

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
 Data File : BF128523.D
 Acq On : 27 May 2022 21:59
 Operator : CG\JU
 Sample : N2930-17
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P006-SS002-0006-01

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: BF128523.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.069	470	473	485	rVB	110333	133551	2.56%	0.363%
2	5.457	533	539	542	rBV	4312068	4275027	81.82%	11.606%
3	6.457	703	709	712	rBV	3777790	4457734	85.32%	12.102%
4	6.834	770	773	777	rVB	1529622	1364393	26.11%	3.704%
5	7.398	863	869	872	rBV	3104808	3060287	58.57%	8.308%
6	8.116	986	991	995	rBV	1947285	1801935	34.49%	4.892%
7	9.198	1169	1175	1178	rBV	5608680	5224967	100.00%	14.184%
8	9.875	1284	1290	1293	rBV	2404270	1947008	37.26%	5.286%
9	10.663	1417	1424	1427	rBV	3357355	2998618	57.39%	8.140%
10	11.363	1539	1543	1546	rBV	2242732	1876409	35.91%	5.094%
11	11.886	1629	1632	1637	rBV	122512	127175	2.43%	0.345%
12	12.674	1763	1766	1777	rBV2	58569	69059	1.32%	0.187%
13	12.951	1809	1813	1816	rBV	4537282	4266477	81.66%	11.582%
14	13.863	1964	1968	1969	rBV	66476	65311	1.25%	0.177%
