

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081123\
 Data File : BF134721.D
 Acq On : 11 Aug 2023 08:39
 Operator : CG\JU
 Sample : PB154756BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB154756BL

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-BF080123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134721.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	7	11	18	rVB	143856	198092	2.99%	0.497%
2	2.257	25	29	36	rVB	55573	73861	1.12%	0.185%
3	5.063	503	506	514	rVB	147699	217191	3.28%	0.545%
4	5.445	565	571	574	rBV	4751869	5153503	77.83%	12.937%
5	6.439	734	740	743	rBV	4168476	5230137	78.99%	13.130%
6	6.798	797	801	804	rBV	1193816	919675	13.89%	2.309%
7	7.363	891	897	900	rBV	3304596	3451408	52.13%	8.664%
8	8.075	1013	1018	1022	rBV	1476457	1235094	18.65%	3.101%
9	9.157	1196	1202	1205	rBV	5663425	5916479	89.36%	14.852%
10	9.833	1311	1317	1320	rBV	1538556	1415886	21.38%	3.554%
11	10.627	1446	1452	1455	rBV	3923782	3943452	59.56%	9.899%
12	11.321	1566	1570	1578	rBV	1745934	1481294	22.37%	3.719%
13	12.921	1837	1842	1845	rBV	6145298	6621188	100.00%	16.622%
