

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121123\
 Data File : BF136492.D
 Acq On : 11 Dec 2023 16:03
 Operator : CG\JU
 Sample : PB157670BL
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB157670BL

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: BF136492.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.463	394	404	407	rBV	3460354	6012576	100.00%	14.427%
2	4.704	440	445	456	rVB	78725	87482	1.45%	0.210%
3	5.069	497	507	510	rBV	2170073	3811919	63.40%	9.147%
4	5.457	567	573	576	rBV	3663704	3791096	63.05%	9.097%
5	5.828	632	636	639	rBV	390157	330500	5.50%	0.793%
6	6.446	733	741	744	rBV	3239259	3953340	65.75%	9.486%
7	6.793	797	800	804	rVB	1023107	793273	13.19%	1.903%
8	7.357	890	896	899	rBV	2127481	2451020	40.76%	5.881%
9	8.069	1012	1017	1021	rBV	1230652	1109305	18.45%	2.662%
10	9.151	1195	1201	1204	rBV	4967048	5004008	83.23%	12.007%
11	9.828	1310	1316	1319	rBV	1597896	1319256	21.94%	3.166%
12	10.622	1445	1451	1455	rBV	3031038	3220281	53.56%	7.727%
13	11.322	1565	1570	1573	rBV	1648190	1435518	23.88%	3.445%
14	12.922	1837	1842	1845	rBV	5387093	5475956	91.08%	13.140%
15	13.969	2016	2020	2024	rBV	1092900	1061374	17.65%	2.547%
16	14.839	2164	2168	2177	rBV2	62701	82635	1.37%	0.198%
17	15.110	2210	2214	2217	rBV	56862	74409	1.24%	0.179%
18	15.274	2237	2242	2255	rVB2	77077	126809	2.11%	0.304%
