

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
 Data File : BF136832.D
 Acq On : 29 Dec 2023 16:42
 Operator : CG\JU
 Sample : 05909-07
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GHL-SS-45

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-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136832.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.034	498	501	510	rVB	31735	42431	1.98%	0.307%
2	5.428	564	568	571	rBV	2051076	1869479	87.06%	13.538%
3	6.434	733	739	741	rBV	1726925	1907181	88.81%	13.811%
4	6.781	794	798	802	rBV	520707	394302	18.36%	2.855%
5	7.346	889	894	897	rBV	1319605	1228829	57.22%	8.899%
6	8.057	1011	1015	1018	rBV	640264	511320	23.81%	3.703%
7	9.134	1193	1198	1202	rBV	2262848	2147377	100.00%	15.551%
8	9.816	1310	1314	1317	rBV	682941	567789	26.44%	4.112%
9	10.610	1445	1449	1452	rBV	1475692	1312239	61.11%	9.503%
10	11.304	1564	1567	1571	rBV	655340	583091	27.15%	4.223%
11	11.839	1655	1658	1675	rBV	107358	166526	7.75%	1.206%
12	12.904	1834	1839	1842	rBV	2123270	1874955	87.31%	13.578%
13	13.963	2015	2019	2028	rVB	392038	396497	18.46%	2.871%
14	14.433	2094	2099	2104	rBV2	44688	54277	2.53%	0.393%
15	14.810	2159	2163	2169	rBV	40317	55416	2.58%	0.401%
16	15.245	2232	2237	2244	rBV2	39309	62284	2.90%	0.451%
17	15.439	2264	2270	2292	rBV	280096	514755	23.97%	3.728%
18	15.751	2318	2323	2329	rBV2	29228	55557	2.59%	0.402%
19	15.922	2348	2352	2358	rVB4	14741	22599	1.05%	0.164%
20	16.351	2420	2425	2433	rVB4	19595	41850	1.95%	0.303%

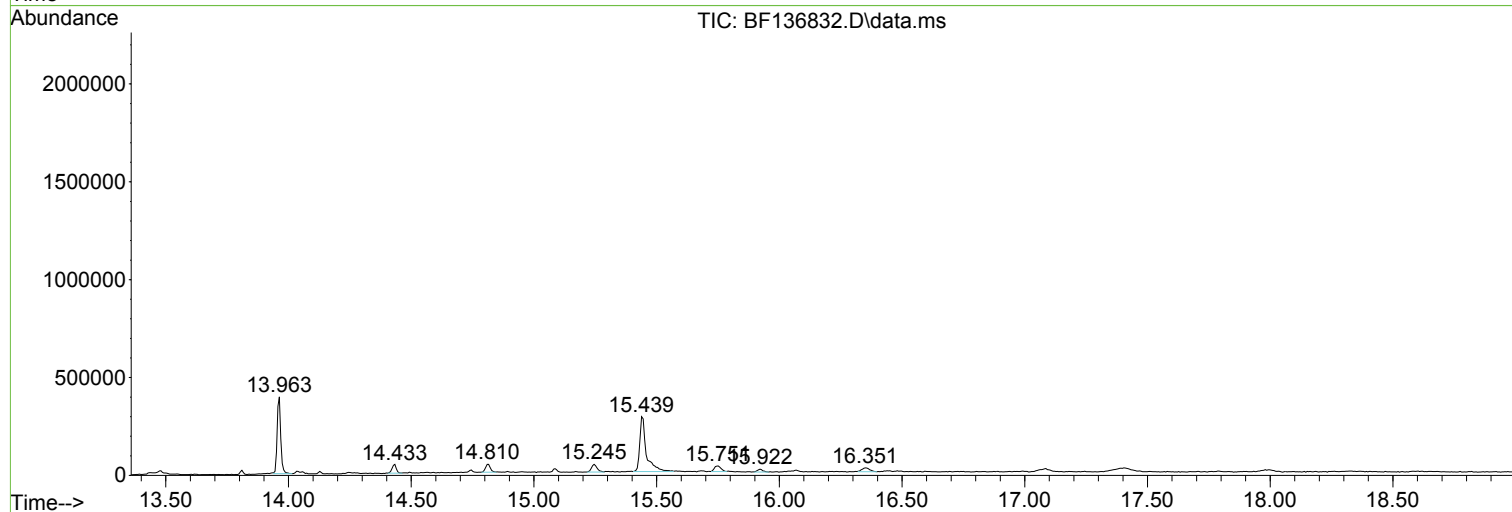
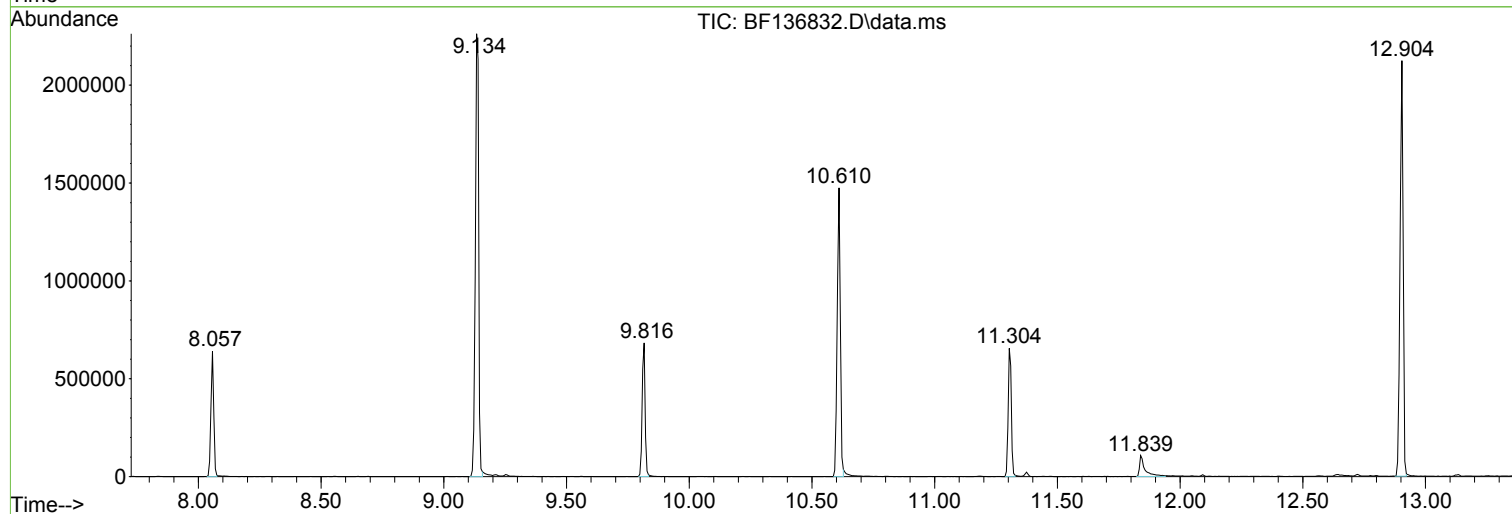
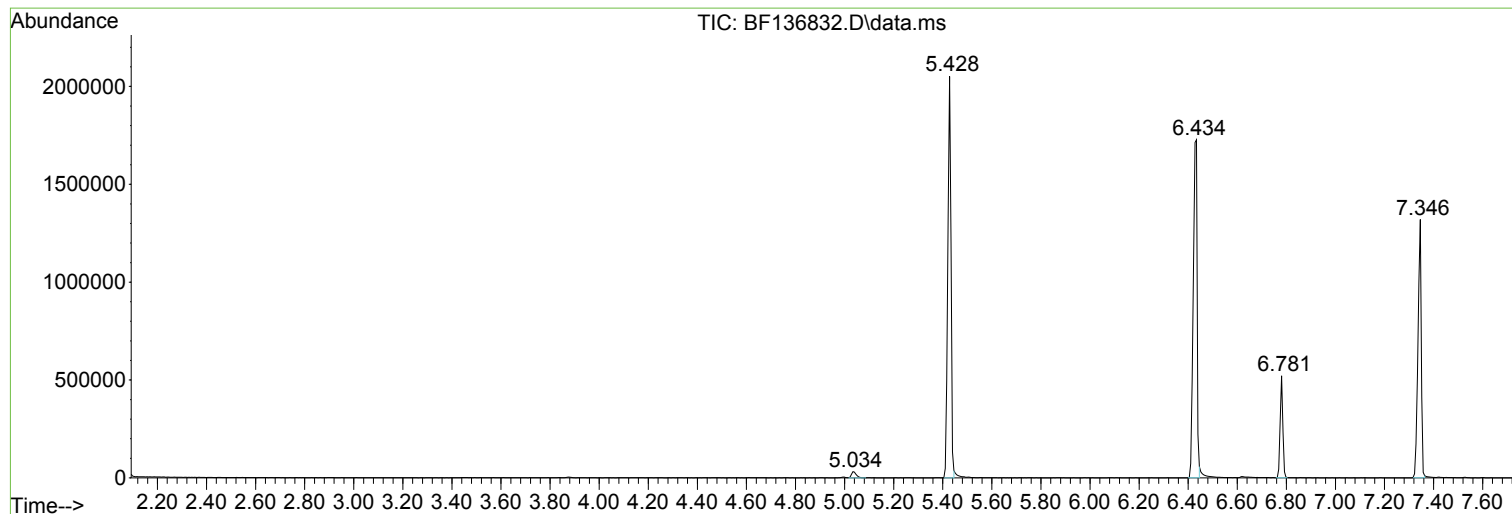
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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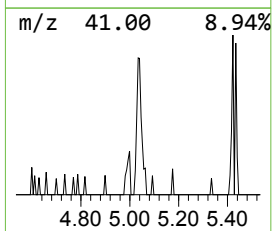