14	13.968	2016	2020	2032	rBV	1281614	1285463	19.41%	3.227%
15	14.062	2032	2036	2046	rVB	172359	188629	2.85%	0.474%
16	14.457	2099	2103	2110	rBV	292901	334484	5.05%	0.840%
17	14.839	2164	2168	2183	rBV2	321558	471010	7.11%	1.182%
18	15.280	2238	2243	2256	rBV2	167773	313178	4.73%	0.786%
19	15.439	2265	2270	2279	rBV	676290	995518	15.04%	2.499%
20	15.792	2325	2330	2341	rBV2	108351	216102	3.26%	0.542%
21	16.404	2428	2434	2442	rBV3	72274	173288	2.62%	0.435%

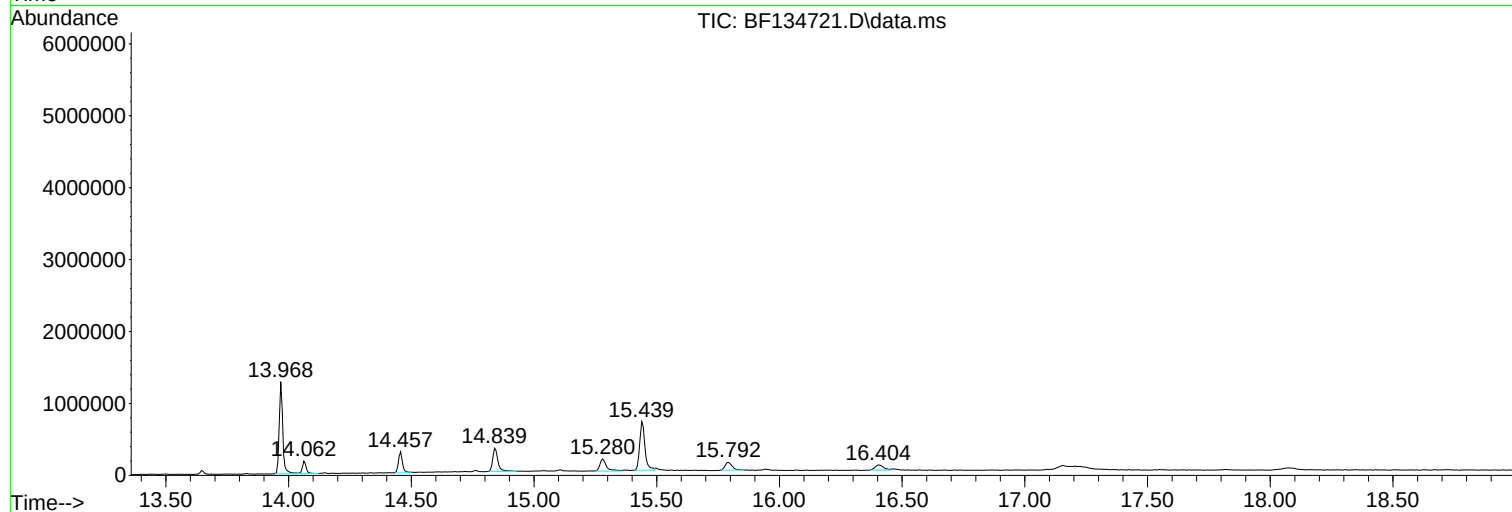
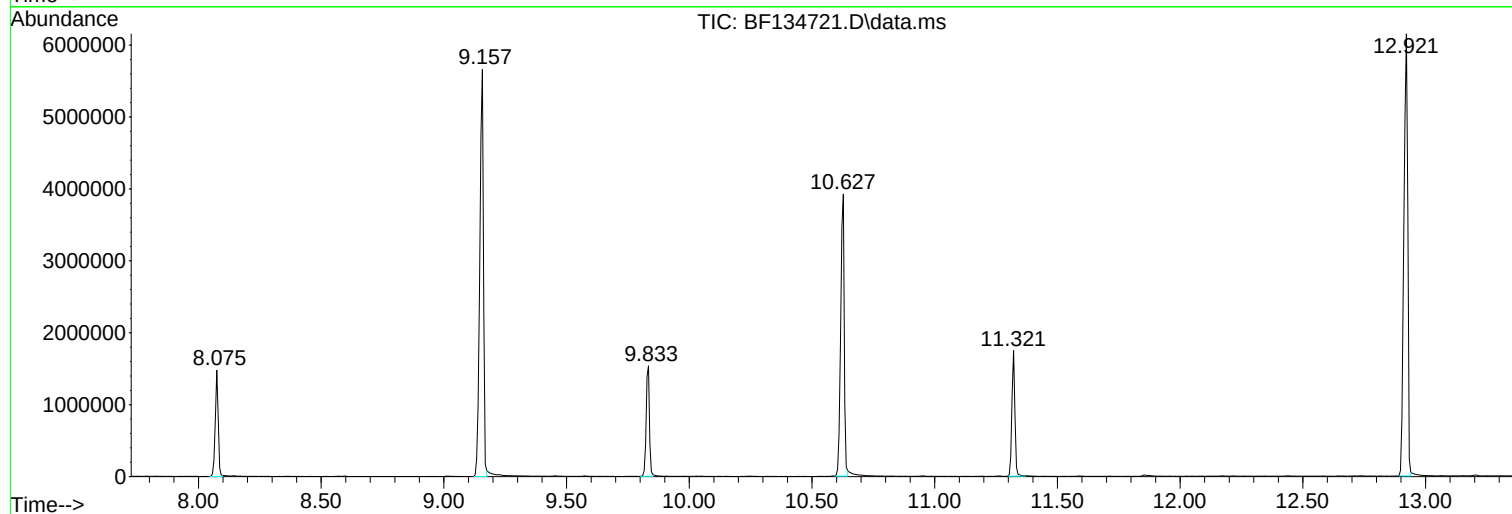
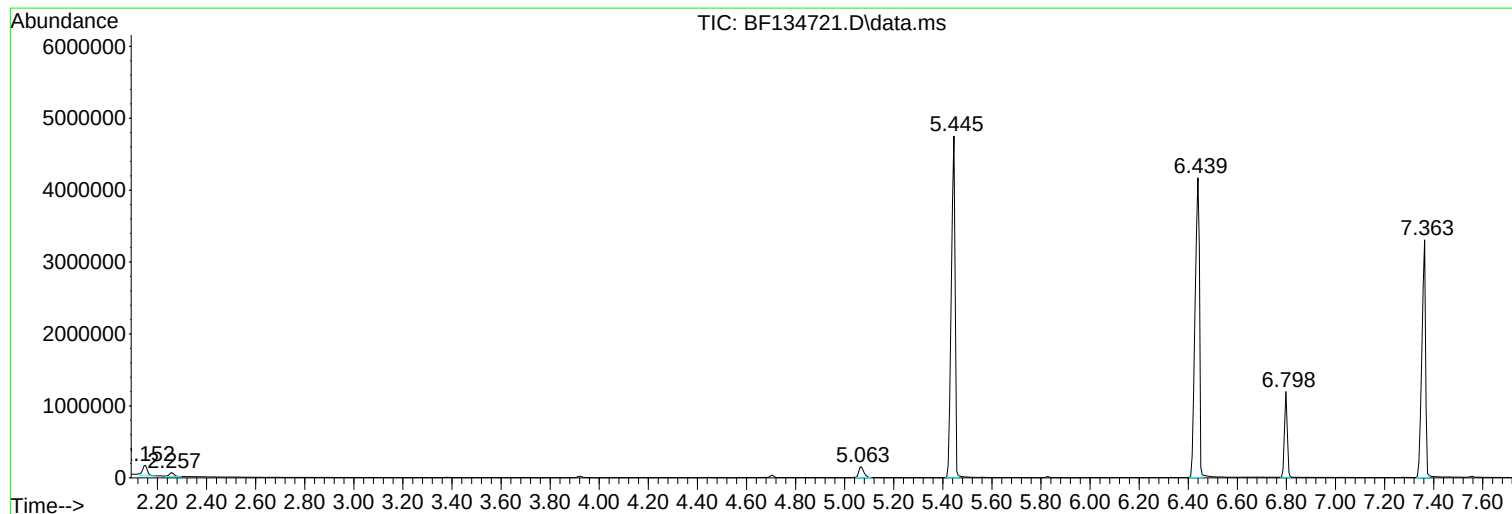
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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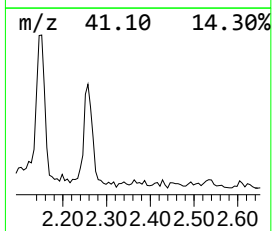
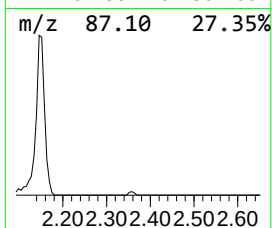
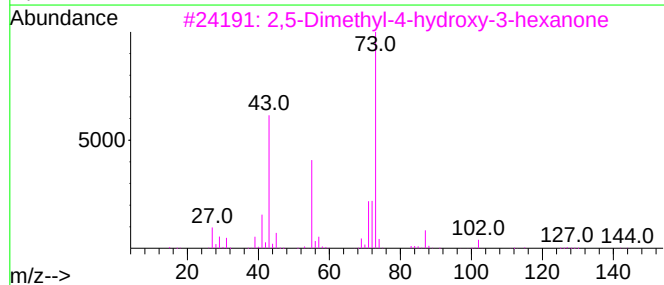
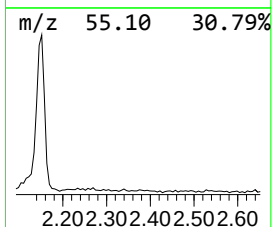
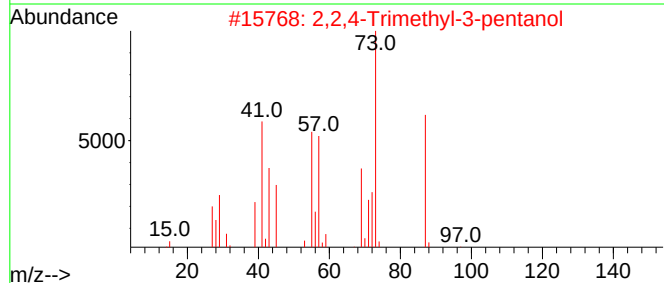
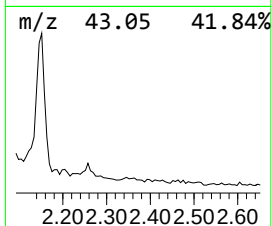
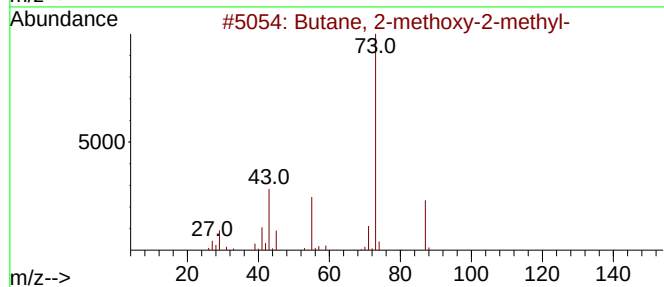
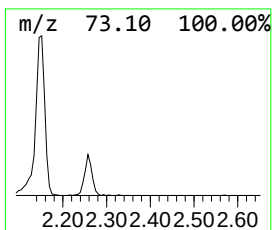
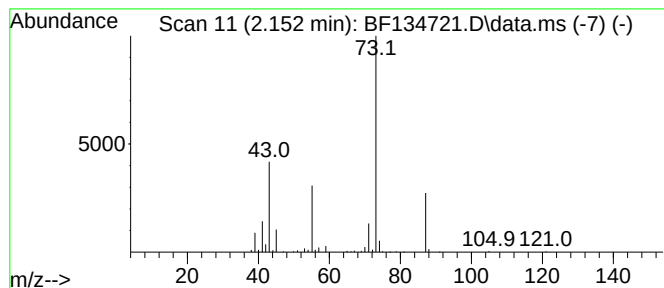
