

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
 Data File : BF128558.D
 Acq On : 28 May 2022 20:08
 Operator : CG\JU
 Sample : N2931-14
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P016-SS001-0006-01

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: BF128558.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.057	467	471	479	rVB	132027	170687	4.30%	0.613%
2	5.451	533	538	541	rBV	3362085	3511577	88.49%	12.603%
3	6.463	704	710	713	rBV	3362751	3481444	87.73%	12.495%
4	6.575	726	729	733	rBV	69841	53199	1.34%	0.191%
5	6.840	770	774	777	rBV	1157555	1003653	25.29%	3.602%
6	7.398	864	869	872	rBV	2574482	2399398	60.46%	8.612%
7	8.116	987	991	995	rBV	1420649	1298092	32.71%	4.659%
8	9.198	1170	1175	1178	rBV	4597647	3968470	100.00%	14.243%
9	9.875	1286	1290	1293	rBV	1742035	1421509	35.82%	5.102%
10	10.663	1420	1424	1427	rBV	2756416	2405484	60.61%	8.633%
11	11.363	1539	1543	1546	rVB	1573094	1335449	33.65%	4.793%
12	11.892	1629	1633	1646	rVB	228542	241225	6.08%	0.866%
13	12.616	1751	1756	1763	rVB2	33809	53177	1.34%	0.191%
14	12.674	1763	1766	1773	rBV2	65936	65645	1.65%	0.236%
15	12.951	1809	1813	1816	rBV	3614581	3131435	78.91%	11.239%
16	13.492	1900	1905	1909	rVB2	55231	60350	1.52%	0.217%
17	13.910	1969	1976	1986	rBV4	70278	205884	5.19%	0.739%
18	14.004	1986	1992	1995	rBV	989291	1073423	27.05%	3.853%
19	14.098	2003	2008	2017	rVB	455465	477959	12.04%	1.715%
20	15.133	2180	2184	2188	rBV	52853	57898	1.46%	0.208%
21	15.468	2235	2241	2246	rBV	744566	943662	23.78%	3.387%
22	15.951	2319	2323	2328	rVB2	39977	63713	1.61%	0.229%
23	16.098	2340	2348	2355	rBV10	33854	121461	3.06%	0.436%
24	16.751	2454	2459	2466	rVB3	81744	149718	3.77%	0.537%
25	17.051	2504	2510	2518	rBV6	24606	65436	1.65%	0.235%
26	18.039	2672	2678	2683	rBV9	20844	52358	1.32%	0.188%
27	18.545	2760	2764	2770	rVB9	23158	50160	1.26%	0.180%

