

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100621\
 Data File : BP007357.D
 Acq On : 06 Oct 2021 16:53
 Operator : CG/JU
 Sample : M4080-05
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 SW-RR-01-(2.0)

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_P\Methods\8270E-BP092121.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP007357.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.440	393	400	419	rBV	1100186	1687437	20.32%	3.971%
2	7.040	665	672	688	rBV	520270	961279	11.58%	2.262%
3	7.857	804	811	819	rBV	486369	779134	9.38%	1.834%
4	9.022	1000	1009	1026	rBV	1454287	2580561	31.08%	6.073%
5	10.469	1246	1255	1273	rBV	34808	114439	1.38%	0.269%
6	10.657	1280	1287	1303	rBV	556583	1017186	12.25%	2.394%
7	13.116	1698	1705	1730	rBV	3885450	6175295	74.37%	14.534%
8	14.492	1932	1939	1960	rBV	821408	1351378	16.28%	3.180%
9	14.934	2006	2014	2033	rBV	1031441	1669516	20.11%	3.929%
10	15.316	2071	2079	2089	rBV	45820	86524	1.04%	0.204%
11	15.986	2186	2193	2220	rBV	2786370	4739570	57.08%	11.155%
12	17.245	2401	2407	2420	rBV	1023567	1650857	19.88%	3.885%
13	18.133	2553	2558	2567	rBV	107202	191114	2.30%	0.450%
14	19.810	2837	2843	2858	rBV	6754328	8302970	100.00%	19.541%