19	15.451	2266	2272	2277	rBV	650521	797727	13.27%	1.914%
20	15.498	2277	2280	2288	rVB	68874	92937	1.55%	0.223%
21	15.786	2323	2329	2338	rBV2	68041	129972	2.16%	0.312%
22	15.951	2352	2357	2362	rVB	51983	76984	1.28%	0.185%
23	16.398	2426	2433	2440	rBV4	53285	130004	2.16%	0.312%
24	16.480	2442	2447	2453	rVB	44093	82851	1.38%	0.199%
25	17.021	2525	2539	2540	rBV	22579	69969	1.16%	0.168%
26	17.145	2557	2560	2569	rVB4	36133	78507	1.31%	0.188%
27	18.068	2708	2717	2726	rBV6	22983	75189	1.25%	0.180%

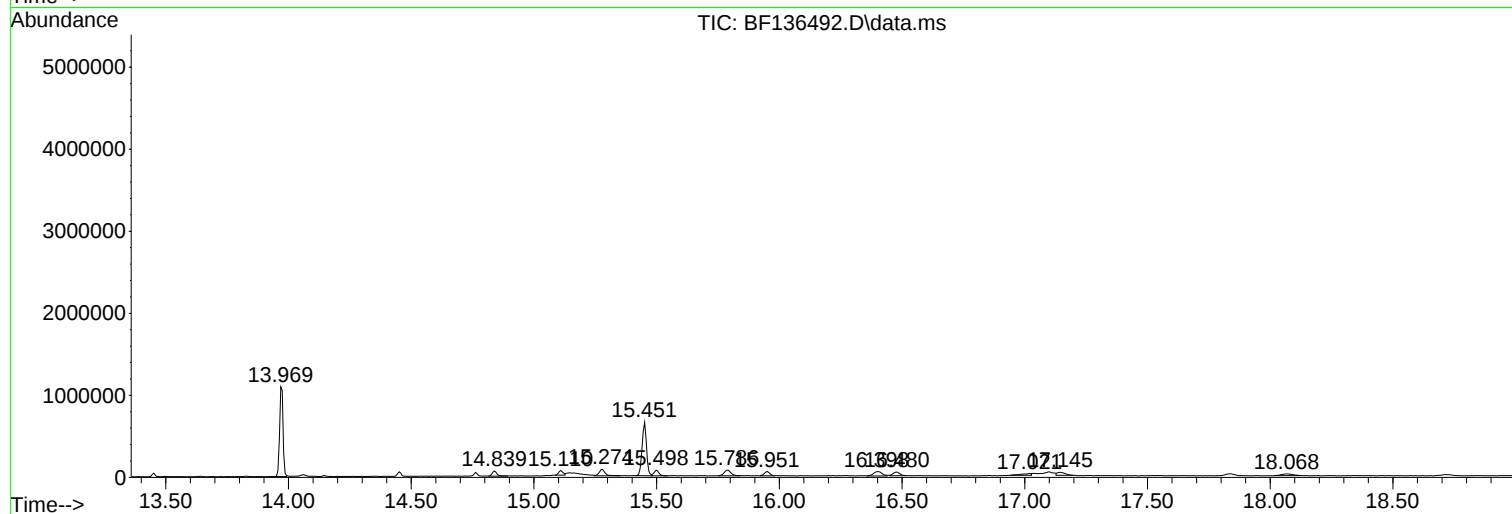
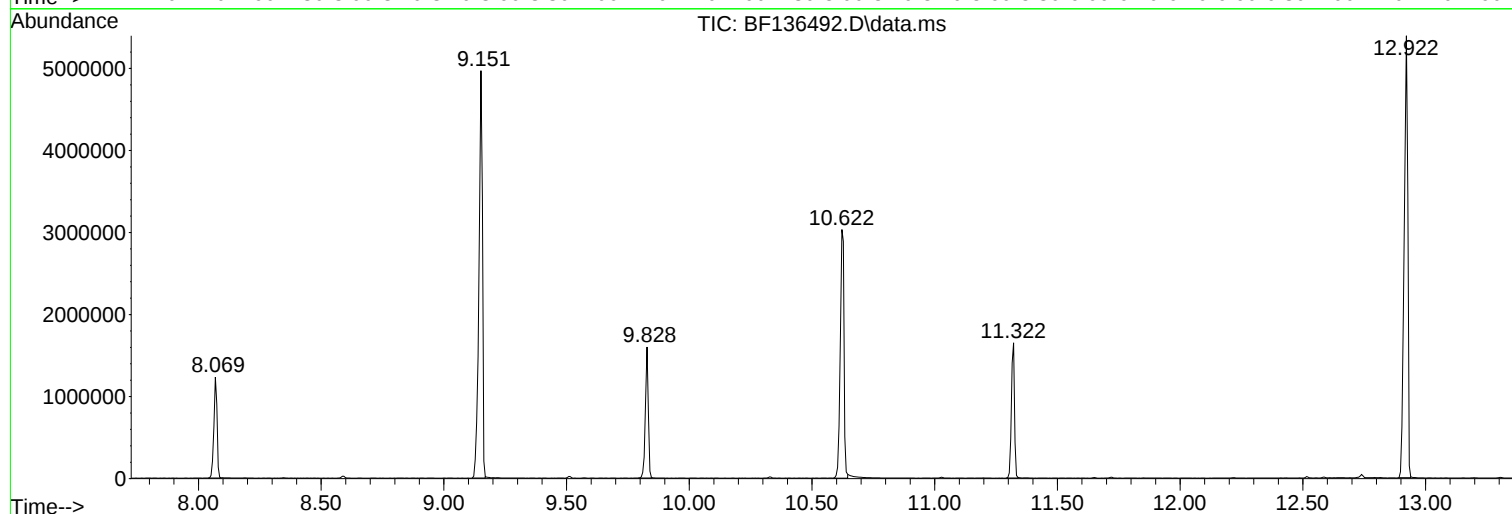
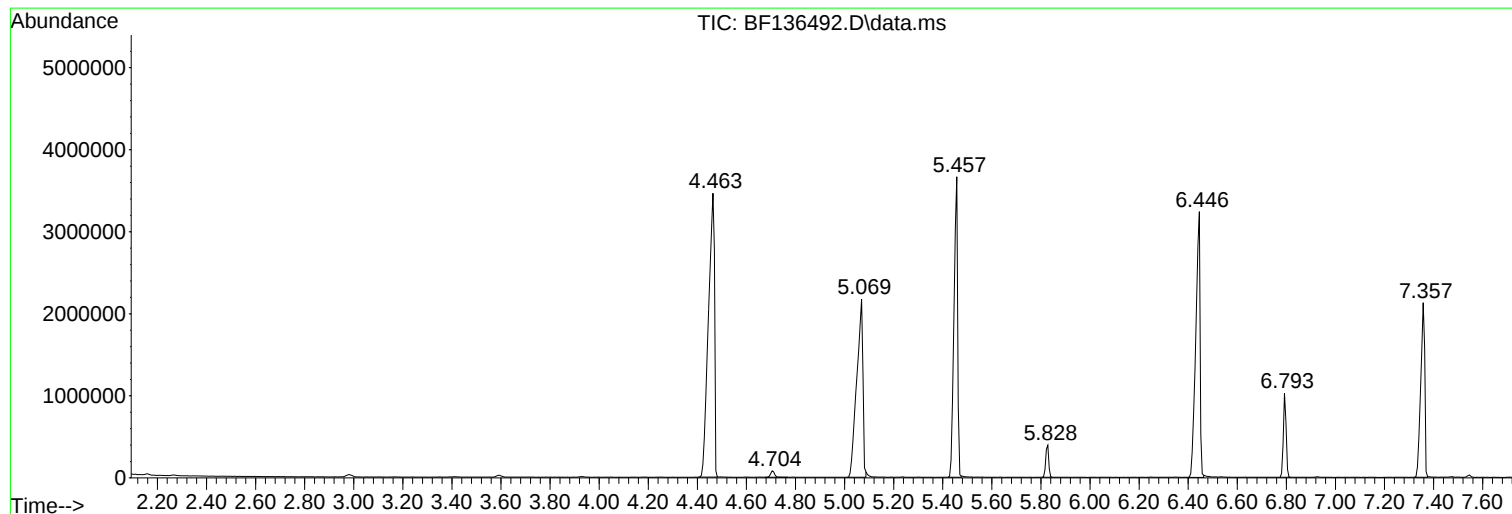
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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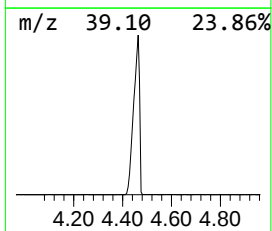
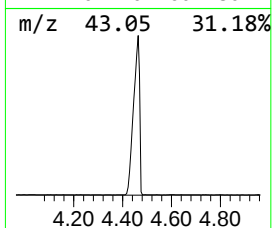
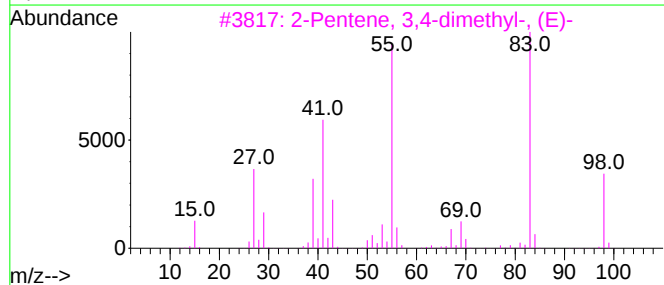
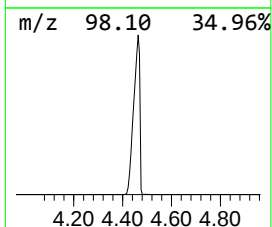
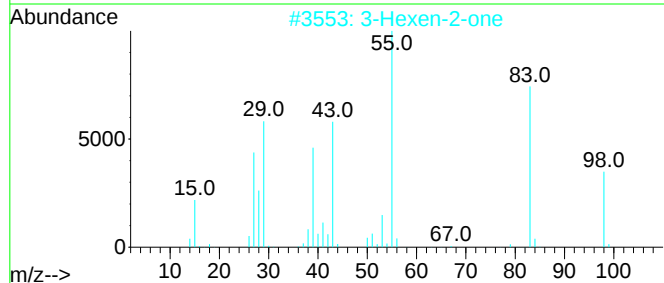
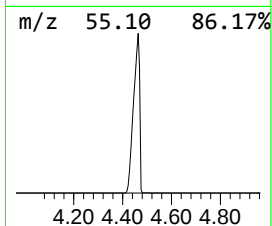
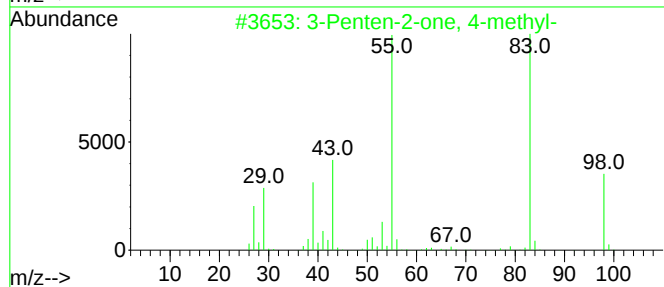
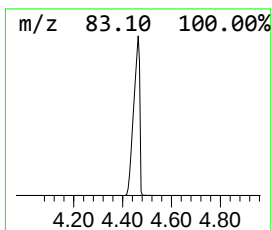
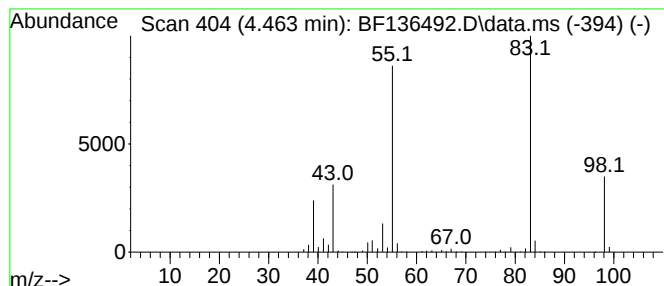
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.463	151.59 ng	6012580	1,4-Dichlorobenzene-d4	6.793

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91	
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91	
