

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
 Data File : BF128506.D
 Acq On : 27 May 2022 13:08
 Operator : CG\JU
 Sample : N2922-06
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P024-SS001-0612-01

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-BF052622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128506.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.081	472	475	484	rVB	55302	75493	1.03%	0.157%
2	5.457	533	539	542	rBV	5076359	5658022	76.99%	11.753%
3	6.463	703	710	713	rBV	4856405	5786949	78.74%	12.021%
4	6.575	726	729	732	rBV	111524	79968	1.09%	0.166%
5	6.834	770	773	777	rVB	1523130	1301324	17.71%	2.703%
6	7.398	864	869	872	rBV	3532870	3993690	54.34%	8.296%
7	8.116	987	991	995	rBV	1944765	1749178	23.80%	3.633%
8	9.198	1169	1175	1178	rBV	6527758	7134432	97.08%	14.820%
9	9.875	1284	1290	1293	rBV	2425172	2083379	28.35%	4.328%
10	10.663	1418	1424	1428	rBV	4138716	4568234	62.16%	9.489%
11	11.363	1539	1543	1546	rBV	2627854	2214199	30.13%	4.599%
12	11.763	1607	1611	1614	rVB	129504	109190	1.49%	0.227%
13	11.857	1623	1627	1630	rBV	134746	136569	1.86%	0.284%
14	11.898	1630	1634	1650	rVB	674102	800624	10.89%	1.663%
15	12.469	1725	1731	1737	rBV	106813	104152	1.42%	0.216%
16	12.616	1751	1756	1762	rVB3	76596	120086	1.63%	0.249%
17	12.680	1764	1767	1780	rVB	225630	247218	3.36%	0.514%
18	12.957	1809	1814	1817	rVB	6774334	7349324	100.00%	15.266%
19	13.922	1969	1978	1986	rBV7	101204	385676	5.25%	0.801%
20	14.004	1987	1992	1995	rVB	1761160	1681830	22.88%	3.494%
21	14.098	2003	2008	2018	rVB	631274	701527	9.55%	1.457%
22	15.463	2235	2240	2246	rBV2	963027	1176501	16.01%	2.444%
23	15.957	2319	2324	2331	rVB2	52465	83499	1.14%	0.173%
24	18.110	2668	2690	2698	rBV2	68557	456956	6.22%	0.949%
25	18.439	2738	2746	2750	rBV6	47601	143375	1.95%	0.298%

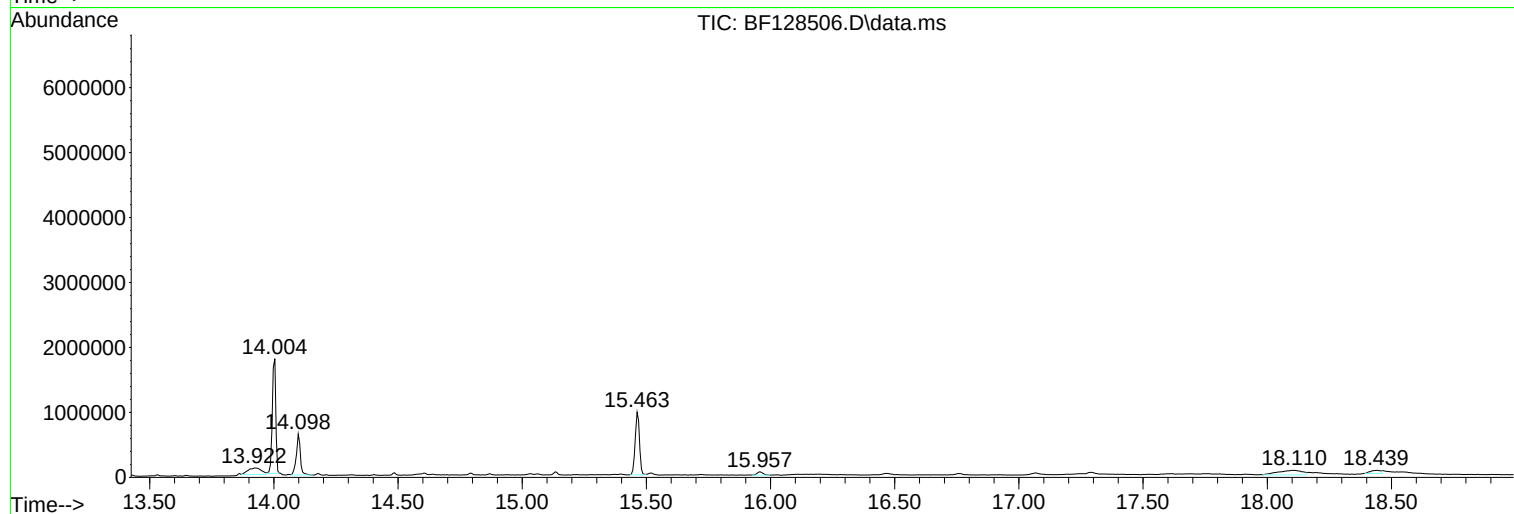
