

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121323\
 Data File : BF136558.D
 Acq On : 14 Dec 2023 02:03
 Operator : CG\JU
 Sample : 05767-04
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-E2-COMP

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: BF136558.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.022	496	499	506	rBV	27617	31537	2.38%	0.227%
2	5.434	564	569	572	rBV	1363136	1225515	92.54%	8.833%
3	6.434	735	739	742	rBV	1369935	1136699	85.84%	8.192%
4	6.792	797	800	804	rBV	489394	404678	30.56%	2.917%
5	7.351	891	895	898	rBV	868827	726751	54.88%	5.238%
6	8.069	1014	1017	1020	rBV	546938	464122	35.05%	3.345%
7	9.145	1197	1200	1204	rBV	1487710	1273057	96.13%	9.175%
8	9.480	1255	1257	1260	rBV2	18488	15758	1.19%	0.114%
9	9.675	1287	1290	1296	rBV2	32672	43756	3.30%	0.315%
10	9.827	1312	1316	1319	rBV	572960	438660	33.13%	3.162%
11	10.616	1447	1450	1461	rVB	776133	671167	50.68%	4.837%
12	11.316	1566	1569	1572	rBV	489780	449102	33.91%	3.237%
13	11.339	1572	1573	1577	rVV	112875	84409	6.37%	0.608%
14	11.392	1577	1582	1585	rVB	36754	38860	2.93%	0.280%
15	11.551	1602	1609	1613	rBV3	10870	19417	1.47%	0.140%
16	11.821	1651	1655	1657	rBV	21711	22510	1.70%	0.162%
17	11.857	1657	1661	1665	rBV	129293	135321	10.22%	0.975%
18	11.933	1671	1674	1677	rBV	32804	38216	2.89%	0.275%
19	12.016	1683	1688	1689	rBV4	14363	18687	1.41%	0.135%
20	12.374	1746	1749	1753	rBV	22236	29922	2.26%	0.216%
21	12.533	1773	1776	1780	rBV	277234	268257	20.26%	1.933%
22	12.580	1780	1784	1790	rVB7	23241	44998	3.40%	0.324%
23	12.645	1790	1795	1801	rBV4	47488	76962	5.81%	0.555%
24	12.768	1809	1816	1818	rBV	266962	289102	21.83%	2.084%
25	12.816	1822	1824	1830	rVB4	15859	19697	1.49%	0.142%
26	12.916	1837	1841	1844	rBV	1587946	1324252	100.00%	9.544%
27	12.986	1849	1853	1858	rBV3	21120	37312	2.82%	0.269%
28	13.074	1865	1868	1869	rBV2	18338	19699	1.49%	0.142%
29	13.098	1869	1872	1875	rVB	49796	52988	4.00%	0.382%
30	13.163	1879	1883	1886	rBV2	32970	37228	2.81%	0.268%
31	13.198	1886	1889	1892	rBV2	46409	51029	3.85%	0.368%
32	13.327	1908	1911	1915	rBV	23807	26428	2.00%	0.190%
33	13.498	1937	1940	1942	rBV3	24110	27333	2.06%	0.197%
34	13.751	1980	1983	1984	rBV	21922	17955	1.36%	0.129%
35	13.768	1984	1986	1992	rVV2	48671	58950	4.45%	0.425%
36	13.968	2016	2020	2023	rBV2	533147	664020	50.14%	4.786%

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ClientSampleId :
SP-E2-COMP

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	2028	rVV	160823	123265	9.31%	0.888%
38	14.057	2032	2035	2041	rVB3	101068	148528	11.22%	1.070%
39	14.145	2048	2050	2053	rVB4	30705	25704	1.94%	0.185%
40	14.451	2098	2102	2106	rBV	234120	253264	19.13%	1.825%
41	14.839	2164	2168	2174	rVB	296399	375491	28.35%	2.706%
42	15.021	2195	2199	2202	rBV	148498	226962	17.14%	1.636%
43	15.274	2238	2242	2247	rBV	263164	385043	29.08%	2.775%
44	15.386	2258	2261	2268	rBV	112640	138034	10.42%	0.995%
45	15.451	2268	2272	2276	rBV	265824	352257	26.60%	2.539%
46	15.786	2324	2329	2340	rVB	257125	506052	38.21%	3.647%
47	16.398	2427	2433	2442	rVB2	182066	382845	28.91%	2.759%
48	17.139	2554	2559	2570	rVB4	136339	339285	25.62%	2.445%
49	18.062	2708	2716	2726	rVB2	97079	333857	25.21%	2.406%

