

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110623\
 Data File : BF136154.D
 Acq On : 06 Nov 2023 14:56
 Operator : CG\JU
 Sample : 05257-09
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-3

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-BF103023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136154.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.046	499	503	510	rVB	41207	46954	2.50%	0.332%
2	5.446	566	571	574	rBV	1732439	1591723	84.60%	11.253%
3	6.451	736	742	745	rBV	1688127	1625781	86.41%	11.494%
4	6.816	801	804	807	rBV	724269	550002	29.23%	3.889%
5	7.381	895	900	903	rBV	1256545	1060499	56.37%	7.498%
6	8.098	1018	1022	1025	rBV	962051	717418	38.13%	5.072%
7	9.175	1202	1205	1209	rVB	2193148	1881417	100.00%	13.302%
8	9.298	1222	1226	1229	rBV	28393	25129	1.34%	0.178%
9	9.857	1317	1321	1324	rBV	1014089	795987	42.31%	5.628%
10	10.645	1451	1455	1459	rBV	1420467	1210056	64.32%	8.555%
11	11.345	1571	1574	1577	rBV	902198	764382	40.63%	5.404%
12	11.369	1577	1578	1582	rVB	54927	31952	1.70%	0.226%
13	11.886	1662	1666	1670	rBV2	150661	143472	7.63%	1.014%
14	12.563	1778	1781	1785	rBV	89824	78591	4.18%	0.556%
15	12.674	1795	1800	1806	rBV3	34067	45352	2.41%	0.321%
16	12.792	1813	1820	1823	rBV	82081	81085	4.31%	0.573%