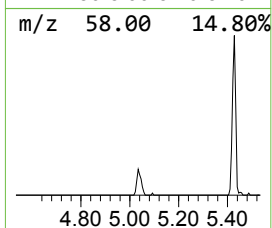
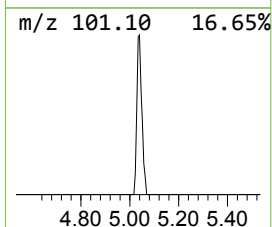
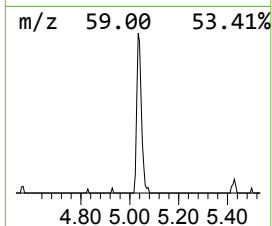
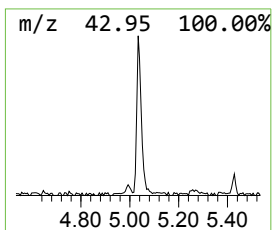
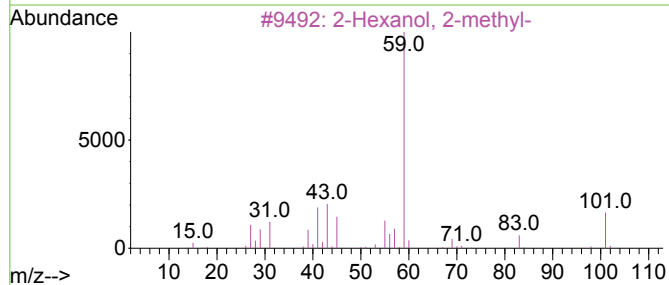
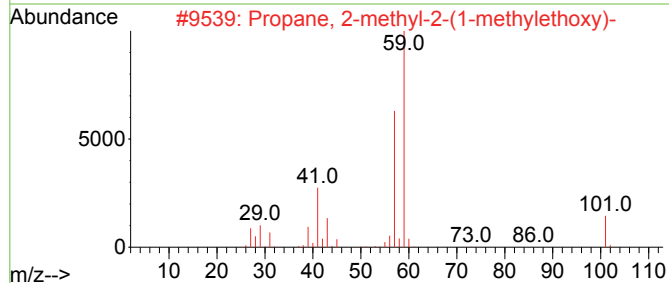
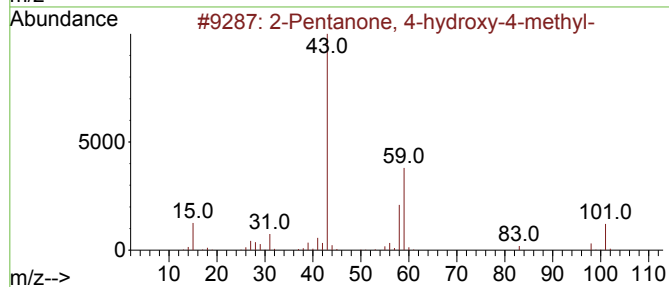
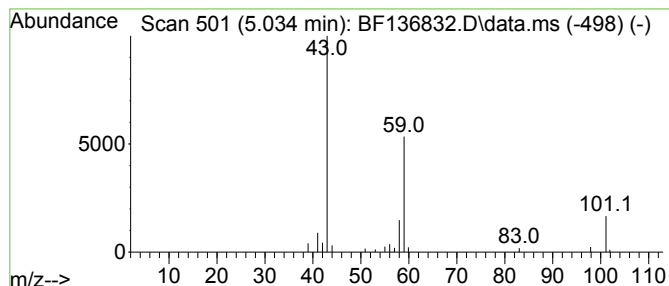
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.034	2.15 ng	42431	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9		



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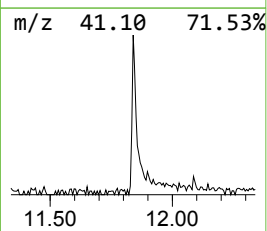
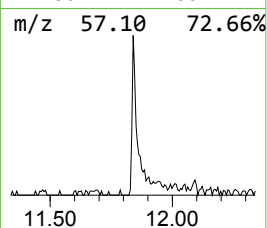
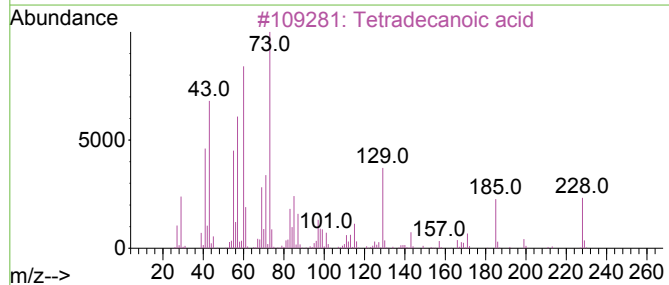
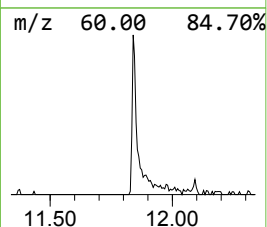
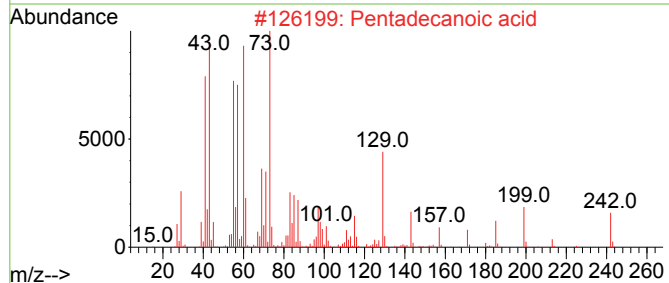
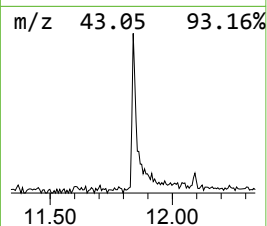
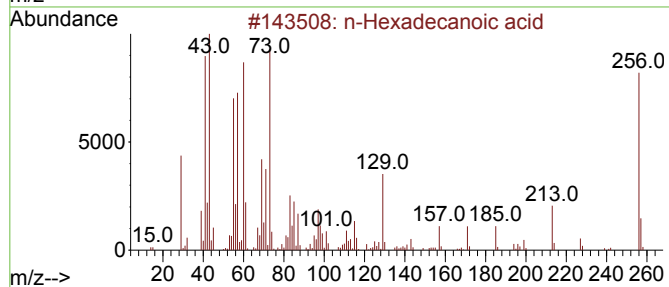
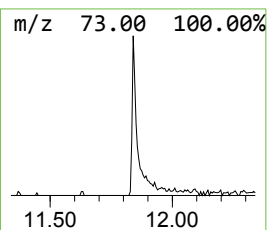
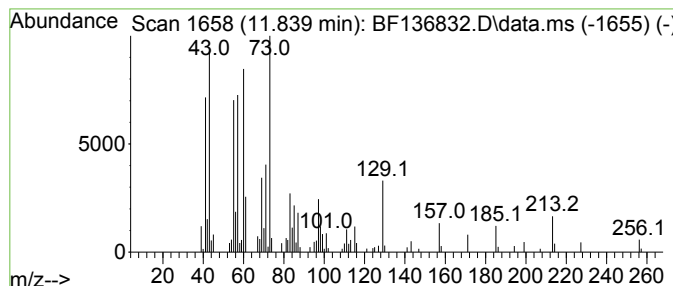