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90	
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86	
5	Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78	



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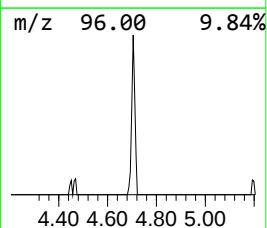
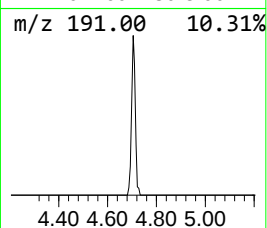
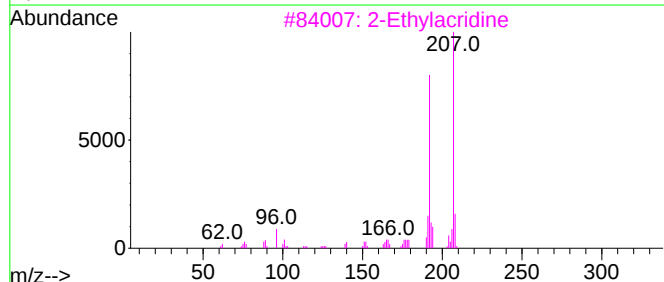
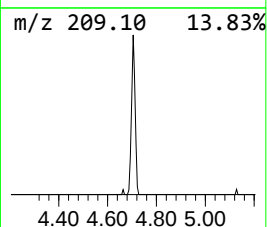
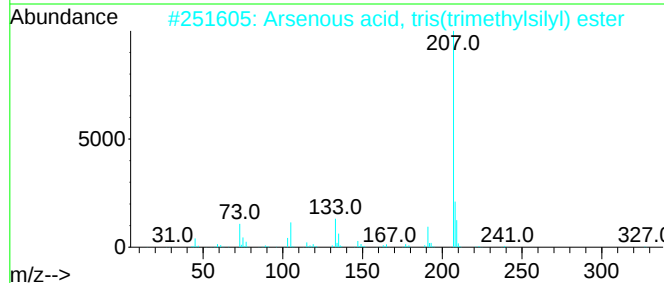
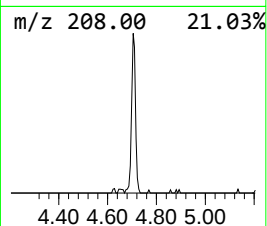
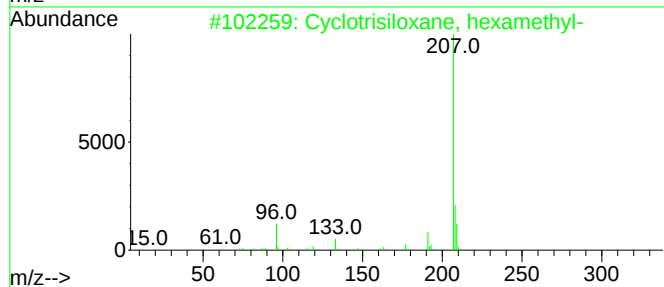
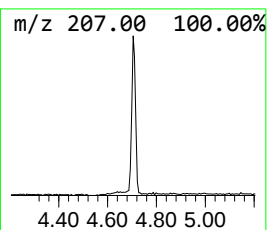
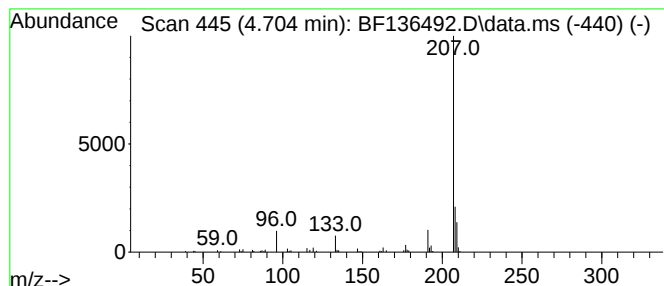
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Cyclotrisiloxane, hexamethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.704	2.21 ng	87482	1,4-Dichlorobenzene-d4	6.793

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotrisiloxane, hexamethyl-	222	C6H18O3Si3	000541-05-9	91
2			Arsenous acid, tris(trimethylsil...	342	C9H27AsO3Si3	055429-29-3	78
3			2-Ethylacridine	207	C15H13N	055751-83-2	45
4			1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	39
5			4-tert-Octylphenol, TMS derivative	278	C17H30OSi	078721-87-6	38



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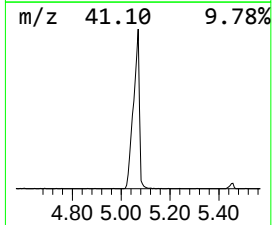
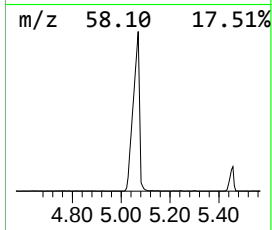
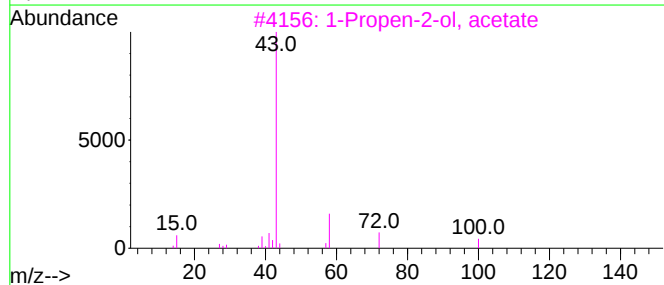