15	20.545	2965	2968	2972	rBV	84390	96353	1.16%	0.227%
16	21.045	3050	3053	3060	rVB3	114878	145044	1.75%	0.341%
17	21.333	3098	3102	3113	rBV	1281539	1877043	22.61%	4.418%
18	21.892	3194	3197	3201	rVB	139736	179786	2.17%	0.423%
19	22.504	3297	3301	3308	rVB	310028	478981	5.77%	1.127%
20	23.192	3413	3418	3425	rVB	473200	882735	10.63%	2.078%
21	23.739	3505	3511	3523	rVB2	888675	1959119	23.60%	4.611%
22	23.998	3550	3555	3565	rVB	604716	1337070	16.10%	3.147%
23	24.962	3712	3719	3730	rVB2	690105	1888310	22.74%	4.444%
24	26.127	3911	3917	3936	rVB2	699156	2338083	28.16%	5.503%

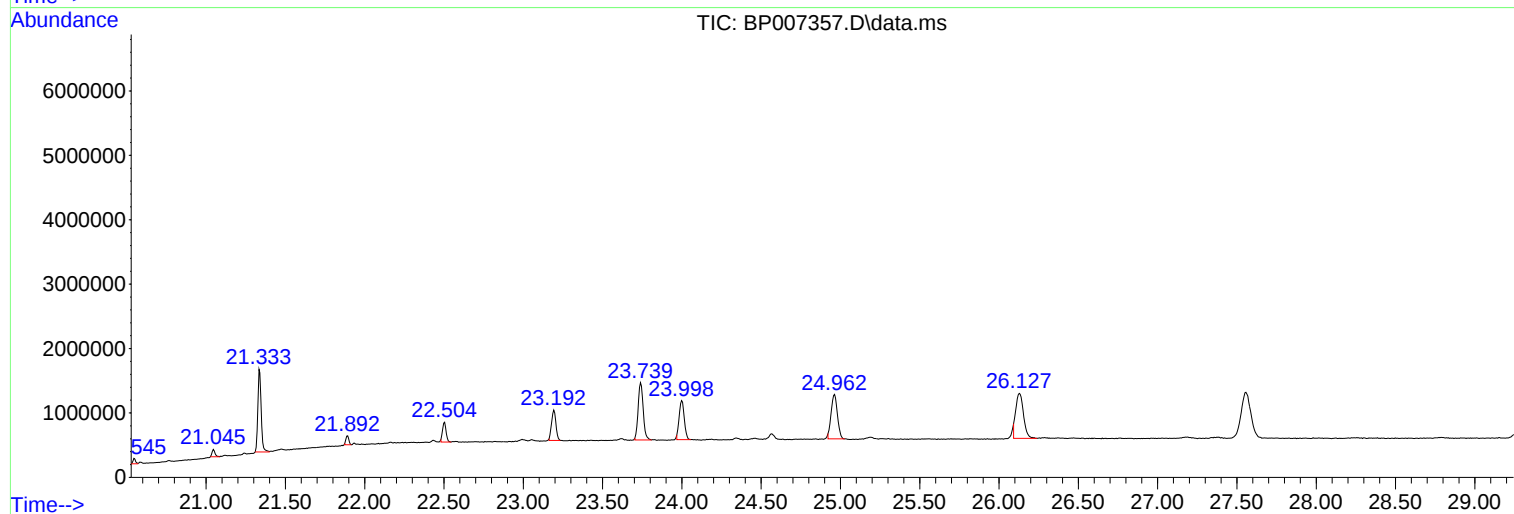
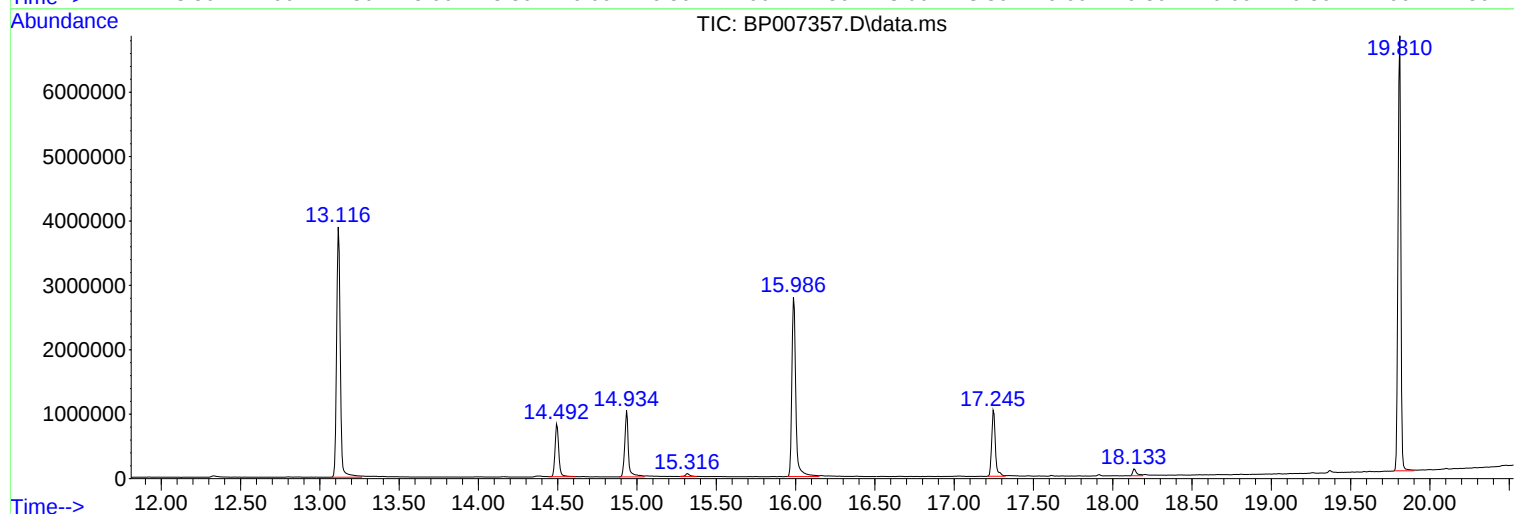
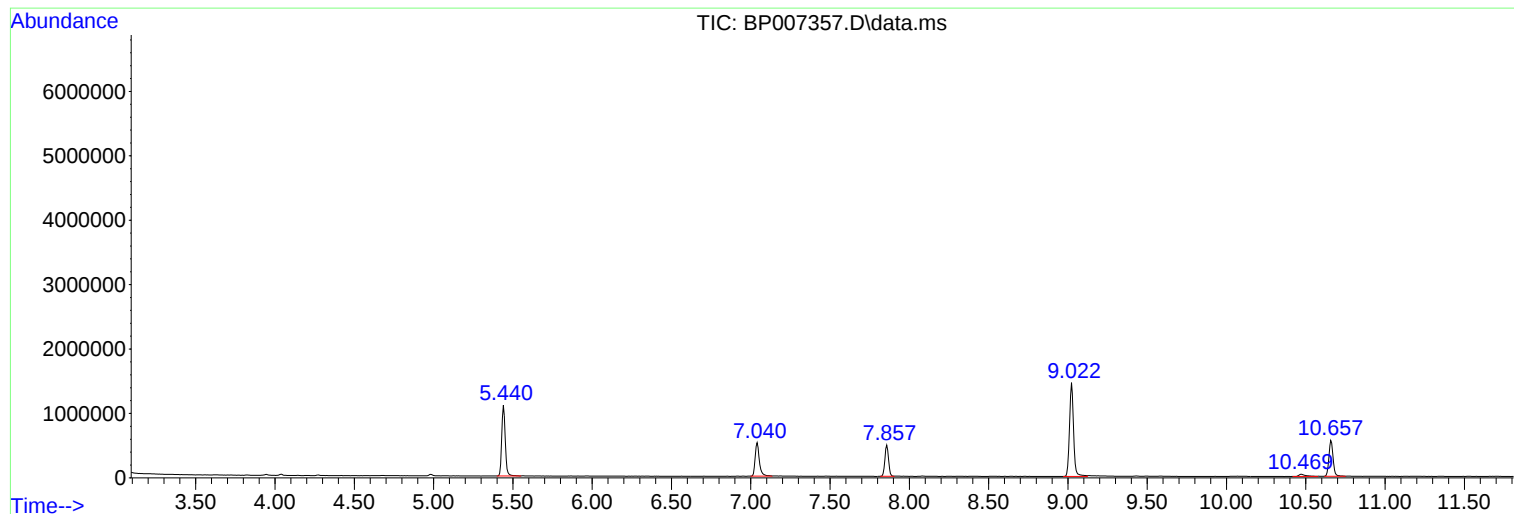
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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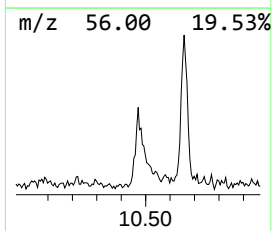
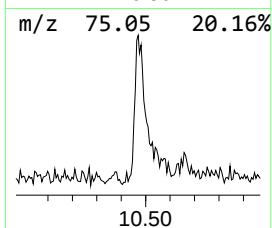
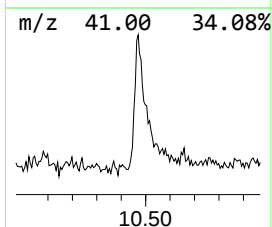
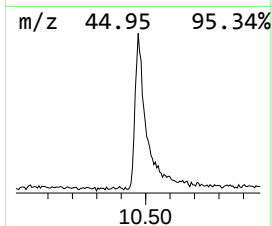
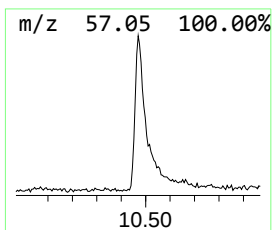
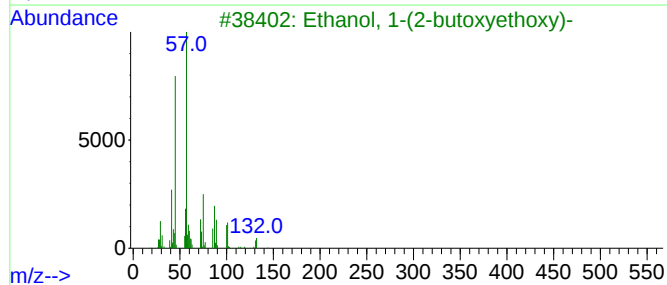
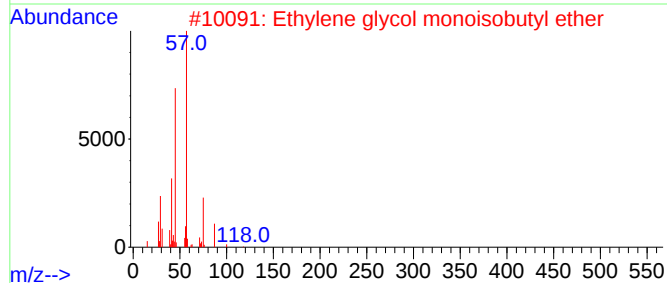
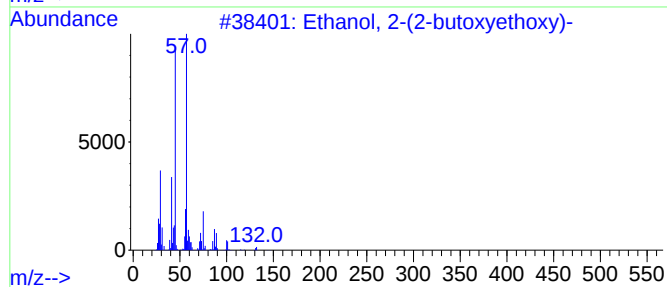
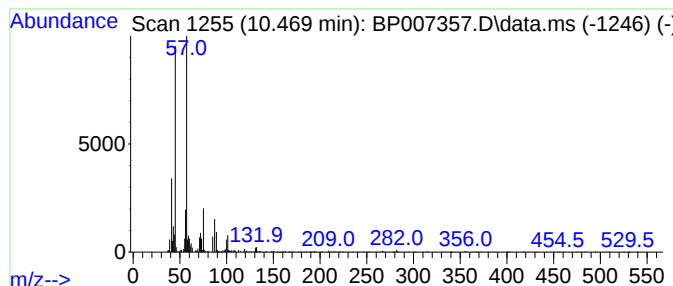