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	5.71 ng	166526	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			Tridecanoic acid	214	C13H26O2	000638-53-9	68
5			Nonanoic acid	158	C9H18O2	000112-05-0	45



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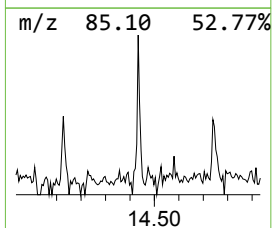
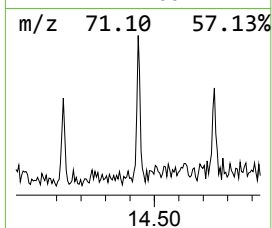
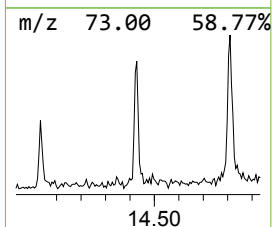
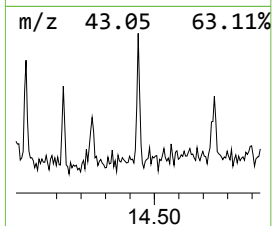
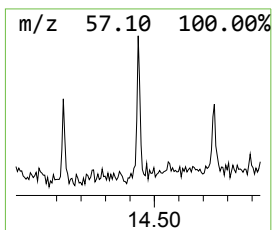
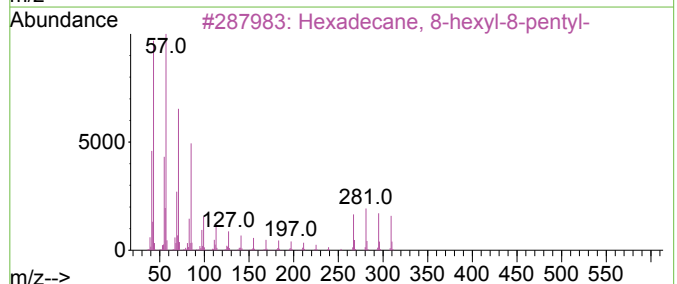
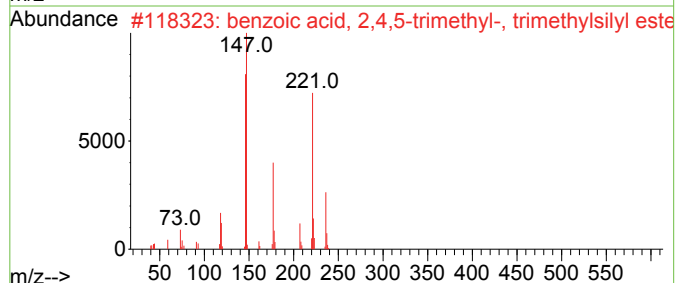
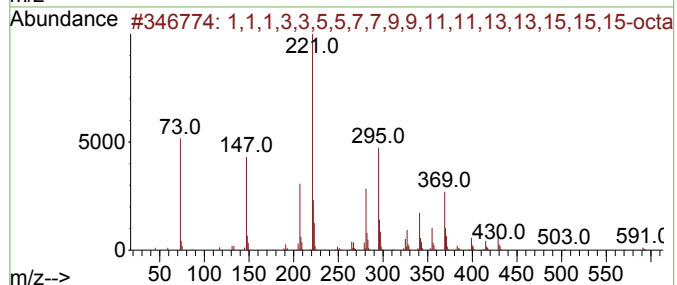
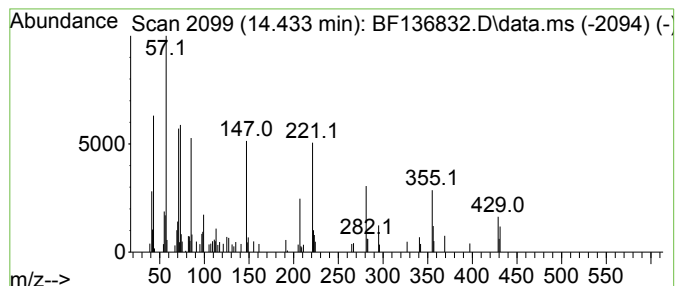
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Peak Number 3 unknown14.433 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.433	2.74 ng	54277	Chrysene-d12	13.963		
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	606	C18H5407Si8	000556-69-4	37	
