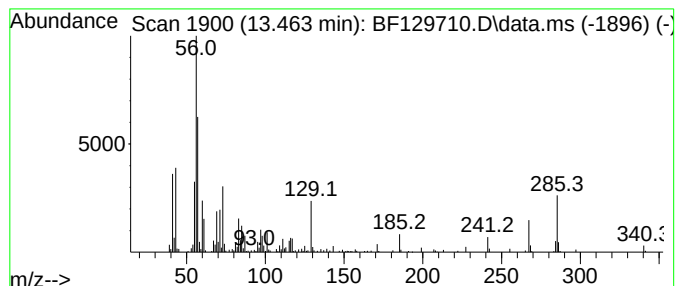
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Octadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.463	2.22 ng	170285	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	93
2			Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	87
3			Butyl myristate	284	C18H36O2	000110-36-1	72
4			Piperidin-4-carboxylic acid	129	C6H11NO2	000498-94-2	38
5			2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	35



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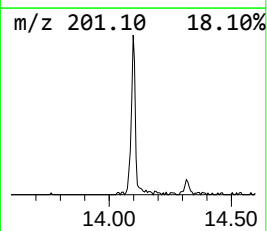
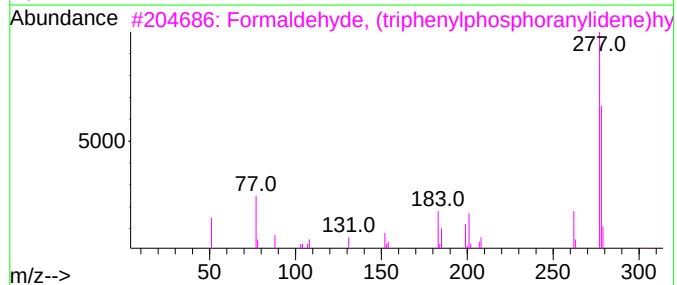
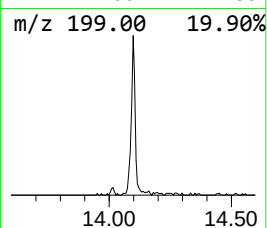
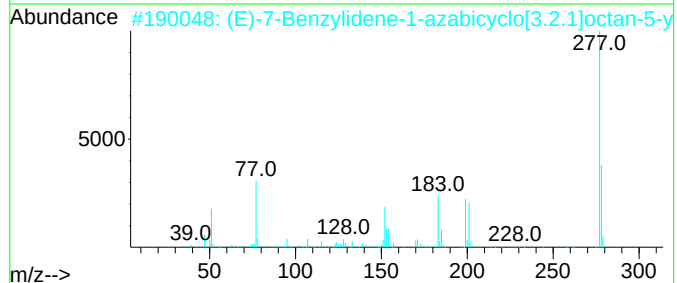
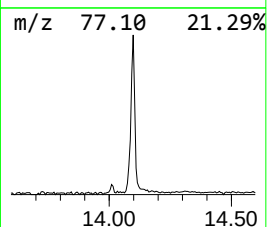
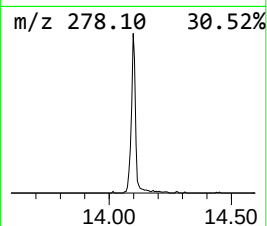
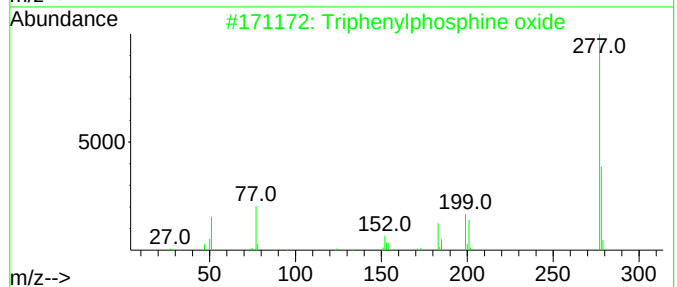
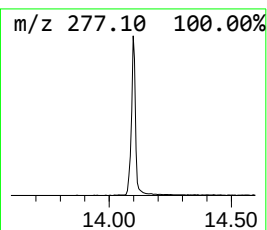
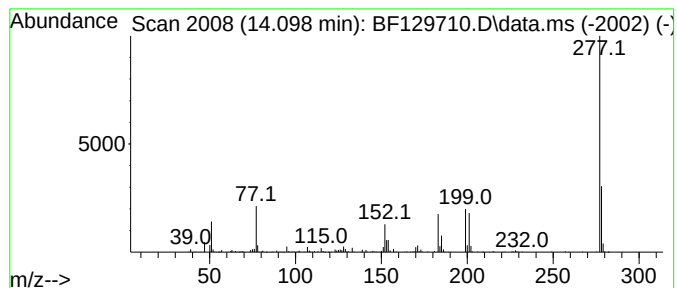
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.098	4.49 ng	344792	Chrysene-d12	14.015

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	76
