

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121223\
 Data File : BF136524.D
 Acq On : 12 Dec 2023 19:28
 Operator : CG\JU
 Sample : 05726-05
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-2

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-BF120523.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136524.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.028	497	500	507	rVB	40335	45377	2.62%	0.289%
2	5.434	565	569	572	rBV	1710112	1518810	87.84%	9.674%
3	6.434	735	739	742	rBV	1533198	1474927	85.30%	9.394%
4	6.793	797	800	804	rBV	559856	468247	27.08%	2.982%
5	7.357	891	896	899	rBV	992643	945885	54.70%	6.025%
6	8.069	1014	1017	1021	rBV	696432	574526	33.23%	3.659%
7	9.151	1196	1201	1204	rBV	2038689	1729148	100.00%	11.013%
8	9.828	1312	1316	1326	rBV	726172	588035	34.01%	3.745%
9	10.622	1447	1451	1466	rBV	953818	891539	51.56%	5.678%
10	11.322	1566	1570	1572	rBV	580046	540044	31.23%	3.440%
11	11.339	1572	1573	1577	rVB	100115	79535	4.60%	0.507%
12	11.822	1652	1655	1658	rBV	29923	27134	1.57%	0.173%
13	11.851	1658	1660	1665	rVV	97137	88065	5.09%	0.561%
14	11.933	1670	1674	1677	rBV	39436	38703	2.24%	0.247%
15	12.122	1699	1706	1708	rBV3	17210	25533	1.48%	0.163%
16	12.375	1744	1749	1752	rBV	34315	36641	2.12%	0.233%
17	12.463	1761	1764	1769	rVB2	21968	26862	1.55%	0.171%
18	12.539	1773	1777	1781	rBV	217925	206919	11.97%	1.318%
19	12.645	1790	1795	1798	rBV2	16510	26464	1.53%	0.169%
20	12.769	1809	1816	1818	rBV	220014	224578	12.99%	1.430%
21	12.816	1822	1824	1829	rVB3	19348	26290	1.52%	0.167%
22	12.916	1837	1841	1844	rBV	1810455	1529007	88.43%	9.739%
23	12.992	1848	1854	1856	rBV2	22736	34002	1.97%	0.217%
24	13.074	1865	1868	1870	rBV2	21952	28334	1.64%	0.180%
25	13.098	1870	1872	1878	rVB	33993	29158	1.69%	0.186%
26	13.163	1878	1883	1886	rBV3	22679	34220	1.98%	0.218%
27	13.198	1886	1889	1893	rVV	42182	43747	2.53%	0.279%
28	13.292	1902	1905	1908	rVV	27420	22305	1.29%	0.142%
29	13.327	1908	1911	1914	rVB	23301	21480	1.24%	0.137%
30	13.492	1935	1939	1942	rBV3	19508	28664	1.66%	0.183%
31	13.604	1956	1958	1962	rBV	26227	27550	1.59%	0.175%
32	13.639	1962	1964	1967	rVB	20008	19856	1.15%	0.126%
33	13.721	1973	1978	1981	rBV3	25950	46338	2.68%	0.295%
34	13.821	1992	1995	1999	rVB2	30179	38085	2.20%	0.243%
35	13.898	2003	2008	2010	rBV5	16218	30772	1.78%	0.196%
36	13.974	2016	2021	2023	rBV2	656034	703920	40.71%	4.483%

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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-BF120523.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.998	2023	2025	2030	rVB	135676	119946	6.94%	0.764%
38	14.063	2032	2036	2040	rBV3	84262	113882	6.59%	0.725%
39	14.145	2047	2050	2053	rVB3	22847	23859	1.38%	0.152%
40	14.363	2084	2087	2090	rVB	35490	29604	1.71%	0.189%
41	14.392	2090	2092	2096	rBV2	23036	26100	1.51%	0.166%
42	14.451	2096	2102	2106	rBV	218069	250409	14.48%	1.595%
43	14.839	2163	2168	2176	rBV	254818	353368	20.44%	2.251%
44	15.016	2194	2198	2202	rBV	113779	183674	10.62%	1.170%
45	15.274	2237	2242	2247	rBV	237911	370426	21.42%	2.359%
46	15.321	2247	2250	2256	rVB	77574	118308	6.84%	0.754%
47	15.386	2257	2261	2267	rVB	89602	119816	6.93%	0.763%
48	15.457	2267	2273	2276	rBV	437448	554607	32.07%	3.532%
49	15.786	2324	2329	2341	rVB2	194460	387286	22.40%	2.467%
50	16.398	2427	2433	2443	rBV2	128711	297469	17.20%	1.895%
51	16.945	2523	2526	2533	rVB2	32550	58165	3.36%	0.370%
52	17.145	2553	2560	2574	rVB3	93402	270131	15.62%	1.721%
53	18.068	2708	2717	2728	rVB3	62319	202784	11.73%	1.292%