15	13.892	1969	1973	1986	rVB5	69635	209760	4.01%	0.569%
16	13.998	1987	1991	1994	rBV	1375013	1318606	25.24%	3.580%
17	14.098	2001	2008	2018	rBV	1033180	1302237	24.92%	3.535%
18	14.480	2070	2073	2076	rBV	119820	112824	2.16%	0.306%
19	15.133	2180	2184	2191	rVB	151506	170164	3.26%	0.462%
20	15.463	2235	2240	2245	rBV	882305	1120598	21.45%	3.042%
21	15.721	2280	2284	2290	rVB	51408	73419	1.41%	0.199%
22	15.957	2319	2324	2329	rBV	94543	142763	2.73%	0.388%
23	16.762	2456	2461	2468	rVB6	36068	74062	1.42%	0.201%
24	16.998	2496	2501	2506	rBV5	52473	106230	2.03%	0.288%
25	17.586	2593	2601	2608	rBV5	39521	153519	2.94%	0.417%
26	18.027	2673	2676	2684	rVB8	31829	66984	1.28%	0.182%
27	18.198	2699	2705	2716	rVB3	71922	187756	3.59%	0.510%
28	18.551	2760	2765	2772	rVB5	59003	128965	2.47%	0.350%

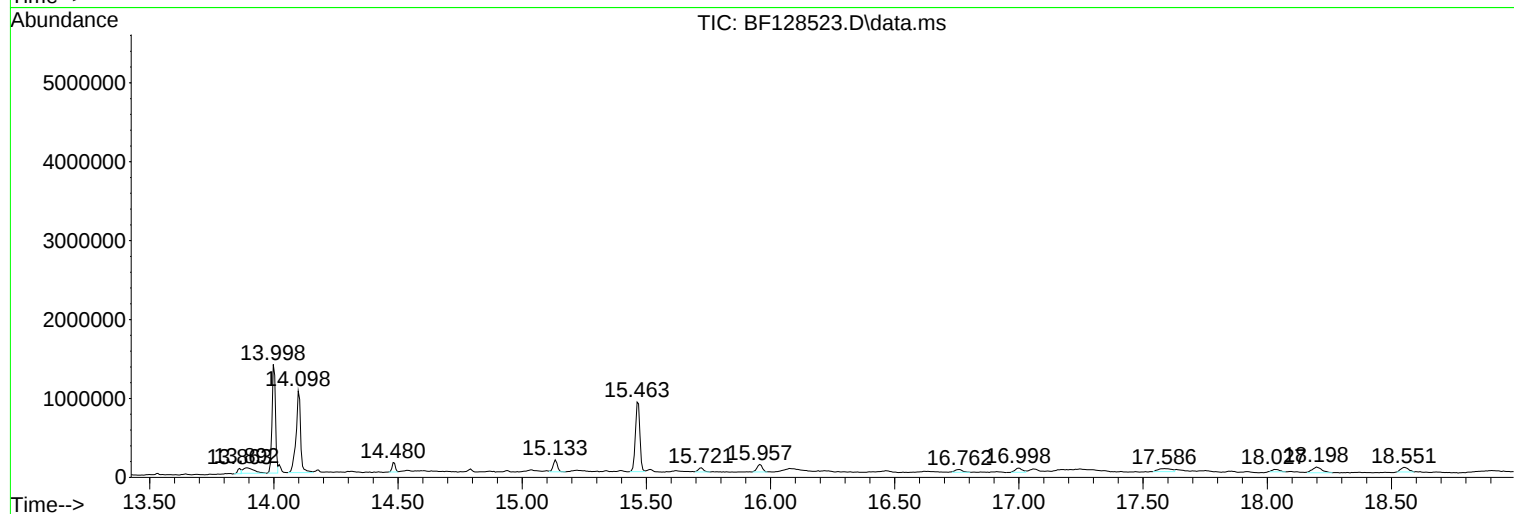
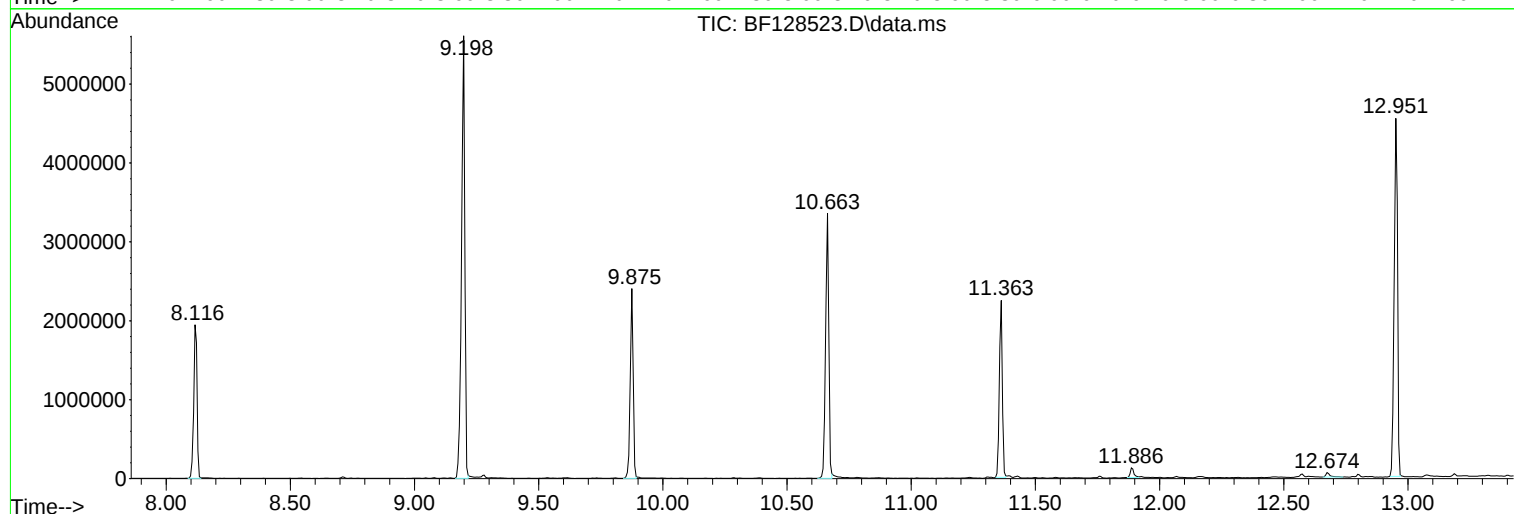
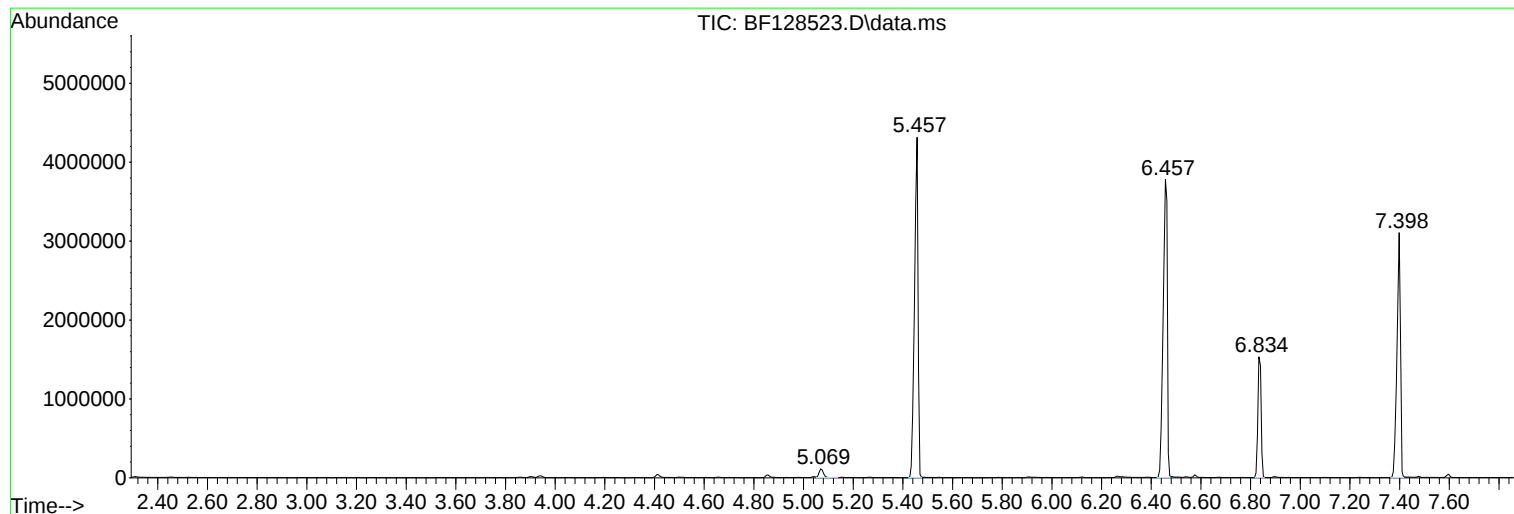
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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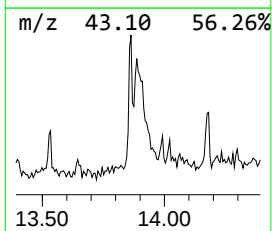
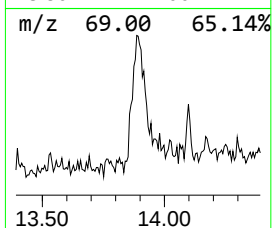