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	59
4			Vanadium, cycloheptatrienyl-(pen...]	277	C17H22V	1000155-20-5	47
5			Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	40



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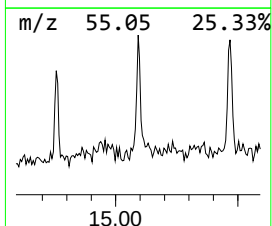
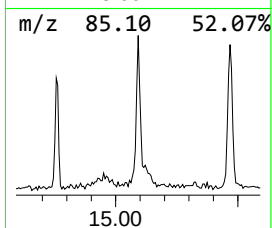
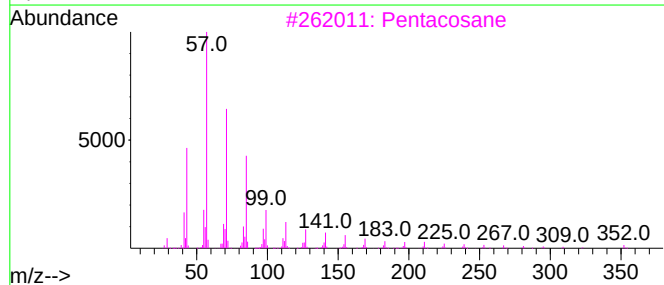
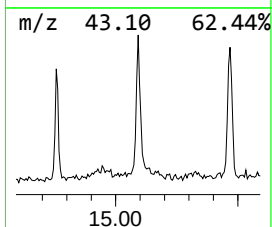
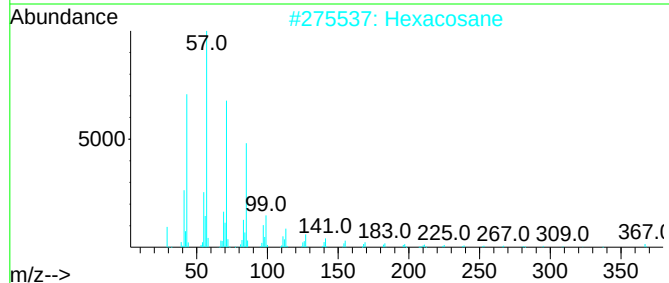
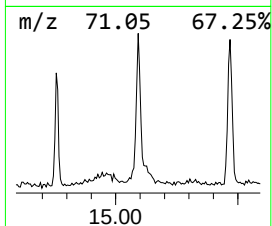
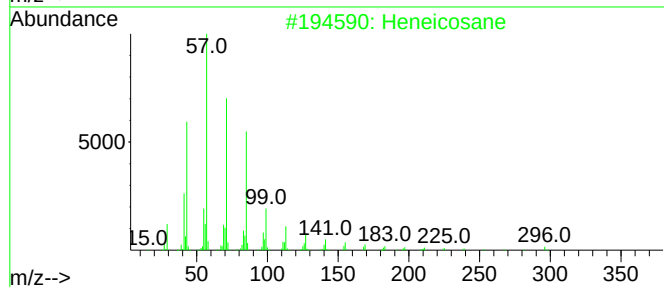
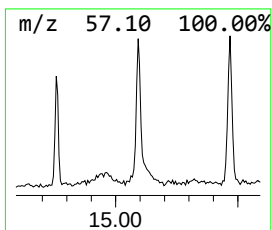
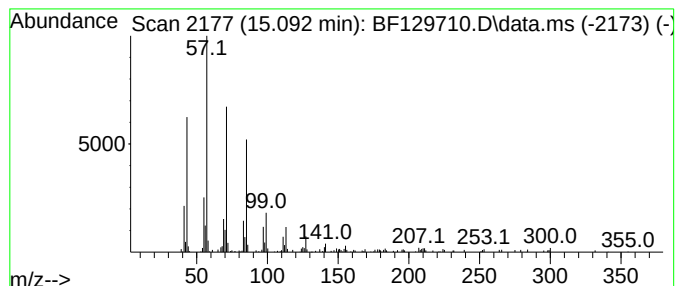
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.092	2.30 ng	150337	Perylene-d12	15.486

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane	296	C21H44	000629-94-7	90
2		Hexacosane	366	C26H54	000630-01-3	90
3		Pentacosane	352	C25H52	000629-99-2	87
4		Docosane, 1-iodo-	436	C22H45I	1000406-31-9	86
5		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	83



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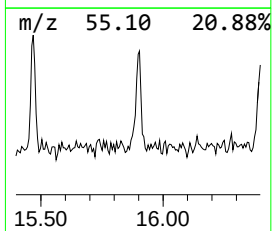