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.469	2.25 ng	114439	Naphthalene-d8	10.657

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	72
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	64
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
5			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	64



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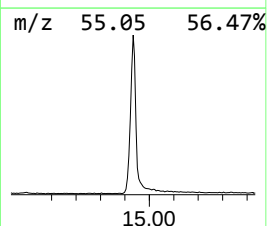
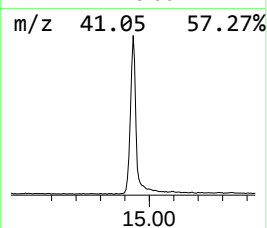
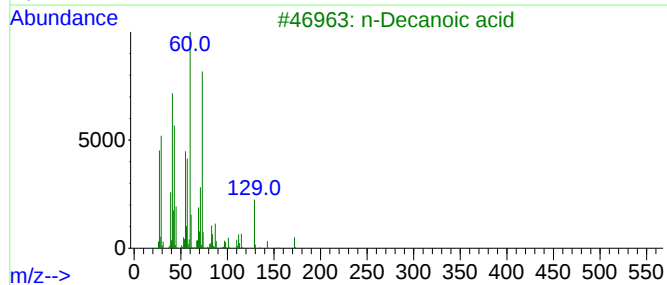
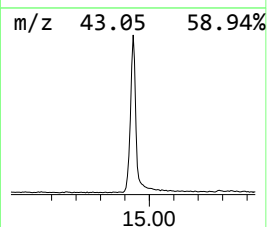
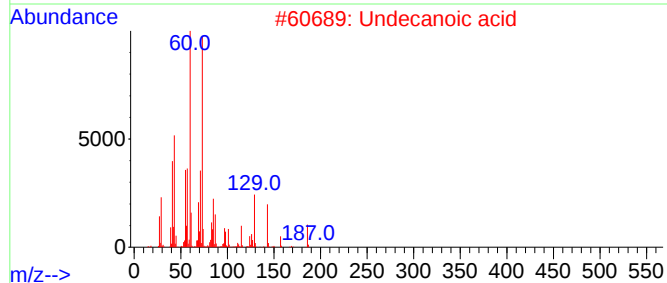
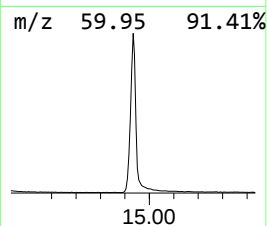
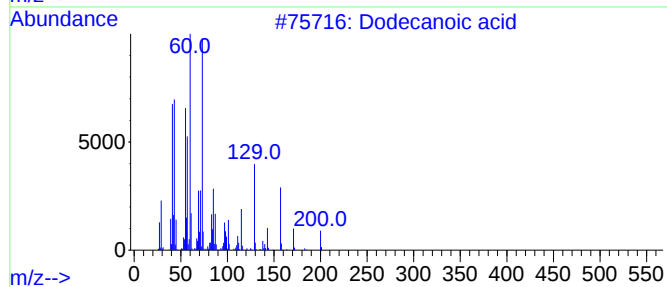
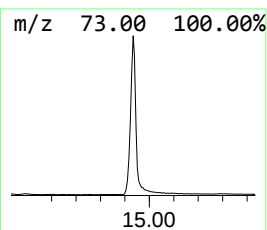
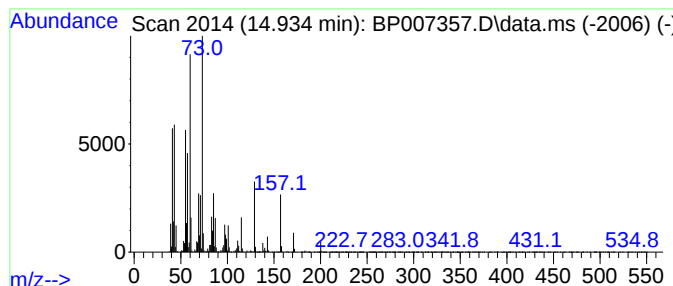
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Peak Number 2 Dodecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.934	24.71 ng	1669520	Acenaphthene-d10	14.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	98
2			Undecanoic acid	186	C11H22O2	000112-37-8	72
3			n-Decanoic acid	172	C10H20O2	000334-48-5	64
4			Nonanoic acid	158	C9H18O2	000112-05-0	58
5			Octanoic acid	144	C8H16O2	000124-07-2	49