2	benzoic acid, 2,4,5-trimethyl-, ...	236	C13H2002Si	1000396-43-7	16	
3	Hexadecane, 8-hexyl-8-pentyl-	380	C27H56	055282-29-6	14	
4	(+)-cis-3,4-Dimethyl-2-phenylte...	207	C12H17NS	092772-63-9	11	
5	4H-Pyrido[1,2-a]pyrimidine-3-car...	221	C11H15N3O2	064399-29-7	11	



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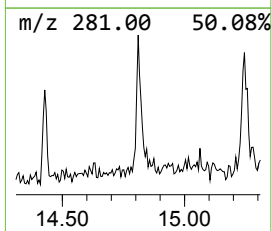
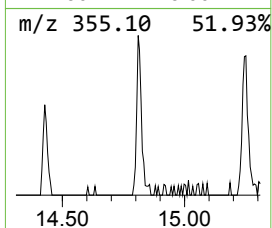
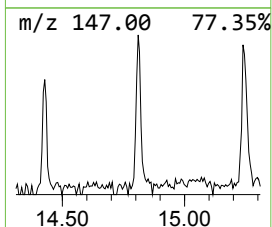
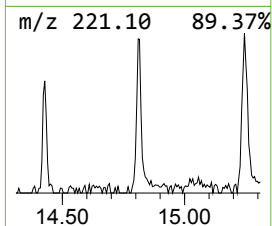
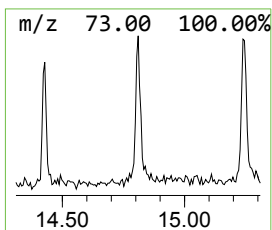
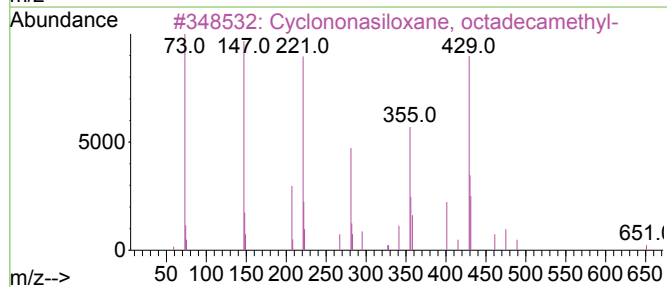
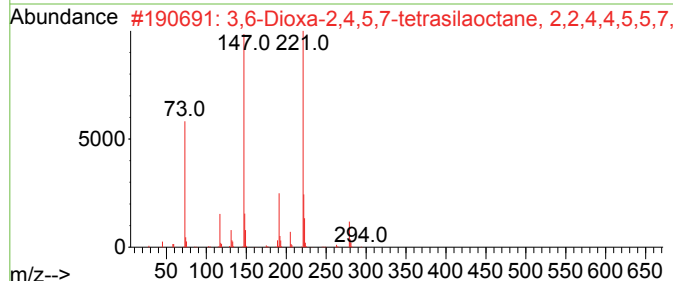
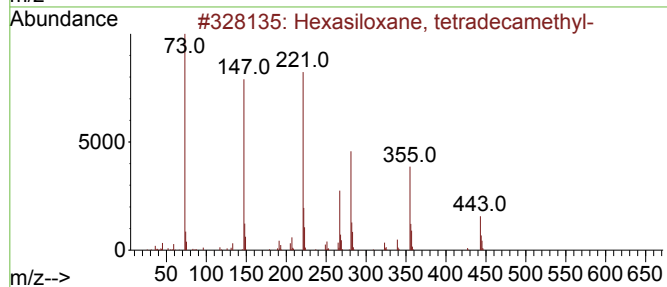
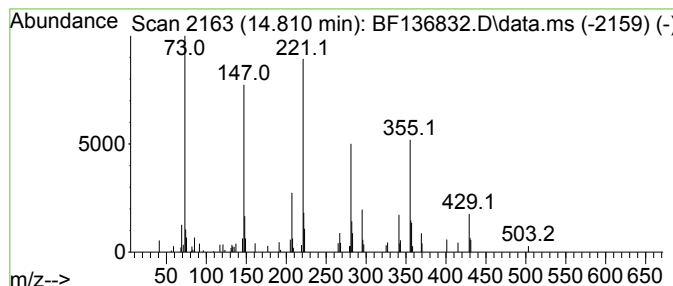
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Peak Number 4 Hexasiloxane, tetradecamethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.810	2.15 ng	55416	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	81