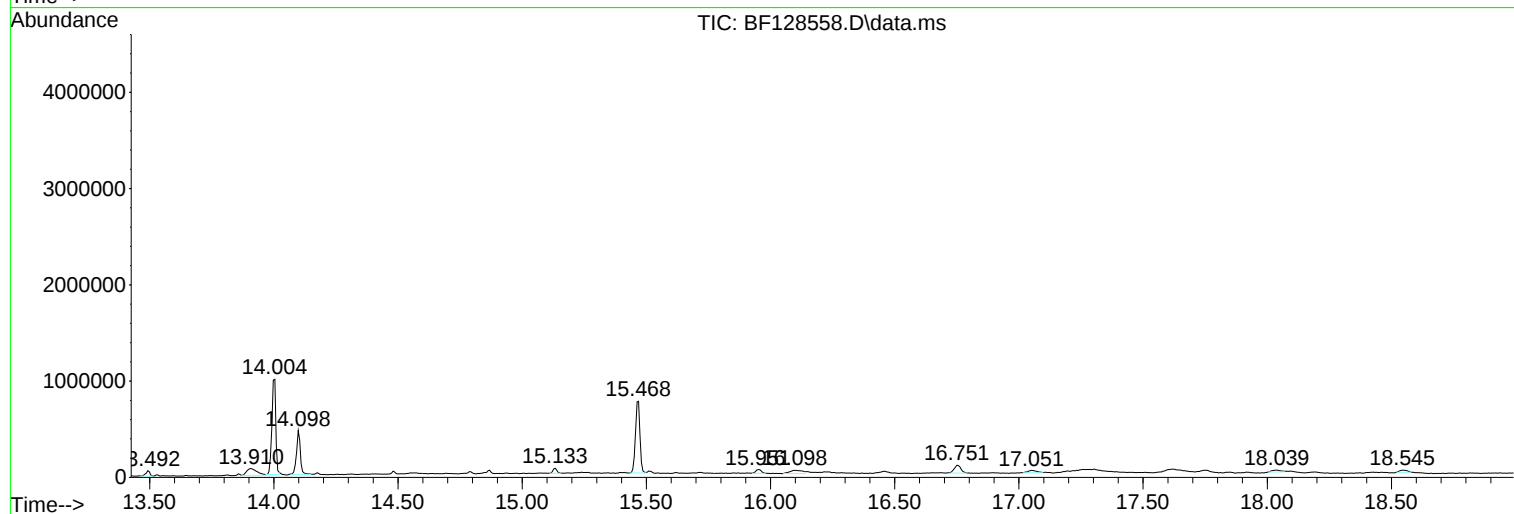
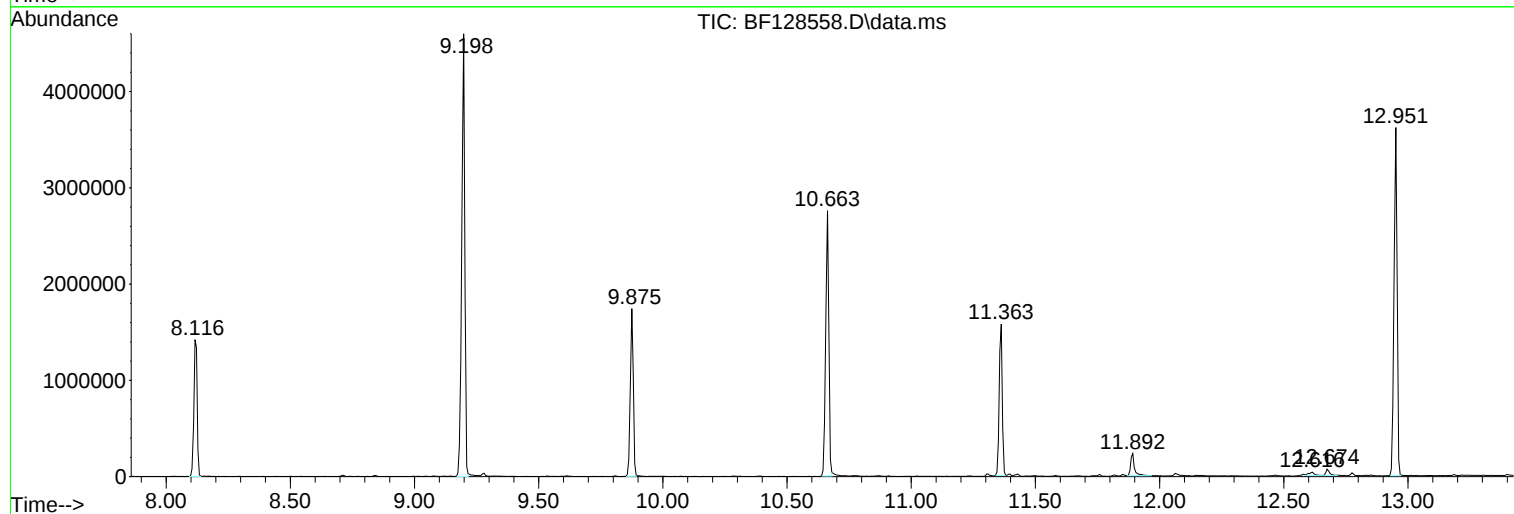
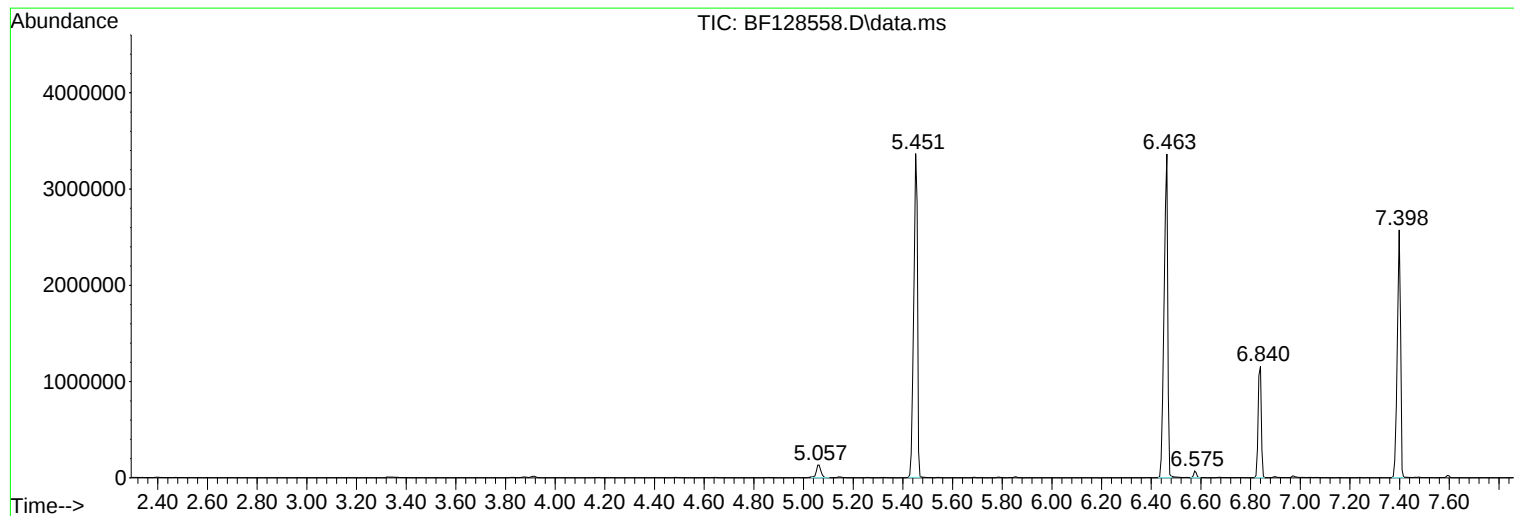
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ClientSampleId :
P016-SS001-0006-01