17	12.945	1842	1846	1850	rBV	1538938	1418250	75.38%	10.027%
18	13.886	2004	2006	2013	rVB7	14354	28507	1.52%	0.202%
19	14.004	2021	2026	2029	rBV	615034	571782	30.39%	4.042%
20	14.027	2029	2030	2033	rVB	43753	22877	1.22%	0.162%
21	14.110	2039	2044	2048	rBV	46898	53411	2.84%	0.378%
22	14.498	2105	2110	2114	rBV2	87144	115622	6.15%	0.817%
23	14.898	2173	2178	2184	rBV2	91306	129624	6.89%	0.916%
24	15.051	2200	2204	2208	rBV	34666	57798	3.07%	0.409%
25	15.163	2219	2223	2226	rVB3	22693	26674	1.42%	0.189%
26	15.251	2232	2238	2242	rBV9	8147	21989	1.17%	0.155%
27	15.351	2250	2255	2262	rVV3	76031	135279	7.19%	0.956%
28	15.421	2264	2267	2274	rVB2	28167	36767	1.95%	0.260%
29	15.492	2274	2279	2287	rBV	482272	567832	30.18%	4.015%
30	15.874	2338	2344	2352	rBV2	53245	103588	5.51%	0.732%
31	16.504	2444	2451	2457	rBV4	36867	83155	4.42%	0.588%
32	17.274	2576	2582	2592	rVB7	25807	74152	3.94%	0.524%
33	18.221	2735	2743	2753	rBV9	14450	47214	2.51%	0.334%

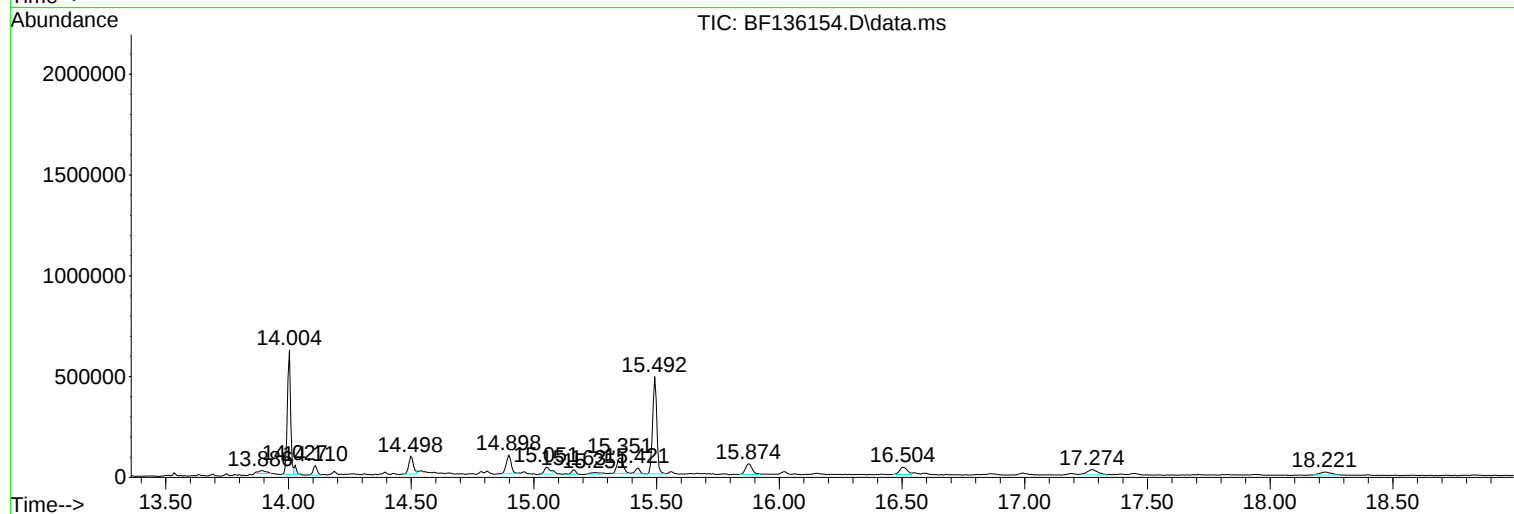
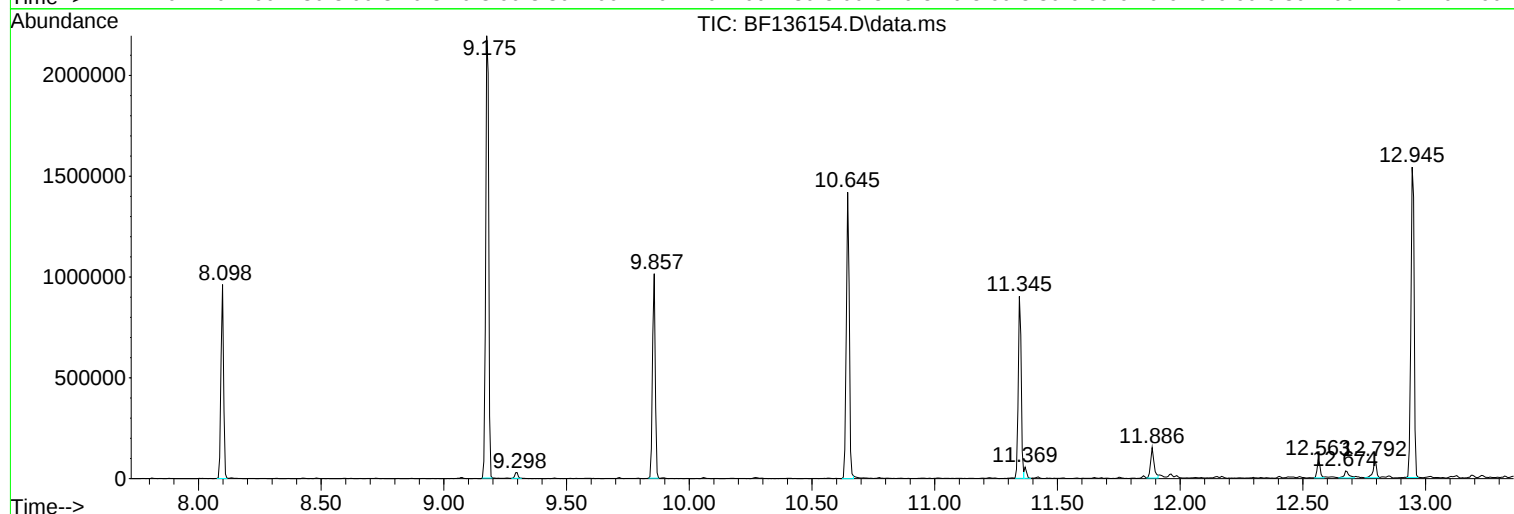
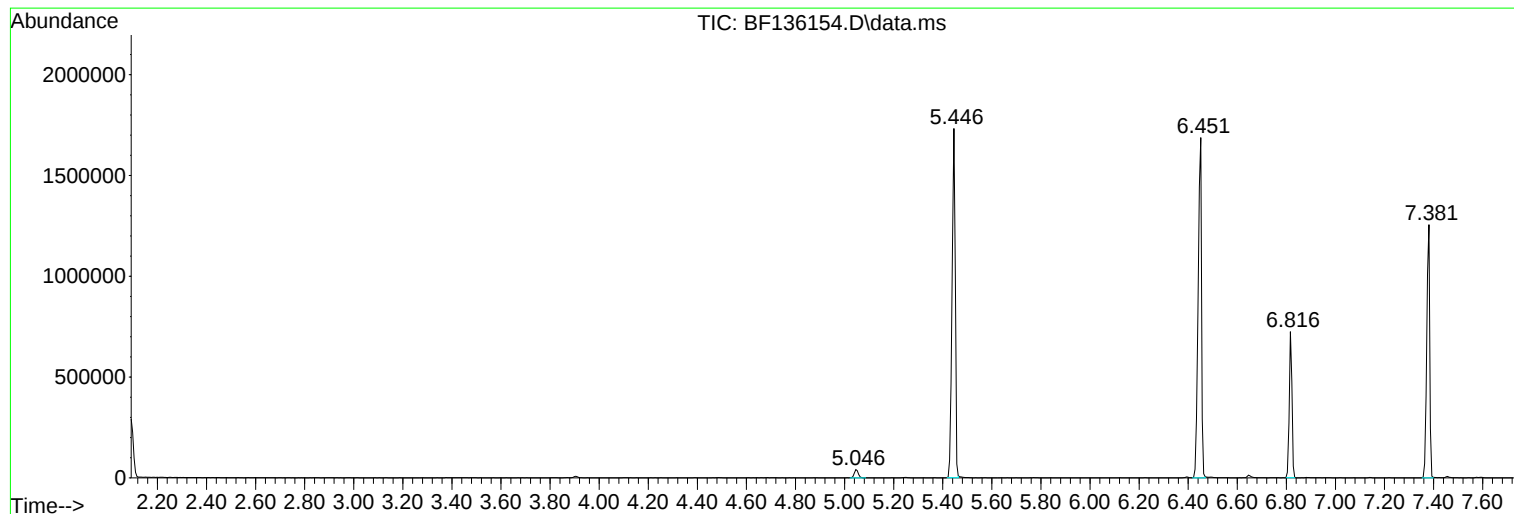
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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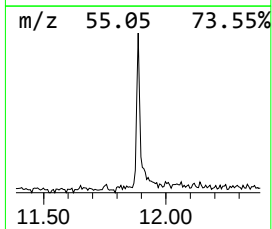
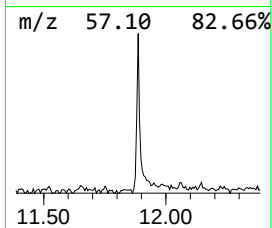