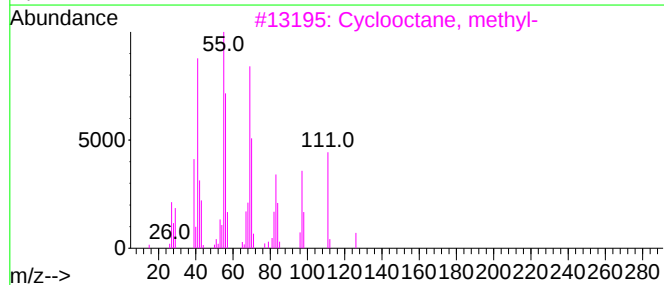
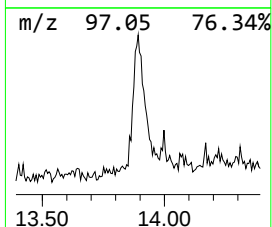
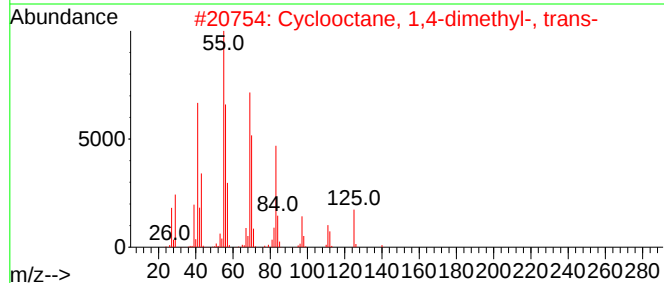
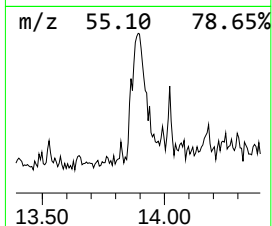
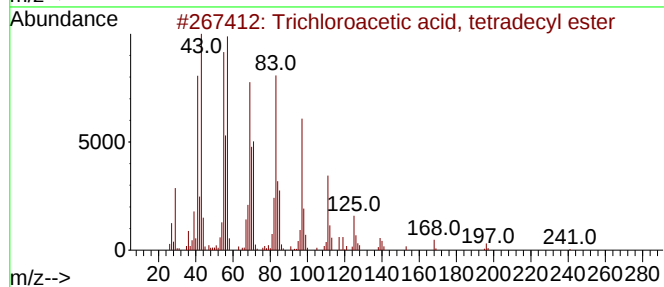
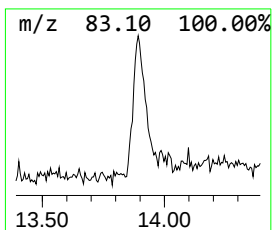
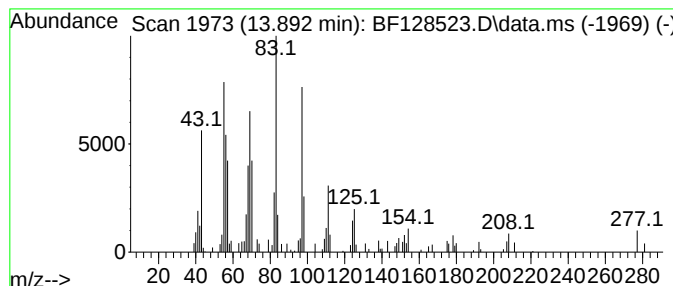
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TIC Library : C:\Database\NIST20.L
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Peak Number 1 Trichloroacetic acid, tetra... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	3.18 ng	209760	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	72
2			Cyclooctane, 1,4-dimethyl-, trans-	140	C10H20	013151-98-9	38
3			Cyclooctane, methyl-	126	C9H18	001502-38-1	38
4			Imidazole, 2-acetamido-	125	C5H7N3O	052737-49-2	27
5			Cyclopentane, 1-ethyl-2-methyl-,...	112	C8H16	000930-89-2	25



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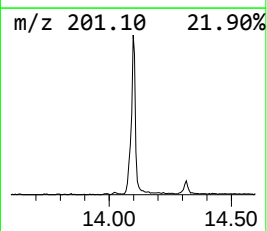
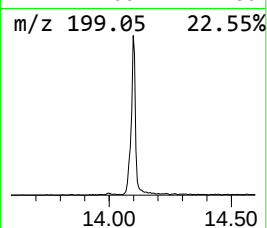
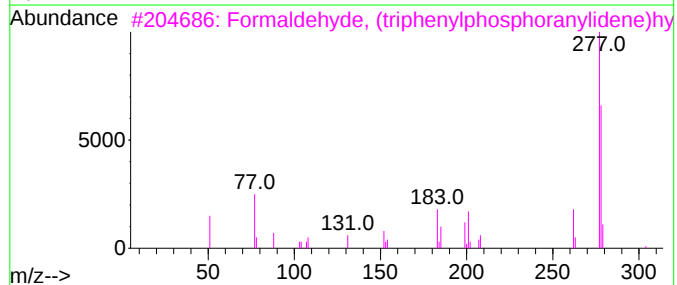
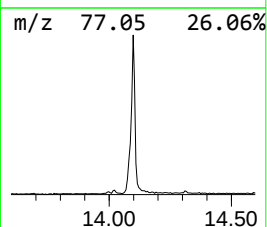
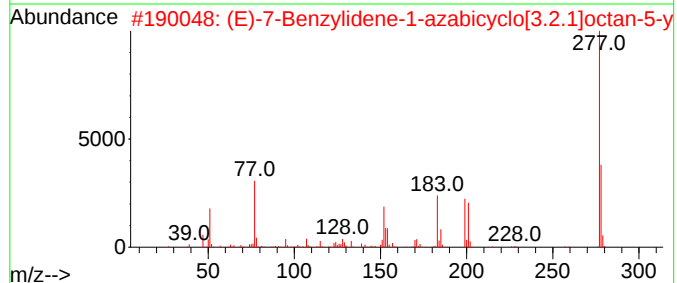