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

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



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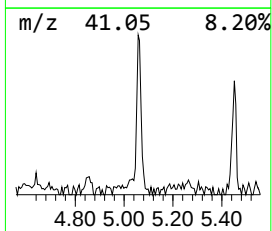
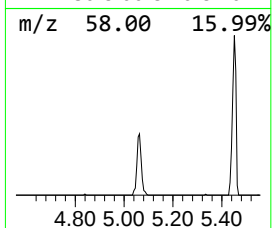
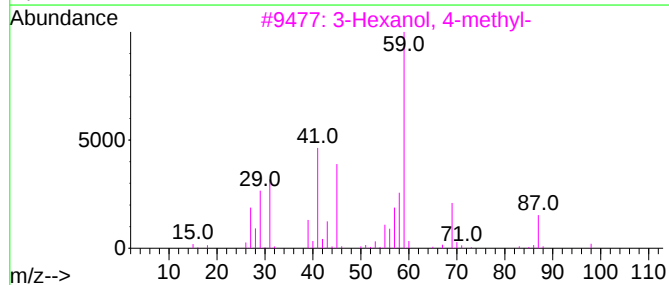
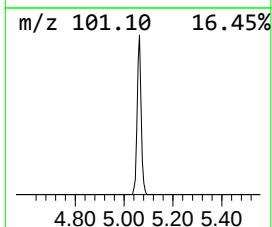
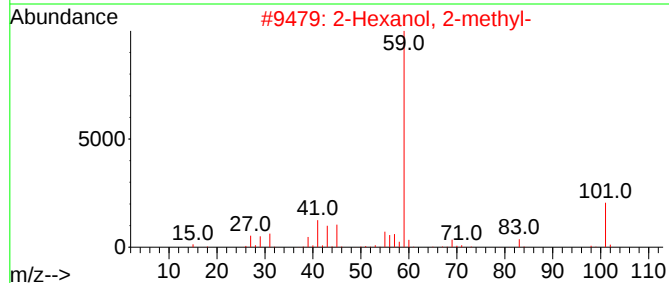
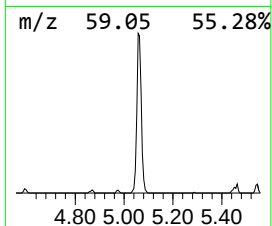
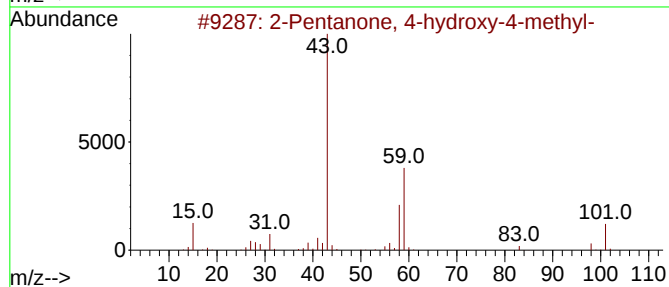
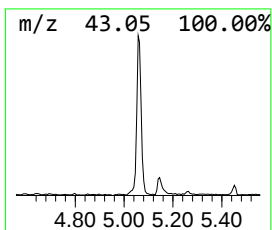
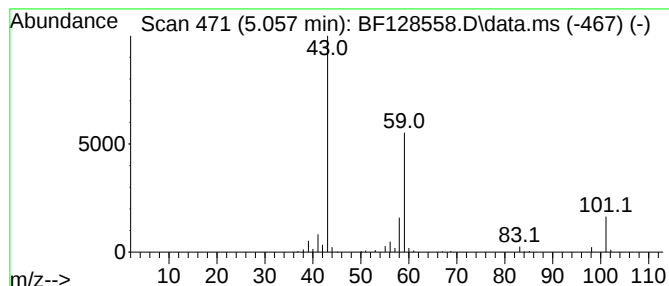
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.057	3.40 ng	170687	1,4-Dichlorobenzene-d4	6.840