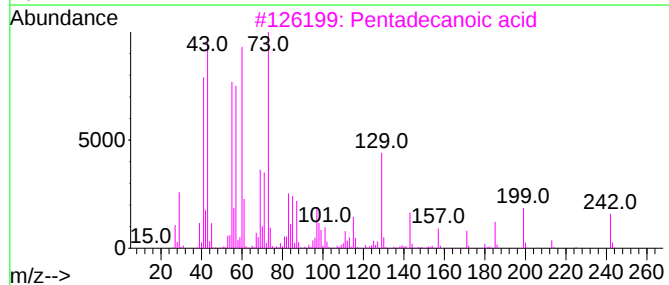
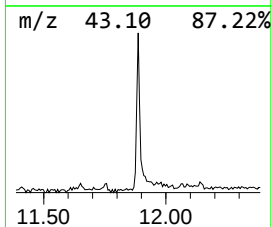
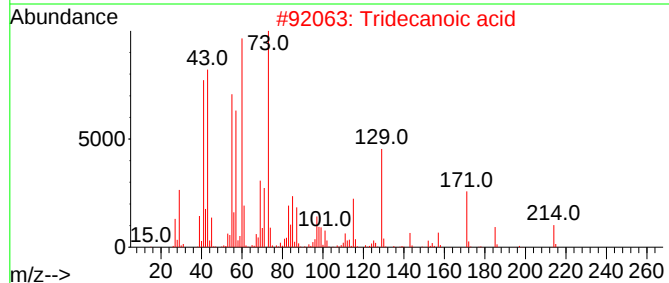
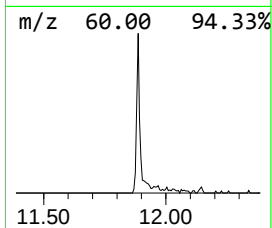
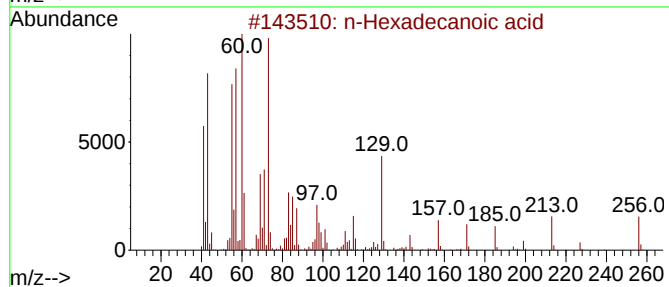
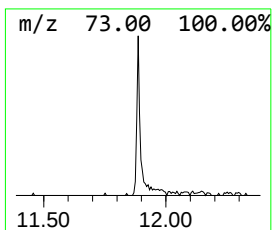
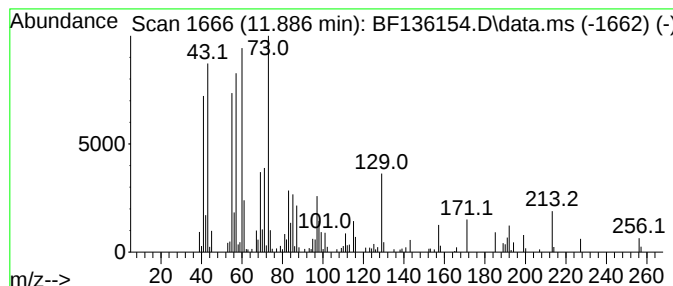
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	3.75 ng	143472	Phenanthrene-d10	11.345

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	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Nonanoic acid	158	C9H18O2	000112-05-0	43



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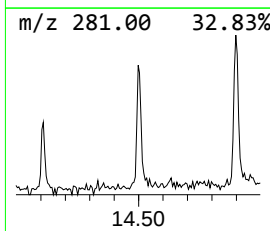
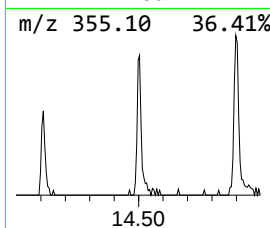
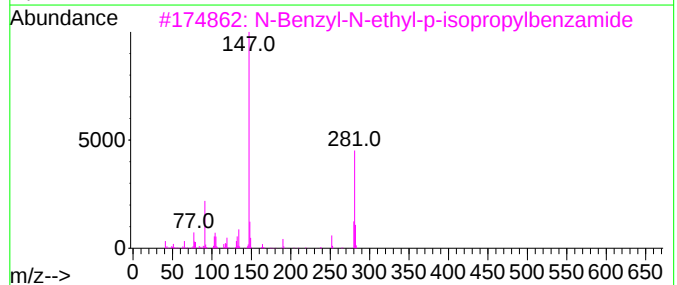
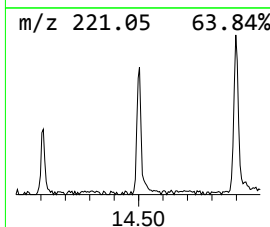
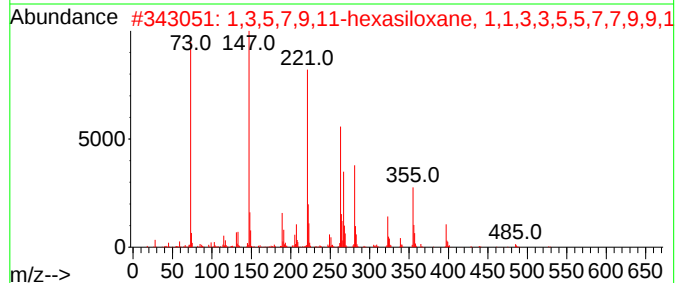
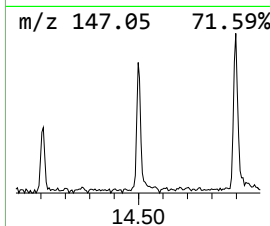
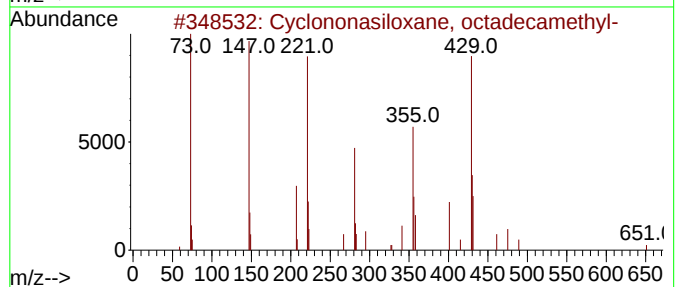
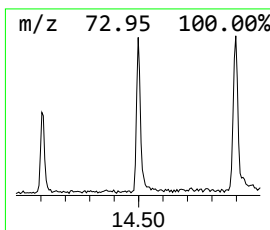
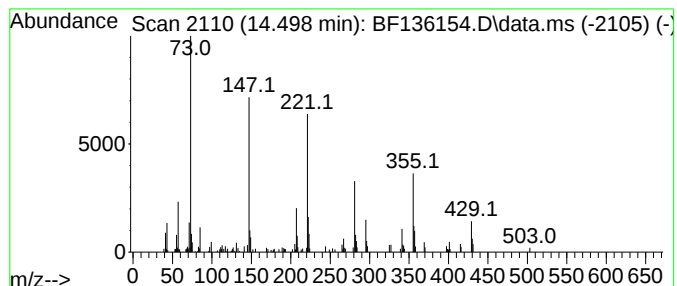
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Cyclononasiloxane, octadeca... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.498	4.04 ng	115622	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	80
2			1,3,5,7,9,11-hexasiloxane, 1,1,3...	542	C20H54O5Si6	1000458-50-7	59
3			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	38