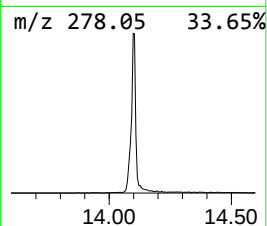
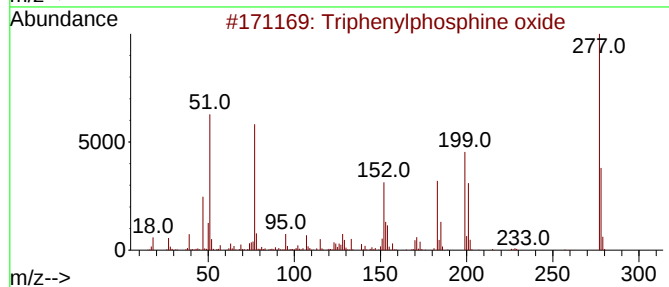
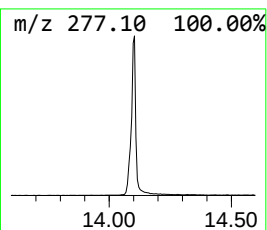
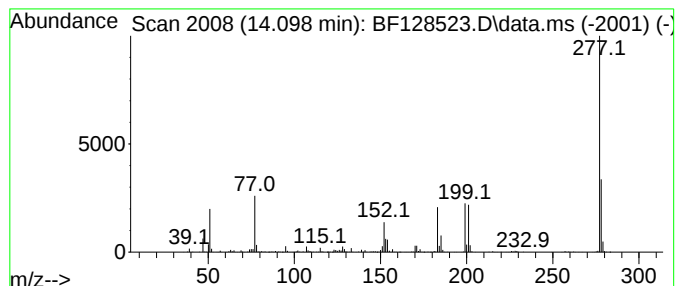
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.098	19.75 ng	1302240	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
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	25



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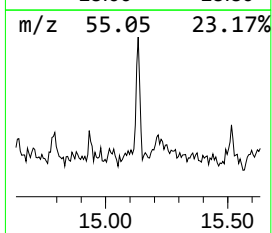
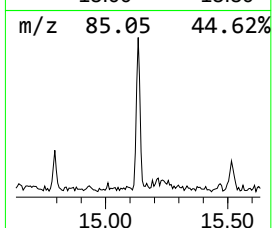
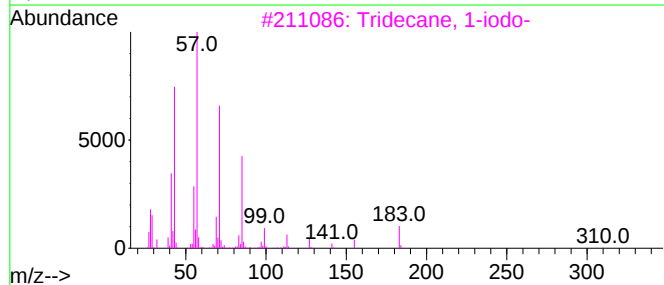
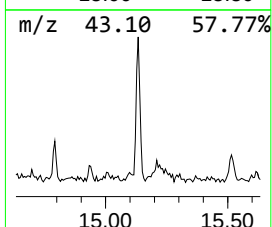
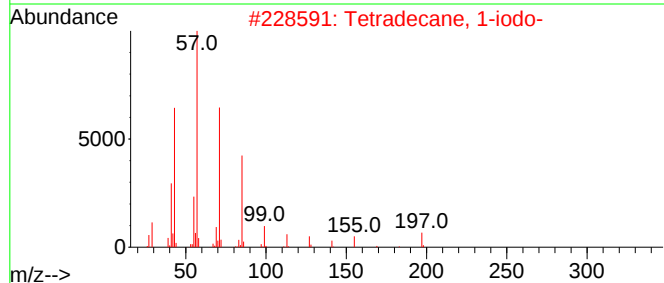
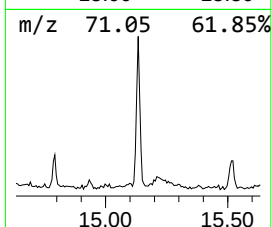
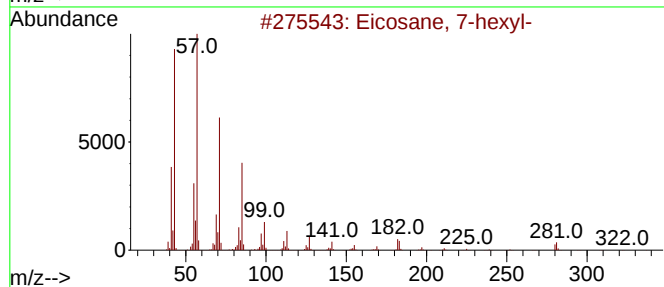
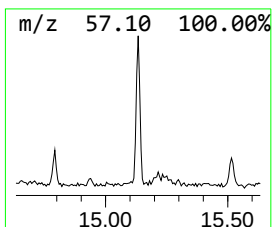
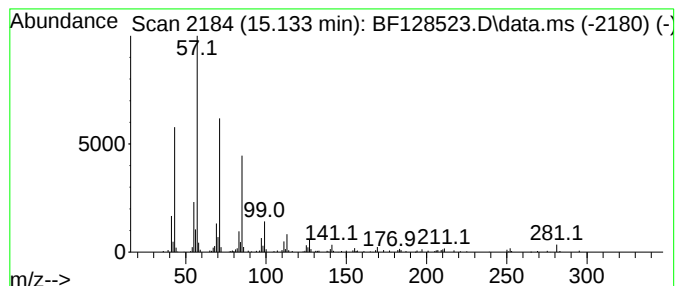
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Eicosane, 7-hexyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.133	3.04 ng	170164	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
2			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	86
3			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80