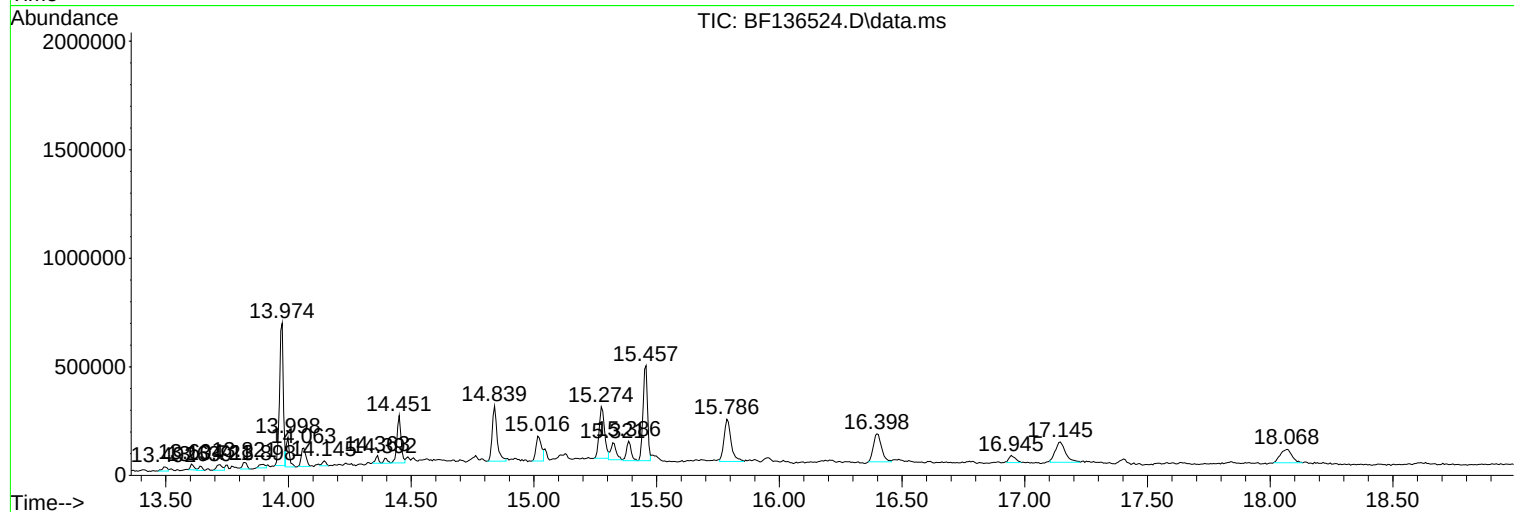
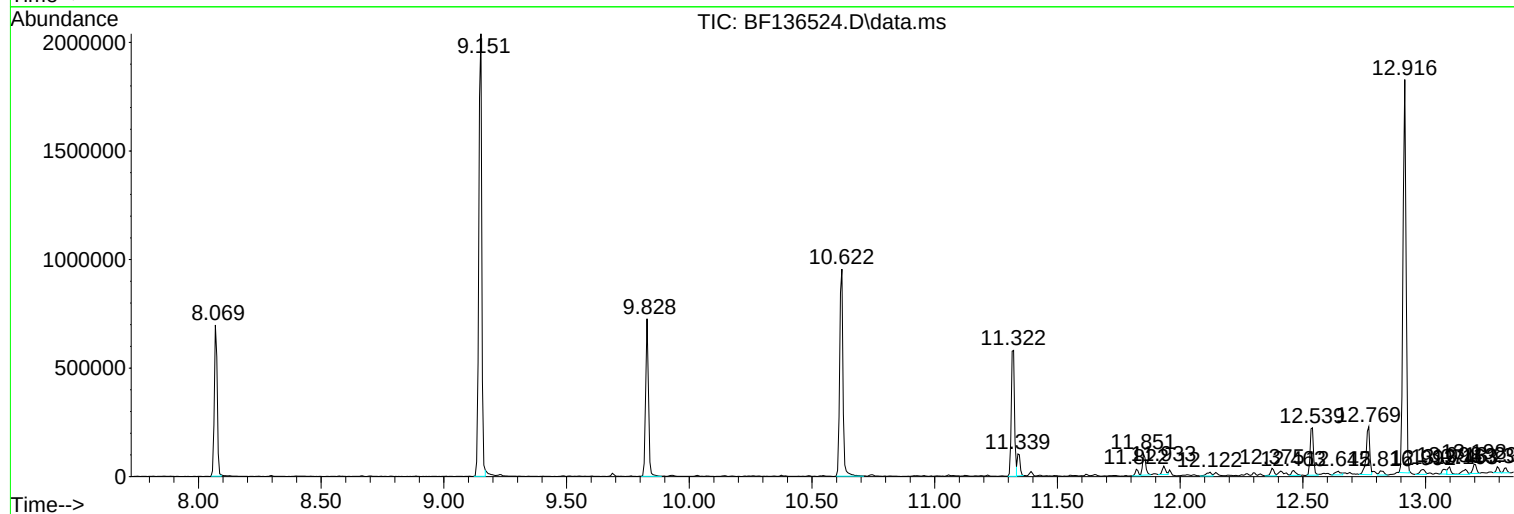
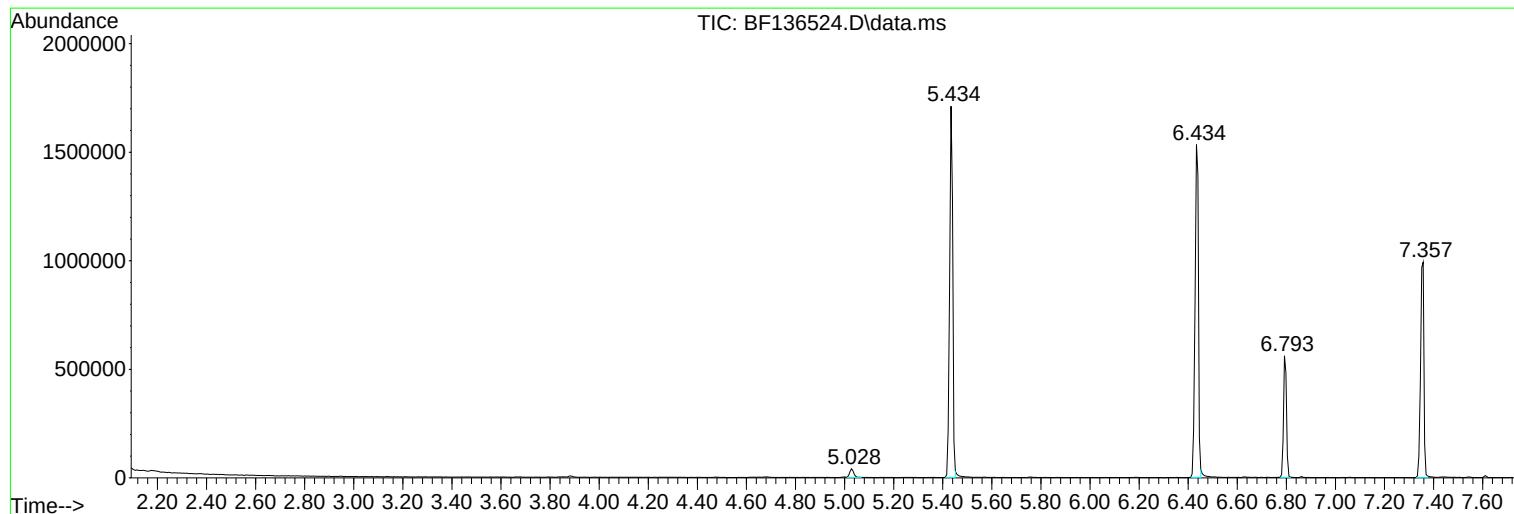
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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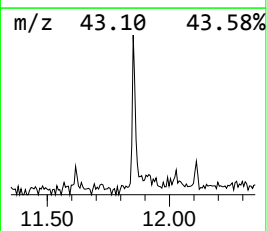
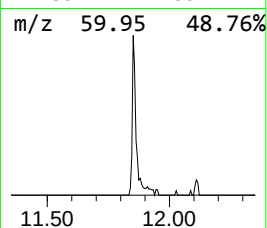
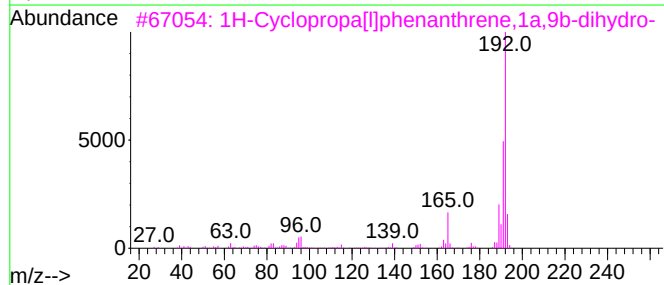
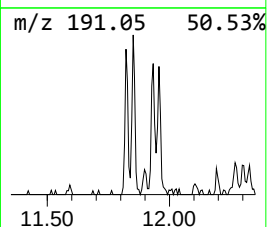
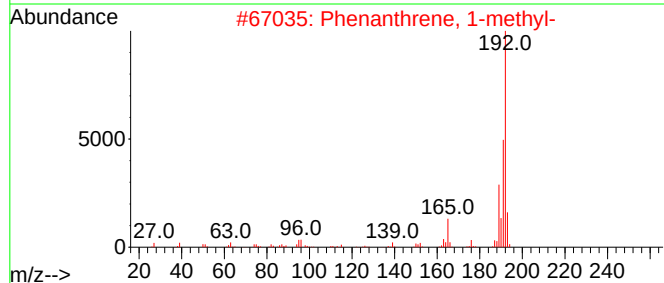
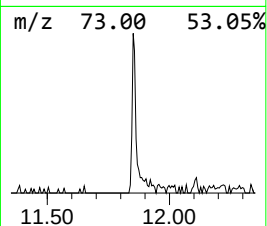
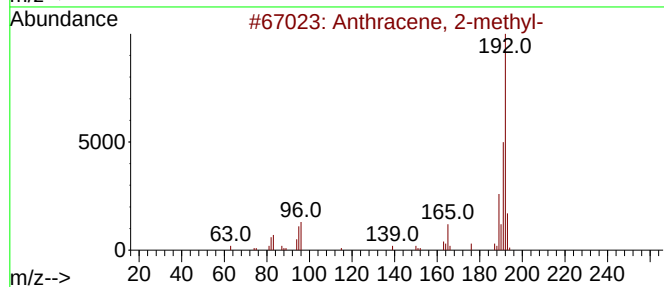
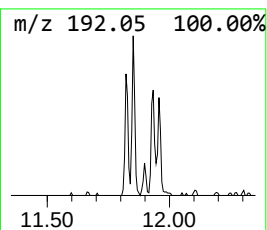
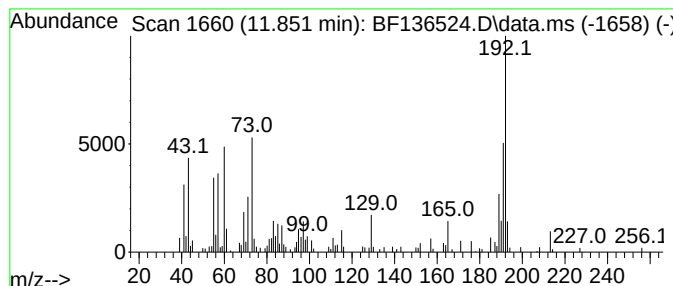
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Anthracene, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.851	3.26 ng	88065	Phenanthrene-d10	11.322