4			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	32
5			2,3-Dimercaptobutane-1,4-diol, 4TMS	442	C16H42O2S2Si4	959295-06-8	27



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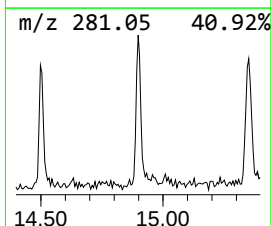
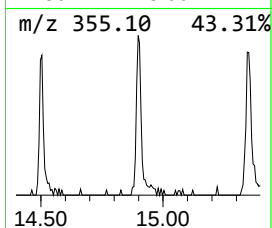
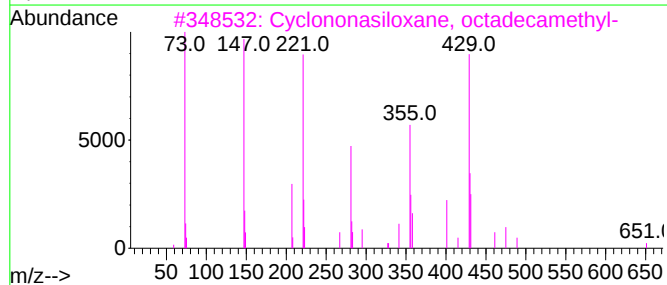
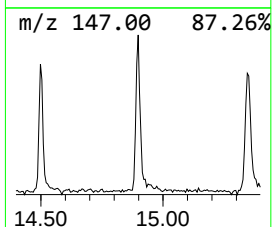
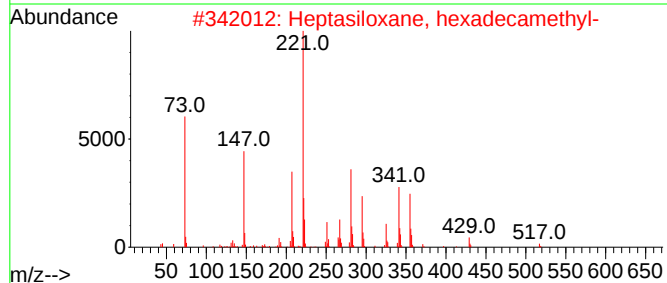
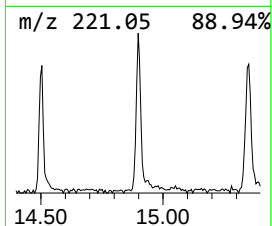
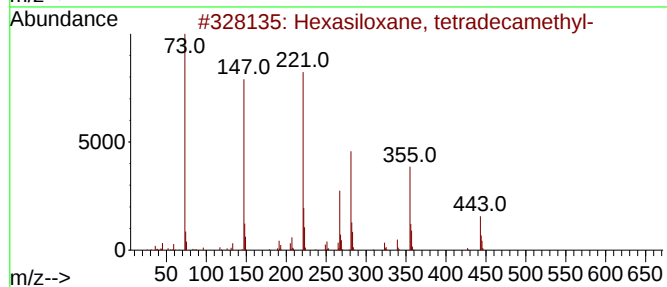
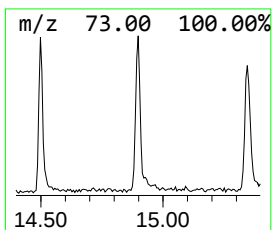
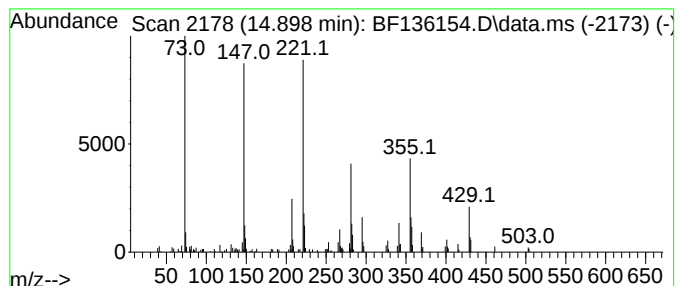
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexasiloxane, tetradecamethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.898	4.57 ng	129624	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	87
2			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	50
3			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	49
4			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	38
5			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	37



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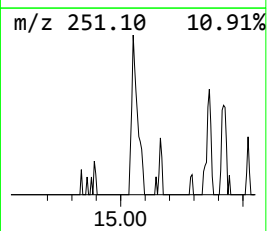
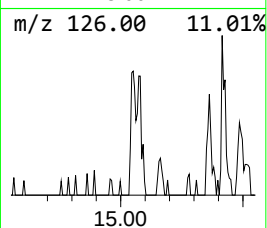
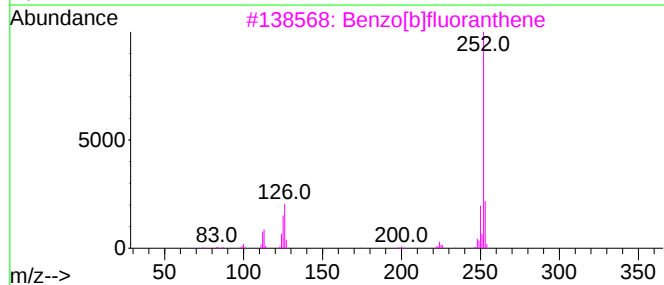
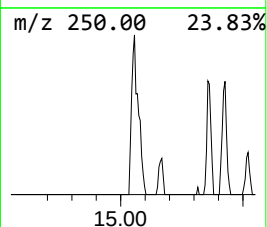