2			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	43
3			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	38
4			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	38
5			Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	30



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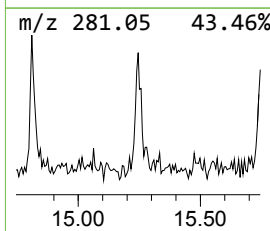
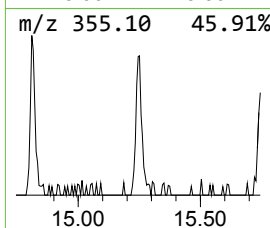
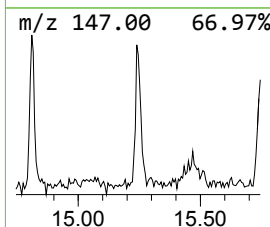
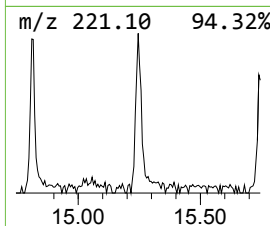
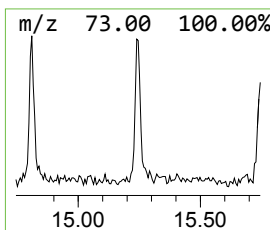
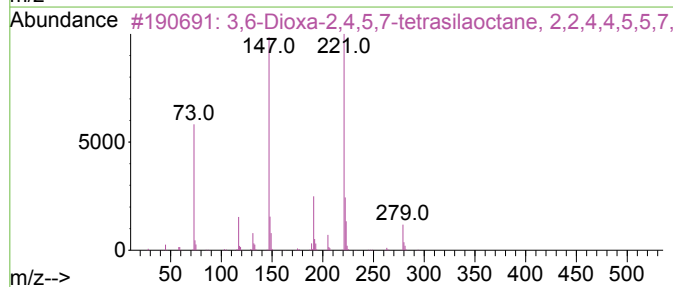
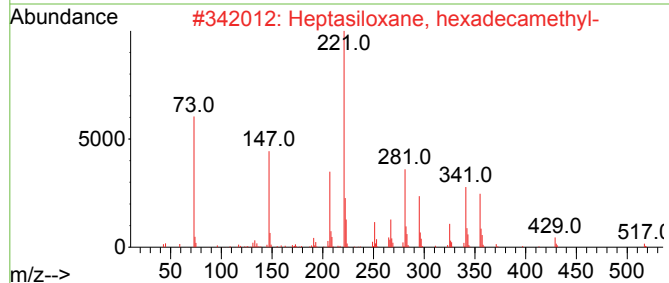
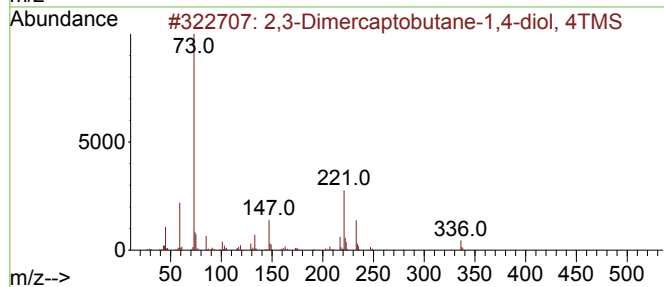
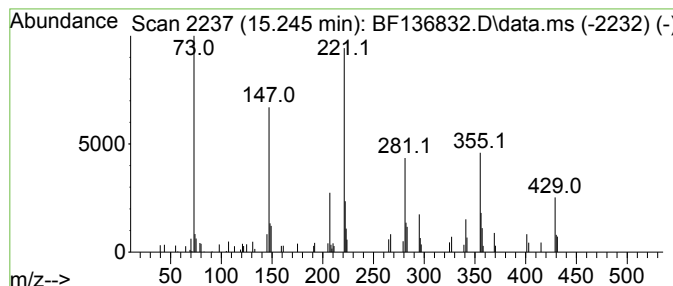
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown15.245 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.245	2.42 ng	62284	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,3-Dimercaptobutane-1,4-diol, 4TMS	442	C16H42O2S2Si4	959295-06-8	38