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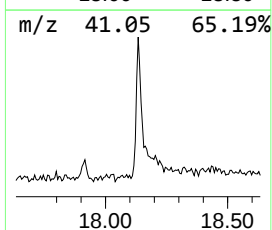
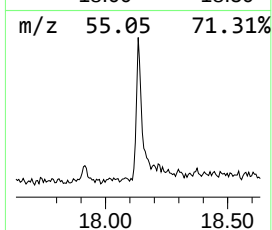
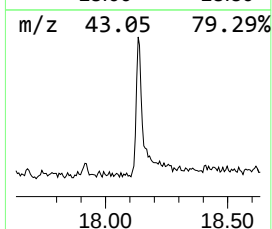
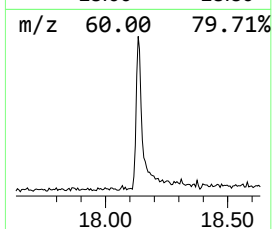
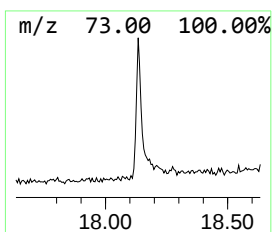
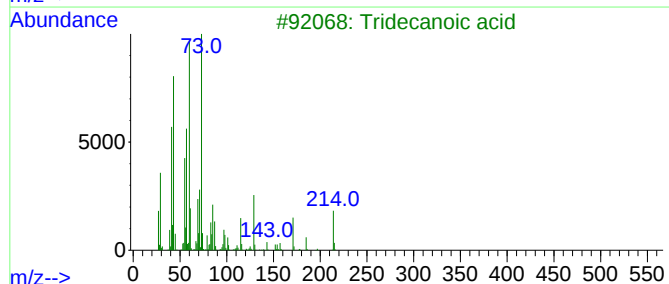
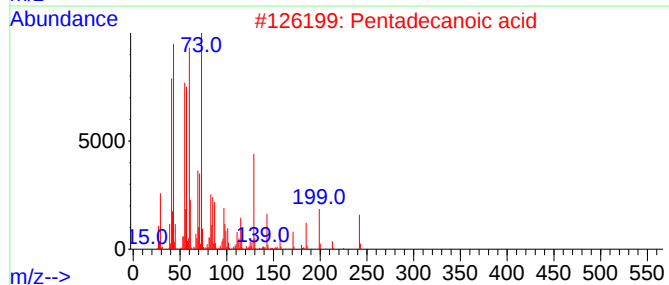
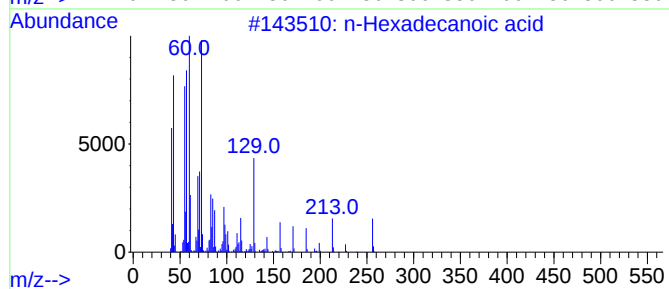
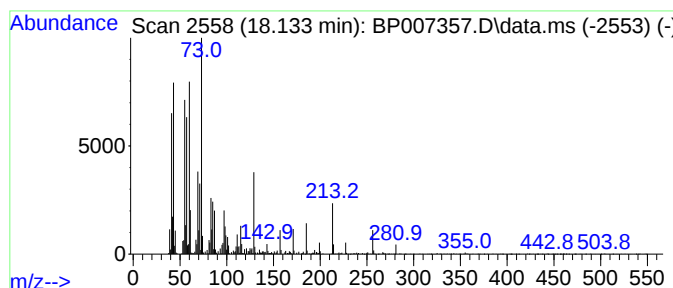
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.133	2.32 ng	191114	Phenanthrene-d10	17.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Tridecanoic acid	214	C13H26O2	000638-53-9	90
4			Octadecanoic acid	284	C18H36O2	000057-11-4	87
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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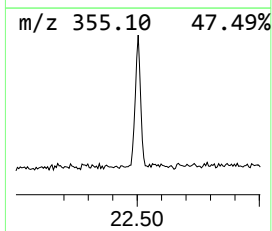
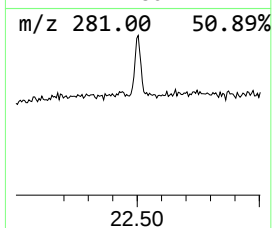
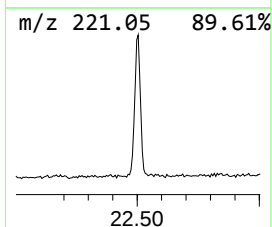
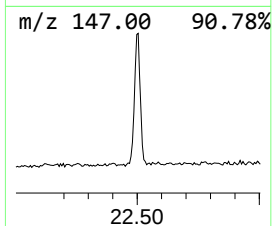
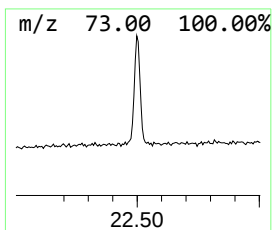
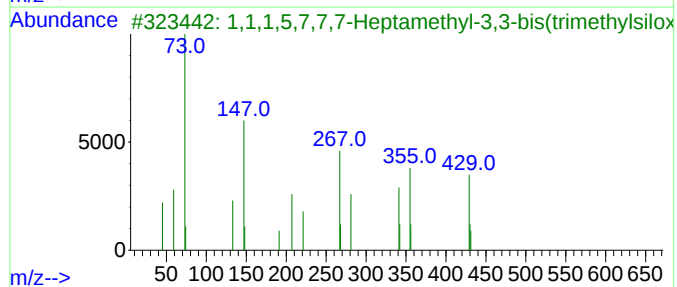
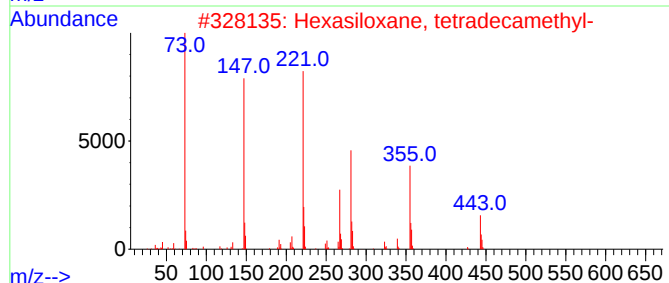
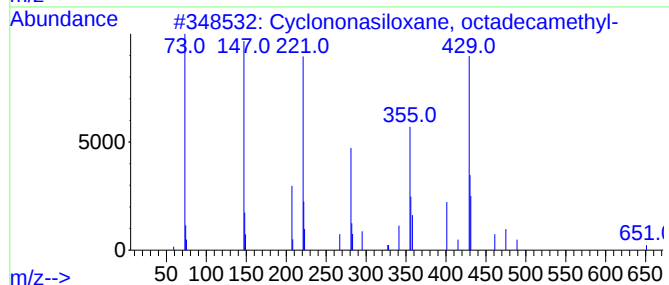
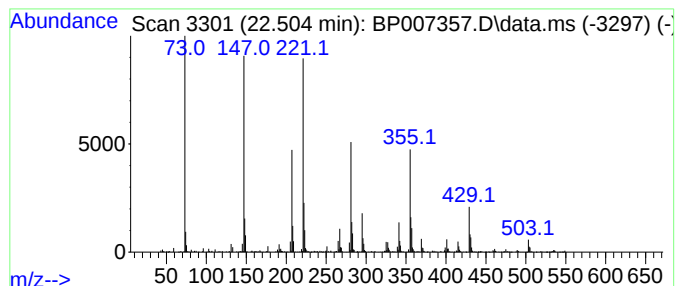