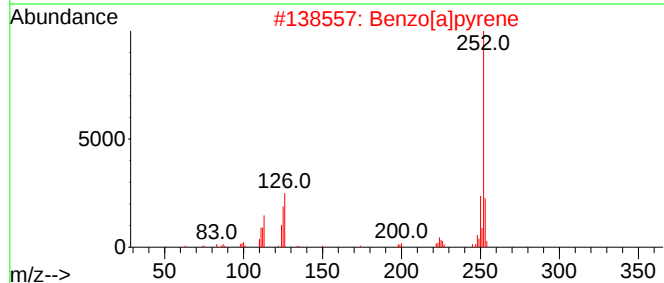
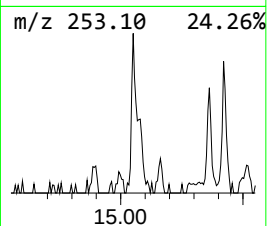
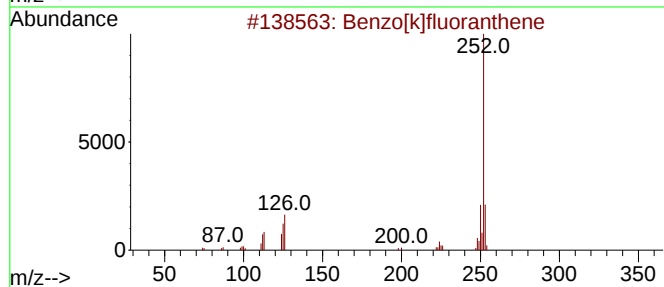
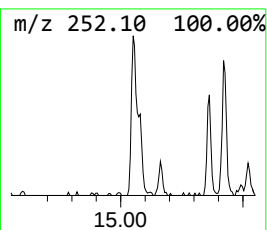
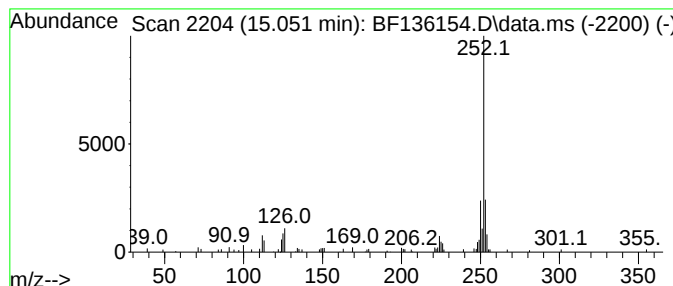
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzo[e]pyrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.051	2.04 ng	57798	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
2			Benzo[a]pyrene	252	C20H12	000050-32-8	93
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	81
4			Benzo[e]pyrene	252	C20H12	000192-97-2	81
5			Perylene	252	C20H12	000198-55-0	81



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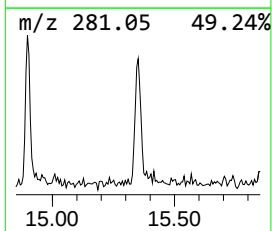
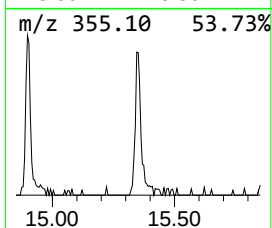
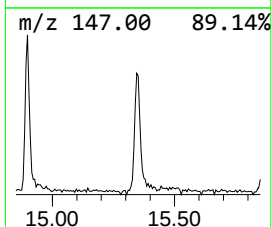
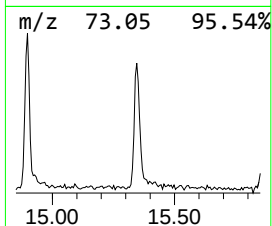
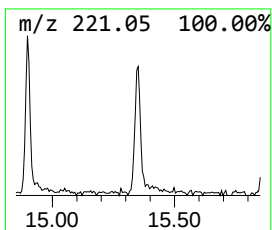
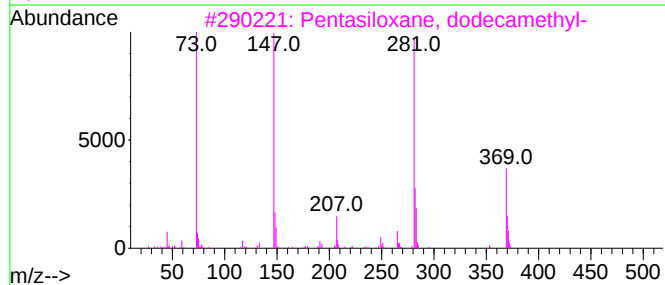
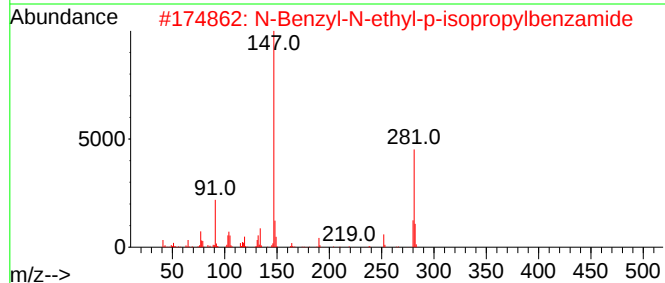
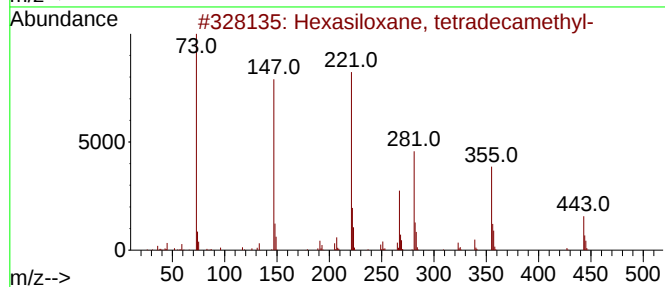
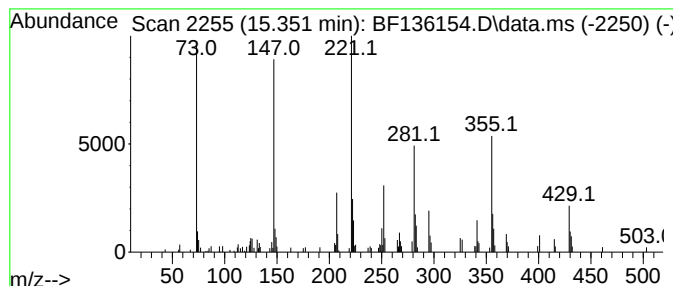
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 N-Benzyl-N-ethyl-p-isopropy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.351	4.76 ng	135279	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	64
2			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	25