2			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	37
3			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	37
4			2,6-Dimethyl-3,4-bis(trimethylsi...	311	C15H29NO2Si2	1000079-52-1	32
5			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	32



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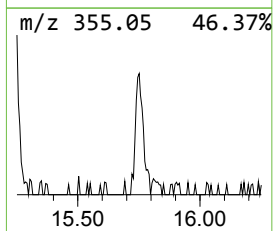
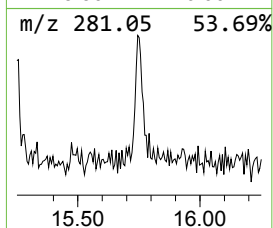
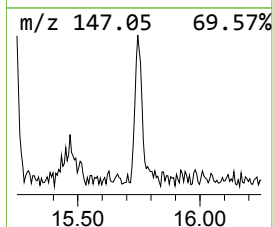
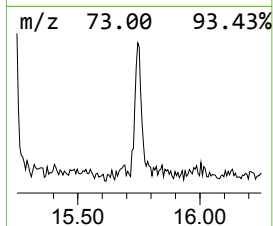
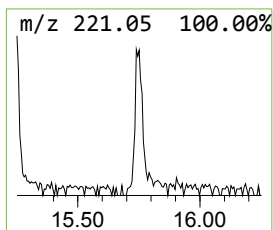
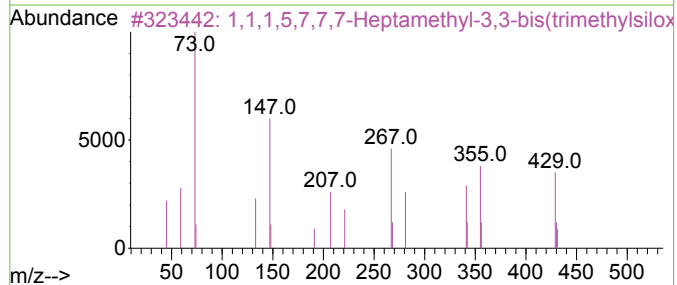
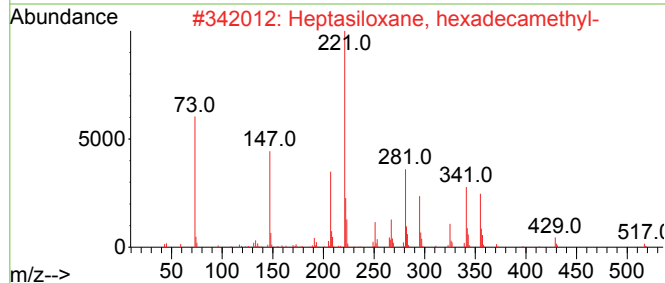
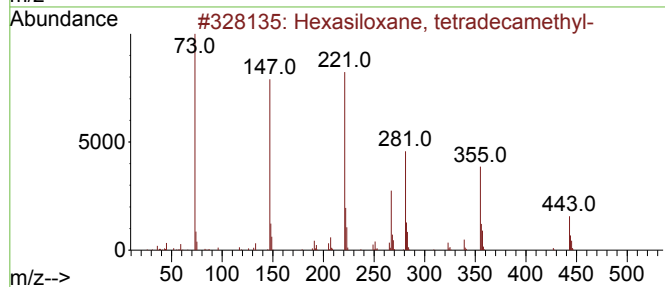
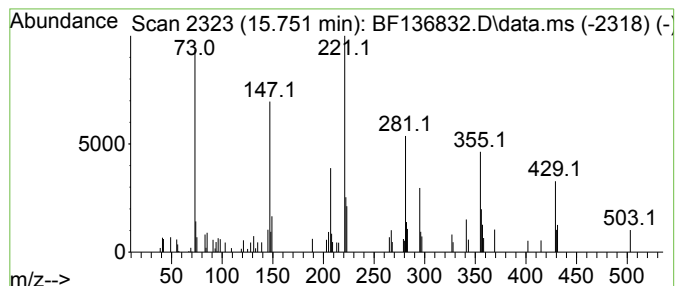
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown15.751 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.751	2.16 ng	55557	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	53
2			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	38
3			1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	38
4			1,1,1,3,3,5,5,7,7,9,11,11,13,1...	606	C18H54O7Si8	000556-69-4	37
5			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136832.D
Acq On : 29 Dec 2023 16:42
Operator : CG\JU
Sample : 05909-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-45

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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
2-Pentanone, 4-...	5.034	2.1	ng	42431	1	6.781	394302	20.0
n-Hexadecanoic ...	11.839	5.7	ng	166526	4	11.304	583091	20.0
unknown14.433	14.433	2.7	ng	54277	5	13.963	396497	20.0
Hexasiloxane, t...	14.810	2.1	ng	55416	6	15.439	514755	20.0
unknown15.245	15.245	2.4	ng	62284	6	15.439	514755	20.0
unknown15.751	15.751	2.2	ng	55557	6	15.439	514755	20.0