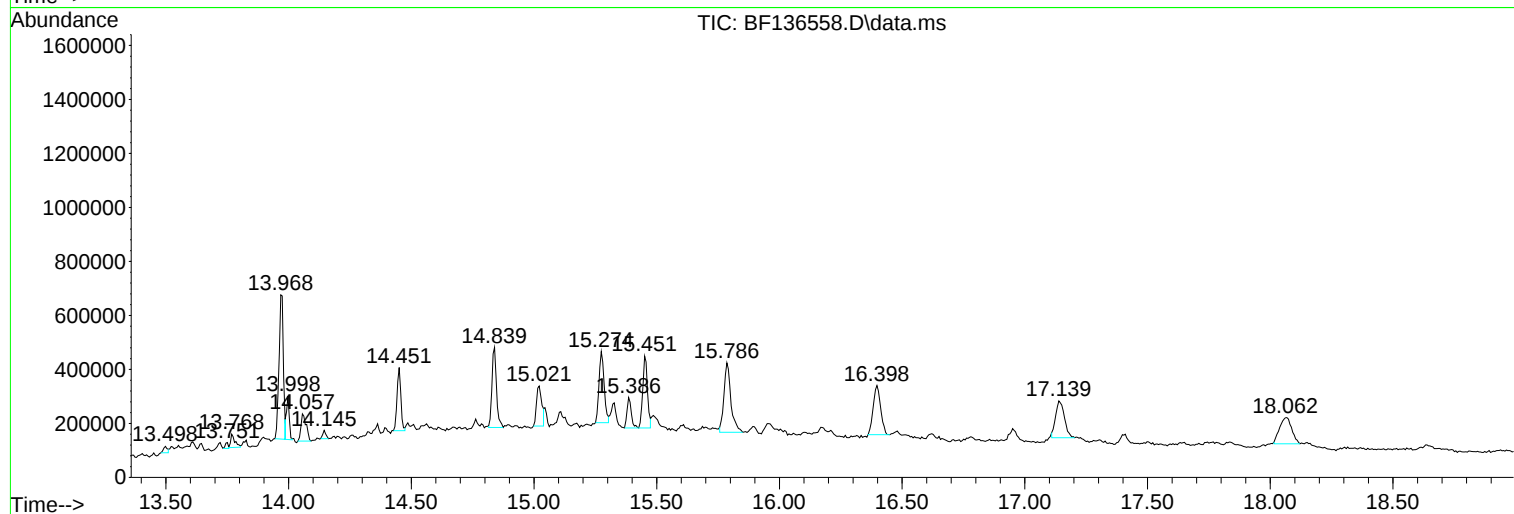
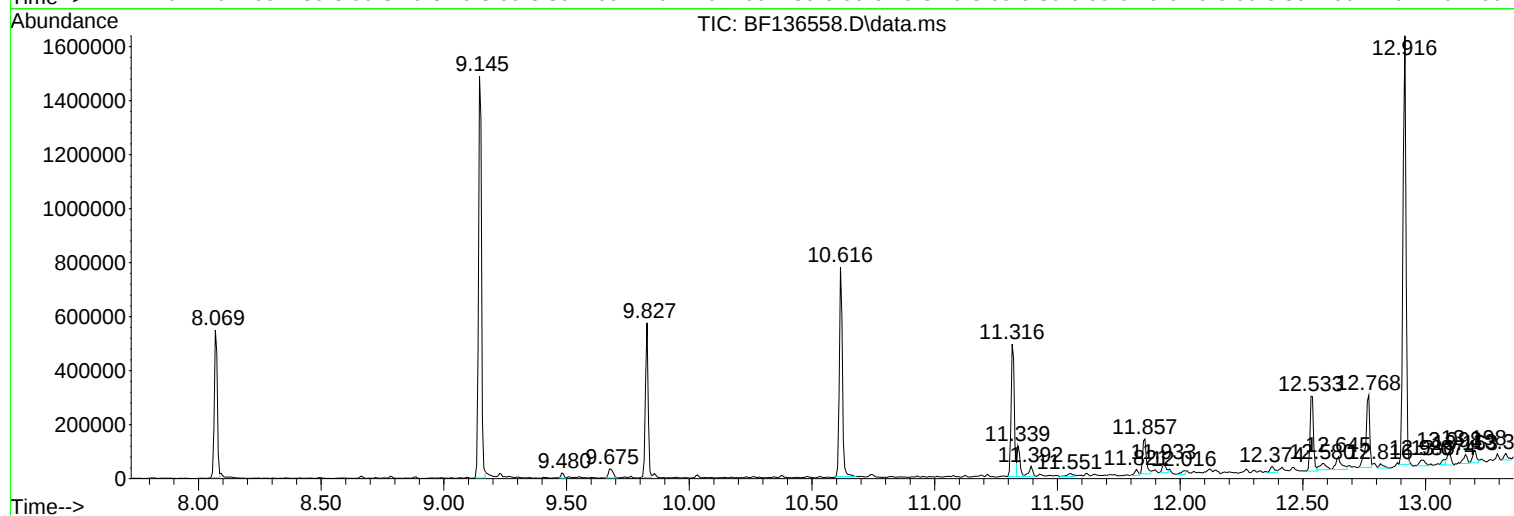
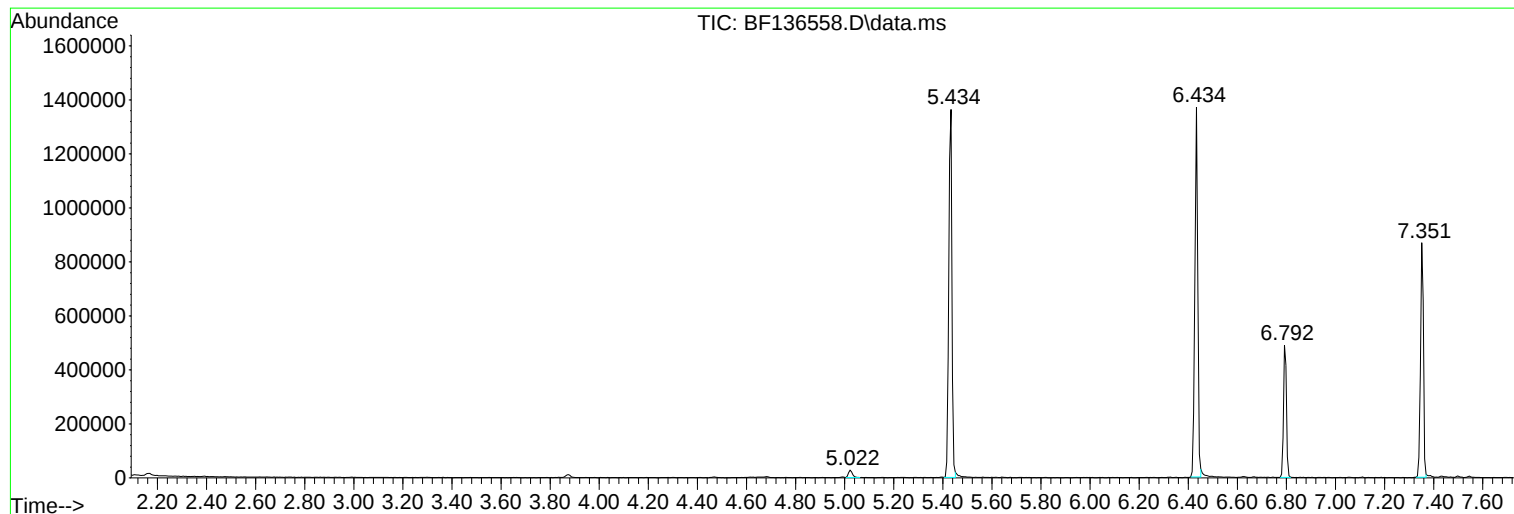
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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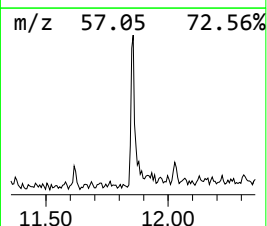
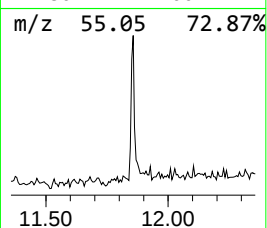
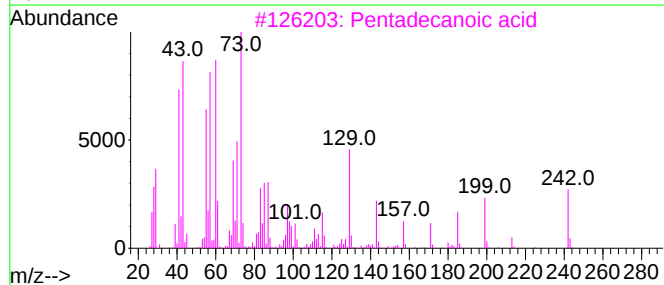
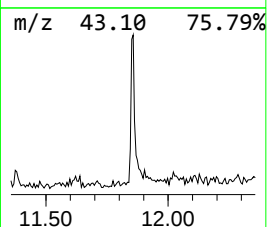
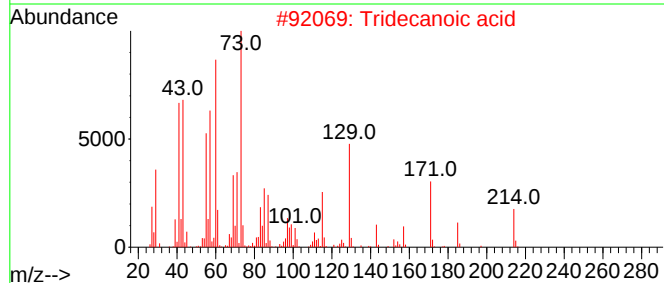
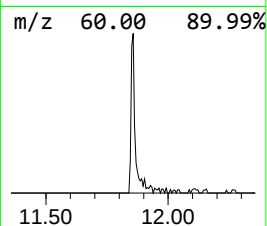
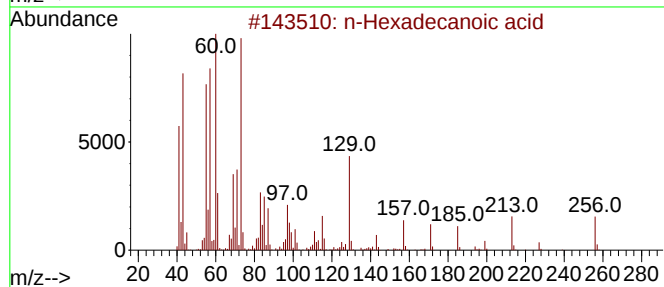
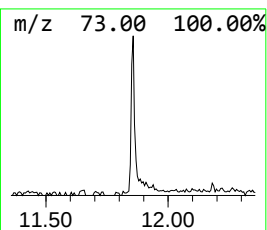
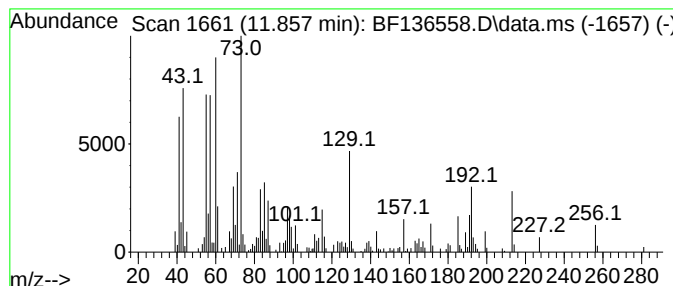
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	6.03 ng	135321	Phenanthrene-d10	11.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	89
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