3			Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	22
4			Indole, 5-(4-methylphenyl)-N-met...	221	C16H15N	1000380-54-7	18
5			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110623\
Data File : BF136154.D
Acq On : 06 Nov 2023 14:56
Operator : CG\JU
Sample : 05257-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-3

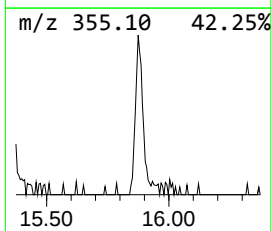
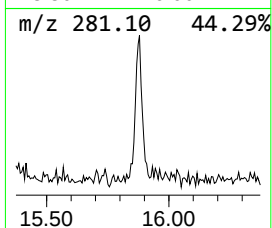
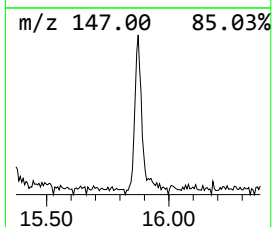
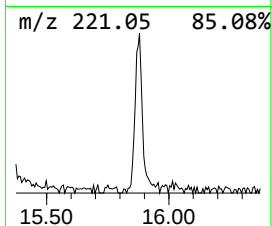
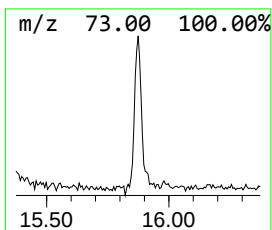
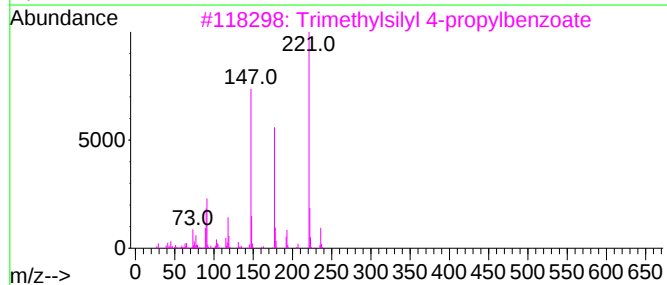
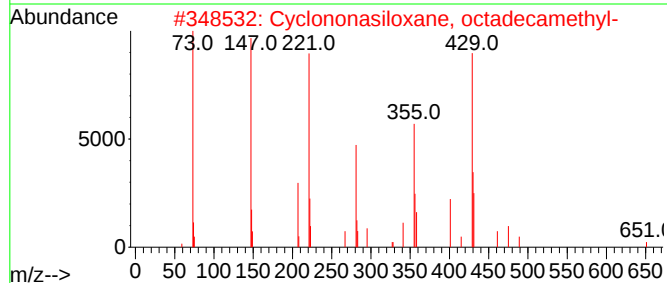
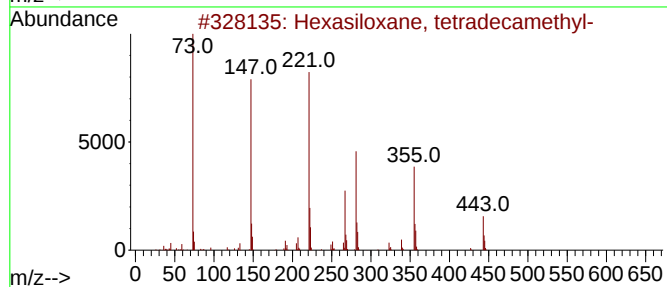
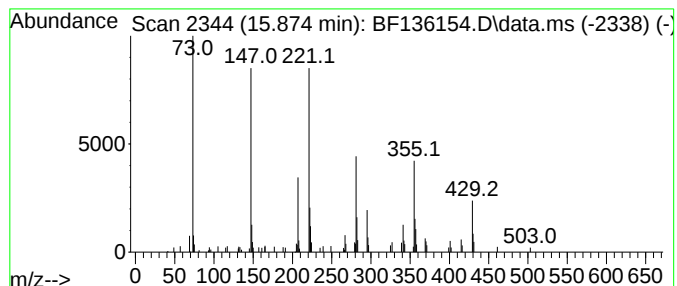
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown15.874 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.874	3.65 ng	103588	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	74
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	52
3			Trimethylsilyl 4-propylbenzoate	236	C13H20O2Si	1000408-13-2	37
4			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	33
5			4-Hydroxybenzyl alcohol, 2TBDMS ...	352	C19H36O2Si2	1000364-43-9	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110623\
Data File : BF136154.D
Acq On : 06 Nov 2023 14:56