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		



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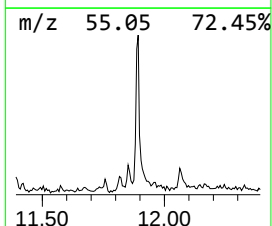
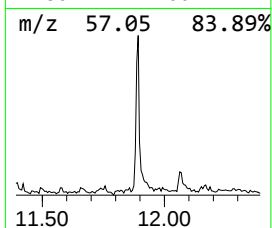
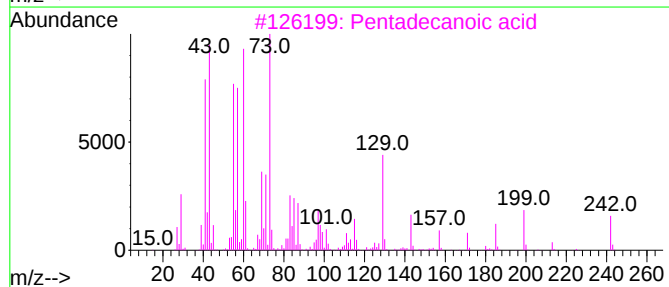
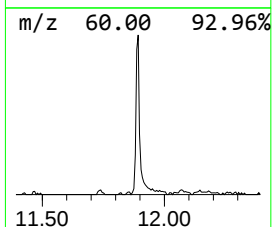
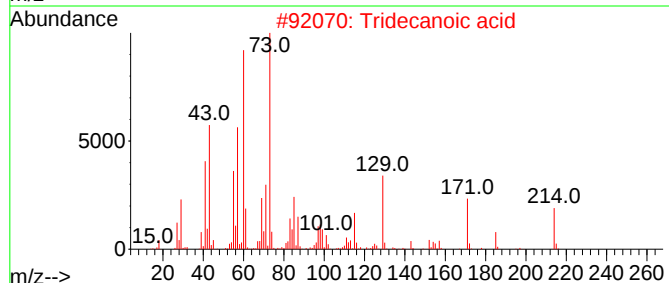
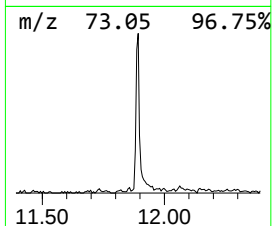
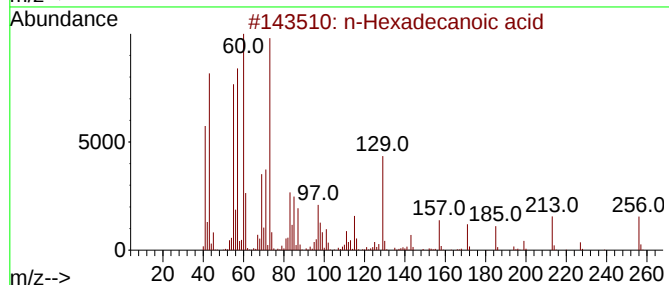
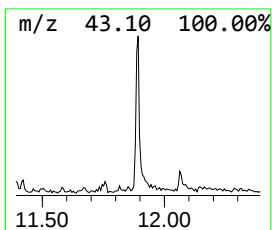
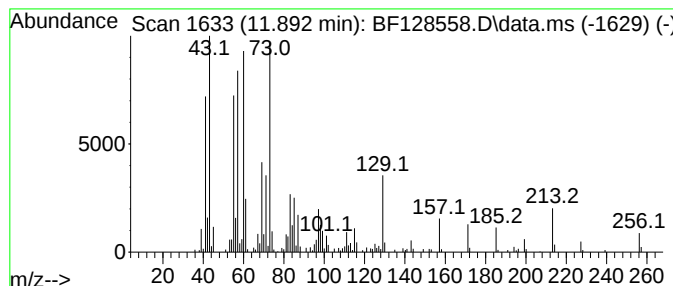
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	3.61 ng	241225	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	89
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	60



