

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM020624\
 Data File : BM043998.D
 Acq On : 06 Feb 2024 18:53
 Operator : MA/JU
 Sample : PB158215BL
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PB158215BL

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_M\Methods\8270-BM020524.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM043998.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.428	223	228	241	rVB	215055	357396	1.84%	0.416%
2	5.034	325	331	346	rVB	1069594	1663675	8.56%	1.937%
3	5.493	402	409	425	rBV	4189363	6338970	32.62%	7.382%
4	7.087	673	680	697	rVB	4251640	6602268	33.97%	7.689%
5	7.922	815	822	829	rVB	699687	1120595	5.77%	1.305%
6	9.092	1013	1021	1033	rBV	2231050	3814961	19.63%	4.443%
7	10.722	1290	1298	1307	rBV	911978	1568208	8.07%	1.826%
8	13.192	1711	1718	1727	rBV	5958503	8779432	45.17%	10.224%
9	14.563	1944	1951	1958	rBV	1442444	2117341	10.89%	2.466%
10	16.057	2199	2205	2223	rVB	4265421	5760053	29.64%	6.708%
11	17.315	2412	2419	2429	rBV	2062591	2909426	14.97%	3.388%
12	19.956	2862	2868	2876	rBV	16611190	19434776	100.00%	22.633%
13	21.515	3128	3133	3138	rBV	3483901	4667260	24.01%	5.435%
14	21.556	3138	3140	3147	rVB	409379	480940	2.47%	0.560%
15	22.139	3235	3239	3249	rBV	573254	870456	4.48%	1.014%
16	22.774	3342	3347	3353	rVB	878478	1364836	7.02%	1.589%
17	23.486	3462	3468	3479	rVB	1069792	2040133	10.50%	2.376%
18	23.927	3535	3543	3556	rVB	2503649	5279372	27.16%	6.148%
19	24.321	3603	3610	3625	rVB	1060483	2470349	12.71%	2.877%
20	25.321	3772	3780	3791	rVB2	933730	2632421	13.54%	3.066%
21	26.538	3978	3987	4001	rVB2	873017	2986213	15.37%	3.478%