Operator : CG\JU
Sample : 05257-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-3

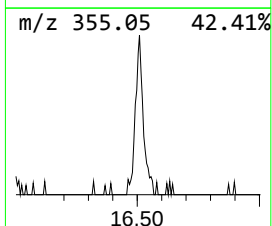
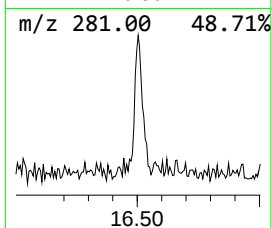
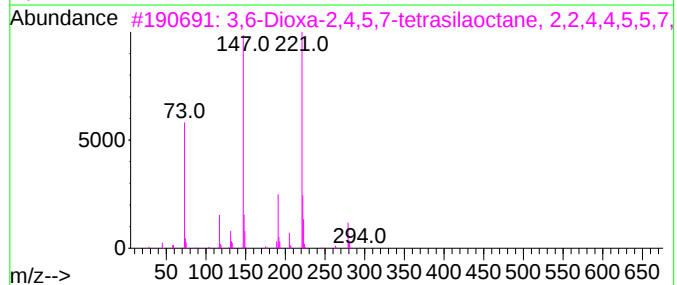
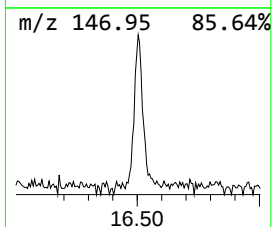
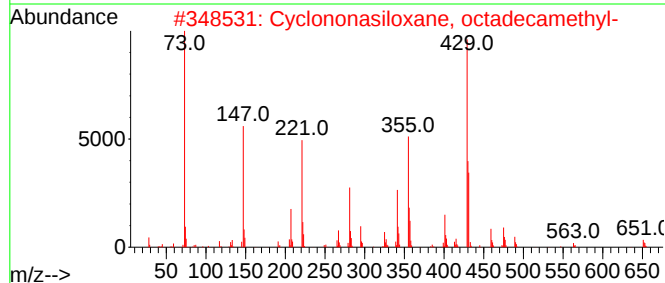
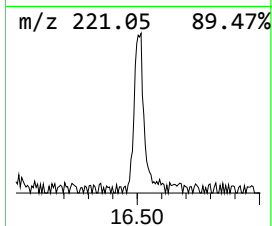
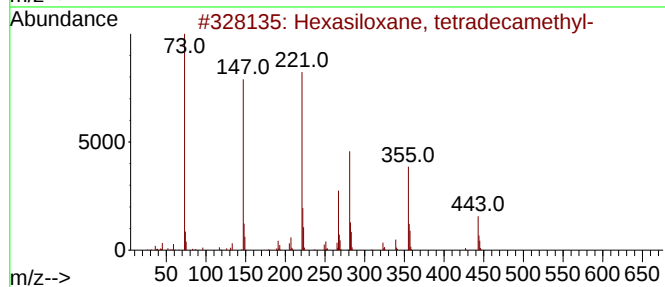
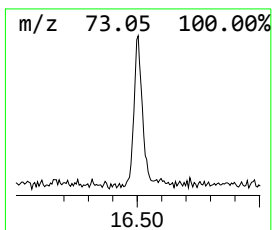
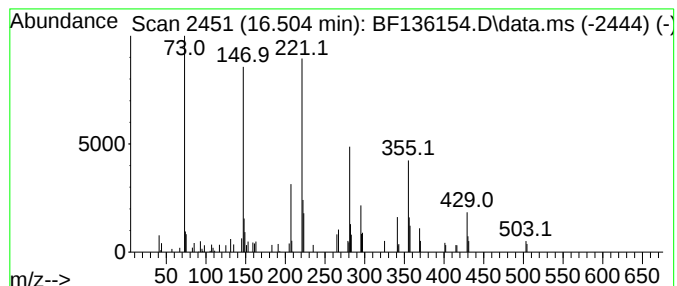
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown16.504 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.504	2.93 ng	83155	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	83
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	56
3			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	37
4			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	37
5			1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110623\
Data File : BF136154.D
Acq On : 06 Nov 2023 14:56
Operator : CG\JU
Sample : 05257-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-3

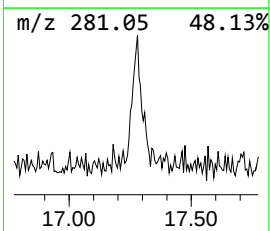
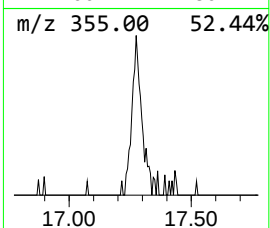
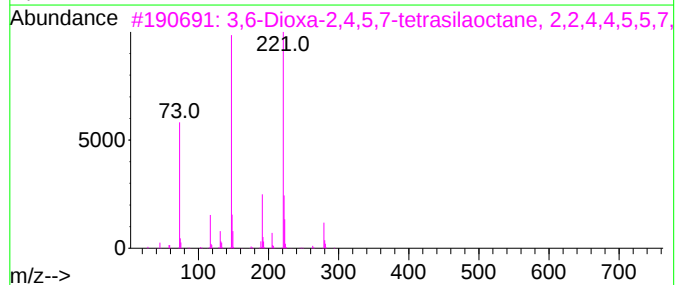
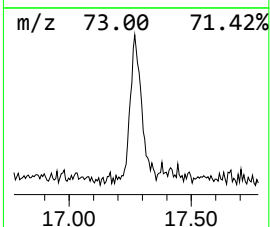
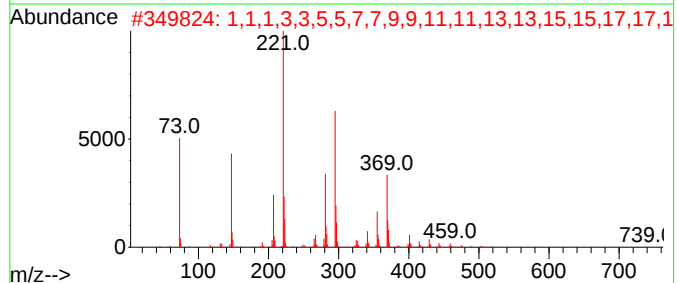