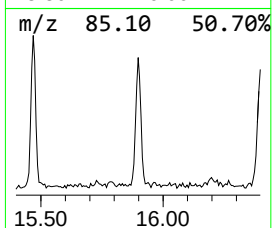
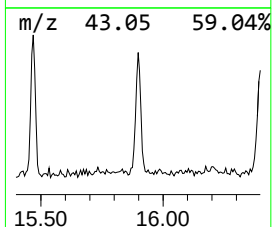
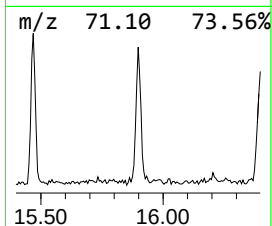
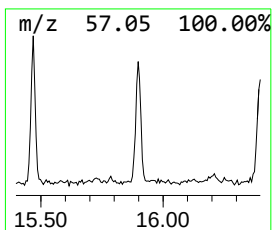
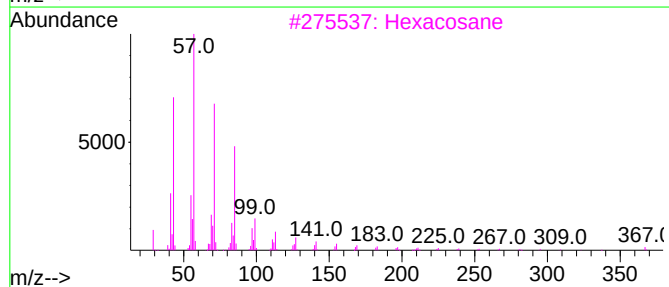
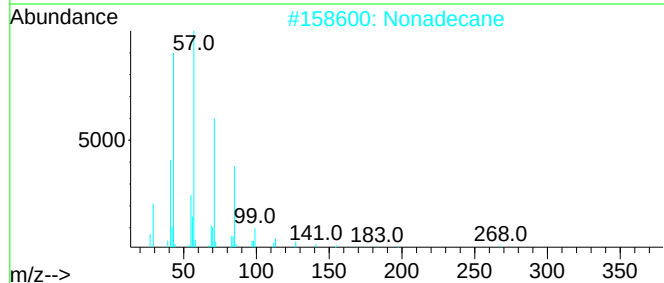
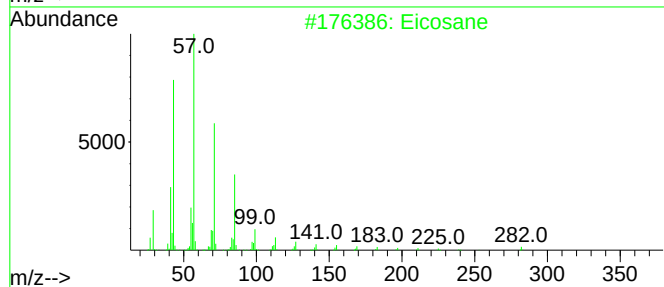
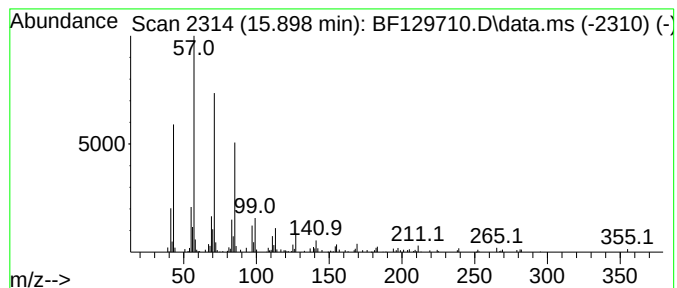
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Peak Number 5 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.898	2.02 ng	132019	Perylene-d12	15.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	95
2			Nonadecane	268	C19H40	000629-92-5	91
3			Hexacosane	366	C26H54	000630-01-3	91
4			Heneicosane	296	C21H44	000629-94-7	91
5			Tetracosane, 11-decyl-	479	C34H70	055429-84-0	91



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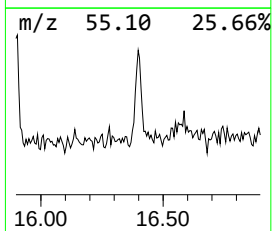
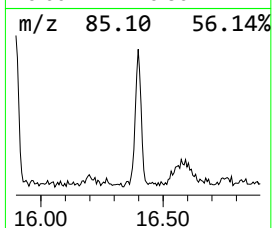
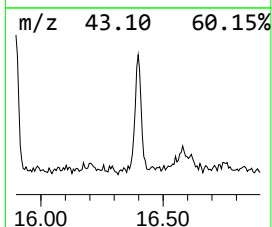
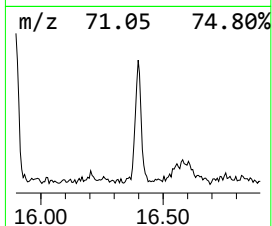
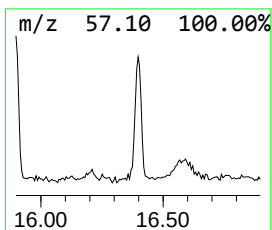