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Peak Number 4 Hexasiloxane, tetradecamethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.504	5.10 ng	478981	Chrysene-d12	21.333

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	83
2			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	76
3			1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	50
4			3,6-Dioxo-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	49
5			Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	27



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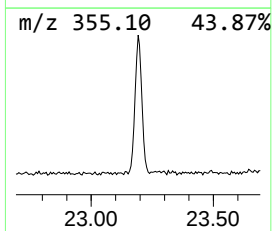
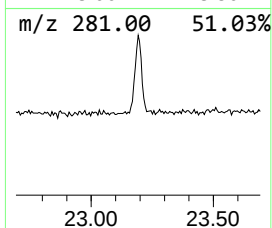
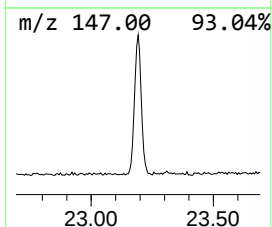
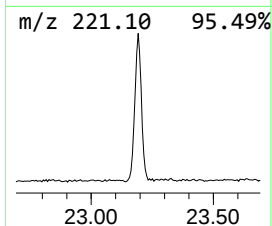
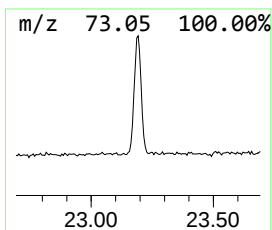
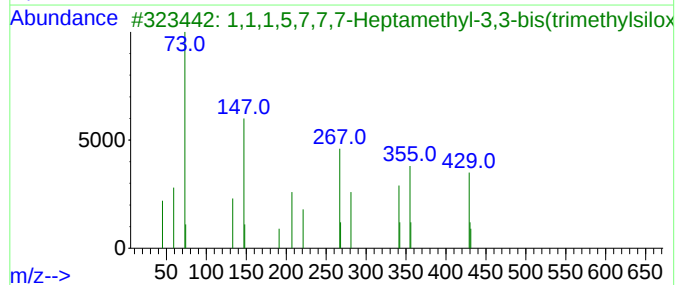
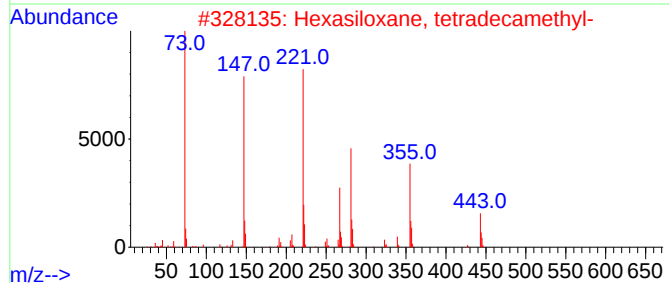
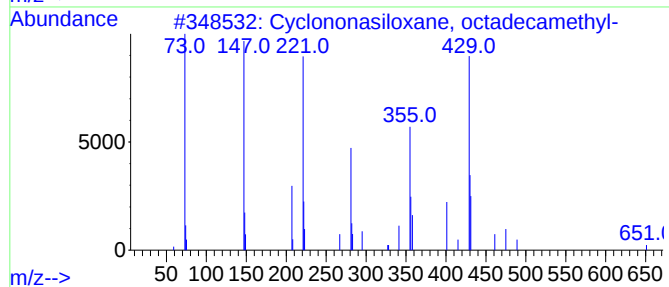
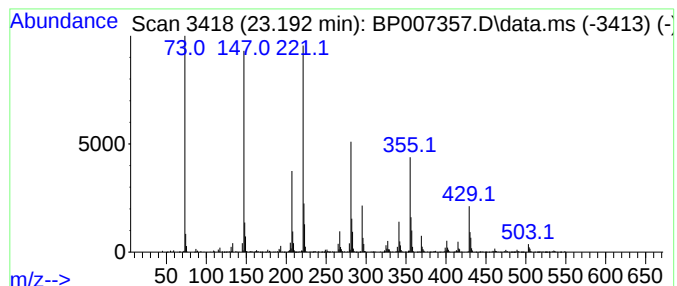
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Peak Number 5 unknown23.192 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.192	9.01 ng	882735	Perylene-d12	23.739

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			1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	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