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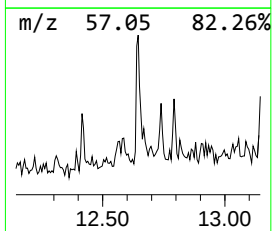
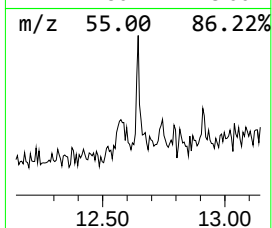
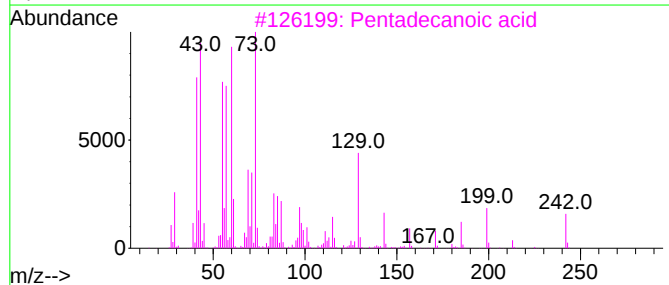
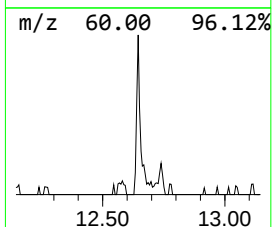
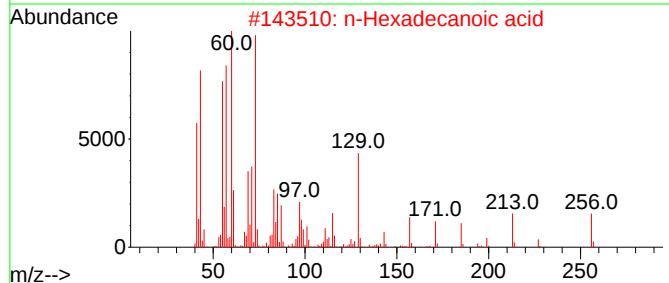
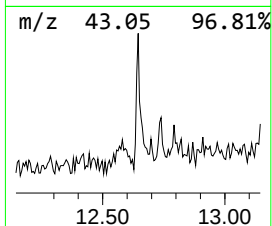
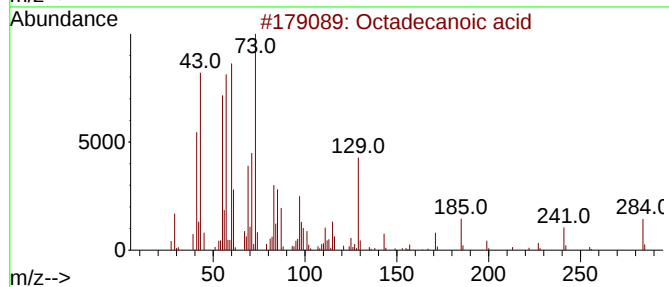
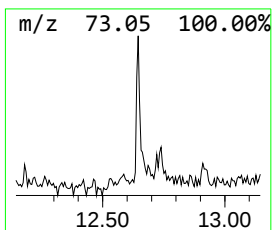
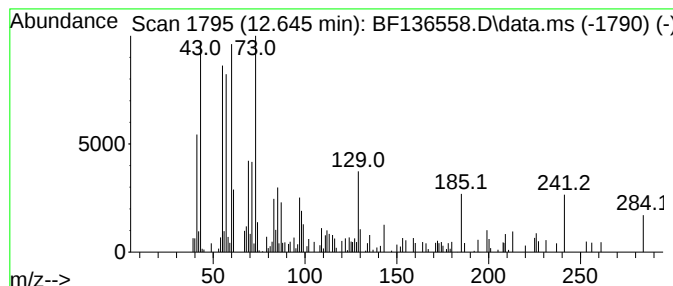
Instrument :
BNA_F
ClientSampleId :
SP-E2-COMP

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 2 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.645	3.43 ng	76962	Phenanthrene-d10		11.316	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octadecanoic acid		284	C18H36O2	000057-11-4	95
2	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	93
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	68
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	59
5	n-Decanoic acid		172	C10H20O2	000334-48-5	53



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Misc :
ALS Vial : 20 Sample Multiplier: 1