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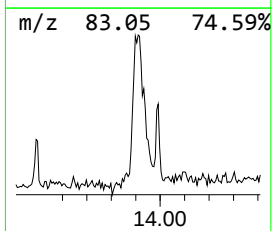
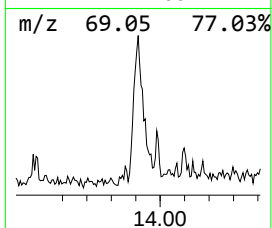
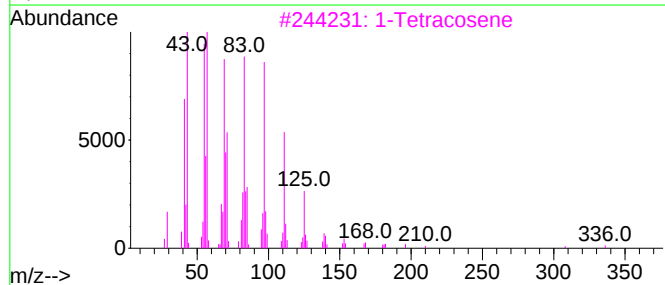
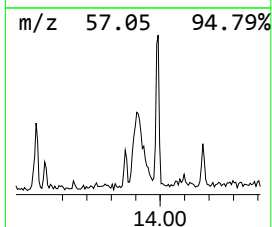
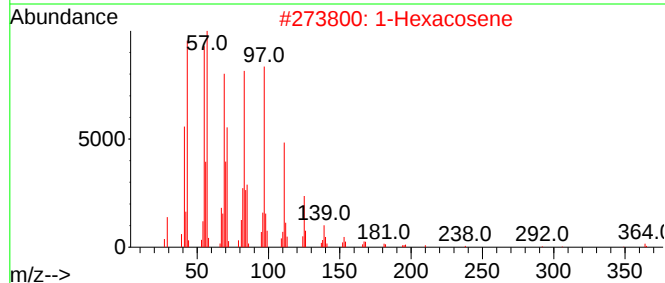
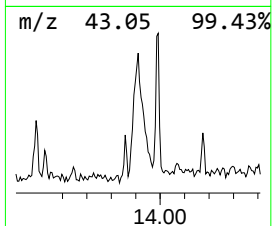
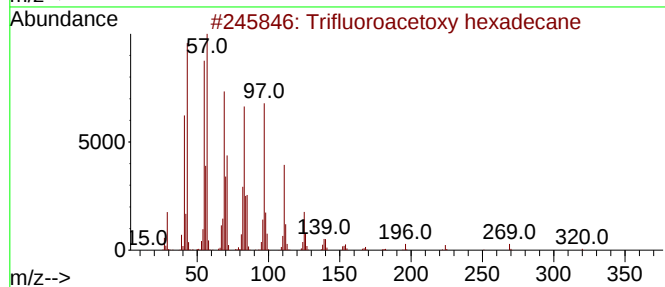
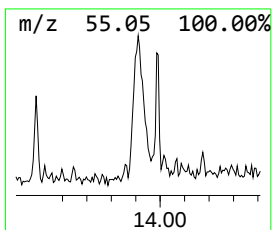
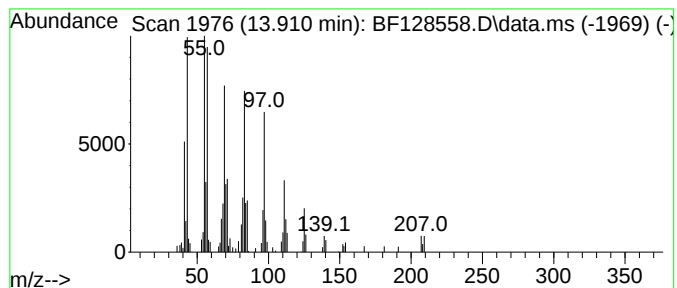
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Trifluoroacetoxy hexadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	3.84 ng	205884	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2			1-Hexacosene	364	C26H52	018835-33-1	91
3			1-Tetracosene	336	C24H48	010192-32-2	90
4			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	90
5			Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	90