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Anthracene, 2-methyl-	192	C15H12	000613-12-7	94
2		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	92
3		1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	90
4		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	90
5		1H-Indene, 1-phenyl-	192	C15H12	001961-96-2	90



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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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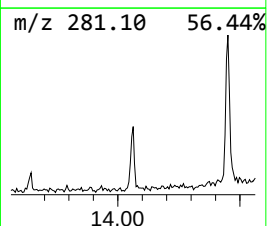
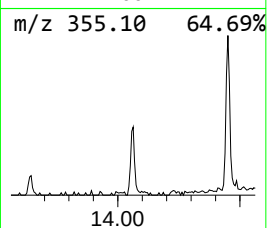
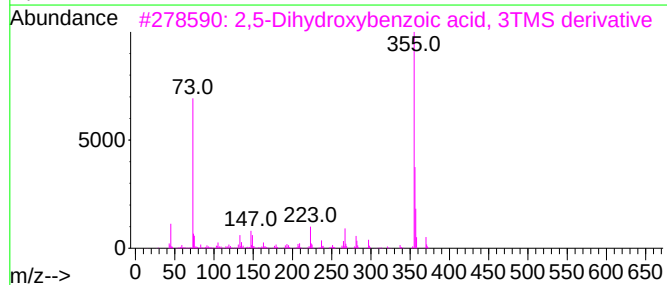
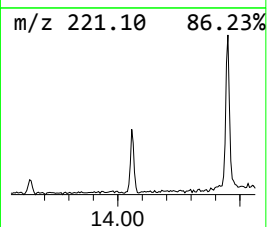
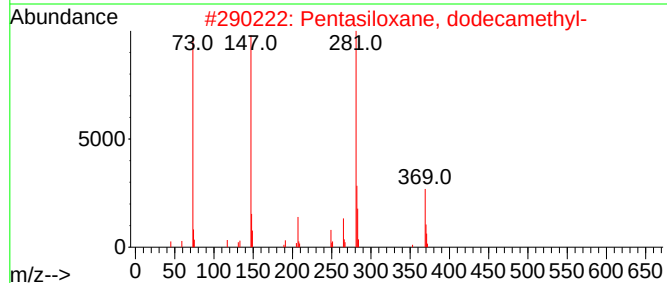
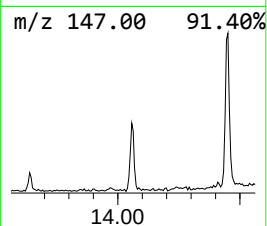
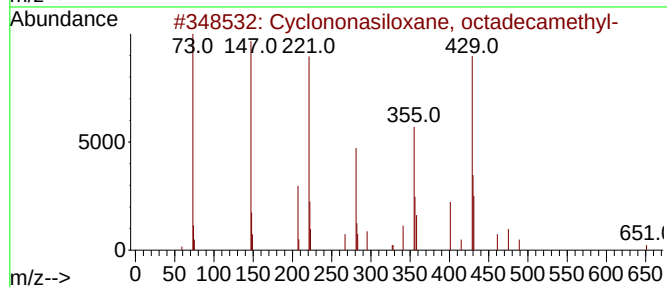
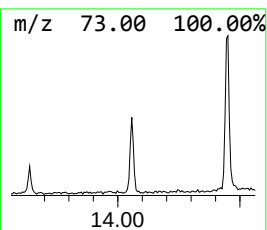
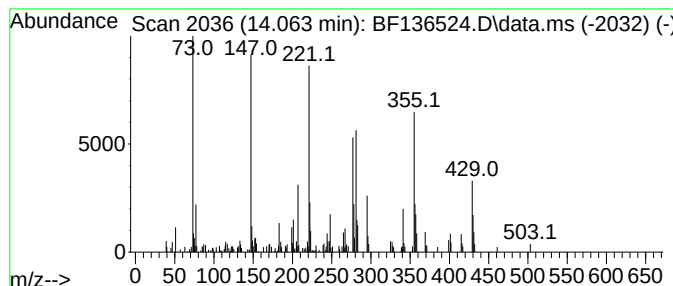
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Cyclononasiloxane, octadeca... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.063	3.24 ng	113882	Chrysene-d12	13.974