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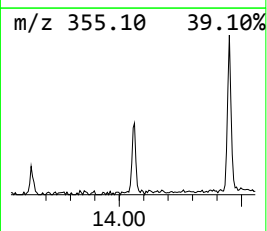
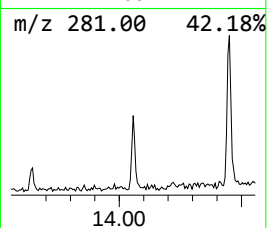
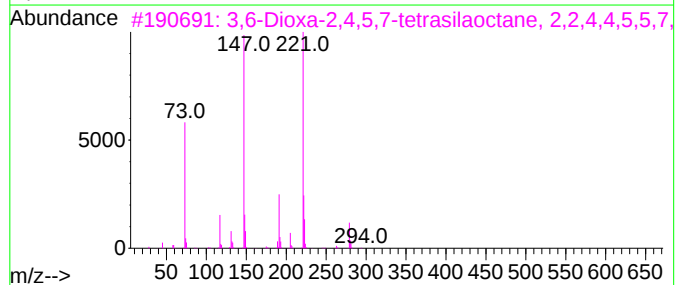
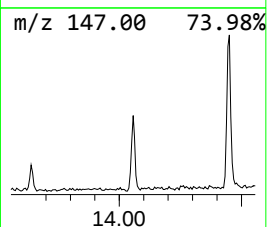
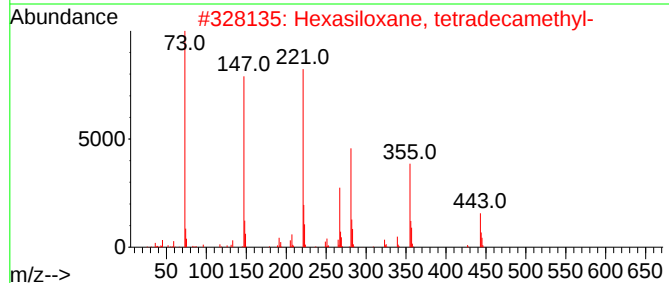
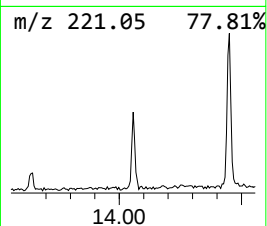
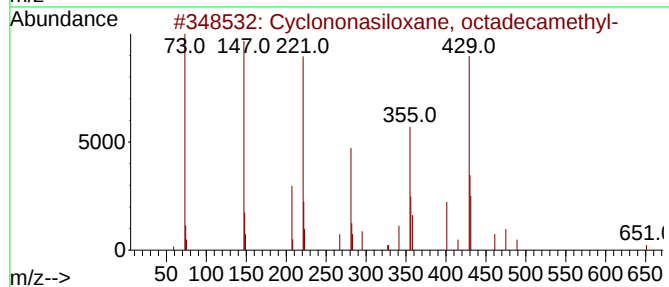
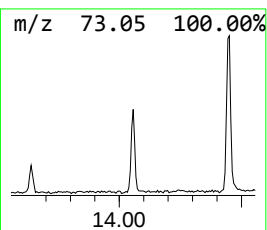
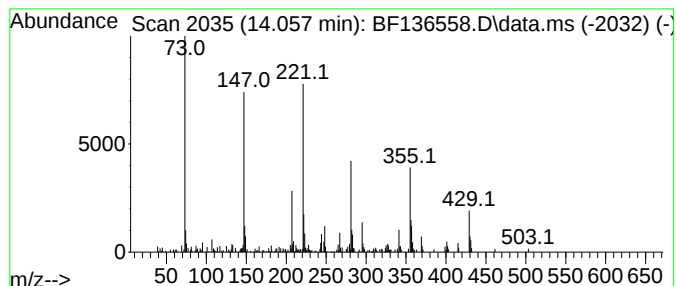
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Cyclononasiloxane, octadeca... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.057	4.47 ng	148528	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	78
2			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	72
3			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	43
4			Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	38
5			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	27



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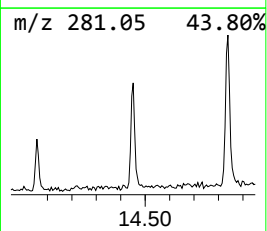
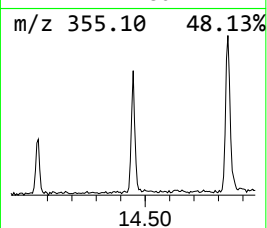
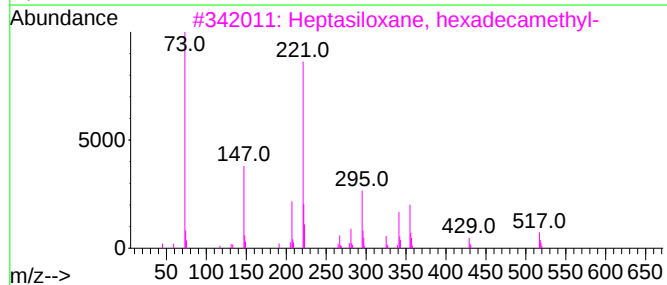
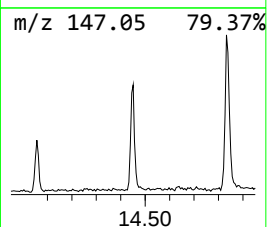
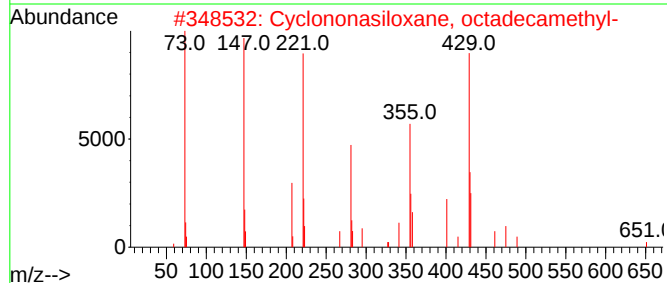
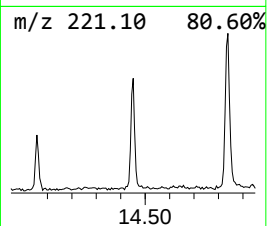
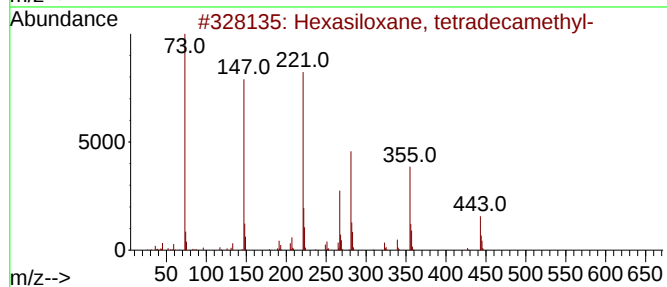
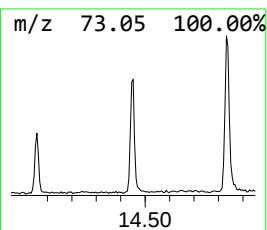
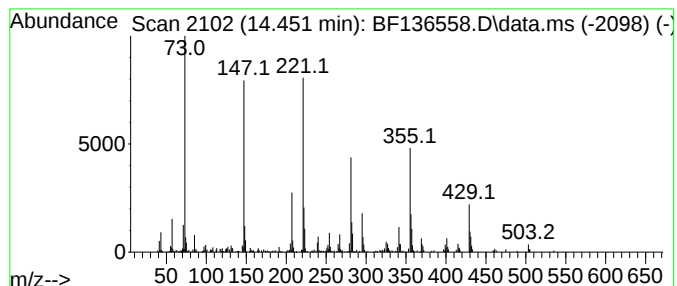
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexasiloxane, tetradecamethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.451	7.63 ng	253264	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	72
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	72
3			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	41
4			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	38
5			Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	30