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.152	4.31 ng	198092	1,4-Dichlorobenzene-d4	6.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			2,5-Dimethyl-4-hydroxy-3-hexanone	144	C8H16O2	000815-77-0	28
4			2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12



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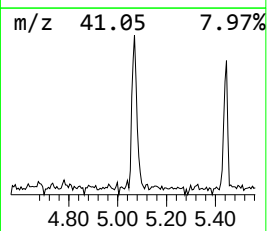
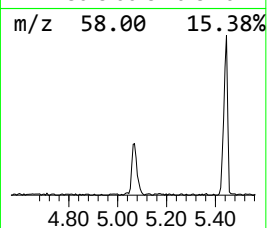
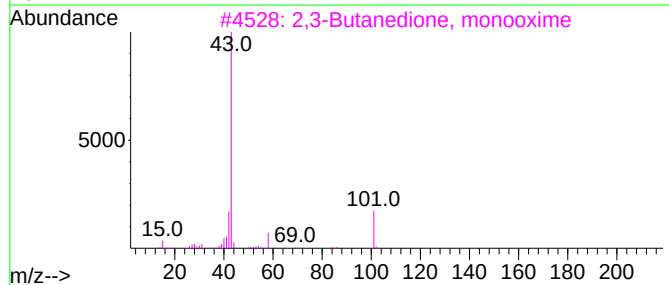
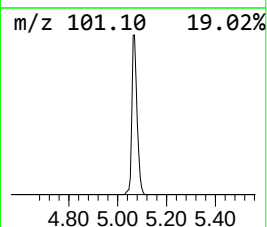
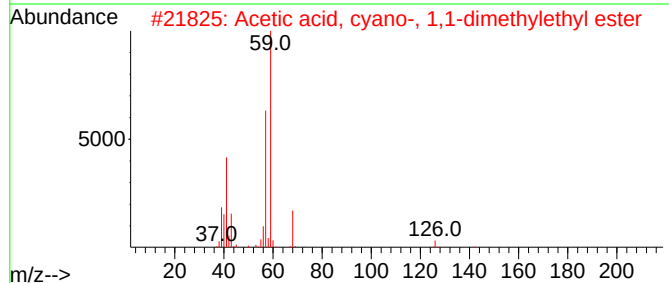
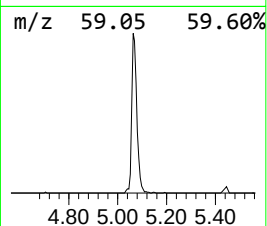
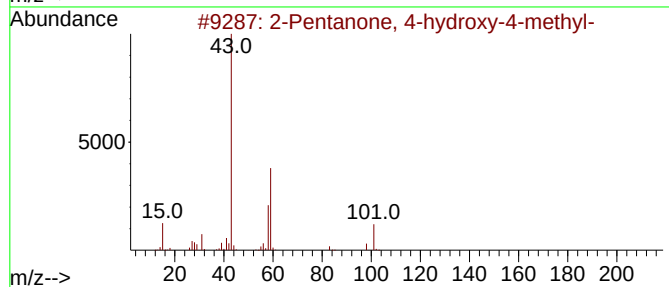
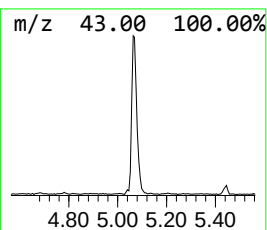
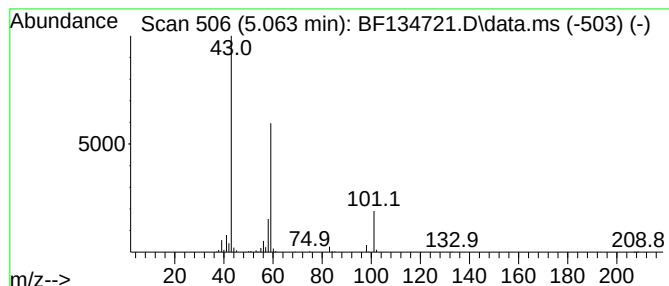
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	4.72 ng	217191	1,4-Dichlorobenzene-d4	6.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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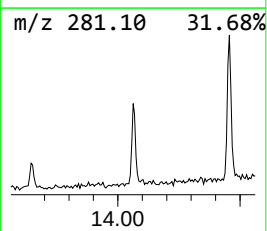
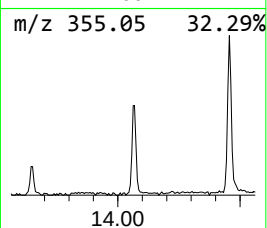
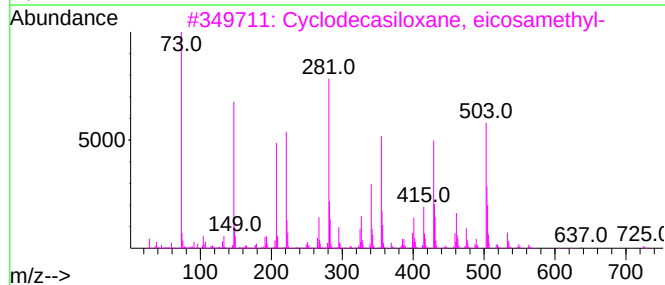
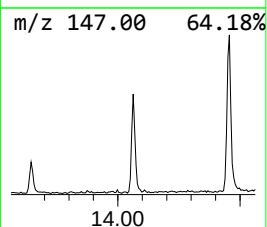
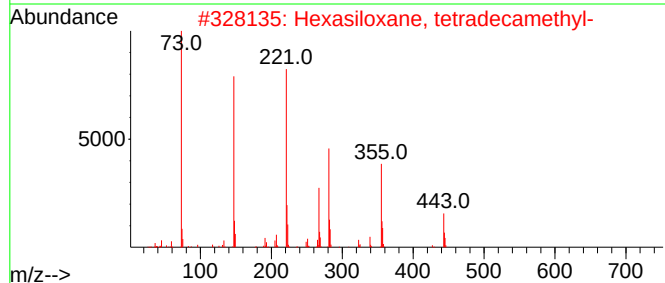
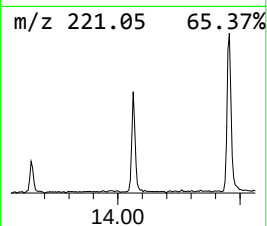
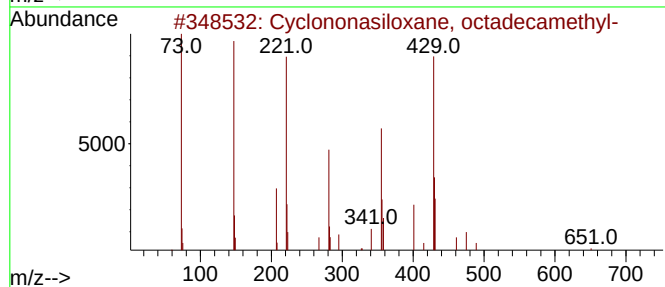
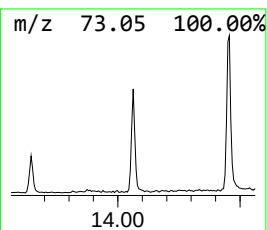