22	28.032	4233	4241	4258	rVB3	621669	2608842	13.42%	3.038%

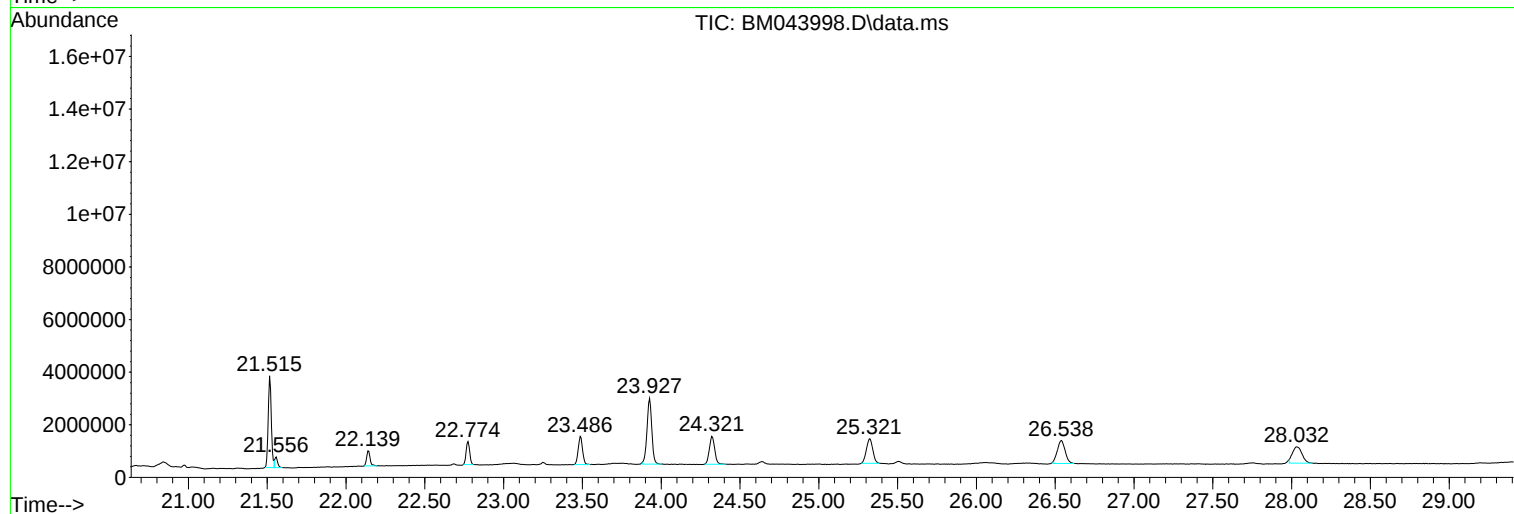
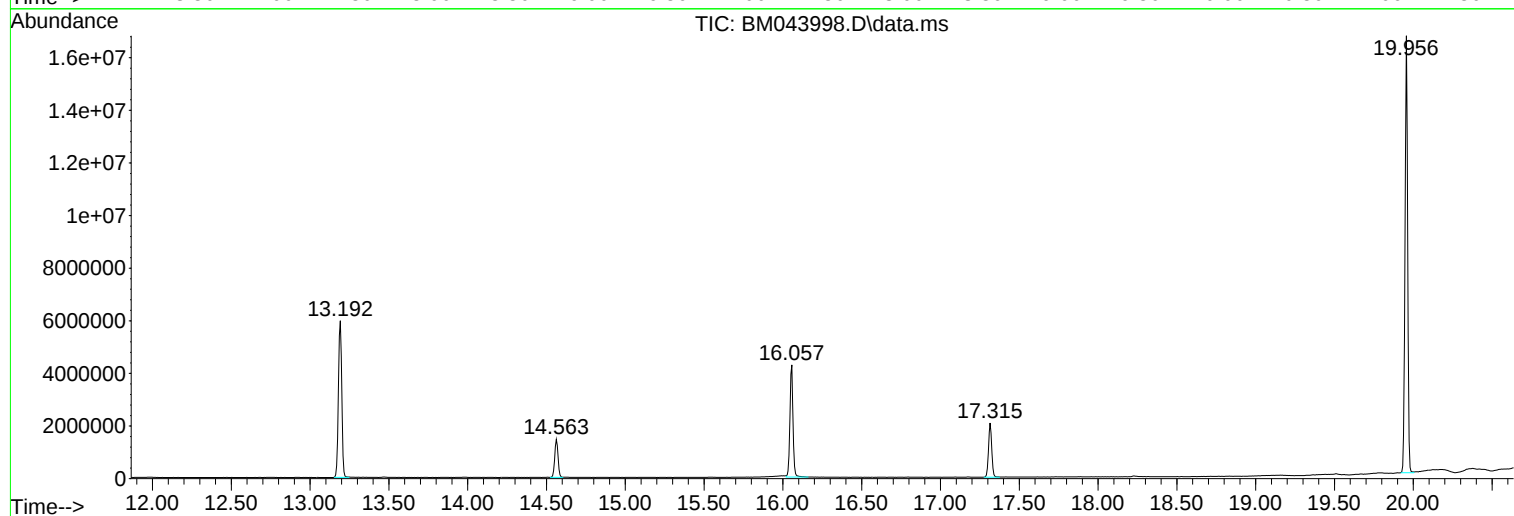
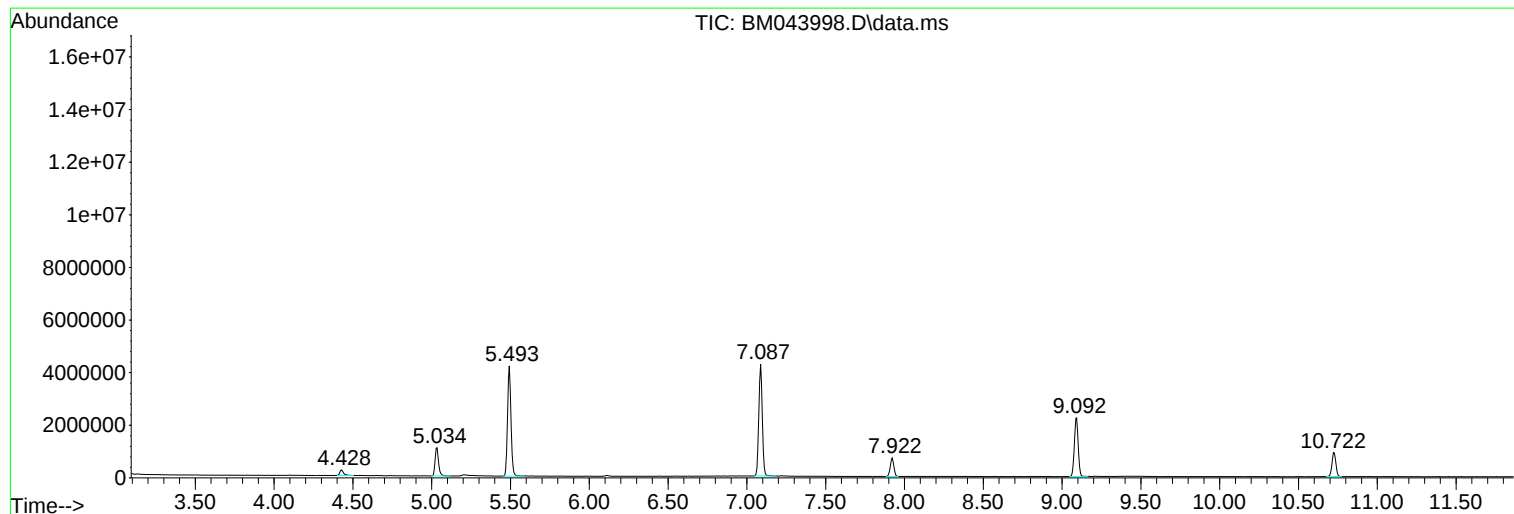
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020524.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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Instrument :
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ClientSampleId :
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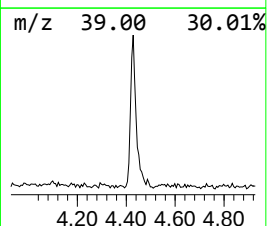
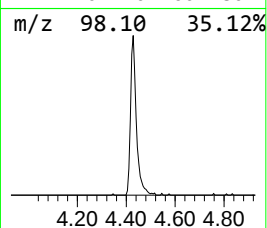
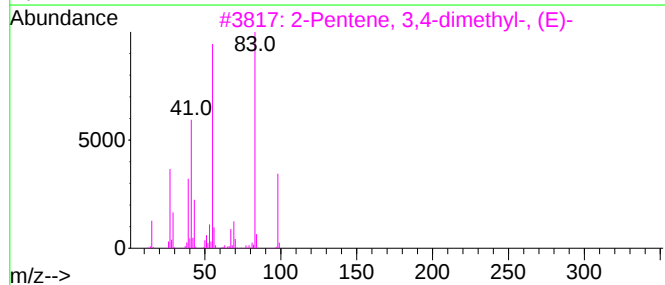
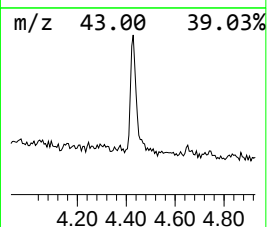
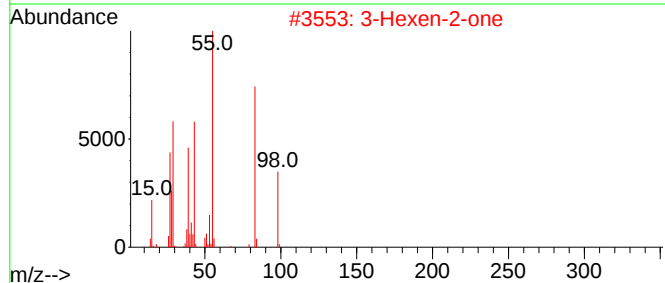
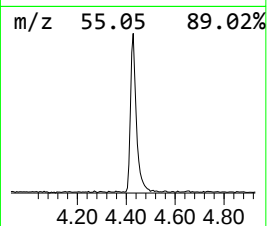
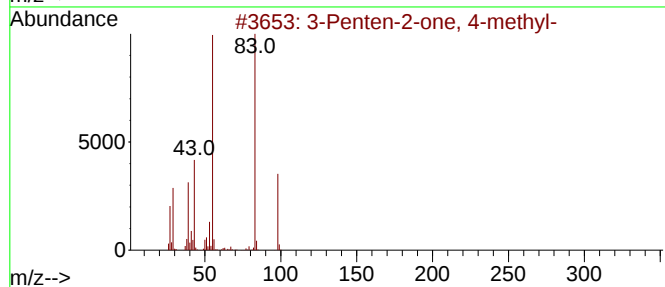
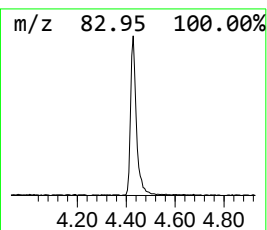