4			Heptacosane	380	C27H56	000593-49-7	68
5			Nonadecane	268	C19H40	000629-92-5	64



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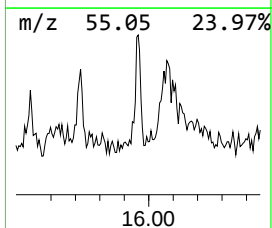
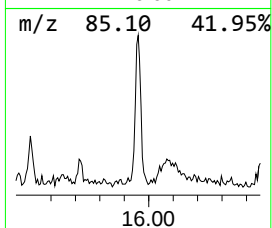
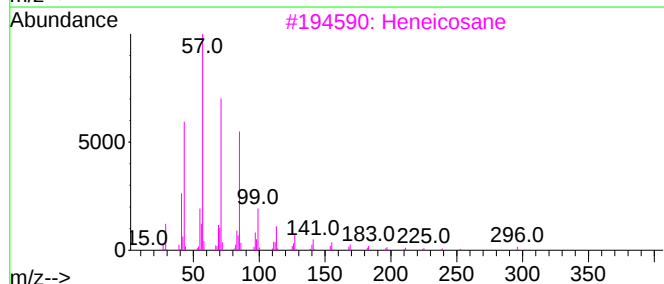
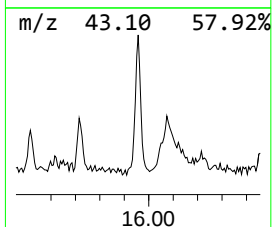
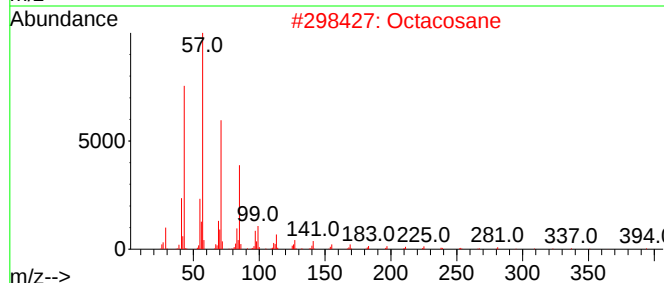
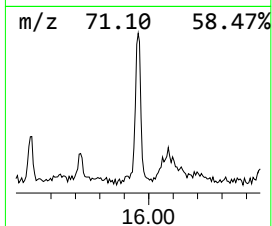
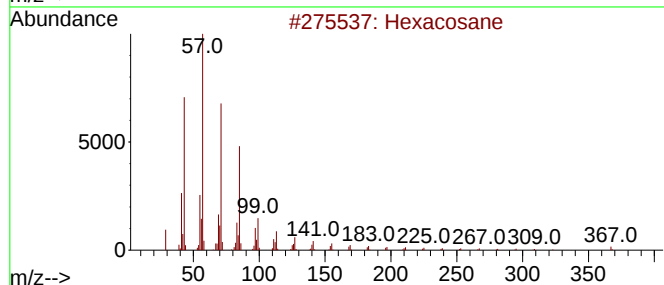
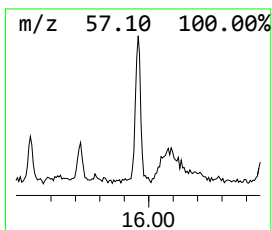
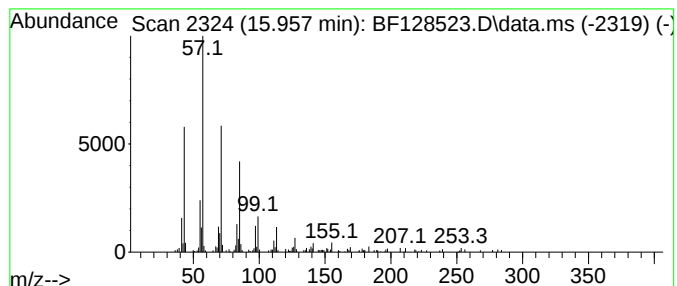
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Peak Number 4 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.957	2.55 ng	142763	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			Octacosane	394	C28H58	000630-02-4	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Nonadecane	268	C19H40	000629-92-5	90
5			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87



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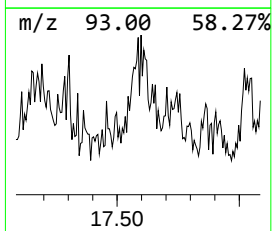
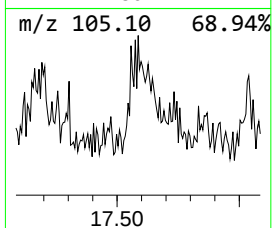
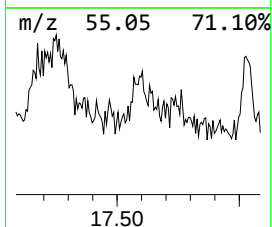
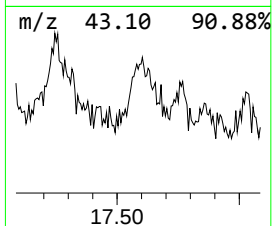