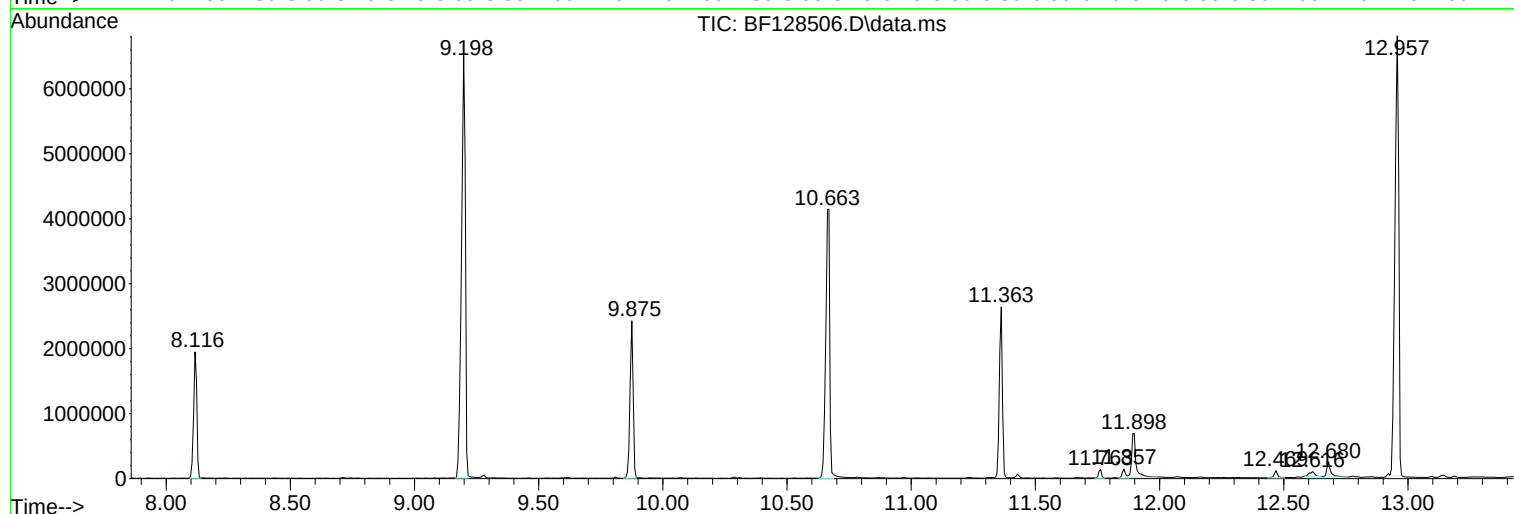
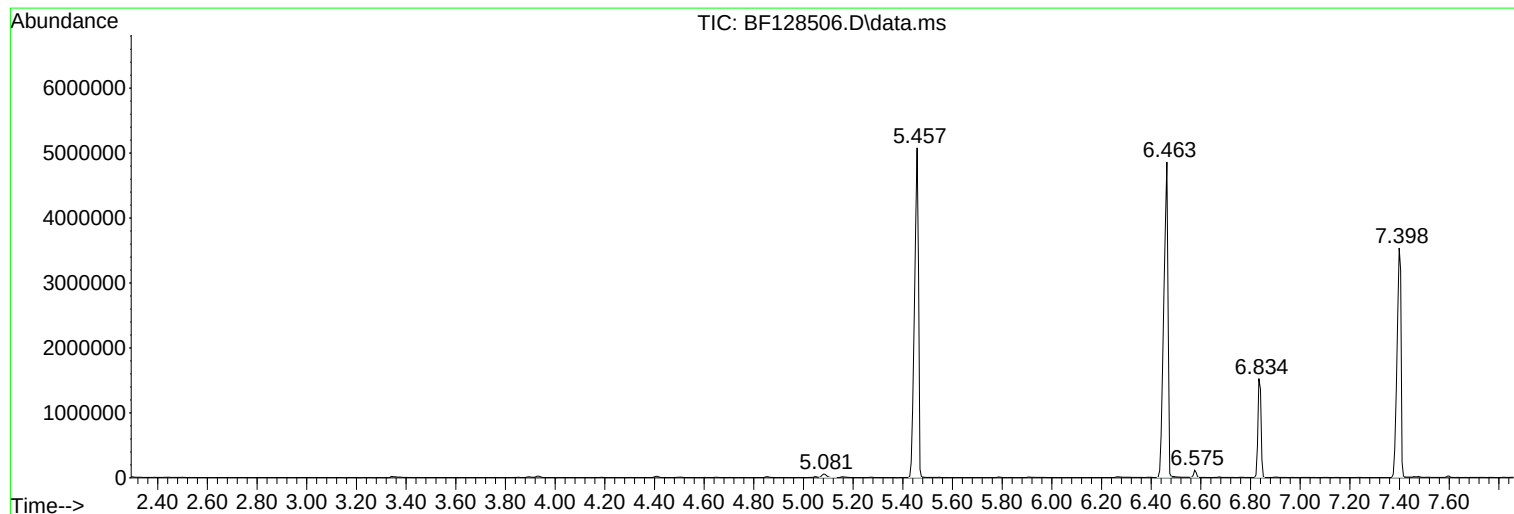
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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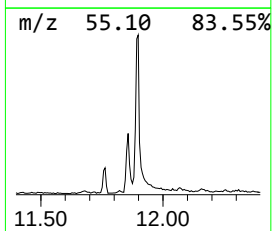
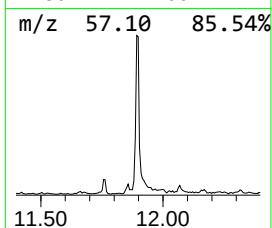
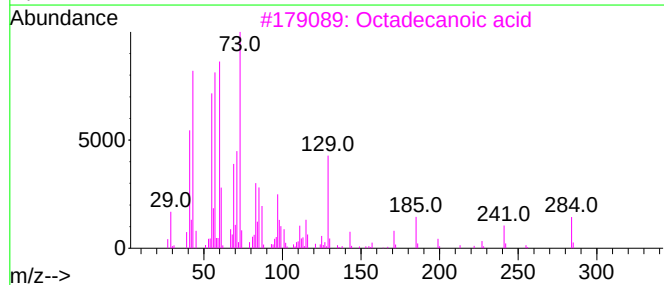
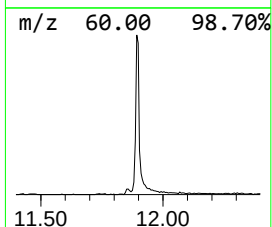
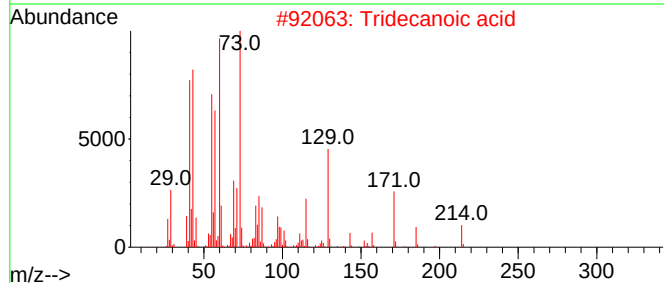
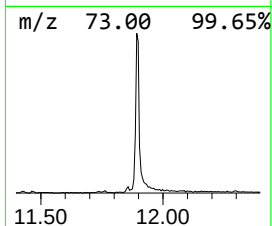
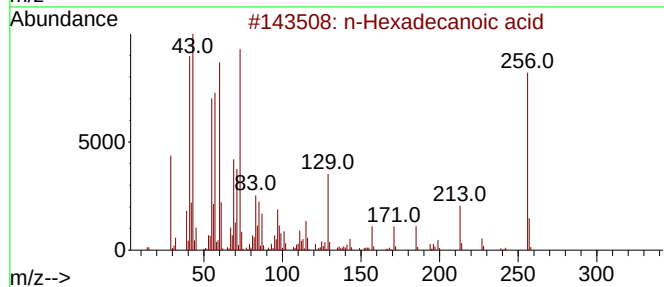
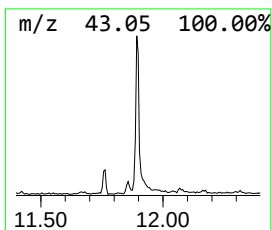
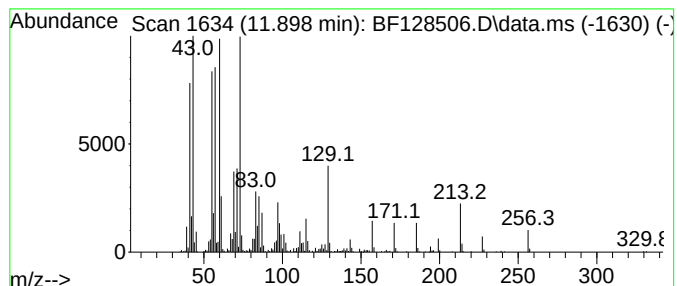
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	7.23 ng	800624	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Octadecanoic acid	284	C18H36O2	000057-11-4	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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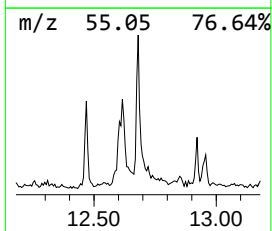
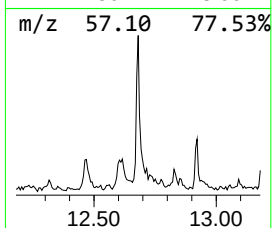