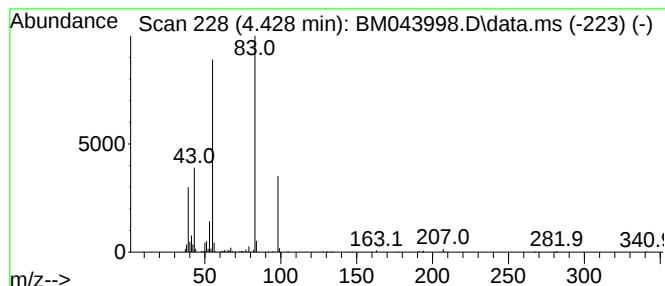
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.428	6.38 ng	357396	1,4-Dichlorobenzene-d4	7.922

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	93
2		3-Hexen-2-one	98	C6H10O	000763-93-9	90
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
5		Cyclohexane, methyl-	98	C7H14	000108-87-2	80



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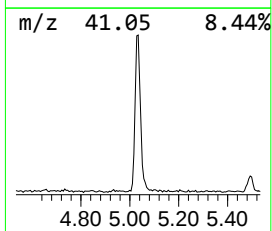
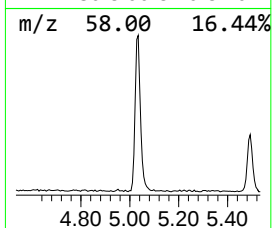
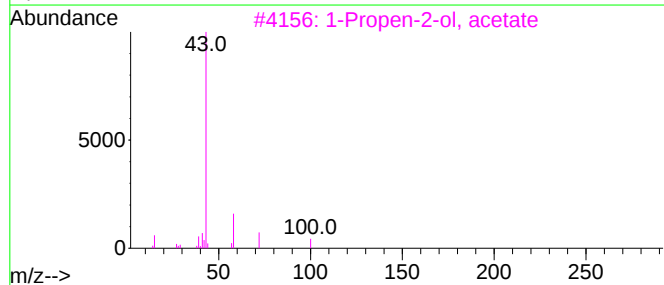
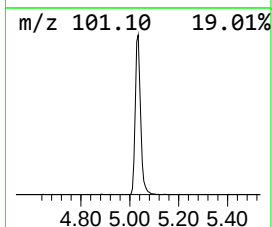
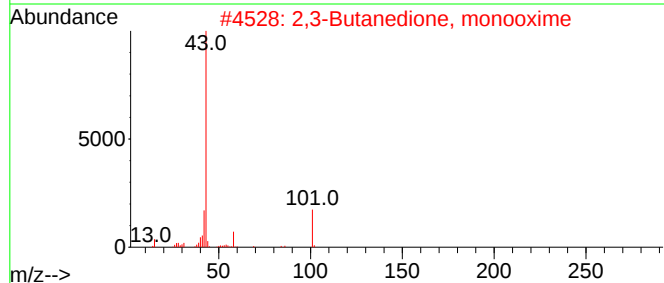
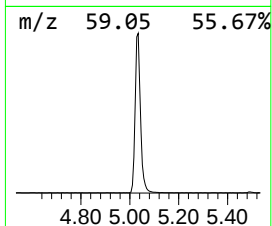
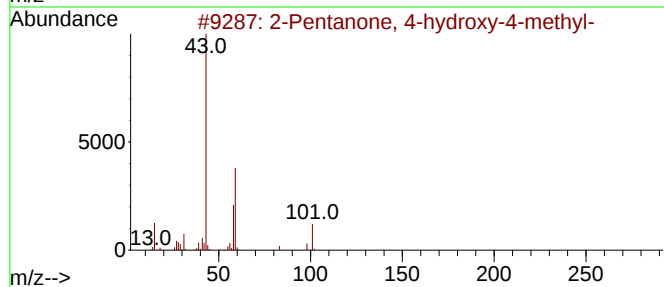
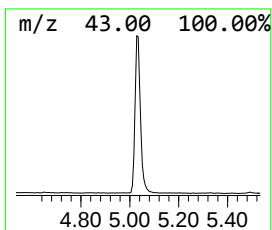
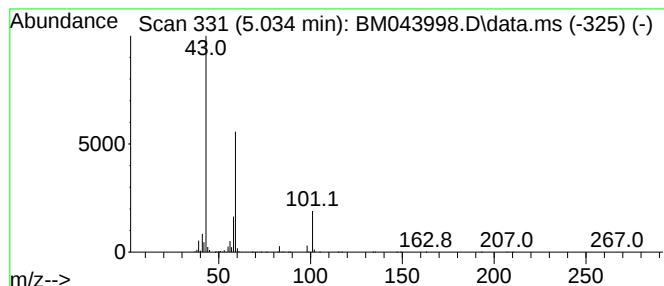
Instrument :