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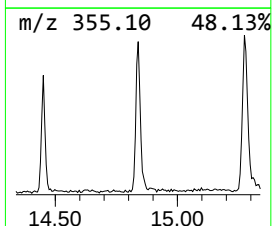
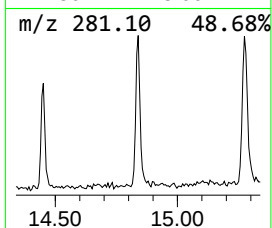
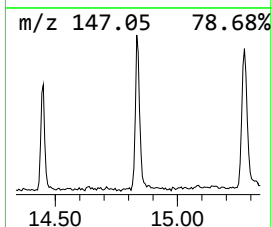
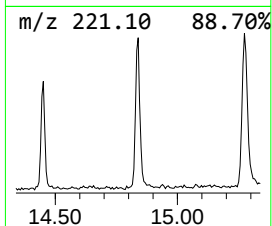
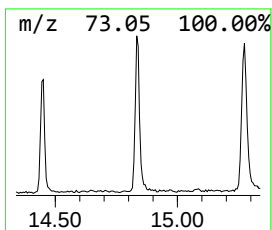
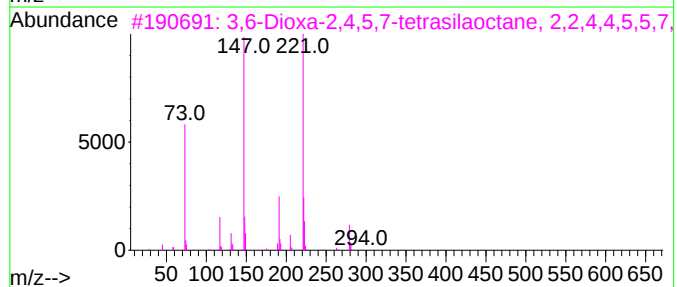
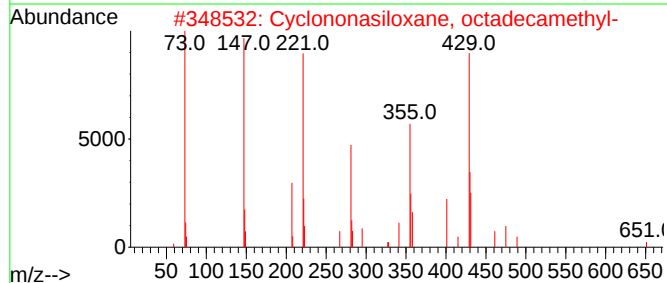
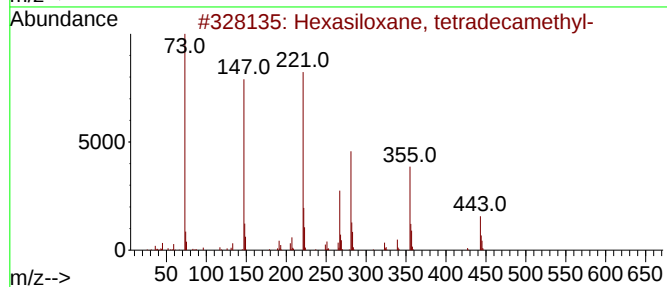
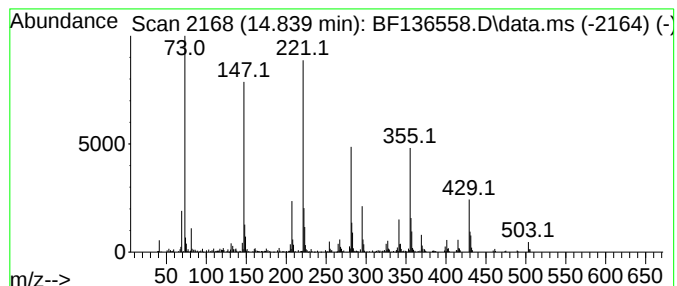
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown14.839 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.839	21.32 ng	375491	Perylene-d12	15.451

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	58
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			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	28



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121323\
Data File : BF136558.D
Acq On : 14 Dec 2023 02:03
Operator : CG\JU
Sample : 05767-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