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	59
2		Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	25
3		2,5-Dihydroxybenzoic acid, 3TMS ...	370	C16H30O4Si3	003618-20-0	25
4		N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	22
5		Triisobutyl(3-phenylpropoxy)silane	334	C21H38OSi	1000282-18-2	22



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ALS Vial : 18 Sample Multiplier: 1

Instrument :
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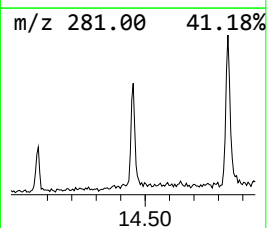
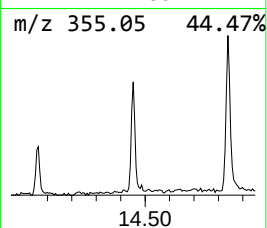
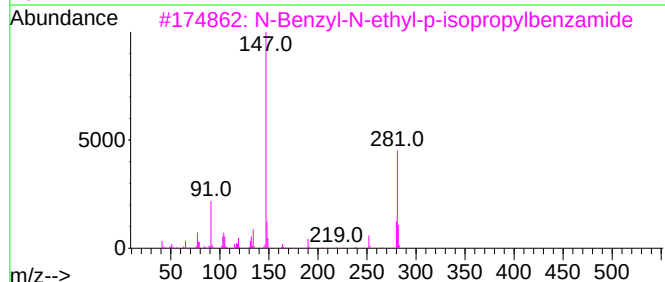
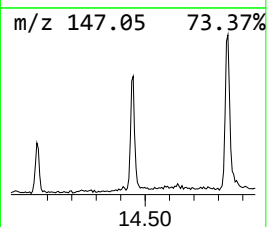
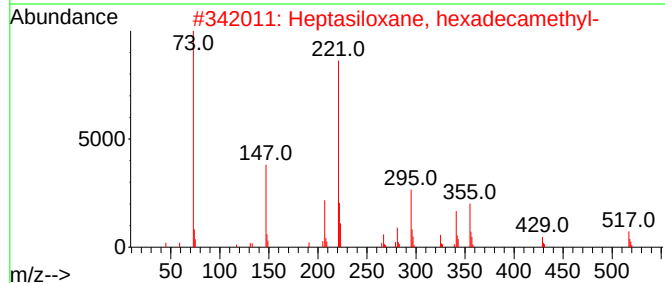
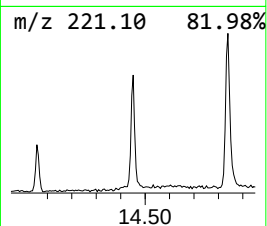
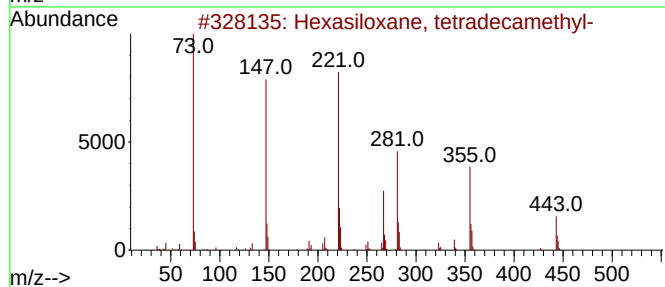
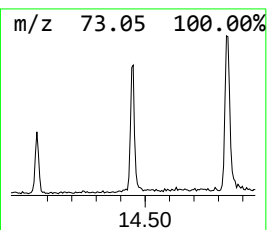
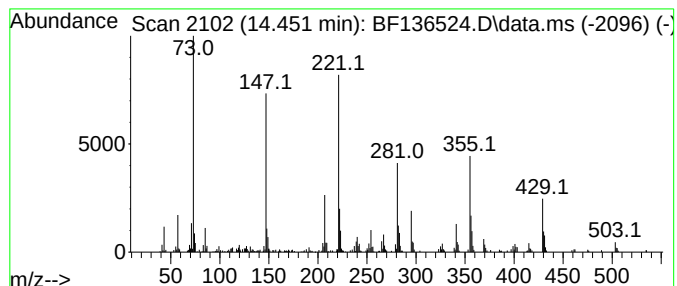
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexasiloxane, tetradecamethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.451	7.11 ng	250409	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	72
2			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	38
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	37
5			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	32



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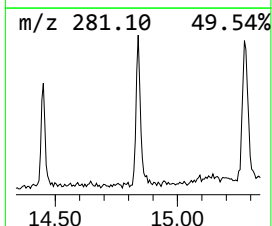
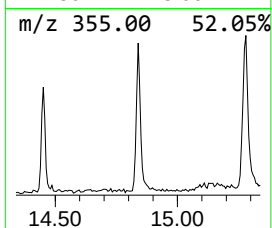
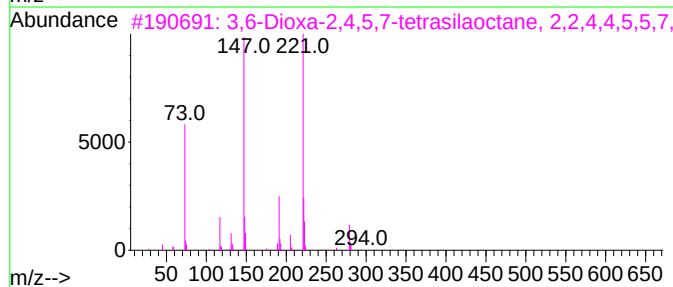
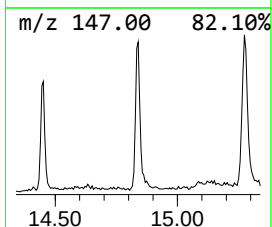
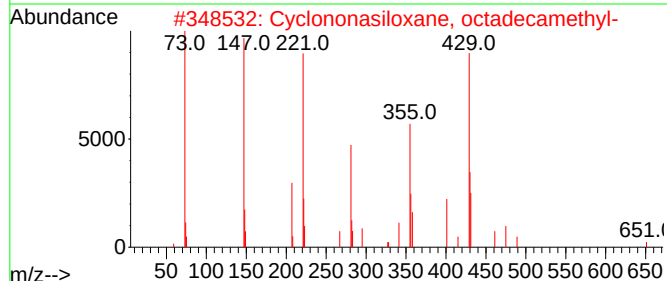
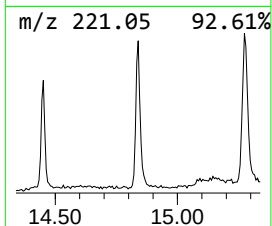
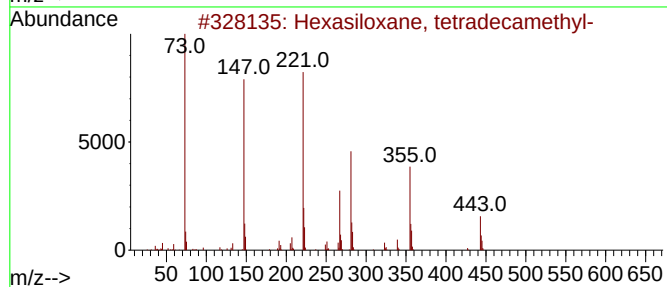
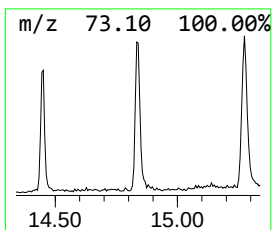
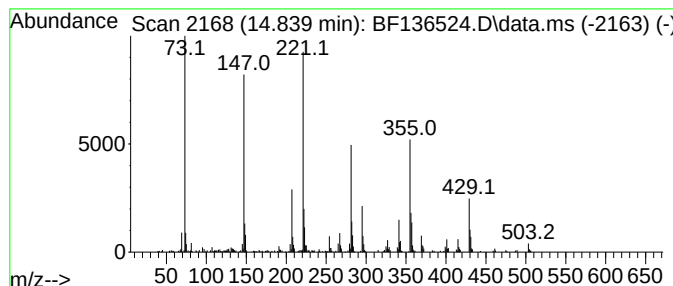
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown14.839 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.839	12.74 ng	353368	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	81
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	64
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			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	25