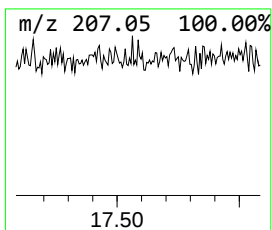
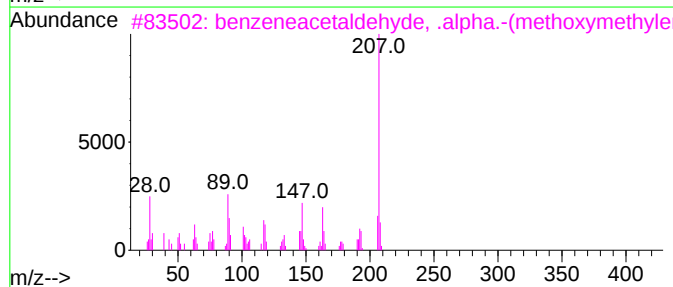
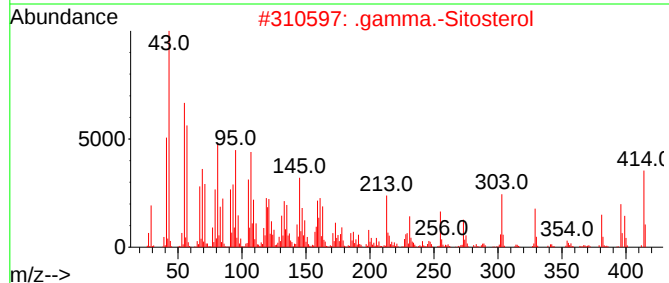
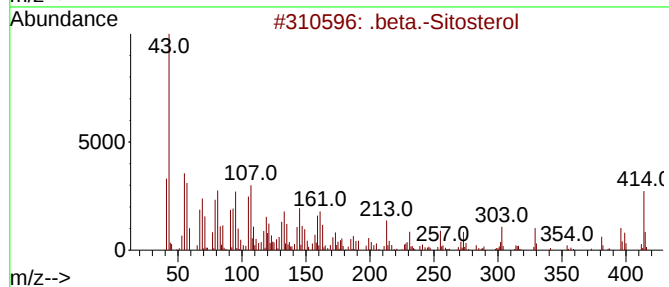
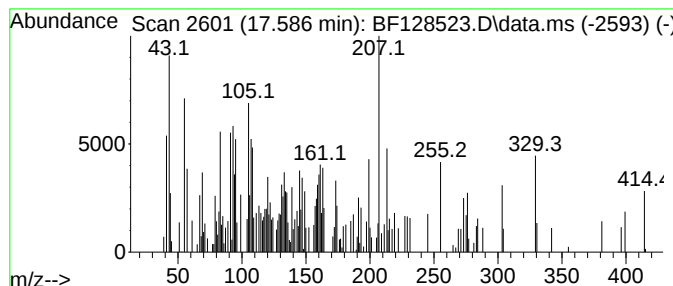
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Peak Number 5 .beta.-Sitosterol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.586	2.74 ng	153519	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.	beta.-Sitosterol	414	C29H50O	000083-46-5	62	
2	.	gamma.-Sitosterol	414	C29H50O	000083-47-6	20	
3	benzeneacetaldehyde, .alpha.-(me...	207	C10H9NO4	1000396-10-6	18		
4	5,7-Dimethyl-2-thioxo-2,3-dihydr...	207	C9H9N3OS	049600-56-8	15		
5	2,3-Dihydroxy-6-nitroquinoxaline	207	C8H5N3O4	002379-56-8	11		



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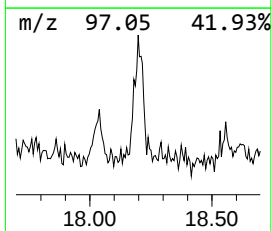
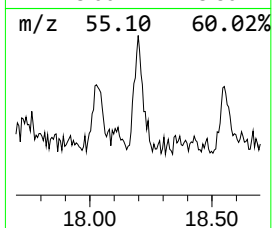
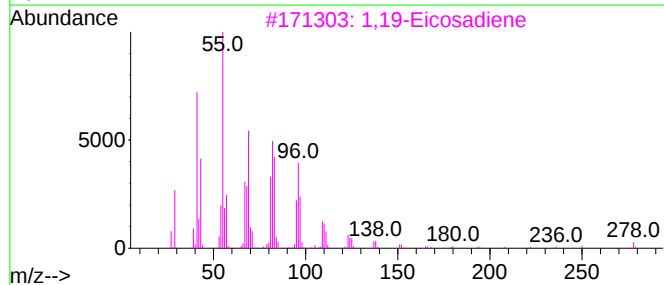
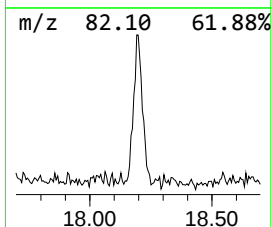
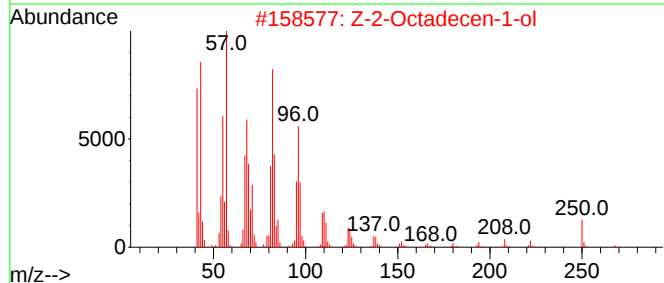
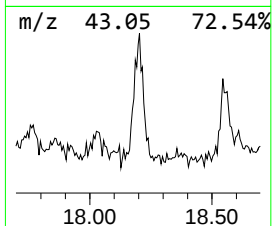
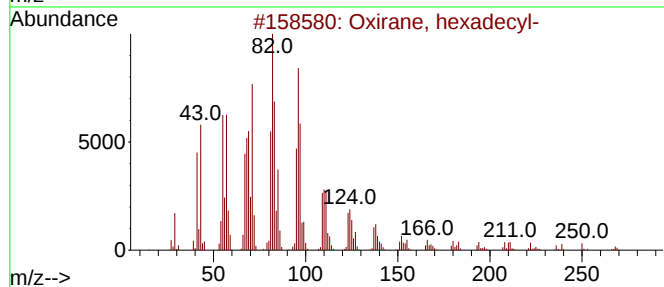
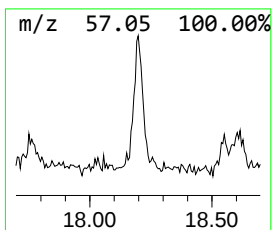