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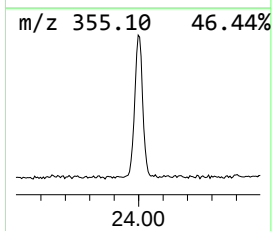
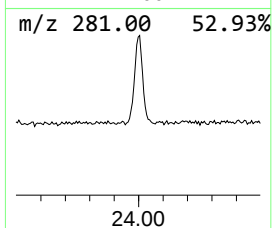
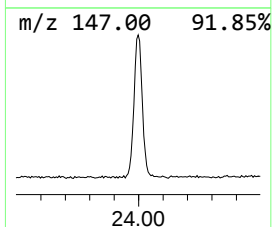
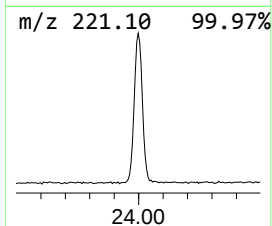
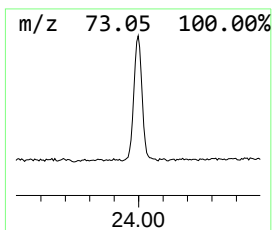
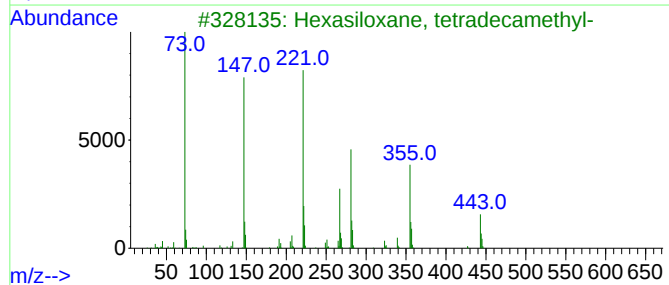
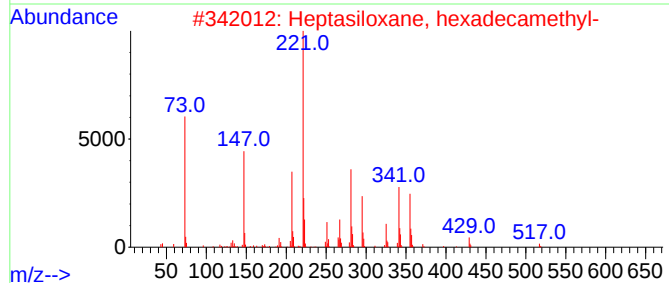
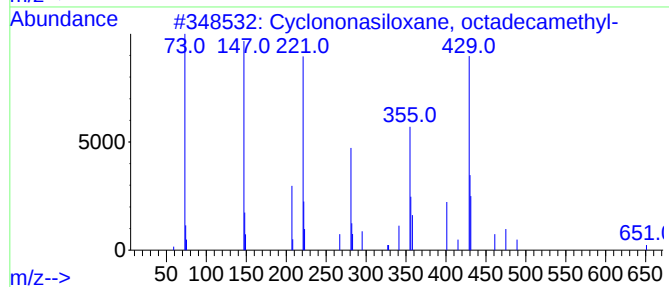
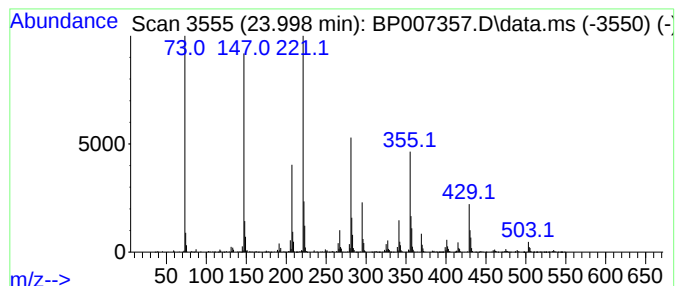
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclononasiloxane, octadeca... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.998	13.65 ng	1337070	Perylene-d12	23.739

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	90
2			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	80
3			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	70
4			1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	50
5			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100621\
Data File : BP007357.D
Acq On : 06 Oct 2021 16:53
Operator : CG/JU
Sample : M4080-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-RR-01-(2.0)

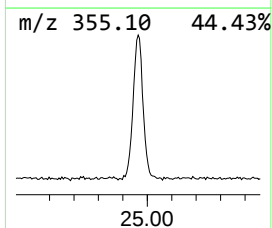
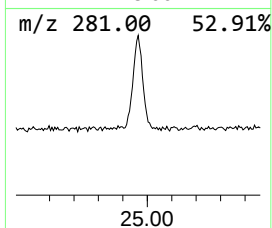
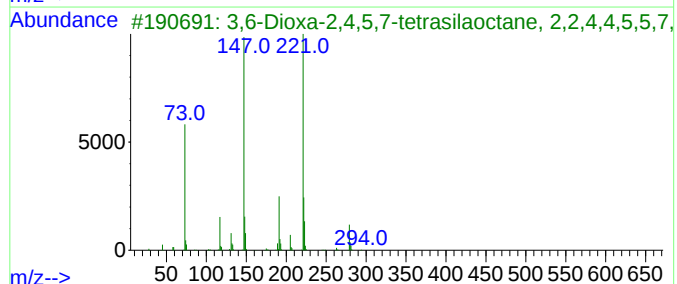
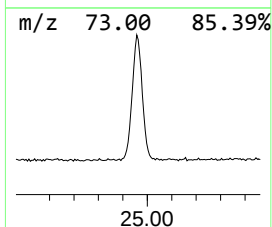