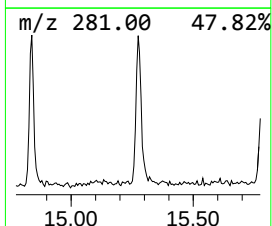
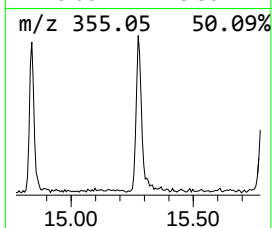
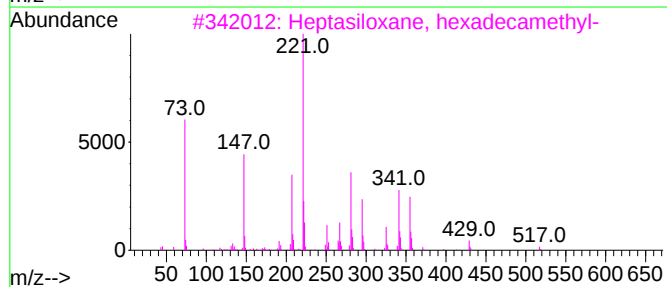
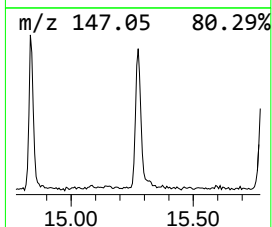
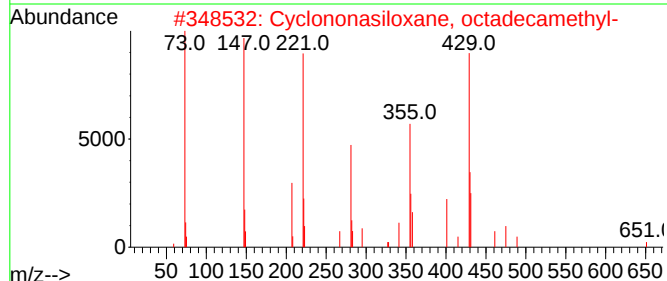
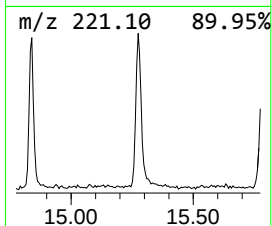
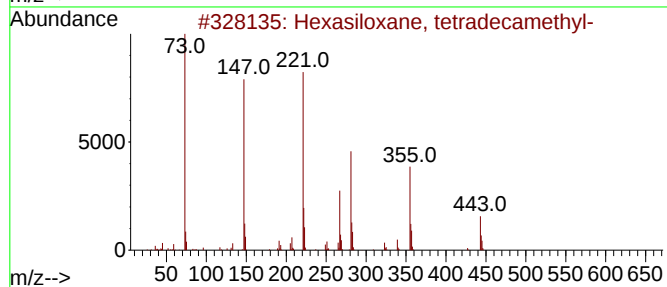
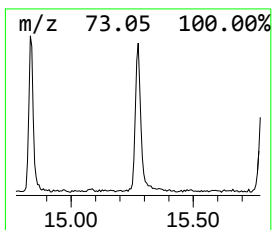
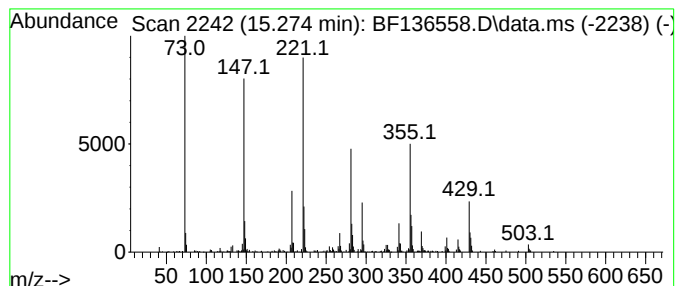
Instrument :
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ClientSampleId :
SP-E2-COMP

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 6 Heptasiloxane, hexadecamethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.274	21.86 ng	385043	Perylene-d12		15.451	
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	74
3	Heptasiloxane, hexadecamethyl-		532	C16H48O6Si7	000541-01-5	50
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\BF121323\
Data File : BF136558.D
Acq On : 14 Dec 2023 02:03
Operator : CG\JU
Sample : 05767-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-E2-COMP

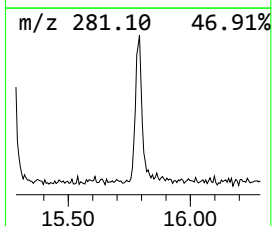
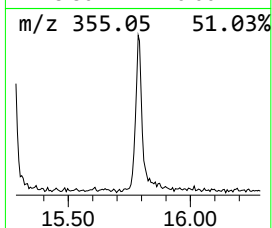
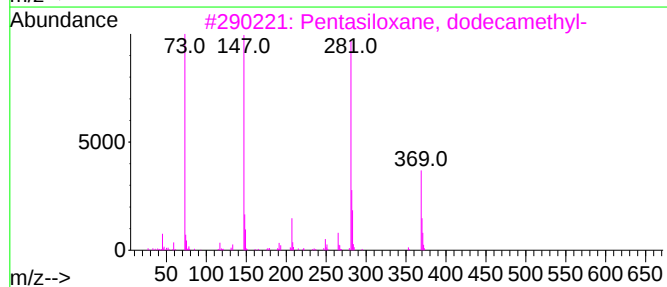
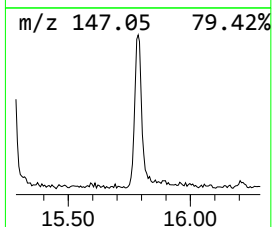
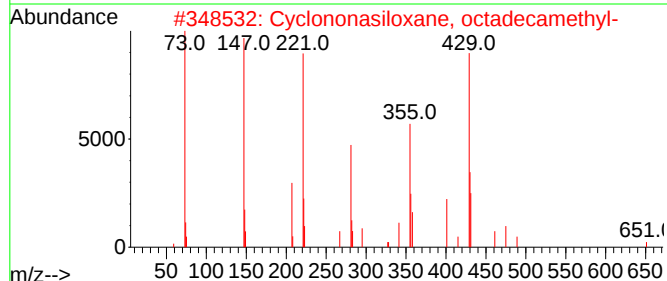
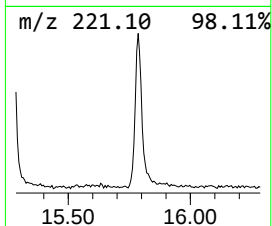
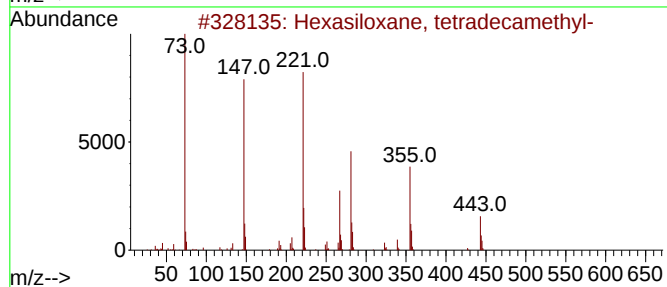
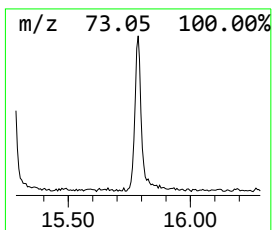
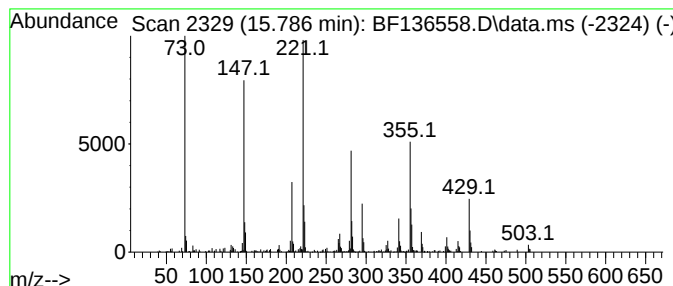
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	28.73 ng	506052	Perylene-d12	15.451

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	42
3		Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	25
4		Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	25
5		3-Hydroxyphthalic anhydride, TMS...	236	C11H12O4Si	1000468-34-8	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121323\
Data File : BF136558.D
Acq On : 14 Dec 2023 02:03
Operator : CG\JU
Sample : 05767-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-E2-COMP