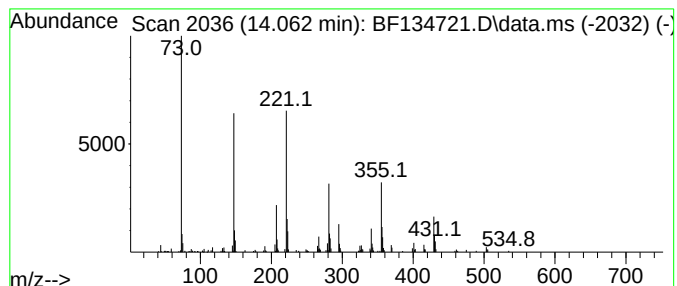
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Peak Number 3 Cyclononasiloxane, octadeca... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.063	2.93 ng	188629	Chrysene-d12	13.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	91
2			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	81
3			Cyclodecasiloxane, eicosamethyl-	740	C20H60O10Si10	018772-36-6	38
4			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	27
5			Octasiloxane, 1,1,3,3,5,5,7,7,9,...	578	C16H50O7Si8	019095-24-0	16



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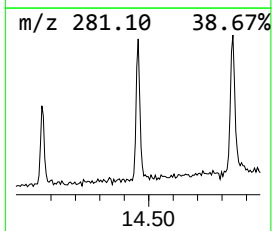
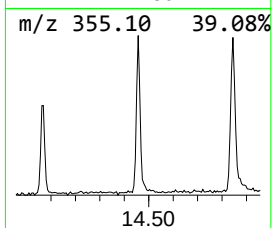
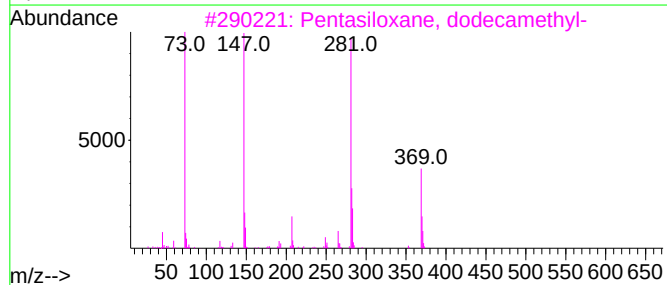
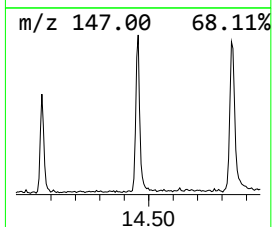
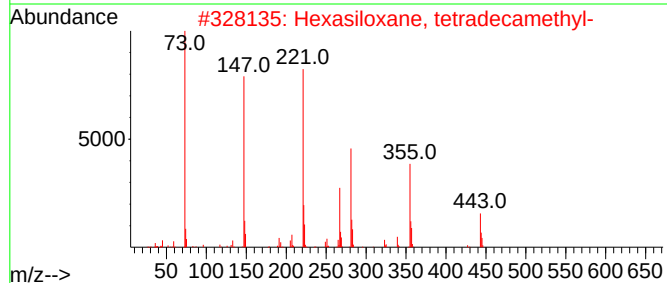
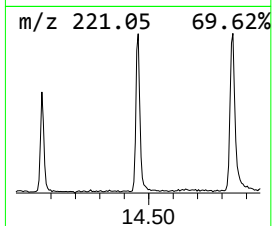
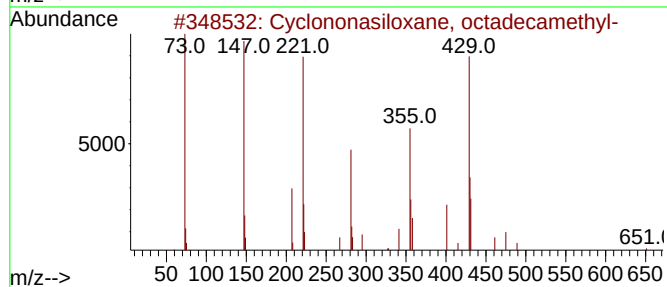
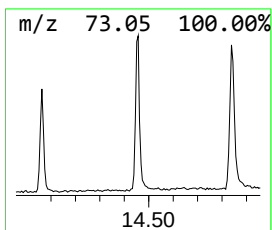
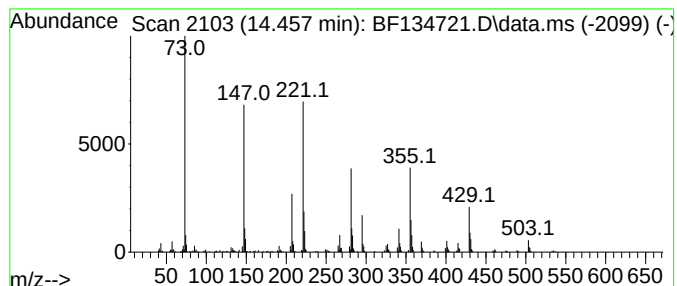
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Peak Number 4 Hexasiloxane, tetradecamethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.457	5.20 ng	334484	Chrysene-d12	13.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	91