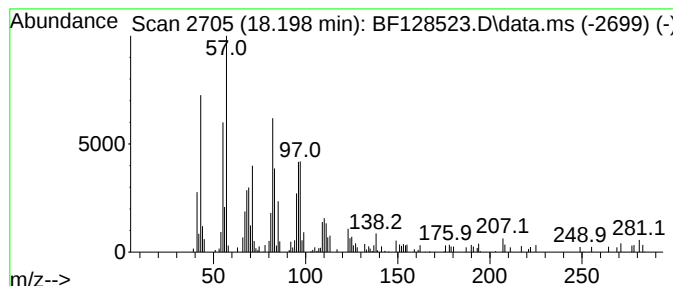
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Oxirane, hexadecyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.198	3.35 ng	187756	Perylene-d12	15.463

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	90
2		Z-2-Octadecen-1-ol	268	C18H36O	1000131-11-0	64
3		1,19-Eicosadiene	278	C20H38	014811-95-1	60
4		Eicosanal	296	C20H40O	002400-66-0	52
5		16-Heptadecenal	252	C17H32O	1010144-57-9	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
Data File : BF128523.D
Acq On : 27 May 2022 21:59
Operator : CG\JU
Sample : N2930-17
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P006-SS002-0006-01

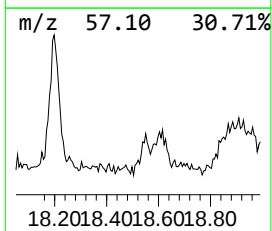
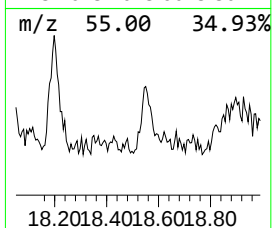
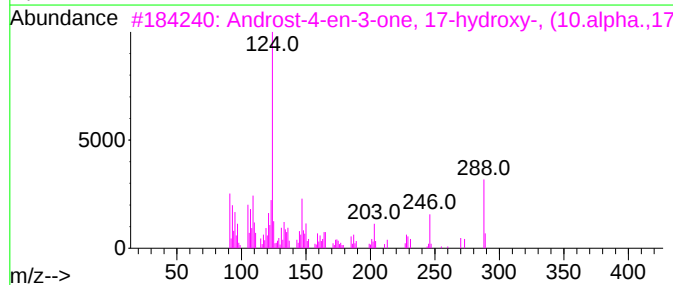
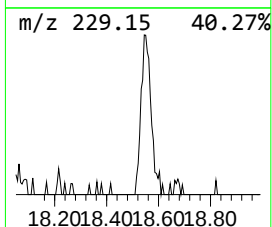
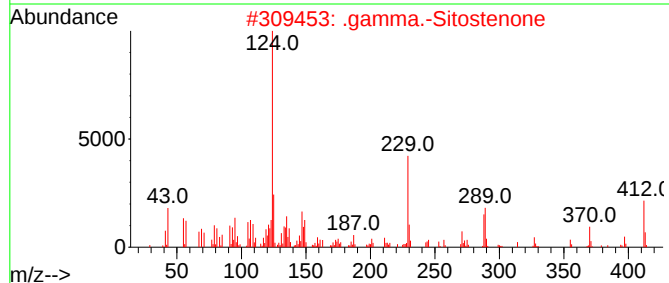
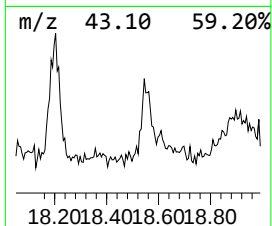
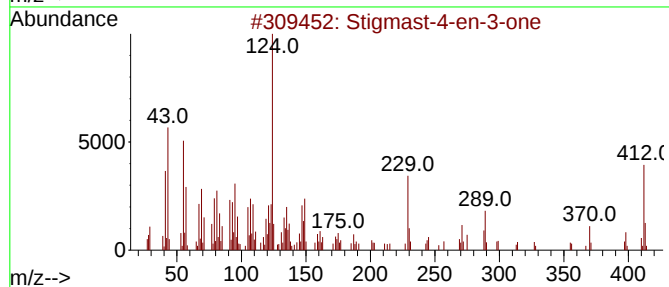
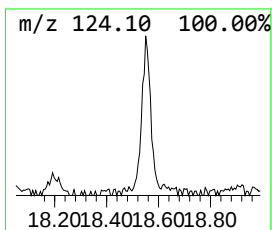
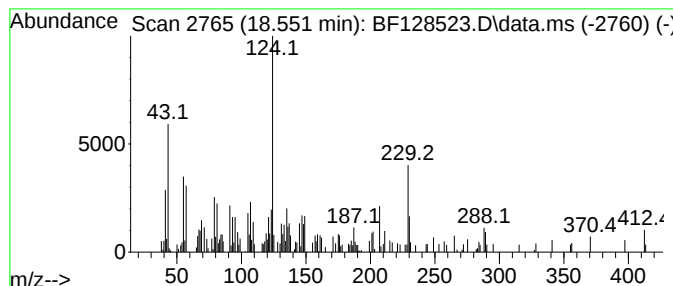