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.034	29.69 ng	1663680	1,4-Dichlorobenzene-d4			7.922
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	59
2	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	16
3	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	12
4	5-Hexen-2-one		98	C6H10O	000109-49-9	9
5	Morpholine, 4-methyl-		101	C5H11NO	000109-02-4	9



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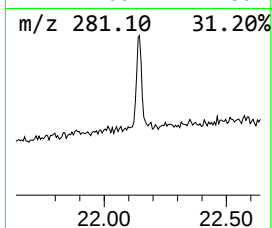
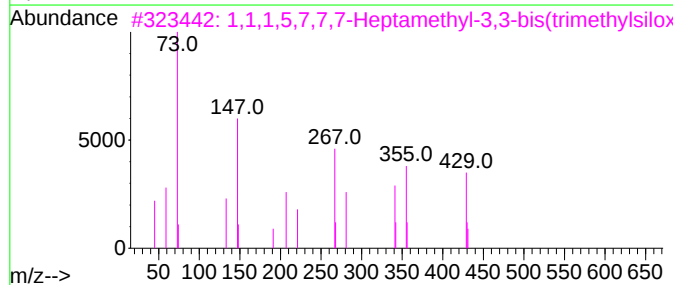
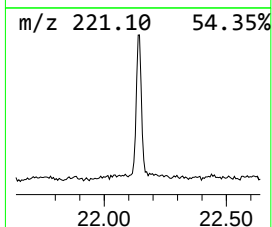
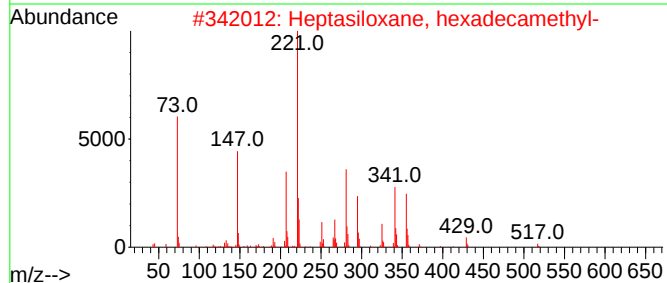
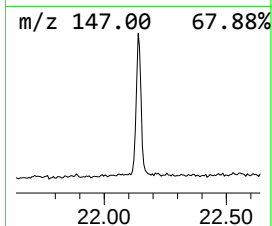
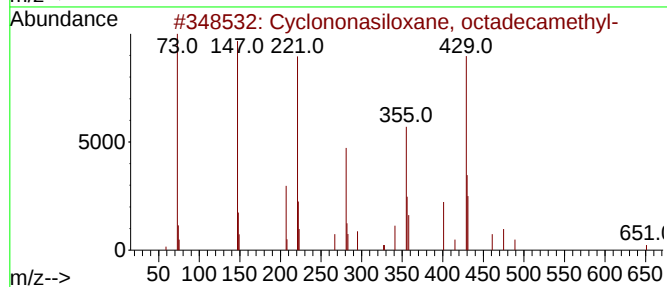
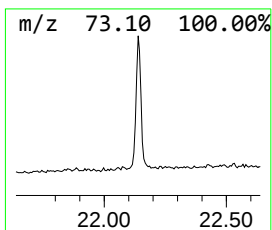
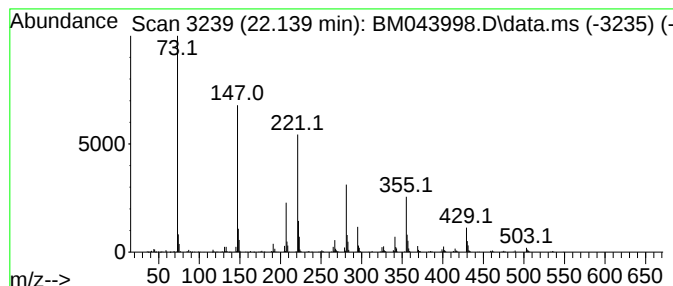