2			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	74
3			Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	27
4			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	22
5			N-[4-(Aminosulfonyl)phenyl]propa...	444	C18H36N2O3SSi3	1000500-82-8	22



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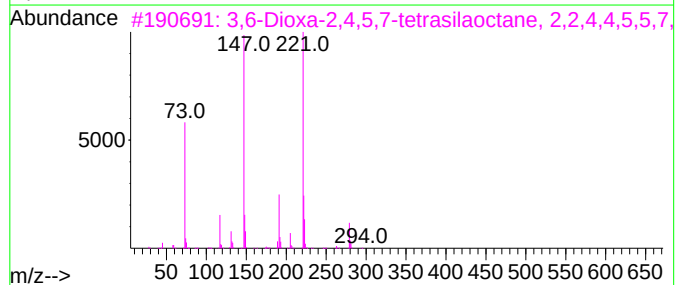
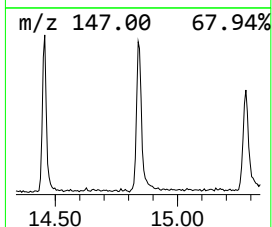
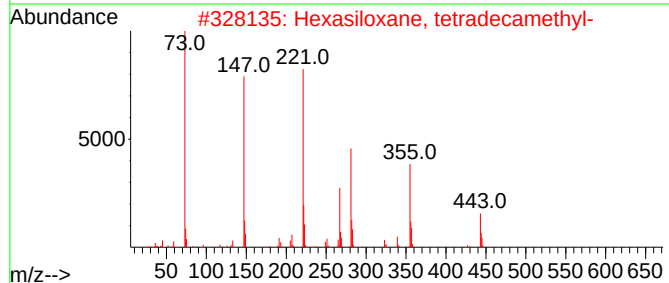
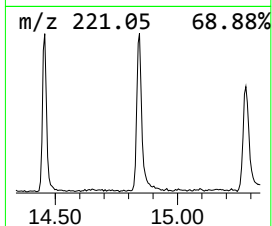
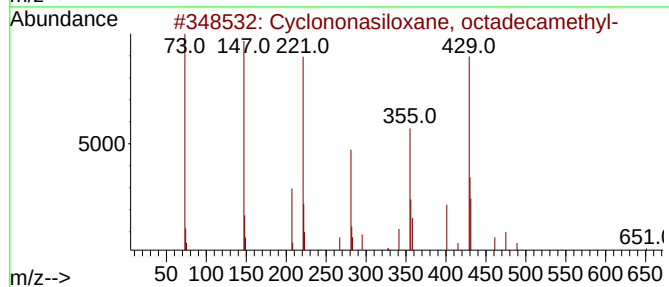
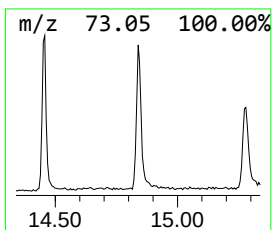
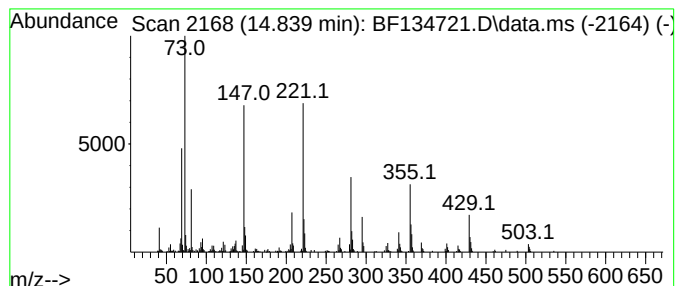
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown14.839 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.839	9.46 ng	471010	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	87
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			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	38
5			1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	754	C22H66O9Si10	000556-70-7	22