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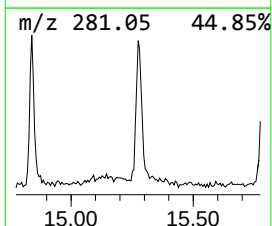
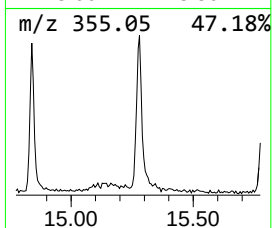
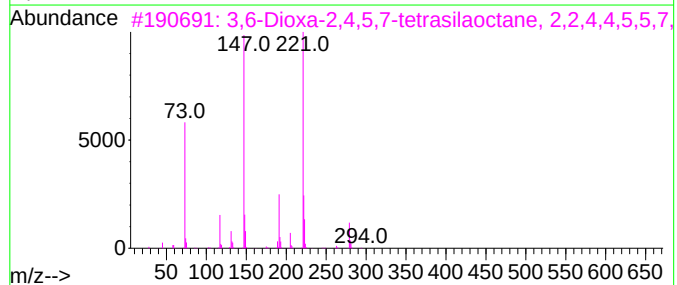
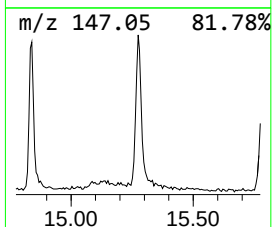
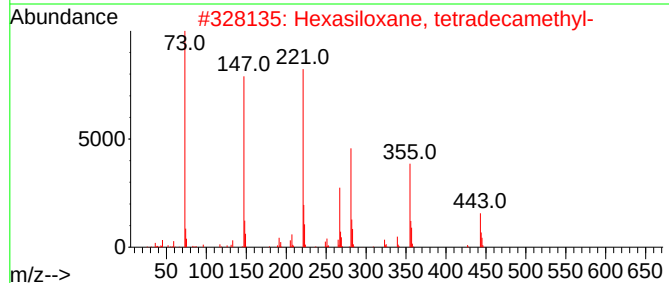
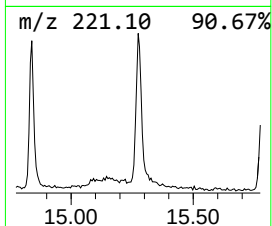
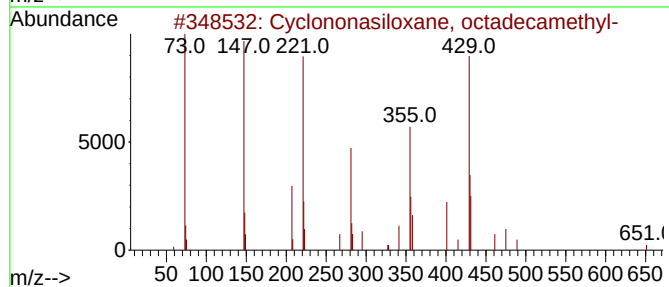
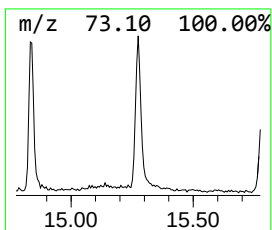
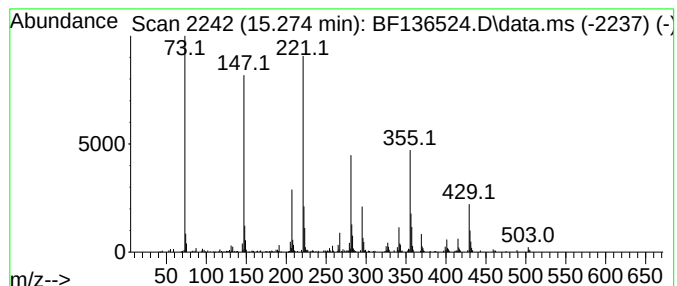
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown15.274 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.274	13.36 ng	370426	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	72
2			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	72
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	32
5			3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121223\
Data File : BF136524.D
Acq On : 12 Dec 2023 19:28
Operator : CG\JU
Sample : 05726-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2