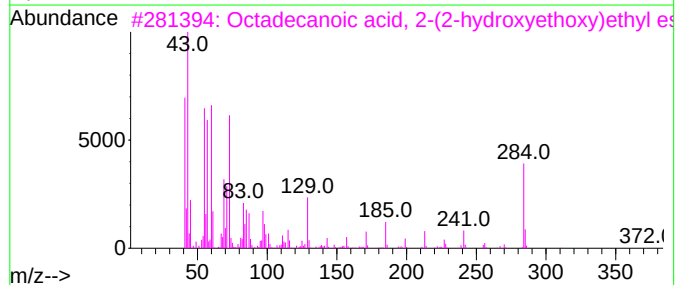
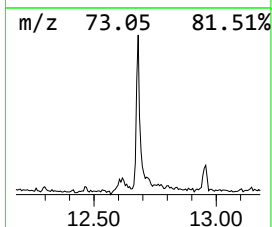
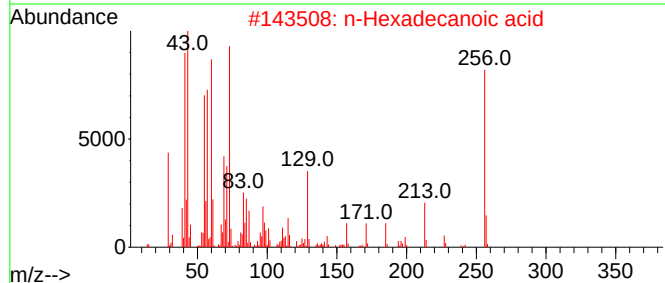
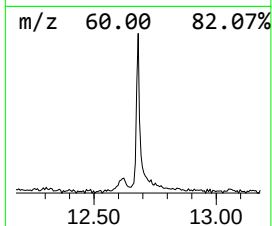
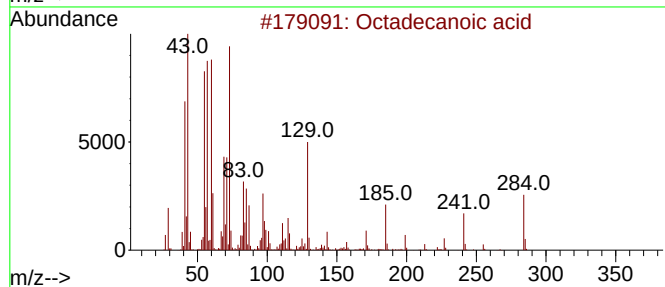
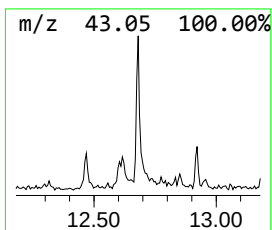
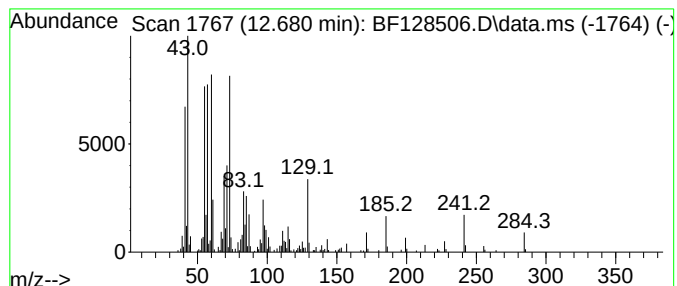
Instrument :
BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.680	2.23 ng	247218	Phenanthrene-d10	11.363	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62



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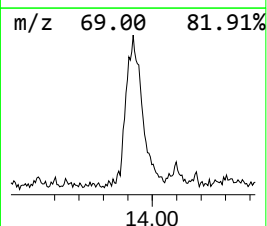
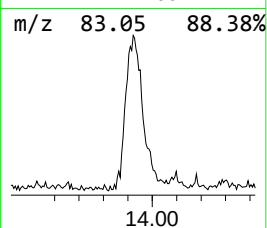
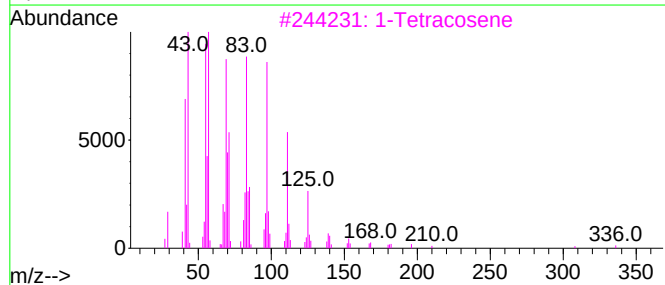
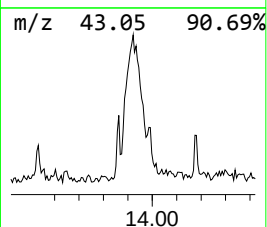
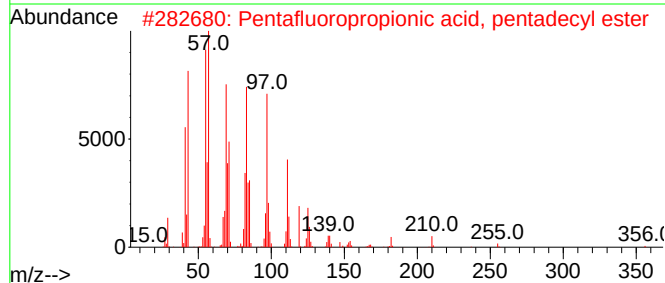
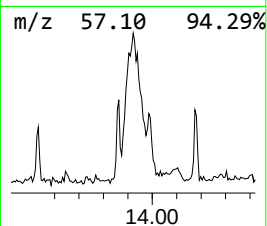
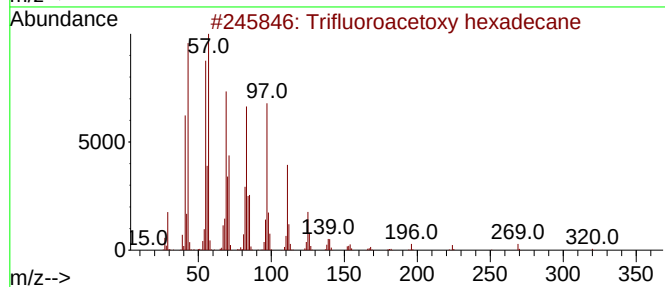
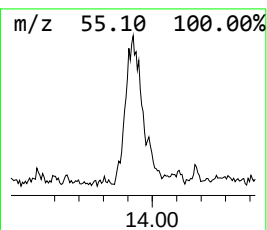
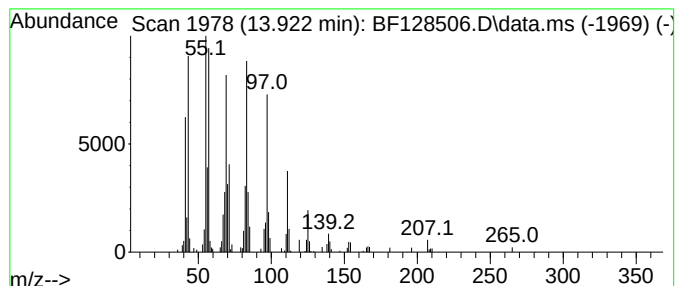