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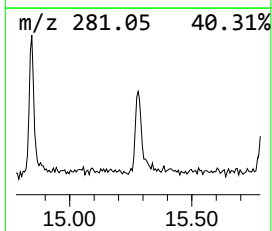
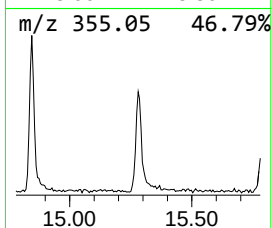
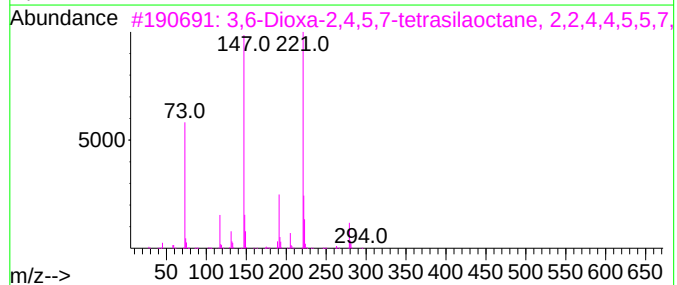
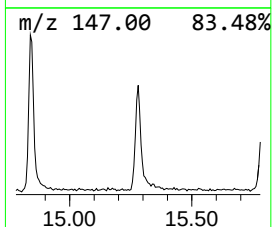
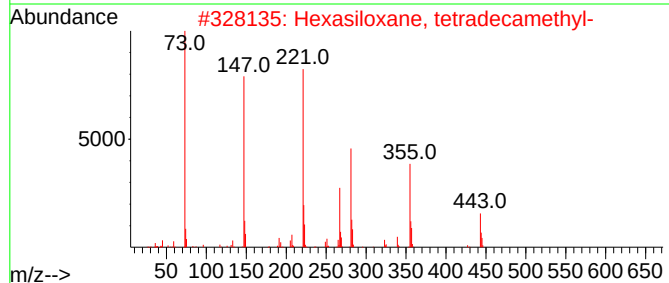
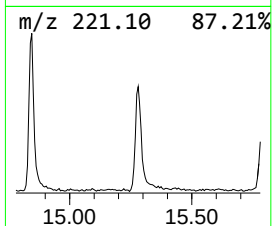
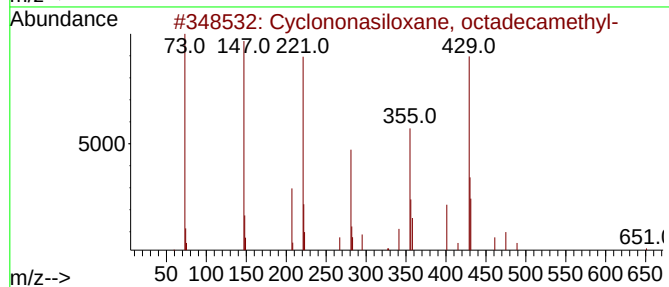
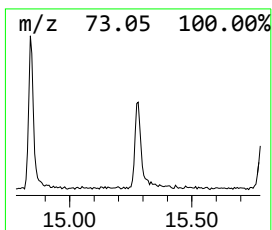
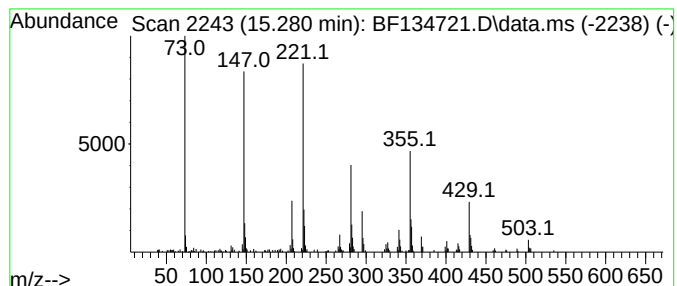
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown15.280 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.280	6.29 ng	313178	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	76
2			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	74
3			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	38
4			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	30
5			Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081123\
Data File : BF134721.D
Acq On : 11 Aug 2023 08:39
Operator : CG\JU
Sample : PB154756BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB154756BL

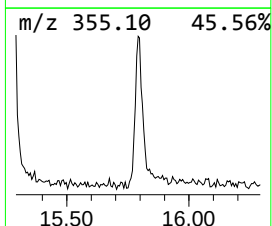
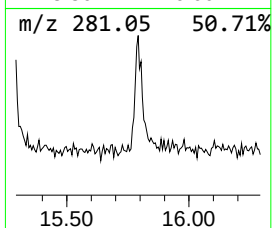
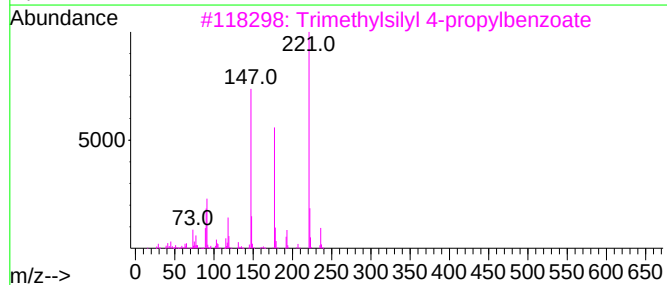
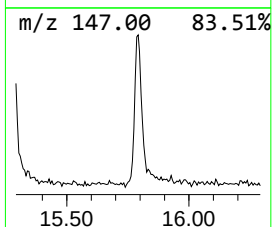