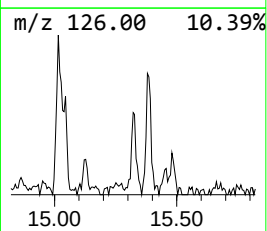
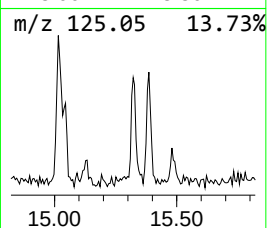
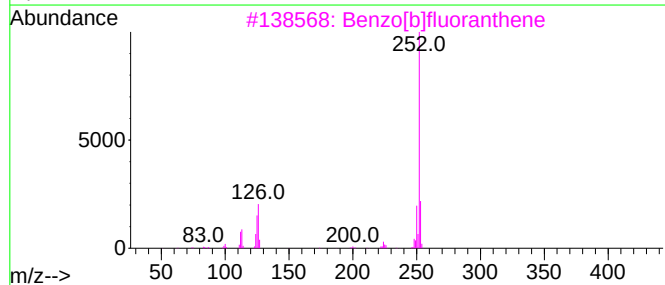
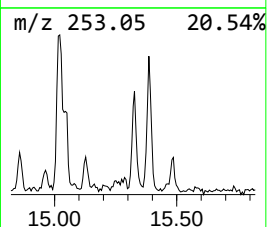
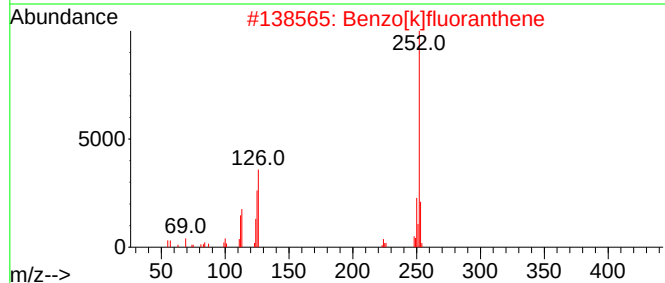
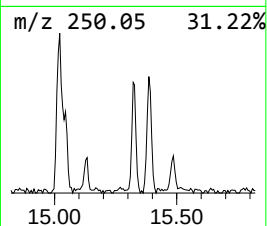
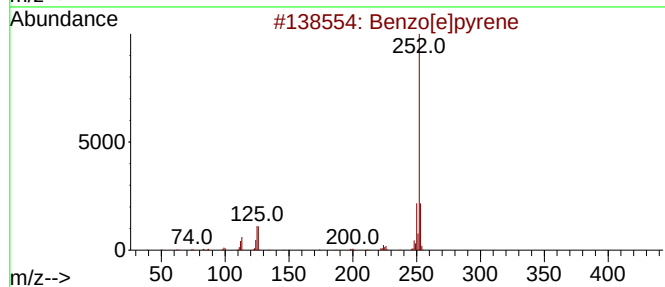
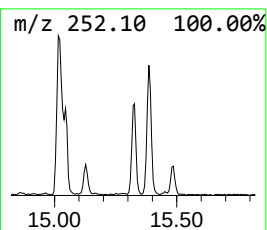
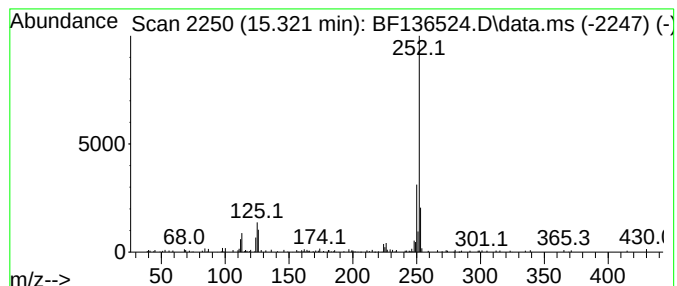
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzo[e]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.321	4.27 ng	118308	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	96
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	90
4			Benzo[j]fluoranthene	252	C20H12	000205-82-3	89
5			Perylene	252	C20H12	000198-55-0	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121223\
Data File : BF136524.D
Acq On : 12 Dec 2023 19:28
Operator : CG\JU
Sample : 05726-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2

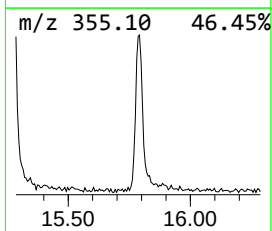
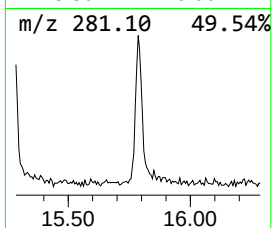
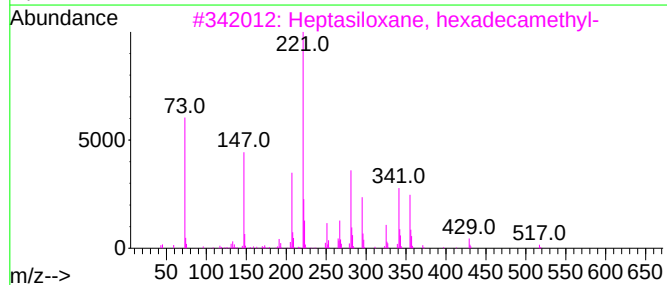
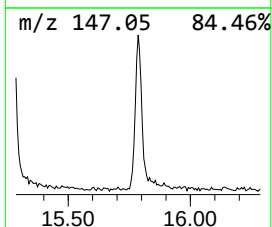
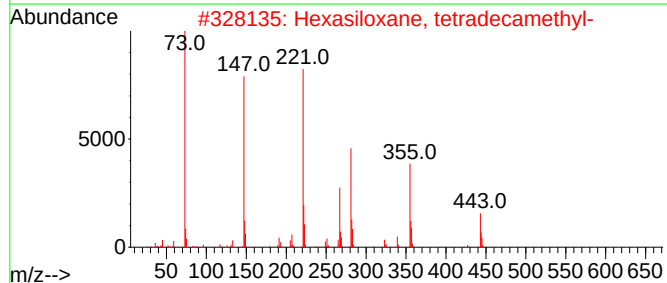
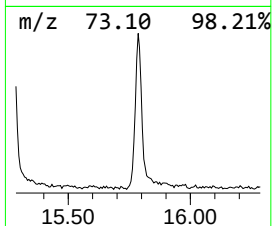
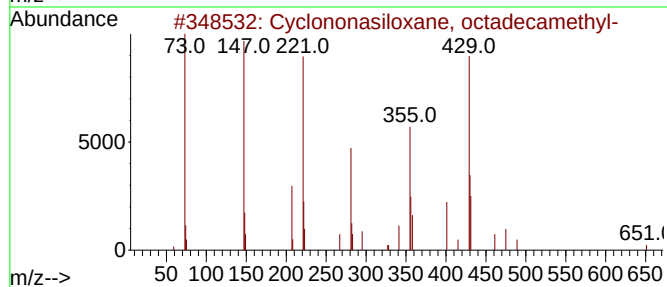
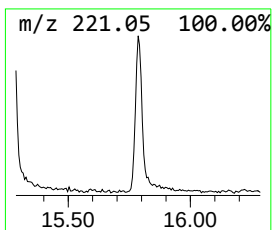
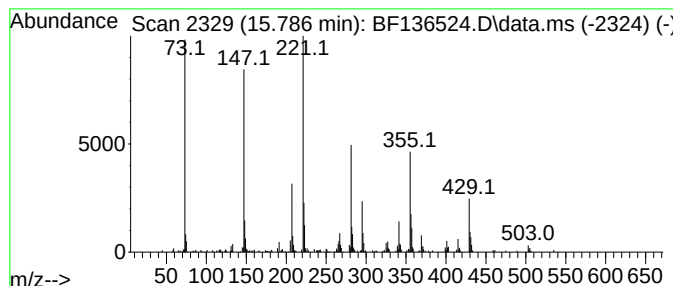
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown15.786 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.786	13.97 ng	387286	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	90
2			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	74
3			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	47
4			3,6-Dioxo-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	37
5			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121223\
Data File : BF136524.D
Acq On : 12 Dec 2023 19:28
Operator : CG\JU
Sample : 05726-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2