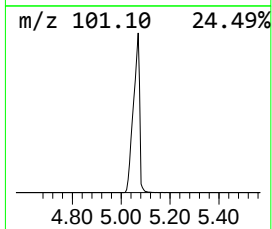
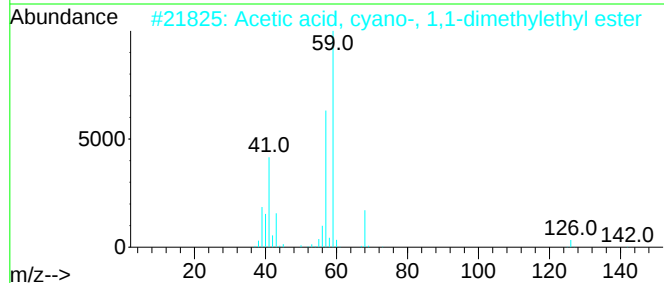
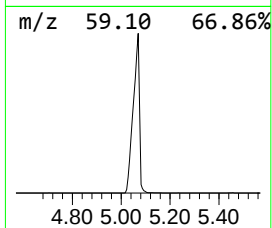
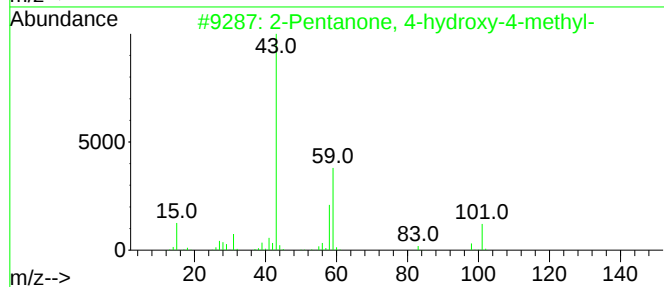
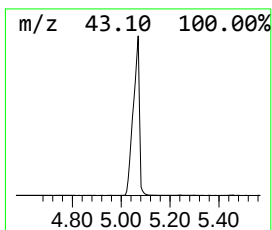
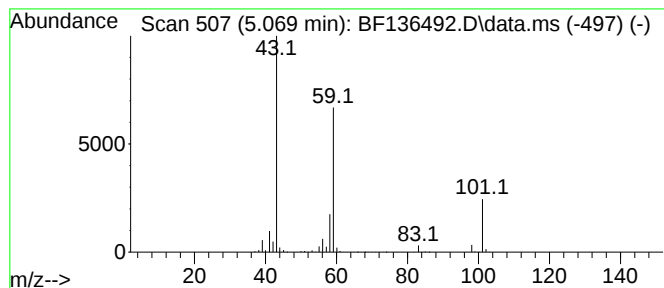
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.069	96.11 ng	3811920	1,4-Dichlorobenzene-d4	6.793	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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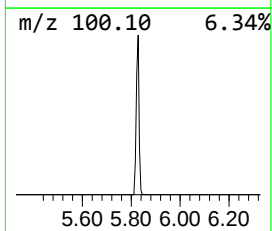
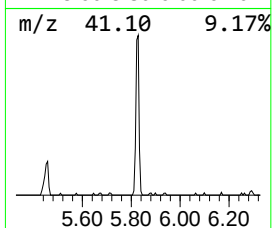
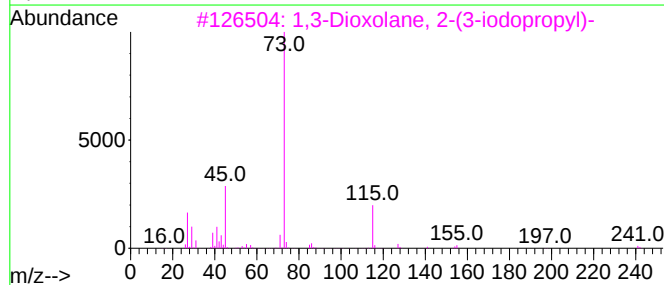
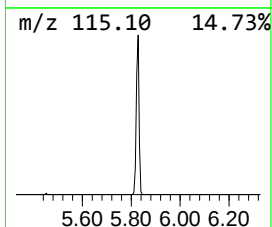
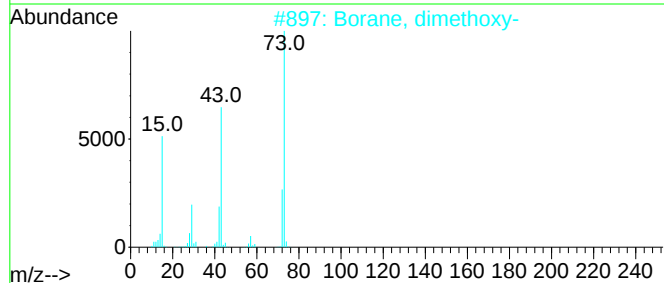
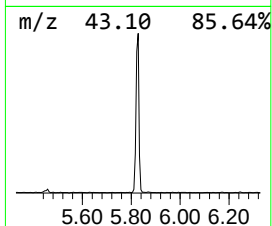
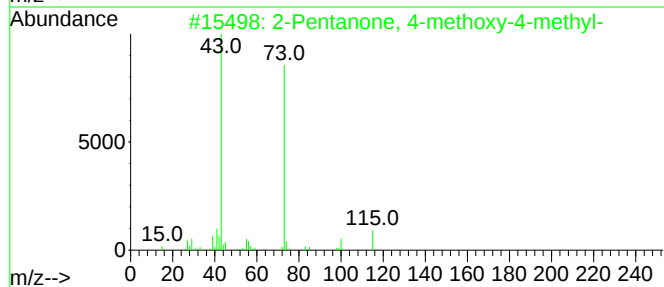
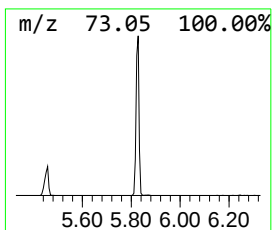
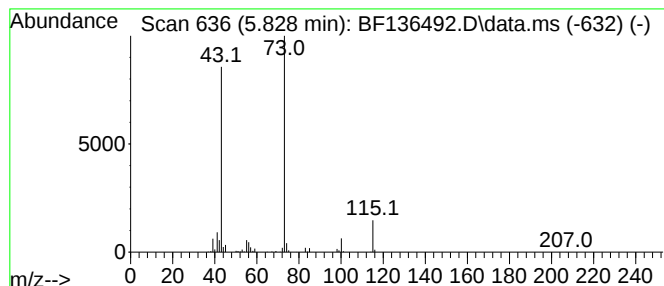
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Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.828	8.33 ng	330500	1,4-Dichlorobenzene-d4	6.793

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	38
3			1,3-Dioxolane, 2-(3-iodopropyl)-	242	C6H11IO2	058135-25-4	28
4			3-Hexanol, acetate	144	C8H16O2	040780-64-1	25
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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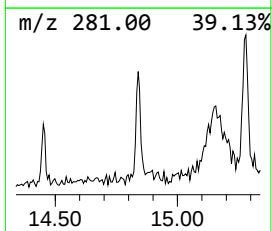