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Cyclononasiloxane, octadeca... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.139	3.73 ng	870456	Chrysene-d12	21.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	81
2			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	64
3			1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	40
4			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	37
5			N-[4-(Aminosulfonyl)phenyl]propa...	444	C18H36N2O3SSi3	1000500-82-8	22



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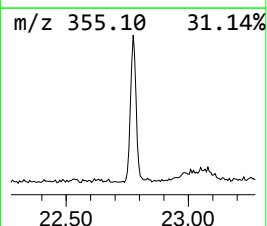
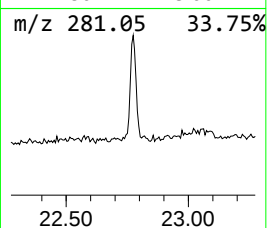
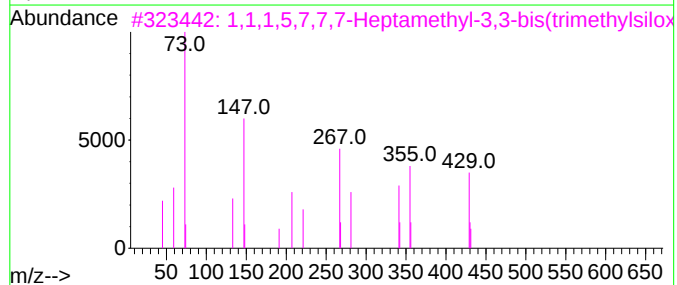
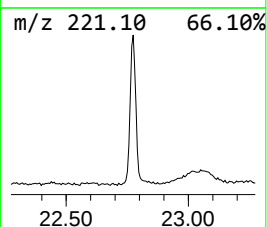
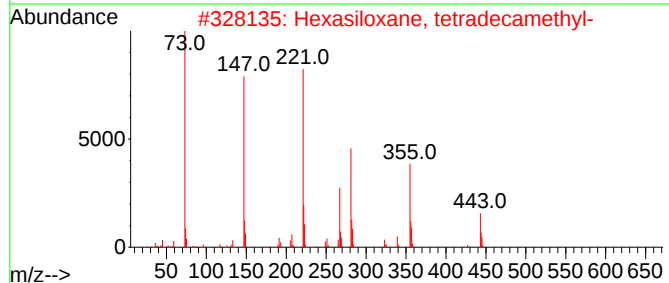
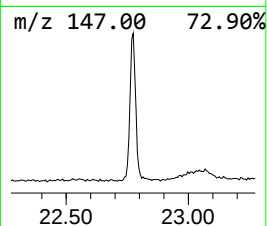
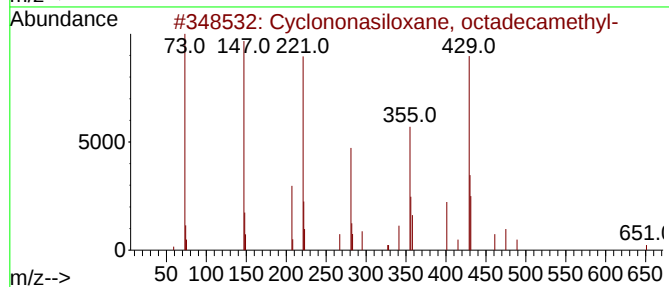