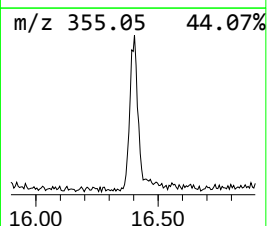
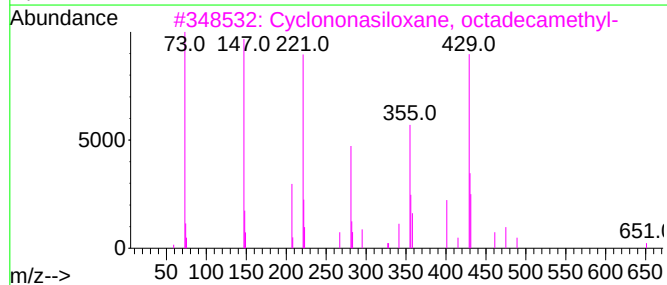
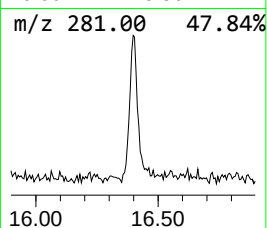
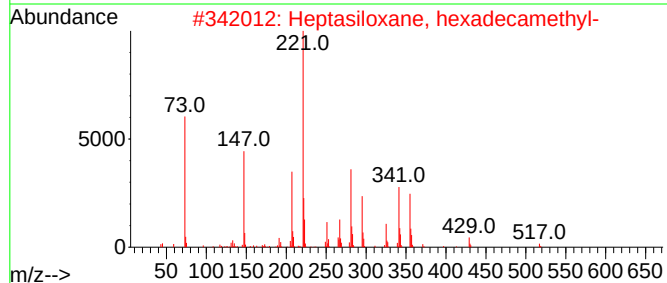
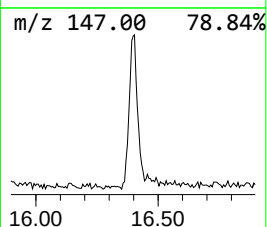
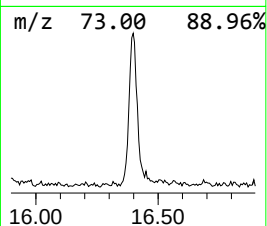
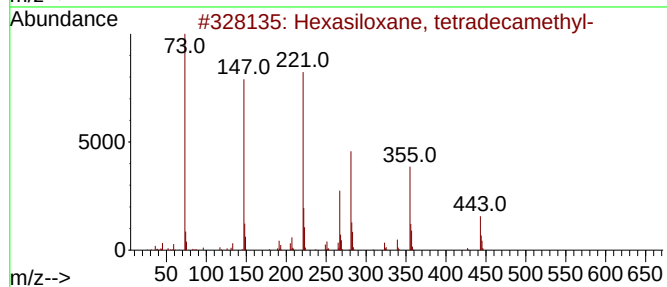
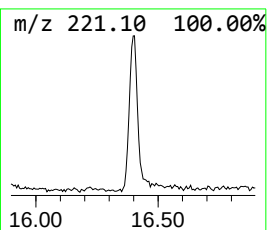
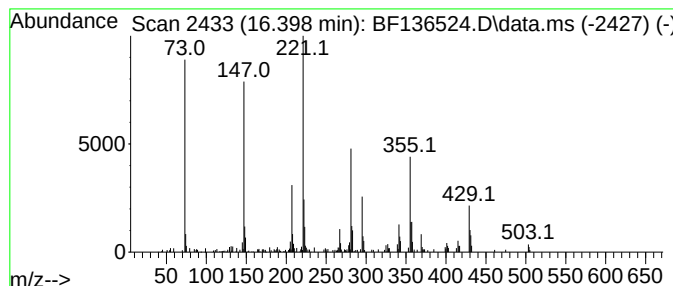
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown16.398 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.398	10.73 ng	297469	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	64
2			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	47
3			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	47
4			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	37
5			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121223\
Data File : BF136524.D
Acq On : 12 Dec 2023 19:28
Operator : CG\JU
Sample : 05726-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2

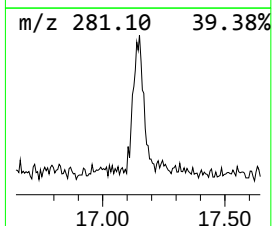
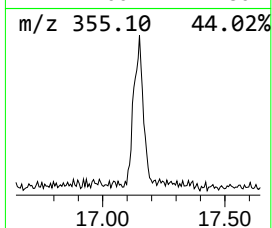
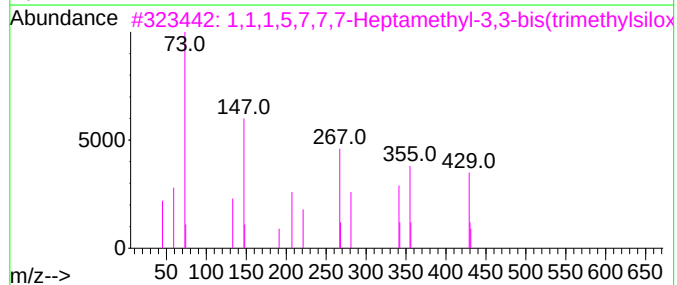
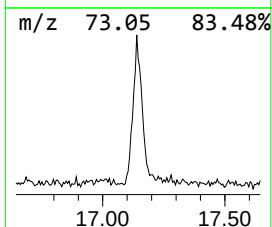
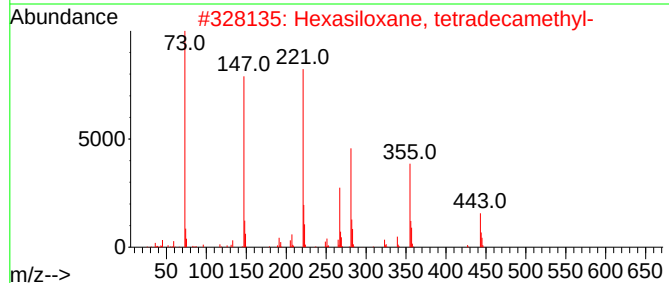
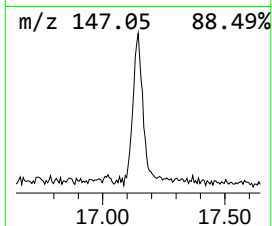
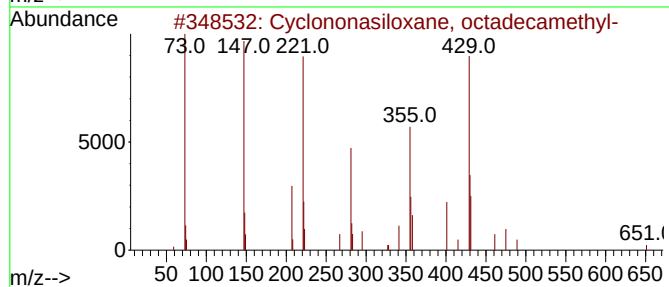
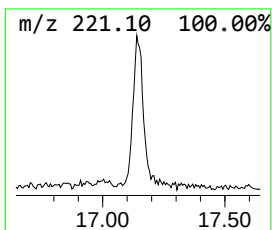
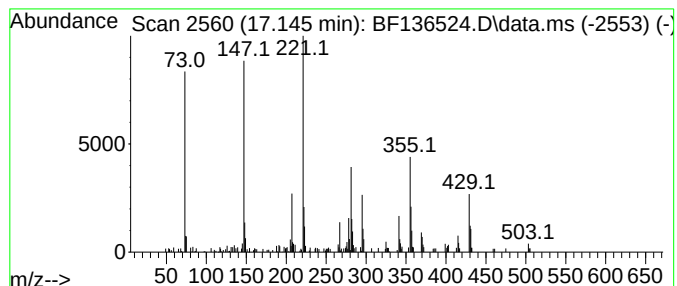
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown17.145 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.145	9.74 ng	270131	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	86
2			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	64
3			1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	50
4			2-Methyl-6-tert-butylphenol, TBD...	278	C17H30O5Si	1000467-05-0	25
5			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121223\
Data File : BF136524.D
Acq On : 12 Dec 2023 19:28
Operator : CG\JU
Sample : 05726-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2