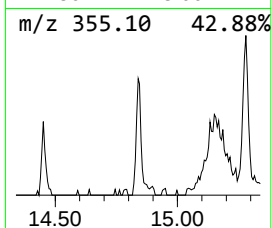
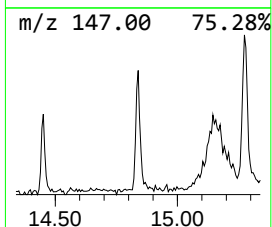
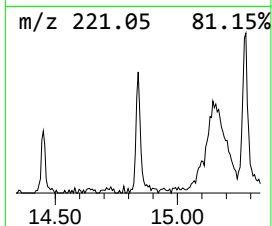
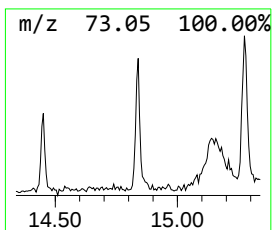
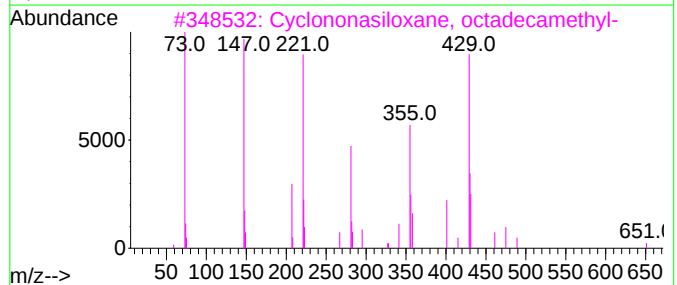
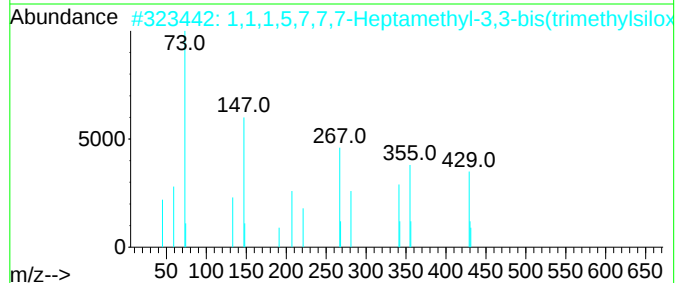
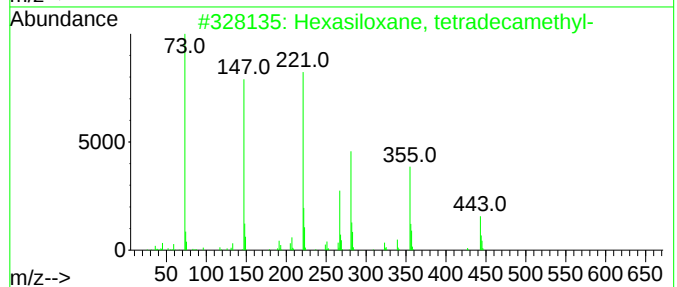
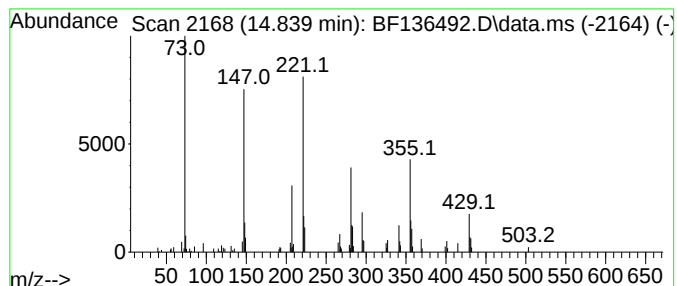
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Peak Number 5 Hexasiloxane, tetradecamethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.839	2.07 ng	82635	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	83
2			1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	42
3			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	40
4			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	38
5			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	38



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ClientSampleId :
PB157670BL

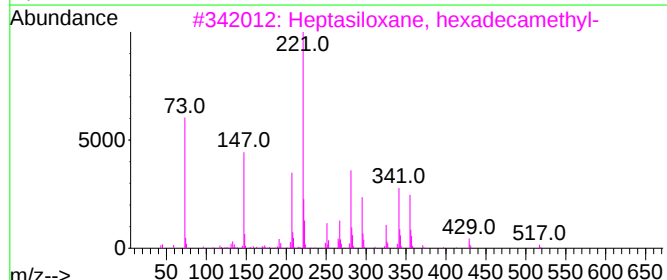
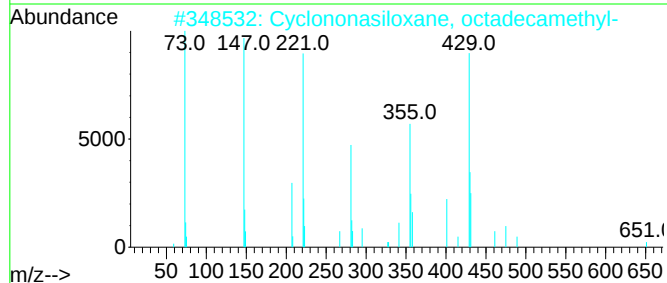
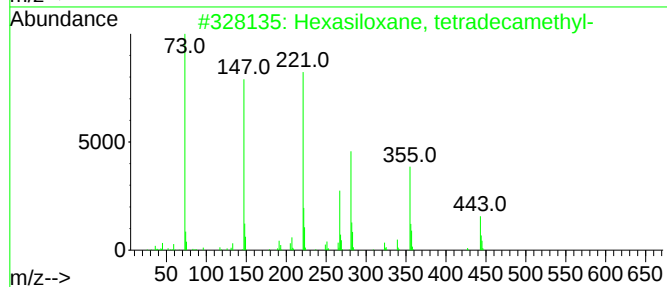
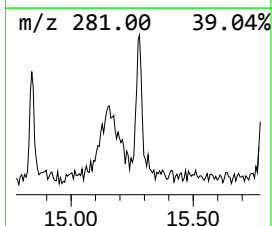
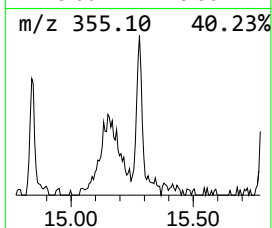
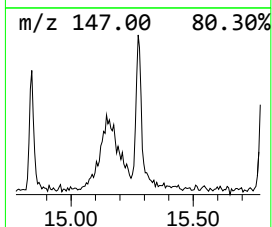
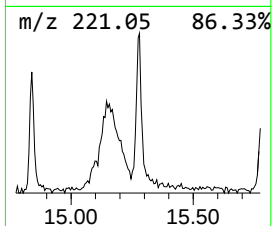
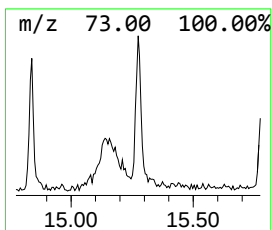
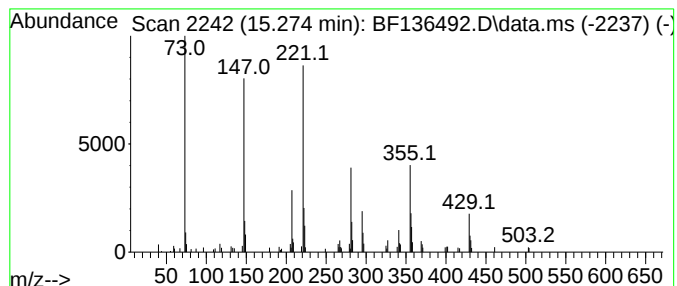