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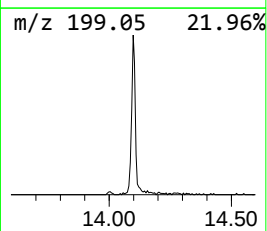
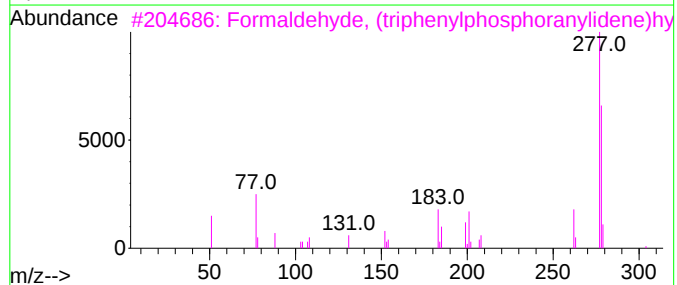
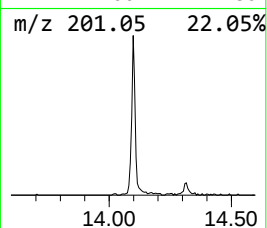
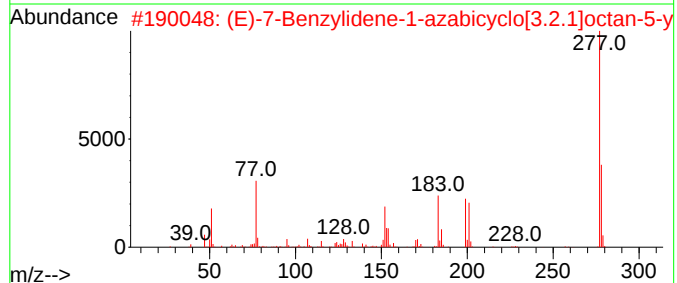
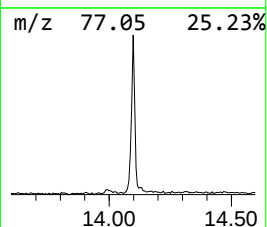
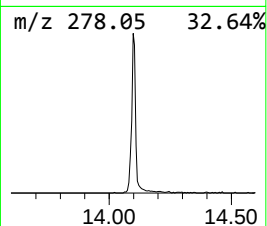
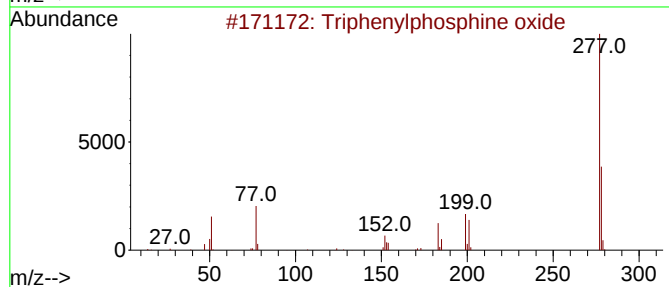
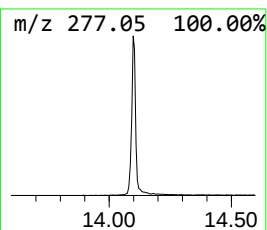
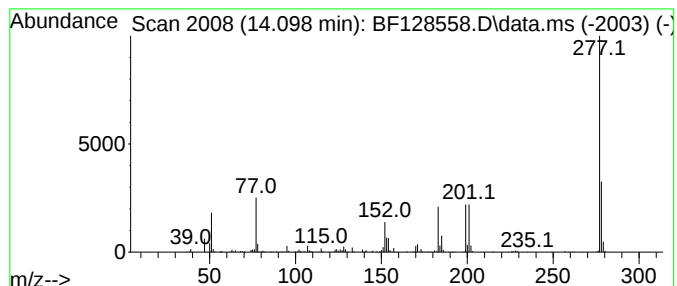
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Peak Number 4 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.098	8.91 ng	477959	Chrysene-d12	14.004

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	91
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	64
4			Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	37
5			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	35