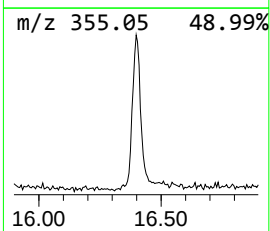
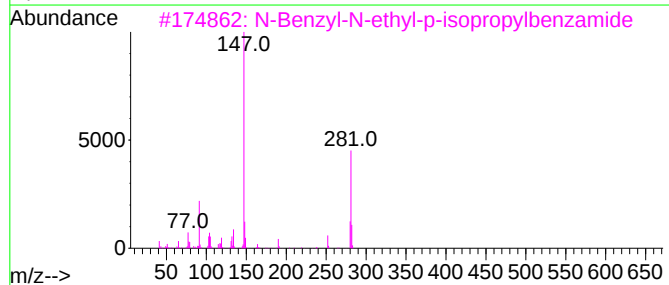
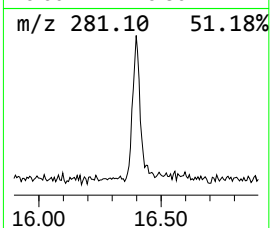
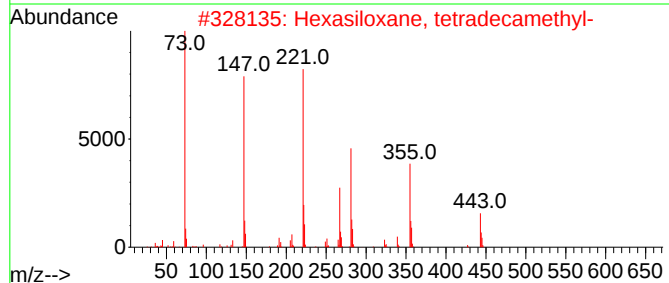
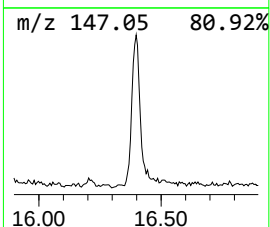
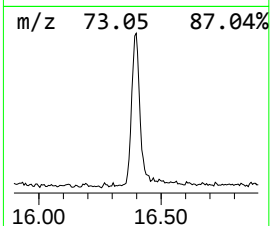
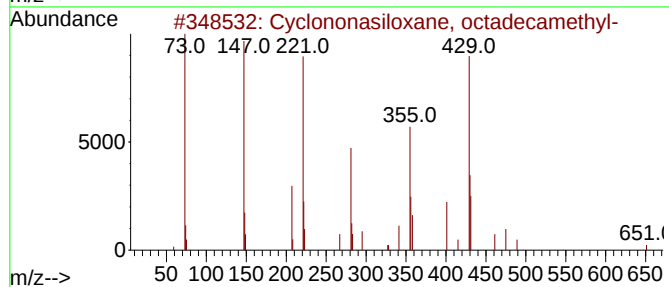
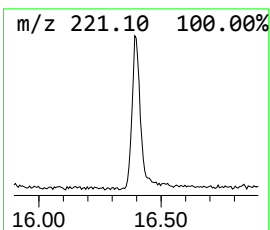
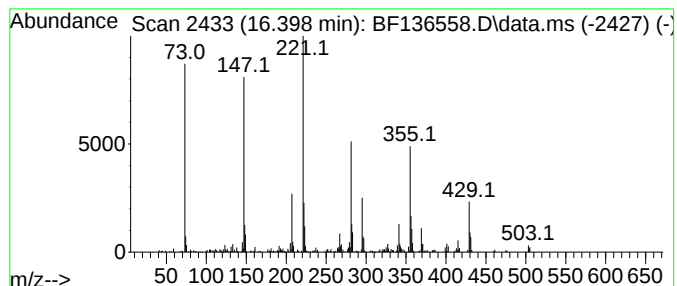
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown16.398 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.398	21.74 ng	382845	Perylene-d12	15.451

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	64
3			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	25
4			Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	25
5			Phthalic acid, 2TMS derivative	310	C14H22O4Si2	002078-22-0	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121323\
Data File : BF136558.D
Acq On : 14 Dec 2023 02:03
Operator : CG\JU
Sample : 05767-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-E2-COMP

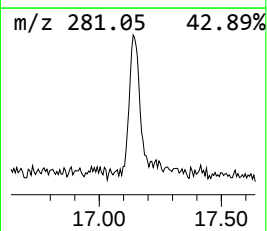
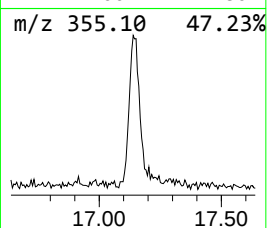
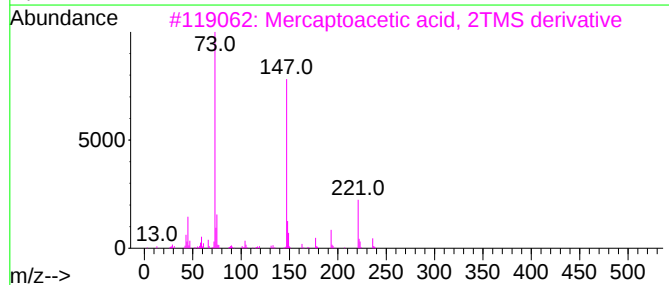
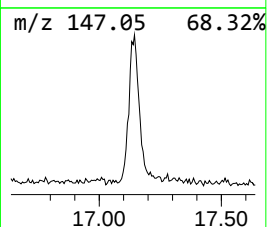
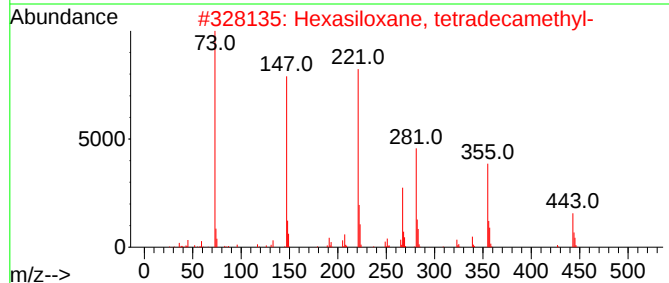
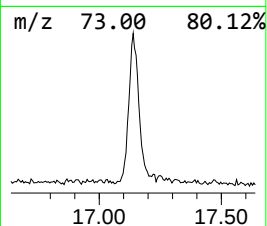
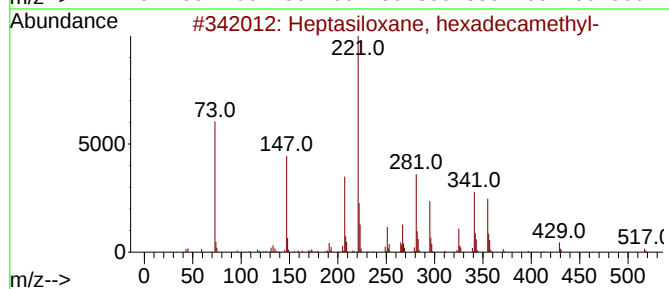
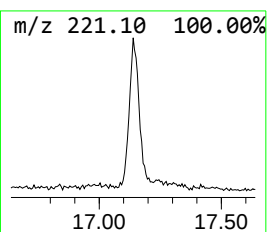
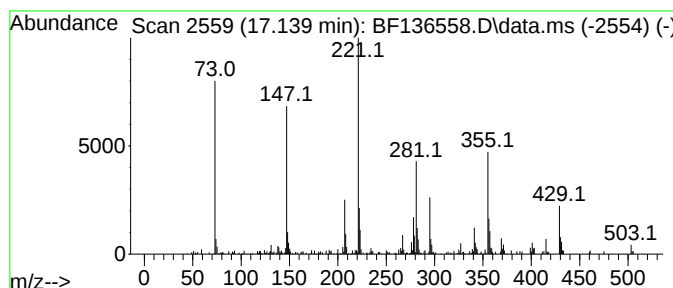
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown17.139 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.139	19.26 ng	339285	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	50
2			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	49
3			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	32
4			Boric acid, 3TMS derivative	278	C9H27B03Si3	004325-85-3	27
5			Bis(4-tert-butyltrimethylsiloxy)b...	458	C26H42O3Si2	1000431-17-0	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121323\
Data File : BF136558.D
Acq On : 14 Dec 2023 02:03
Operator : CG\JU
Sample : 05767-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-E2-COMP