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.922	4.59 ng	385676	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
3			1-Tetracosene	336	C24H48	010192-32-2	91
4			Behenic alcohol	326	C22H46O	000661-19-8	91
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	91



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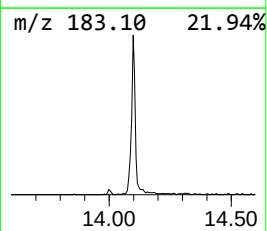
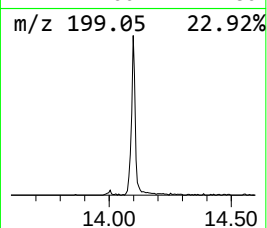
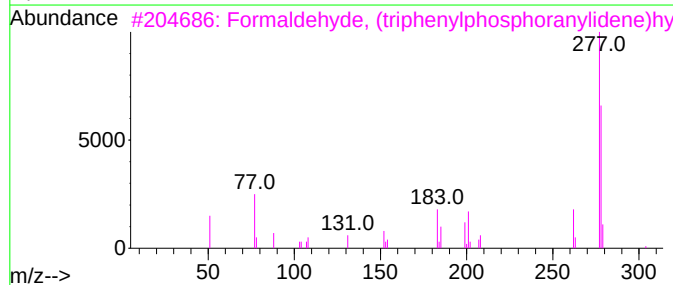
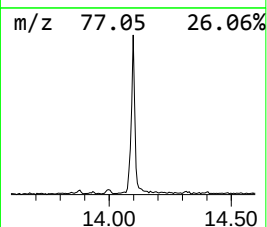
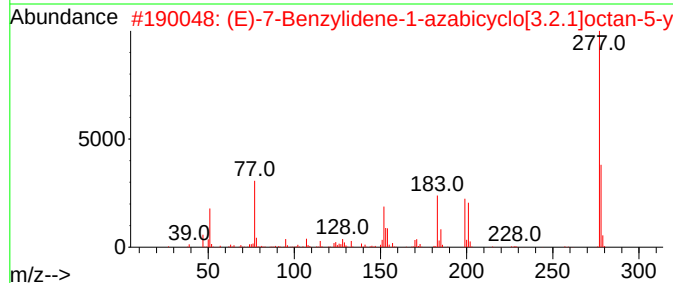
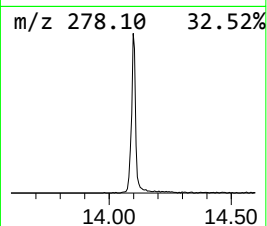
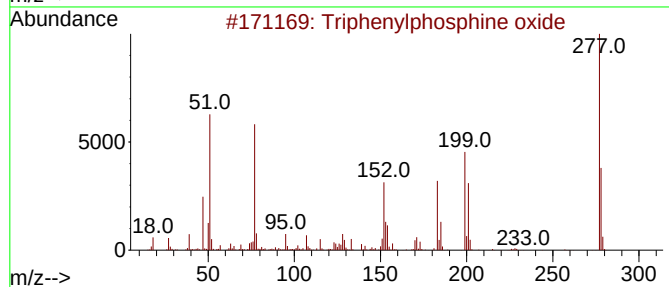
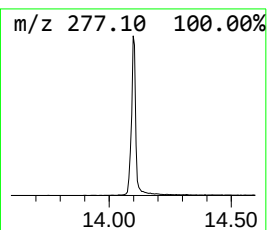
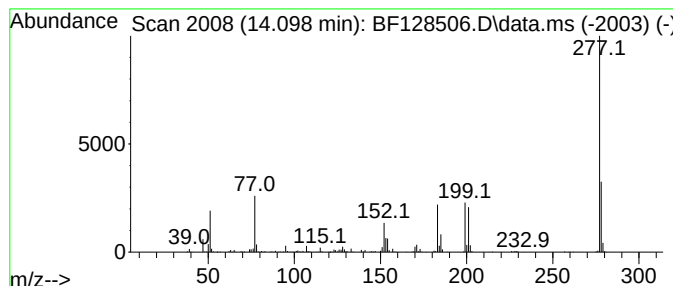
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Peak Number 4 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.098	8.34 ng	701527	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	96
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	81