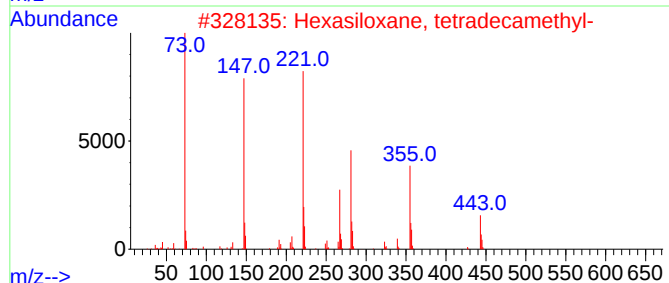
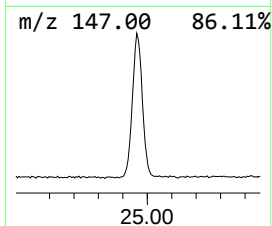
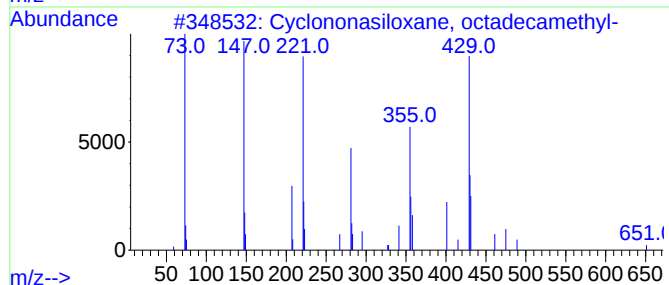
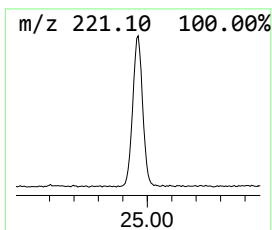
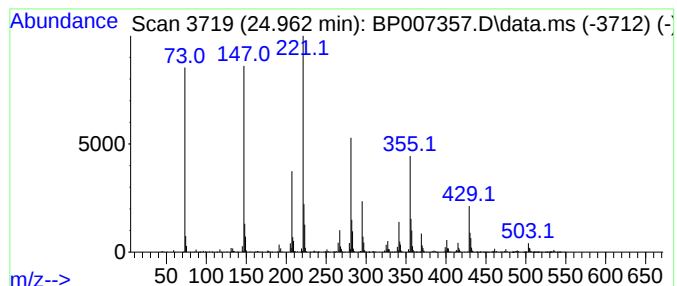
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown24.962 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.962	19.28 ng	1888310	Perylene-d12	23.739

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	81
3			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	46
4			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	37
5			Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100621\
Data File : BP007357.D
Acq On : 06 Oct 2021 16:53
Operator : CG/JU
Sample : M4080-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

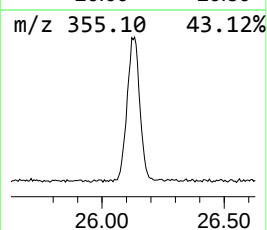
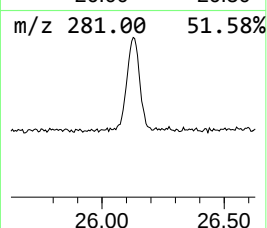
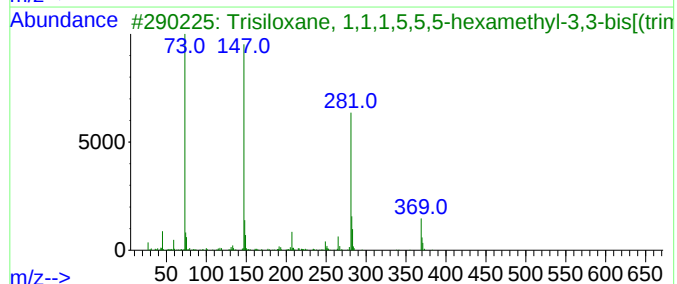
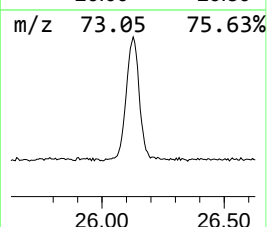
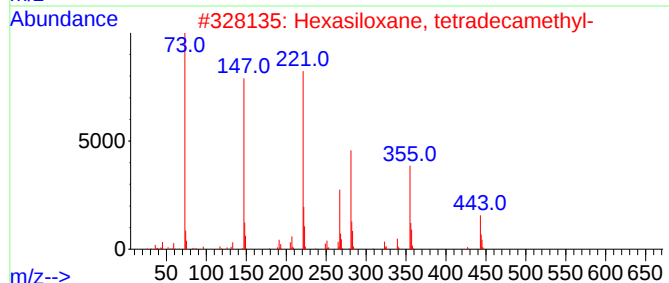
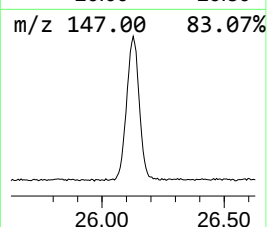
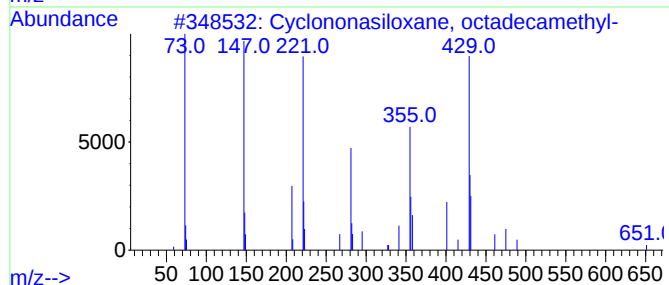
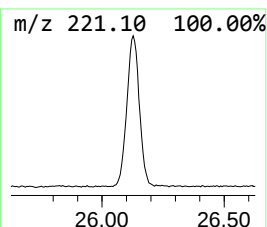
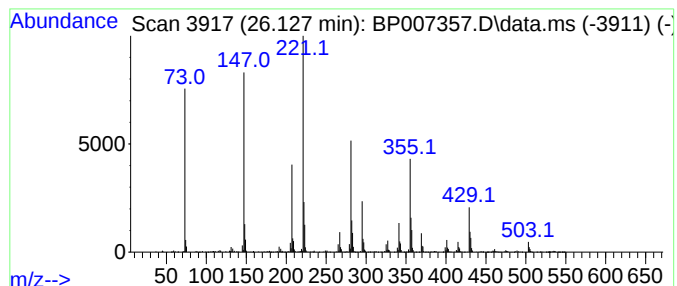
Instrument :
BNA_P
ClientSampleId :