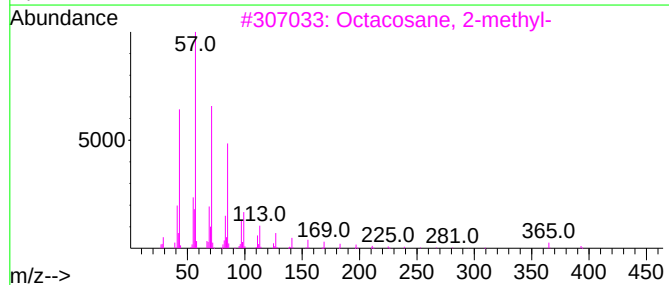
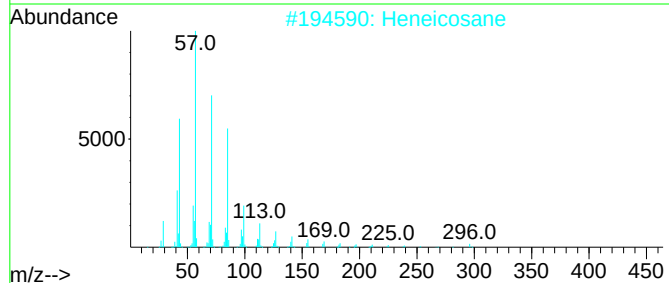
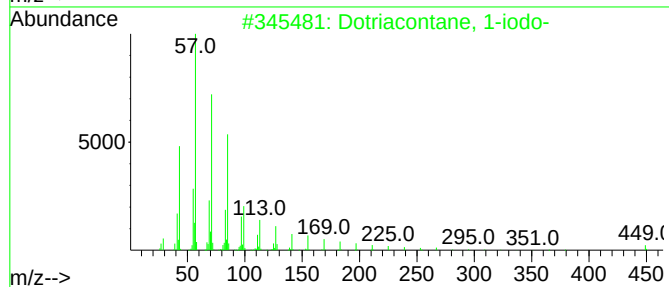
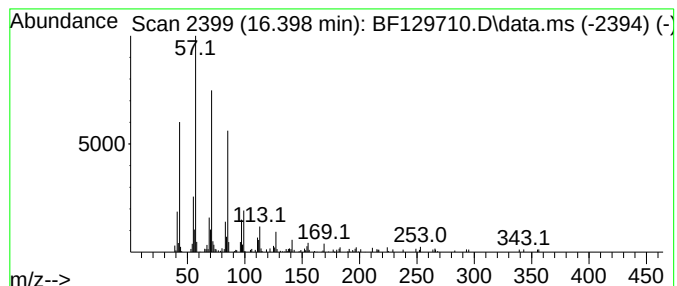
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Dotriacontane, 1-iodo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.398	2.18 ng	142600	Perylene-d12	15.486

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4		Tetracosane	338	C24H50	000646-31-1	91
5		Docosane, 11-butyl-	366	C26H54	013475-76-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081122\
Data File : BF129710.D
Acq On : 11 Aug 2022 11:06
Operator : CG\JU
Sample : PB146625BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB146625BL

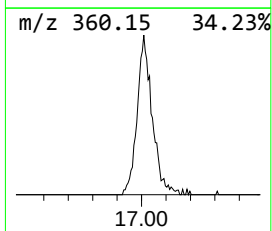
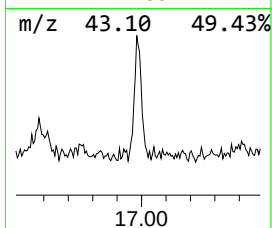
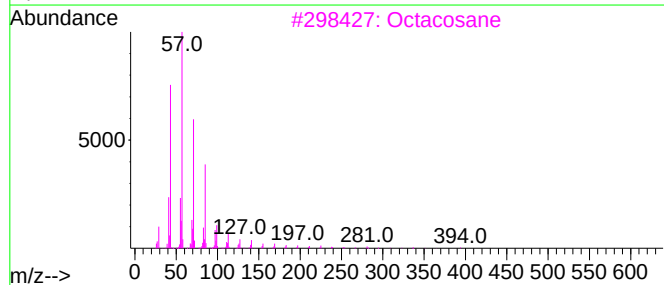
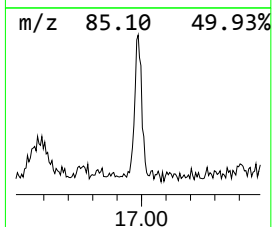
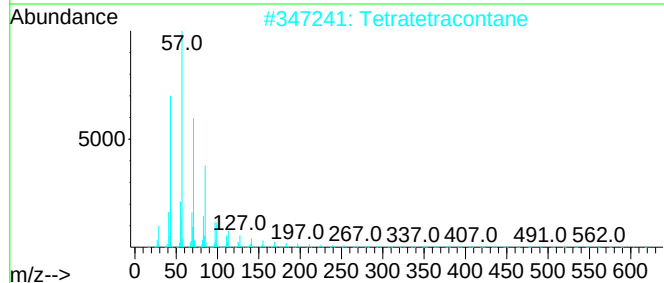
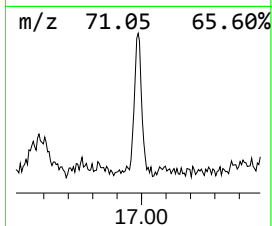
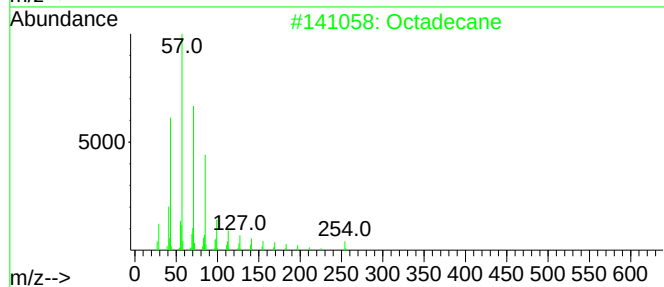
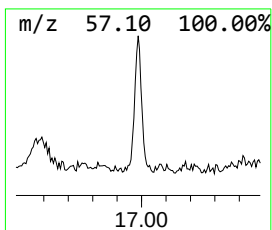
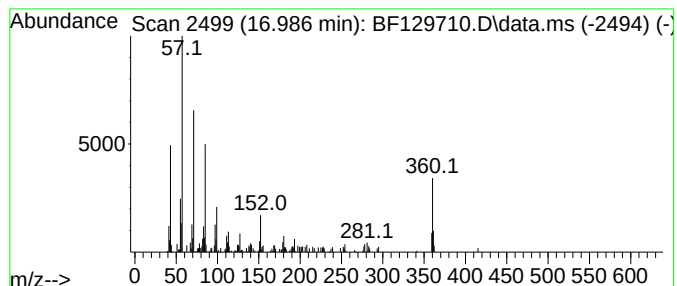
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.986	3.12 ng	204450	Perylene-d12	15.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	78
2			Tetratetracontane	619	C44H90	007098-22-8	53
3			Octacosane	394	C28H58	000630-02-4	53
4			Pentacosane	352	C25H52	000629-99-2	52
5			1-Iodoundecane	282	C11H23I	004282-44-4	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081122\
Data File : BF129710.D
Acq On : 11 Aug 2022 11:06
Operator : CG\JU
Sample : PB146625BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB146625BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.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...	12.757	3.1	ng	238011	5	14.015	1534830	20.0
Octadecanoic ac...	13.463	2.2	ng	170285	5	14.015	1534830	20.0
Triphenylphosph...	14.098	4.5	ng	344792	5	14.015	1534830	20.0
Heneicosane	15.092	2.3	ng	150337	6	15.486	1309060	20.0
Eicosane	15.898	2.0	ng	132019	6	15.486	1309060	20.0
Dotriacontane, ...	16.398	2.2	ng	142600	6	15.486	1309060	20.0
Octadecane	16.986	3.1	ng	204450	6	15.486	1309060	20.0