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	64
4			4-Nitro-4'-methyldiphenylsulfone	277	C13H11N04S	004094-37-5	43
5			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	27



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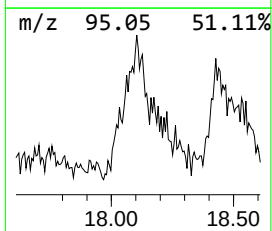
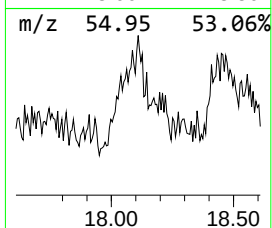
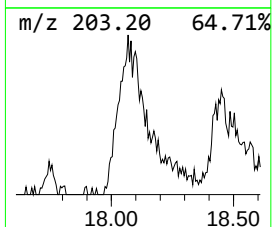
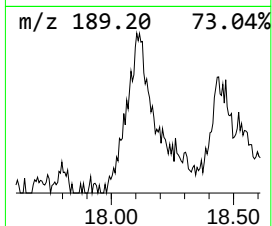
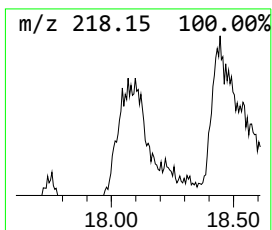
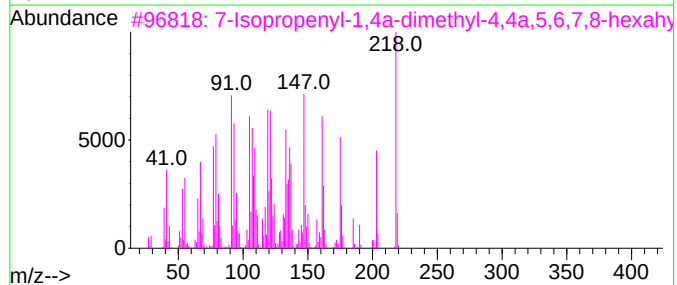
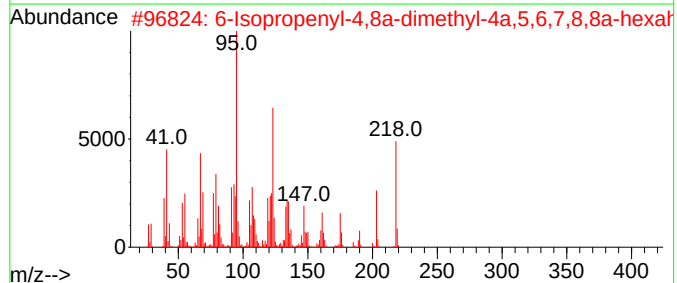
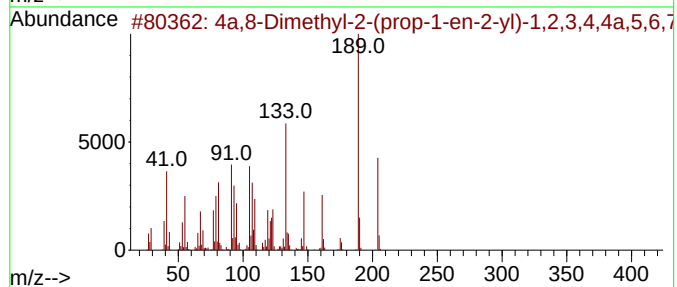
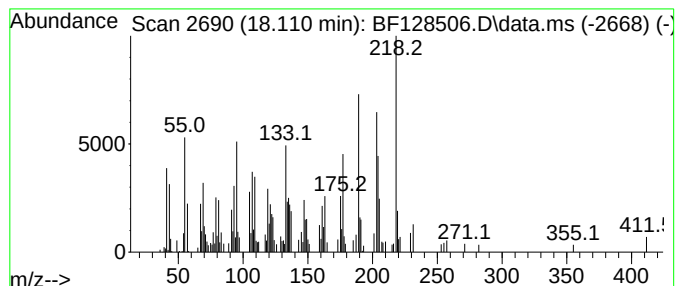
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 4a,8-Dimethyl-2-(prop-1-en-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.110	7.77 ng	456956	Perylene-d12	15.463	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4a,8-Dimethyl-2-(prop-1-en-2-yl)...	204	C15H24	103827-22-1	74