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclononasiloxane, octadeca... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.274	3.18 ng	126809	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	87
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	87
3			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	40
4			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	40
5			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121123\
Data File : BF136492.D
Acq On : 11 Dec 2023 16:03
Operator : CG\JU
Sample : PB157670BL
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB157670BL

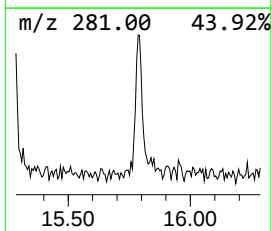
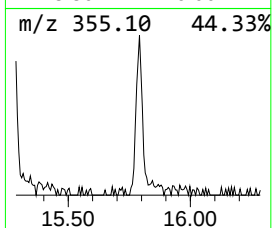
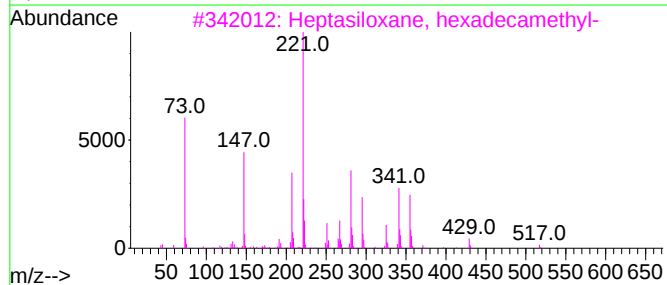
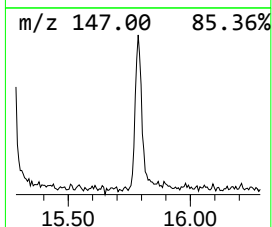
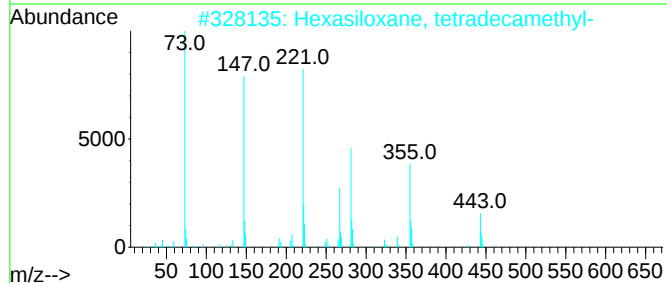
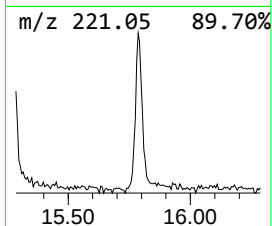
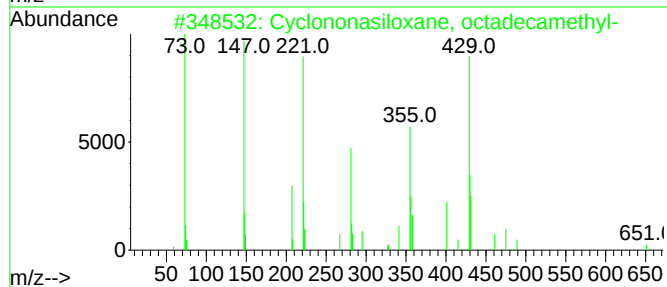
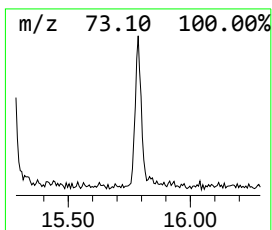
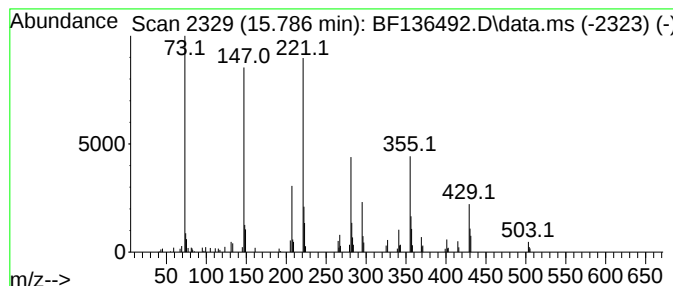
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptasiloxane, hexadecamethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.786	3.26 ng	129972	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	72
3			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	59
4			1,1,1,5,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	38
5			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121123\
Data File : BF136492.D