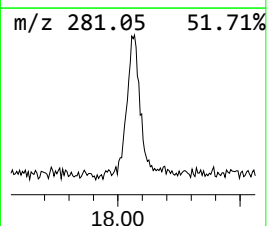
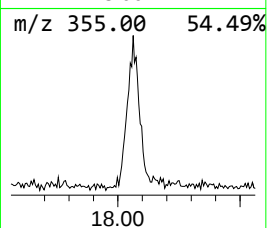
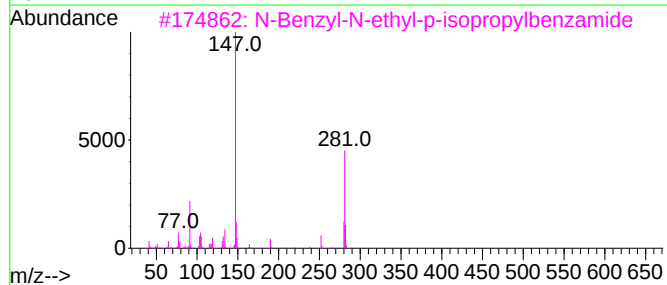
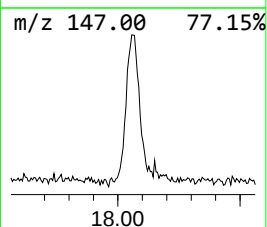
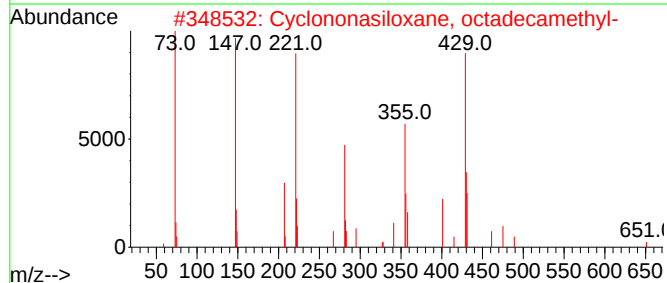
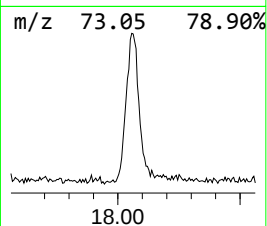
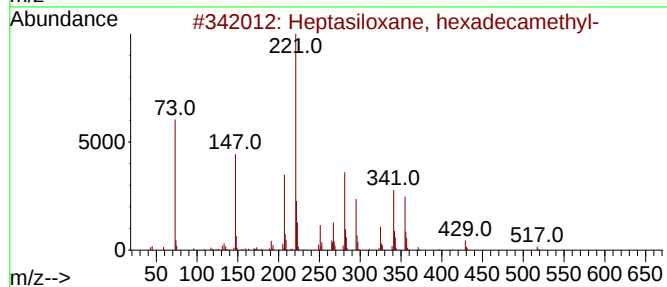
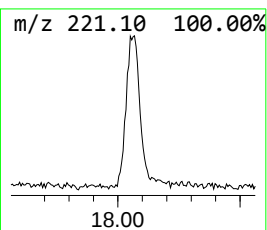
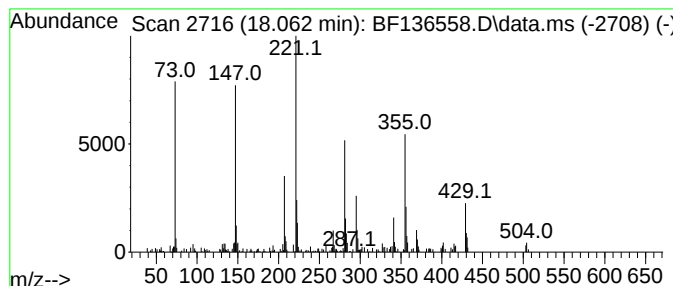
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown18.062 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.062	18.96 ng	333857	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	64
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	47
3			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	25
4			2-Hydrazinyl-5-nitropyridine, 3T...	370	C14H30N4O2Si3	1000478-90-5	25
5			6-Amino-2-(fluoromethylidene)-3-...	355	C19H22FN3OSi	1010408-41-2	15



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121323\
Data File : BF136558.D
Acq On : 14 Dec 2023 02:03
Operator : CG\JU
Sample : 05767-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-E2-COMP

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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Octadecanoic acid	12.645	3.4	ng	76962	4	11.316	449102	20.0
Cyclononasiloxa...	14.057	4.5	ng	148528	5	13.974	664020	20.0
Hexasiloxane, t...	14.451	7.6	ng	253264	5	13.974	664020	20.0
unknown14.839	14.839	21.3	ng	375491	6	15.451	352257	20.0
Heptasiloxane, ...	15.274	21.9	ng	385043	6	15.451	352257	20.0
unknown15.786	15.786	28.7	ng	506052	6	15.451	352257	20.0
unknown16.398	16.398	21.7	ng	382845	6	15.451	352257	20.0
unknown17.139	17.139	19.3	ng	339285	6	15.451	352257	20.0
unknown18.062	18.062	19.0	ng	333857	6	15.451	352257	20.0