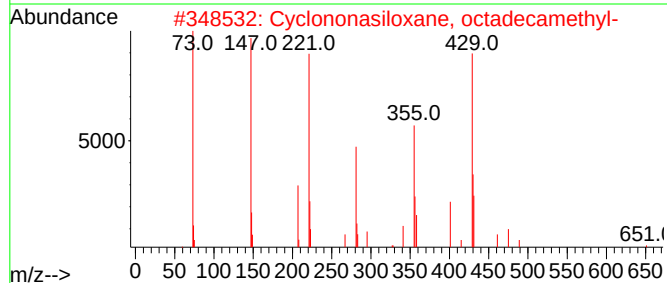
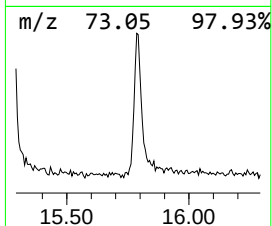
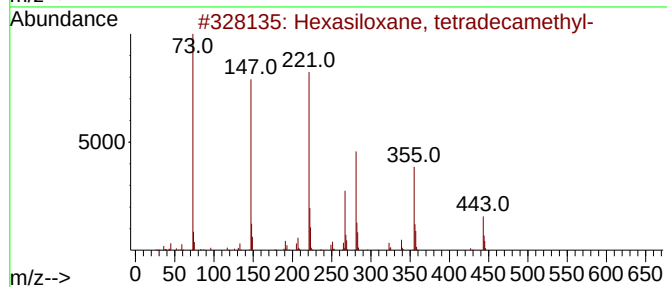
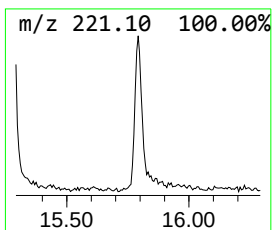
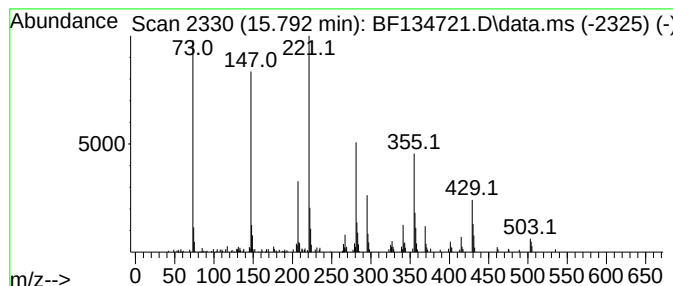
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown15.792 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.792	4.34 ng	216102	Perylene-d12	15.439

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	62
3			Trimethylsilyl 4-propylbenzoate	236	C13H20O2Si	1000408-13-2	37
4			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	37
5			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081123\
Data File : BF134721.D
Acq On : 11 Aug 2023 08:39
Operator : CG\JU
Sample : PB154756BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB154756BL

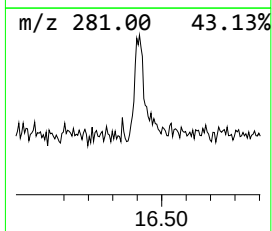
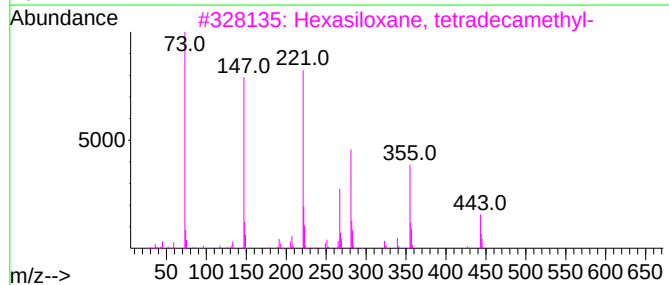
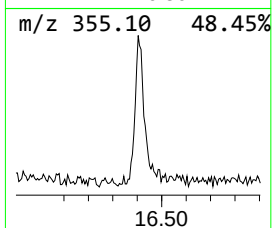
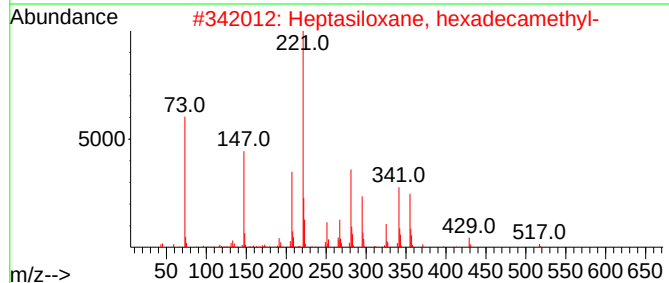
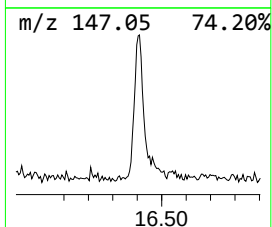
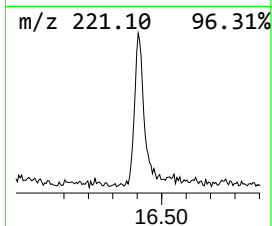
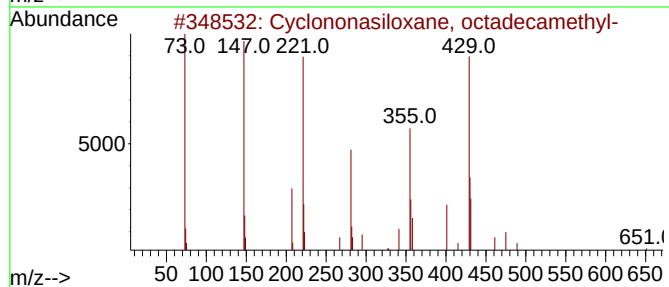
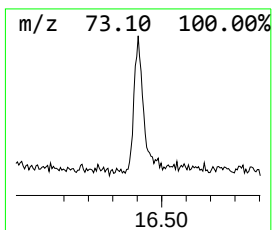