Acq On : 11 Dec 2023 16:03
Operator : CG\JU
Sample : PB157670BL
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB157670BL

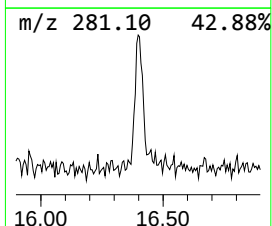
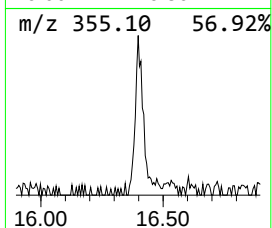
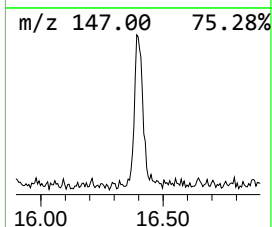
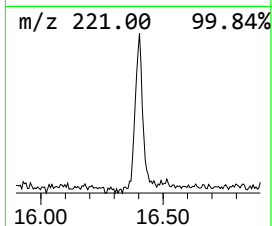
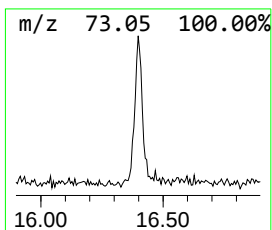
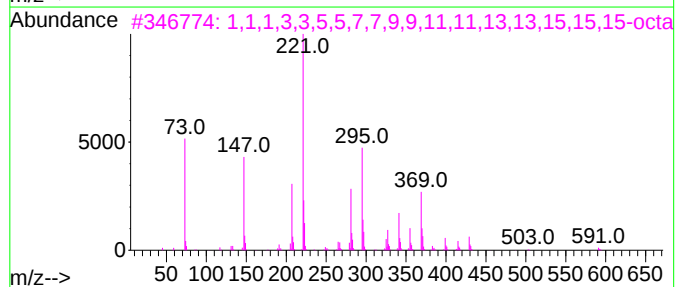
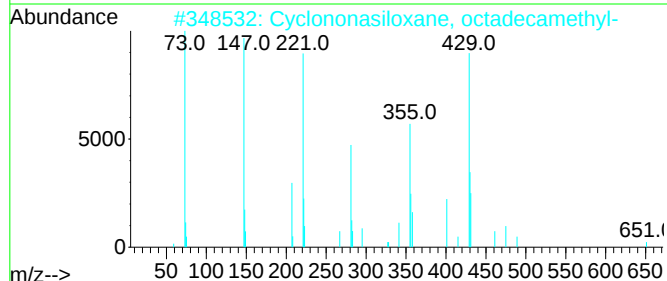
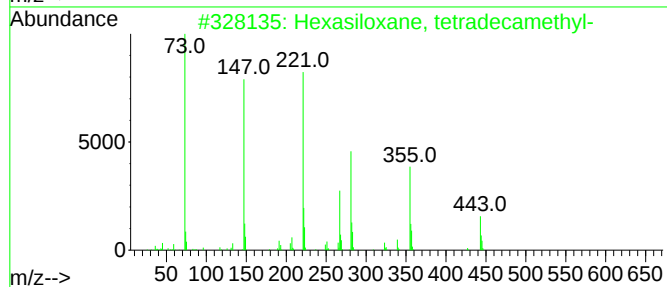
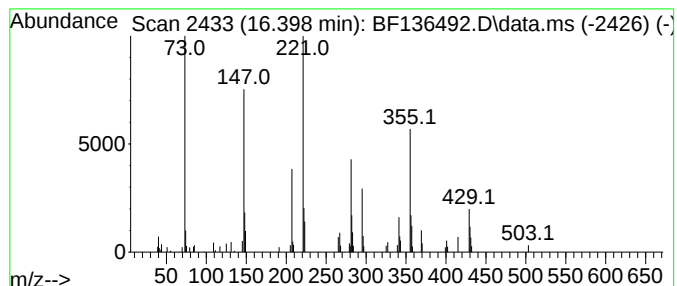
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	3.26 ng	130004	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	58
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	42
3			1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	606	C18H54O7Si8	000556-69-4	25
4			Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	22
5			Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121123\
Data File : BF136492.D
Acq On : 11 Dec 2023 16:03
Operator : CG\JU
Sample : PB157670BL
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB157670BL

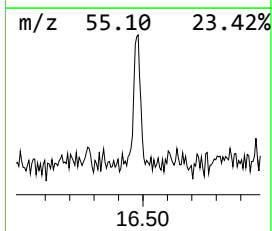
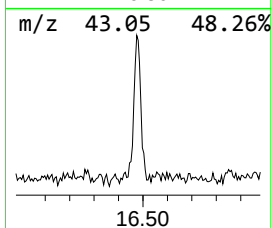
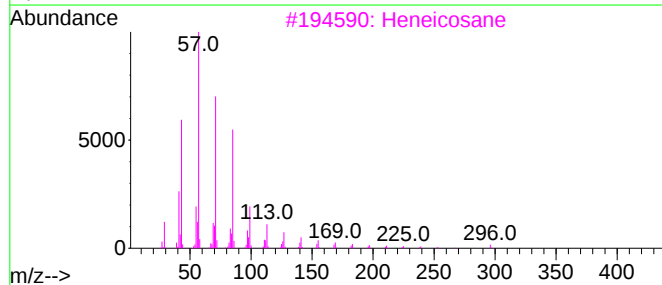
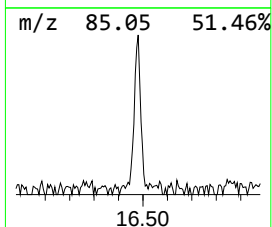
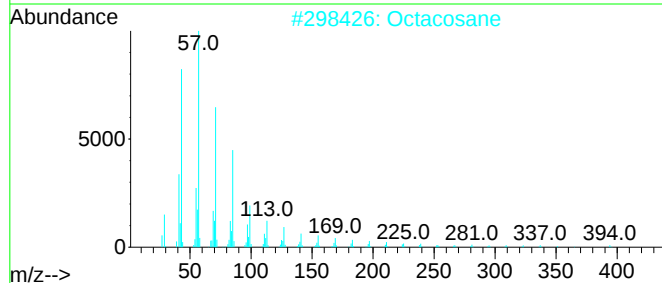
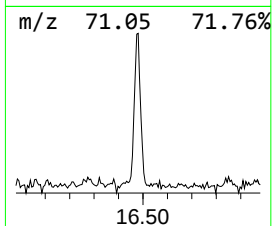
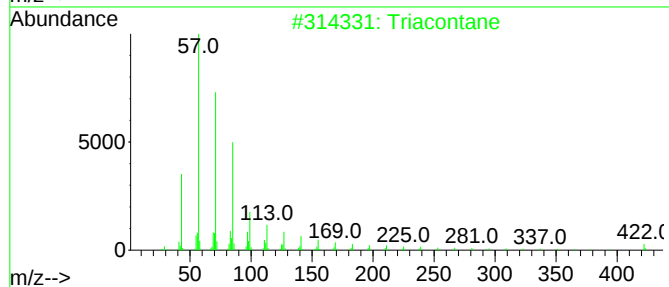