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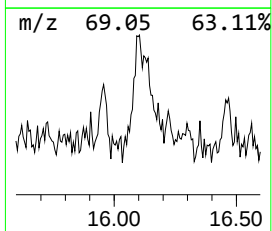
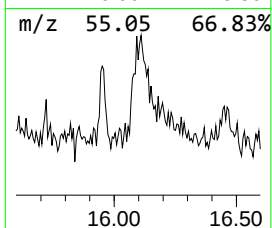
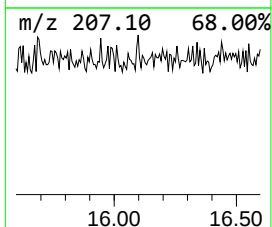
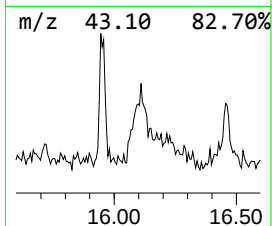
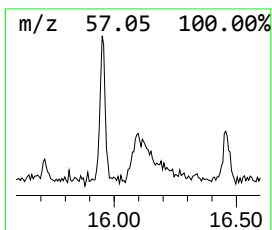
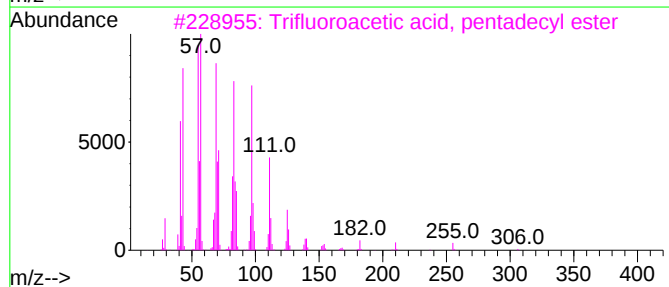
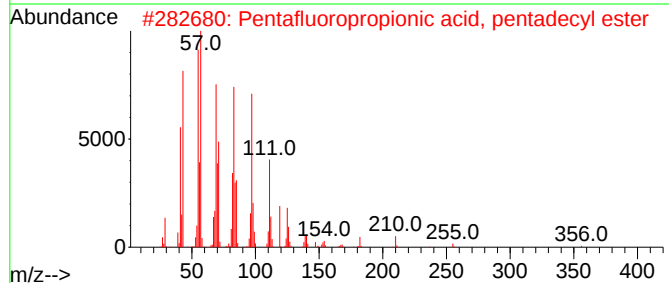
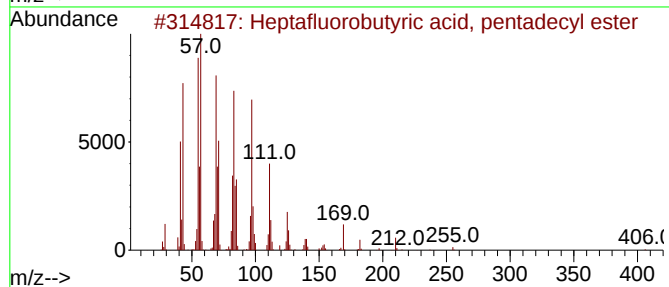
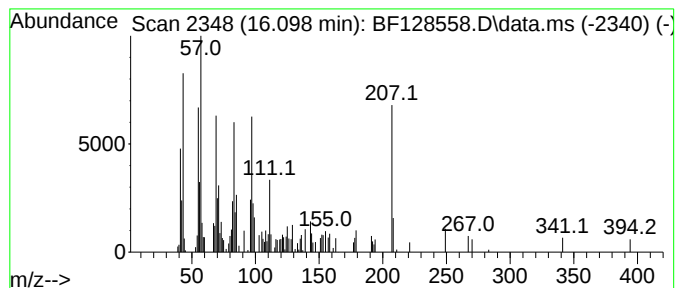
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptafluorobutyric acid, pe... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.098	2.57 ng	121461	Perylene-d12	15.468	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	60
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	60
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	55
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	55
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	53