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Stigmast-4-en-3-one Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.551	2.30 ng	128965	Perylene-d12	15.463

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Stigmast-4-en-3-one	412	C29H48O	001058-61-3	91
2		.gamma.-Sitostenone	412	C29H48O	084924-96-9	89
3		Androst-4-en-3-one, 17-hydroxy-,...	288	C19H28O2	000604-39-7	50
4		Phenol, 2,6-diamino-	124	C6H8N2O	022440-82-0	38
5		5-Heptylresorcinol	208	C13H20O2	000500-67-4	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
Data File : BF128523.D
Acq On : 27 May 2022 21:59
Operator : CG\JU
Sample : N2930-17
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P006-SS002-0006-01

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
Trichloroacetic...	13.892	3.2	ng	209760	5	13.998	1318610	20.0
Triphenylphosph...	14.098	19.8	ng	1302240	5	13.998	1318610	20.0
Eicosane, 7-hexyl-	15.133	3.0	ng	170164	6	15.463	1120600	20.0
Hexacosane	15.957	2.5	ng	142763	6	15.463	1120600	20.0
.beta.-Sitosterol	17.586	2.7	ng	153519	6	15.463	1120600	20.0
Oxirane, hexade...	18.198	3.4	ng	187756	6	15.463	1120600	20.0
Stigmast-4-en-3...	18.551	2.3	ng	128965	6	15.463	1120600	20.0