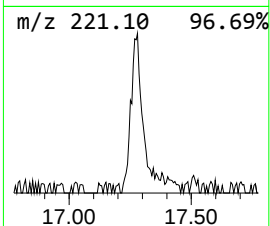
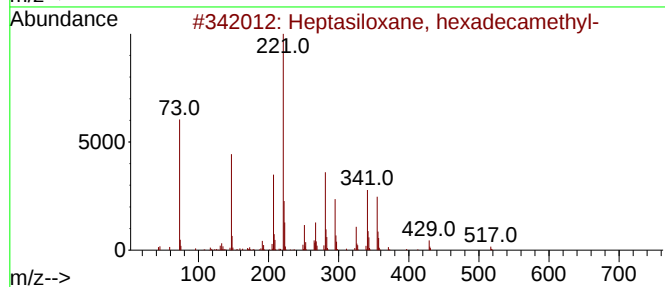
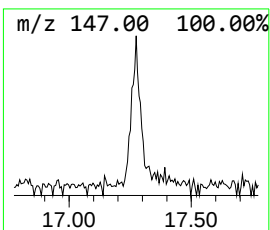
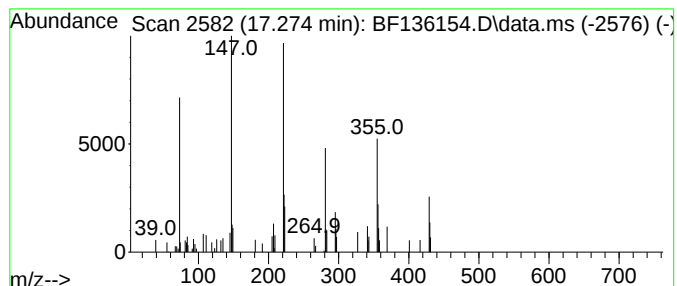
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown17.274 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.274	2.61 ng	74152	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	45
2			1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	754	C22H66O9Si10	000556-70-7	40
3			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	37
4			3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	25
5			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110623\
Data File : BF136154.D
Acq On : 06 Nov 2023 14:56
Operator : CG\JU
Sample : 05257-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.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 ...	11.886	3.8	ng	143472	4	11.345	764382	20.0
Cyclononasiloxa...	14.498	4.0	ng	115622	5	14.004	571782	20.0
Hexasiloxane, t...	14.898	4.6	ng	129624	6	15.492	567832	20.0
Benzo[e]pyrene	15.051	2.0	ng	57798	6	15.492	567832	20.0
N-Benzyl-N-ethy...	15.351	4.8	ng	135279	6	15.492	567832	20.0
unknown15.874	15.874	3.6	ng	103588	6	15.492	567832	20.0
unknown16.504	16.504	2.9	ng	83155	6	15.492	567832	20.0
unknown17.274	17.274	2.6	ng	74152	6	15.492	567832	20.0