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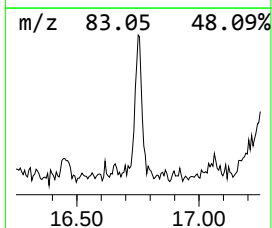
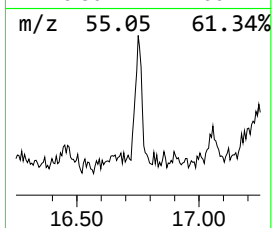
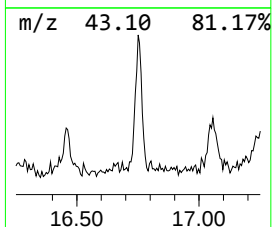
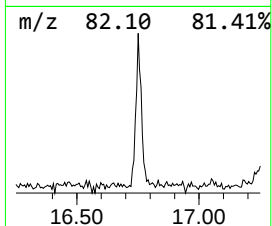
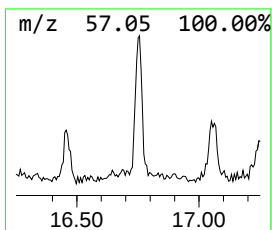
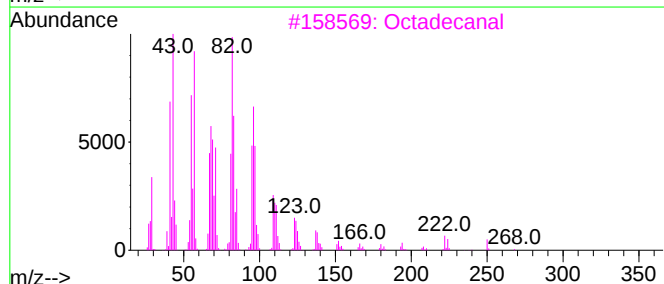
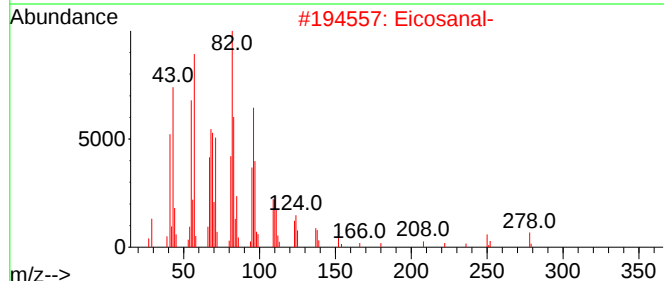
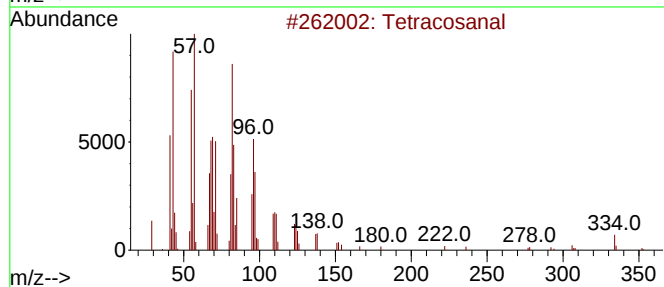
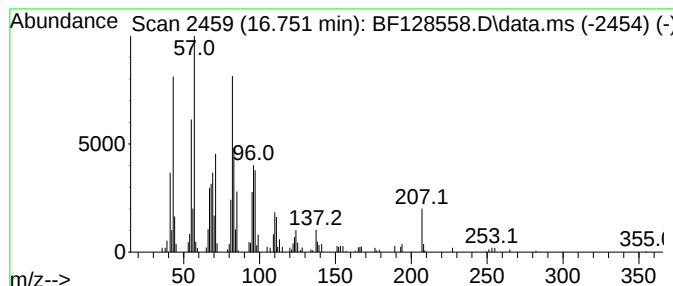
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tetracosanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.751	3.17 ng	149718	Perylene-d12	15.468

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosanal	352	C24H48O	057866-08-7	86
2		Eicosanal-	296	C20H40O	002400-66-0	74
3		Octadecanal	268	C18H36O	000638-66-4	52
4		1,19-Eicosadiene	278	C20H38	014811-95-1	46
5		Cyclohexane, (1-hexyltetradecyl)-	364	C26H52	004443-60-1	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128558.D
Acq On : 28 May 2022 20:08
Operator : CG\JU
Sample : N2931-14
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P016-SS001-0006-01

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

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.057	3.4	ng	170687	1	6.840	1003650	20.0
n-Hexadecanoic ...	11.892	3.6	ng	241225	4	11.363	1335450	20.0
Trifluoroacetox...	13.910	3.8	ng	205884	5	14.004	1073420	20.0
Triphenylphosph...	14.098	8.9	ng	477959	5	14.004	1073420	20.0
Heptafluorobuty...	16.098	2.6	ng	121461	6	15.468	943662	20.0
Tetracosanal	16.751	3.2	ng	149718	6	15.468	943662	20.0