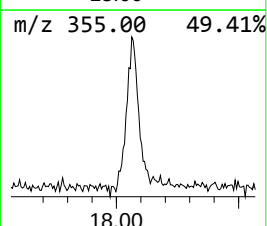
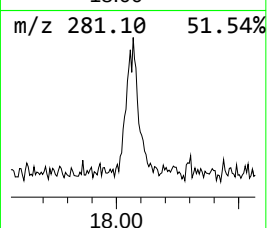
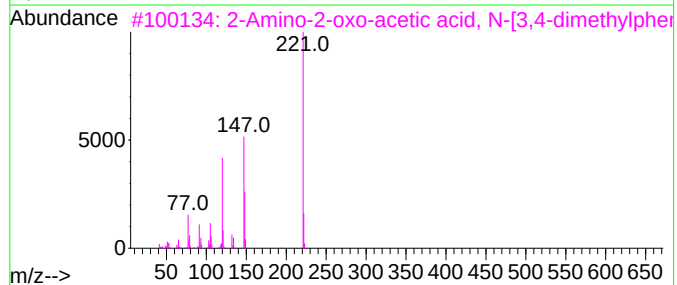
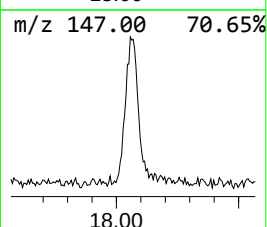
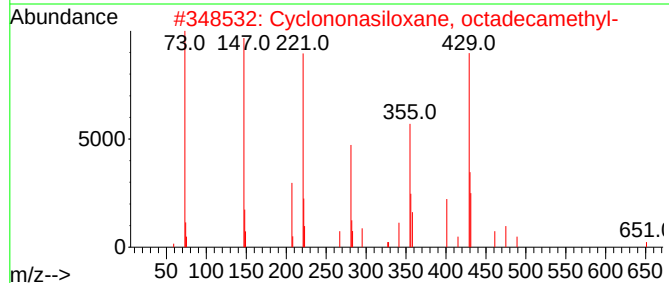
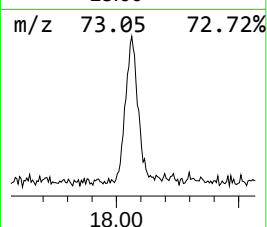
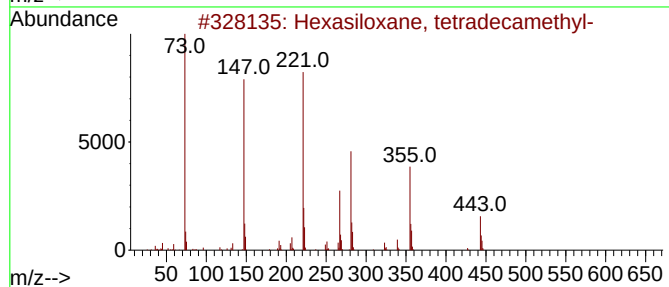
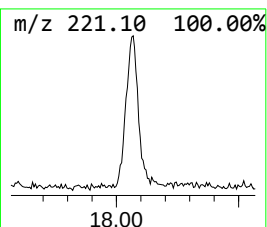
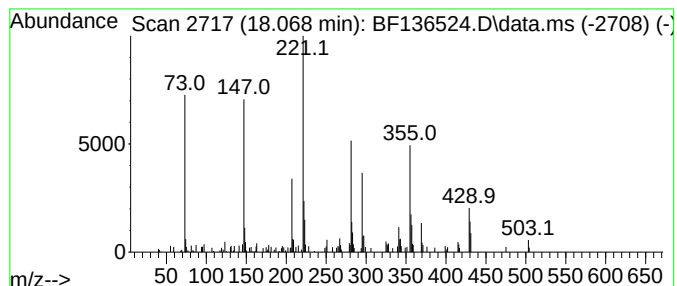
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown18.068 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.068	7.31 ng	202784	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	50
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	38
3			2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	38
4			2-{[2-(Methoxycarbonyl)anilino]c...	371	C19H21NO5Si	1000475-02-2	25
5			1,3(2H,4H)-Isoquinolinedione, 6,...	369	C20H19NO6	1000115-82-7	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121223\
Data File : BF136524.D
Acq On : 12 Dec 2023 19:28
Operator : CG\JU
Sample : 05726-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.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
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Cyclononasiloxa...	14.063	3.2	ng	113882	5	13.974	703920	20.0
Hexasiloxane, t...	14.451	7.1	ng	250409	5	13.974	703920	20.0
unknown14.839	14.839	12.7	ng	353368	6	15.457	554607	20.0
unknown15.274	15.274	13.4	ng	370426	6	15.457	554607	20.0
Benzo[e]pyrene	15.321	4.3	ng	118308	6	15.457	554607	20.0
unknown15.786	15.786	14.0	ng	387286	6	15.457	554607	20.0
unknown16.398	16.398	10.7	ng	297469	6	15.457	554607	20.0
unknown17.145	17.145	9.7	ng	270131	6	15.457	554607	20.0
unknown18.068	18.068	7.3	ng	202784	6	15.457	554607	20.0