2	6-Isopropenyl-4,8a-dimethyl-4a,5...	218	C15H220	086917-79-5	64
3	7-Isopropenyl-1,4a-dimethyl-4,4a...	218	C15H220	000473-08-5	60
4	(E)-2-((8R,8aS)-8,8a-Dimethyl-3,...	218	C15H220	137695-18-2	49
5	5(1H)-Azulenone, 2,4,6,7,8,8a-he...	218	C15H220	006754-66-1	46



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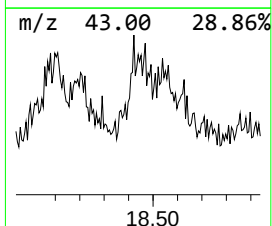
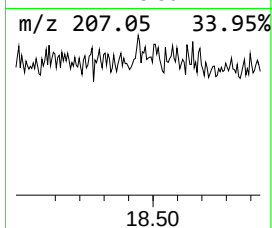
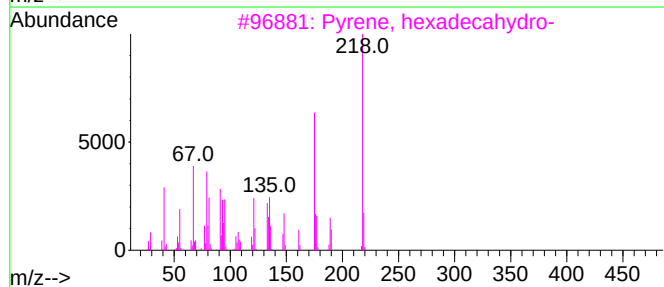
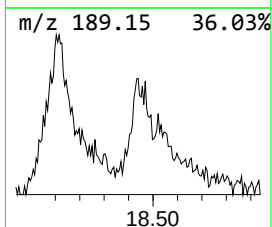
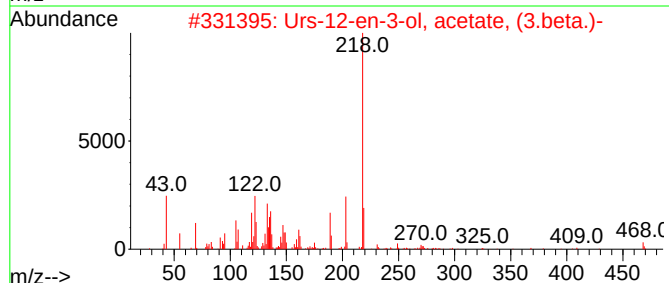
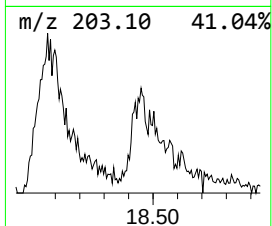
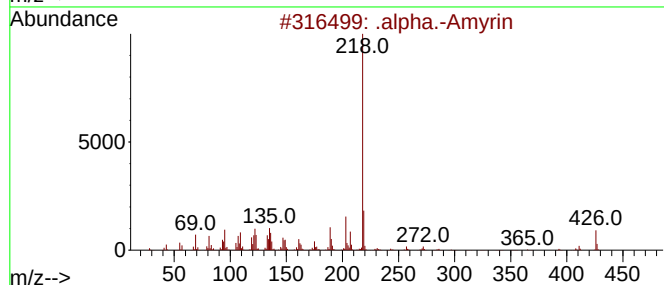
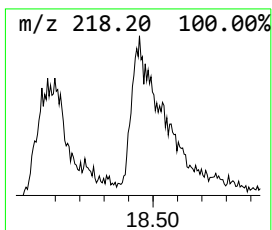
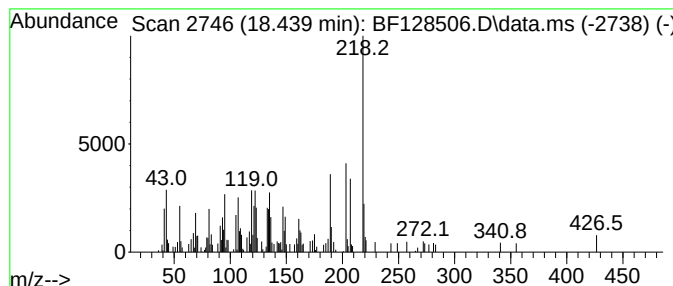
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 .alpha.-Amyrin Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.439	2.44 ng	143375	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.		.alpha.-Amyrin	426	C30H50O	000638-95-9	78
2	Urs-12-en-3-ol, acetate, (3.beta.)-	468	C32H52O2			000863-76-3	52
3	Pyrene, hexadecahydro-	218	C16H26			002435-85-0	50
4	(3aR,4R,7R)-1,4,9,9-Tetramethyl-...	218	C15H22O			003466-15-7	49
5	4H-Benz[de]anthracene, 5,6-dihydro-	218	C17H14			004389-09-7	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
Data File : BF128506.D
Acq On : 27 May 2022 13:08
Operator : CG\JU
Sample : N2922-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P024-SS001-0612-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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
n-Hexadecanoic ...	11.898	7.2	ng	800624	4	11.363	2214200	20.0
Octadecanoic acid	12.680	2.2	ng	247218	4	11.363	2214200	20.0
Trifluoroacetox...	13.922	4.6	ng	385676	5	14.004	1681830	20.0
Triphenylphosph...	14.098	8.3	ng	701527	5	14.004	1681830	20.0
4a,8-Dimethyl-2...	18.110	7.8	ng	456956	6	15.463	1176500	20.0
.alpha.-Amyrin	18.439	2.4	ng	143375	6	15.463	1176500	20.0