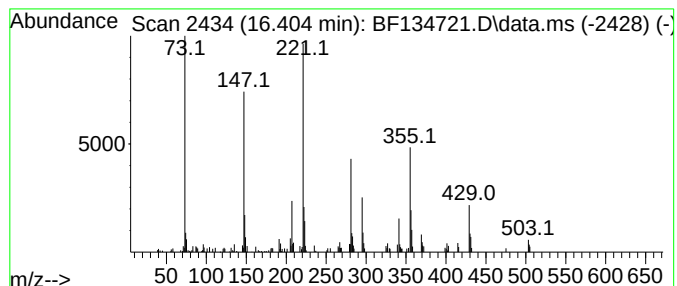
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptasiloxane, hexadecamethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.404	3.48 ng	173288	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	72
2			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	53
3			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	47
4			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	37
5			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081123\
Data File : BF134721.D
Acq On : 11 Aug 2023 08:39
Operator : CG\JU
Sample : PB154756BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB154756BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.152	4.3	ng	198092	1	6.798	919675	20.0
2-Pentanone, 4-...	5.063	4.7	ng	217191	1	6.798	919675	20.0
Cyclononasiloxa...	14.063	2.9	ng	188629	5	13.968	1285460	20.0
Hexasiloxane, t...	14.457	5.2	ng	334484	5	13.968	1285460	20.0
unknown14.839	14.839	9.5	ng	471010	6	15.439	995518	20.0
unknown15.280	15.280	6.3	ng	313178	6	15.439	995518	20.0
unknown15.792	15.792	4.3	ng	216102	6	15.439	995518	20.0
Heptasiloxane, ...	16.404	3.5	ng	173288	6	15.439	995518	20.0