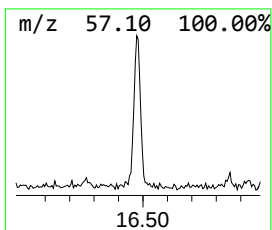
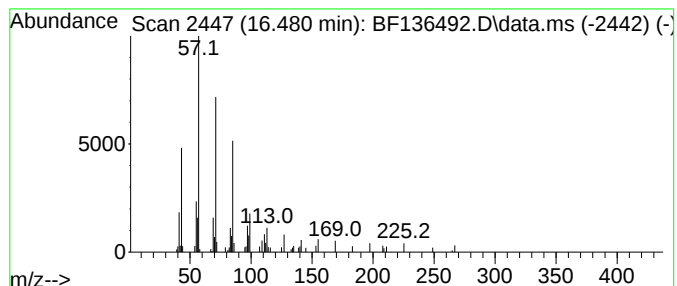
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Triacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.480	2.08 ng	82851	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triacontane	422	C30H62	000638-68-6	91
2			Octacosane	394	C28H58	000630-02-4	90
3			Heneicosane	296	C21H44	000629-94-7	90
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
5			Pentacosane	352	C25H52	000629-99-2	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121123\
Data File : BF136492.D
Acq On : 11 Dec 2023 16:03
Operator : CG\JU
Sample : PB157670BL
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
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\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one,...	4.463	151.6	ng	6012580	1	6.793	793273	20.0
Cyclotrisiloxan...	4.704	2.2	ng	87482	1	6.793	793273	20.0
2-Pentanone, 4-...	5.069	96.1	ng	3811920	1	6.793	793273	20.0
2-Pentanone, 4-...	5.828	8.3	ng	330500	1	6.793	793273	20.0
Hexasiloxane, t...	14.839	2.1	ng	82635	6	15.451	797727	20.0
Cyclononasiloxa...	15.274	3.2	ng	126809	6	15.451	797727	20.0
Heptasiloxane, ...	15.786	3.3	ng	129972	6	15.451	797727	20.0
unknown16.398	16.398	3.3	ng	130004	6	15.451	797727	20.0
triacontane	16.480	2.1	ng	82851	6	15.451	797727	20.0