SW-RR-01-(2.0)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown26.127 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
26.127	23.87 ng	2338080	Perylene-d12	23.739		
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	38
3		Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	22
4		Boric acid, 3TMS derivative	278	C9H27B03Si3	004325-85-3	14
5		Trisiloxane, octamethyl-	236	C8H24O2Si3	000107-51-7	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100621\
Data File : BP007357.D
Acq On : 06 Oct 2021 16:53
Operator : CG/JU
Sample : M4080-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-RR-01-(2.0)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.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
Ethanol, 2-(2-b...	10.469	2.3	ng	114439	2	10.657	1017190	20.0
Dodecanoic acid	14.934	24.7	ng	1669520	3	14.492	1351380	20.0
n-Hexadecanoic ...	18.133	2.3	ng	191114	4	17.245	1650860	20.0
Hexasiloxane, t...	22.504	5.1	ng	478981	5	21.333	1877040	20.0
unknown23.192	23.192	9.0	ng	882735	6	23.739	1959120	20.0
Cyclononasiloxa...	23.998	13.7	ng	1337070	6	23.739	1959120	20.0
unknown24.962	24.962	19.3	ng	1888310	6	23.739	1959120	20.0
unknown26.127	26.127	23.9	ng	2338080	6	23.739	1959120	20.0