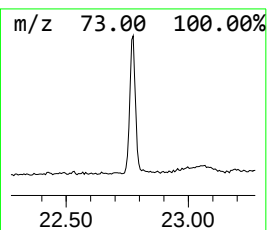
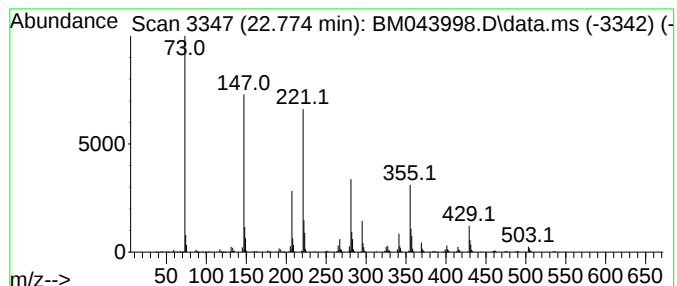
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Peak Number 4 Hexasiloxane, tetradecamethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.774	5.17 ng	1364840	Perylene-d12	23.927

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			1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	59
4			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	47
5			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	37



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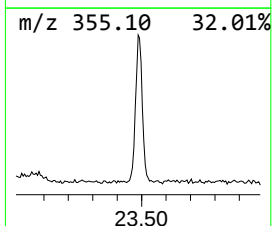
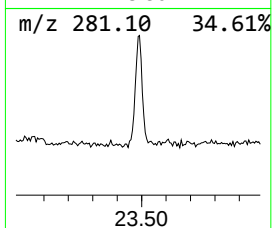
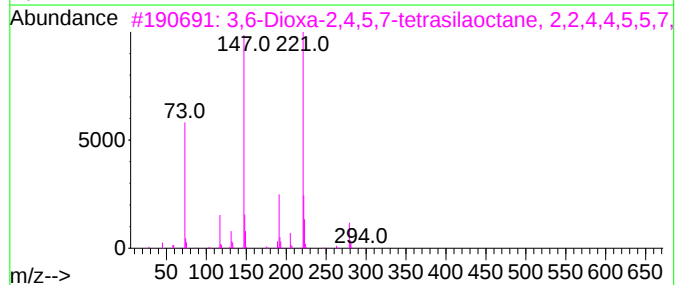
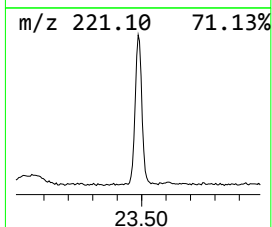
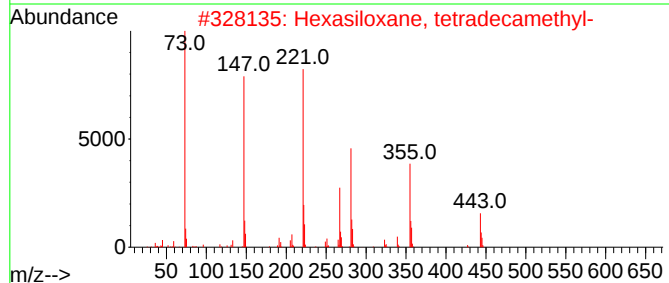
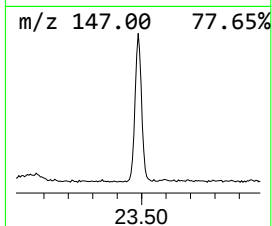
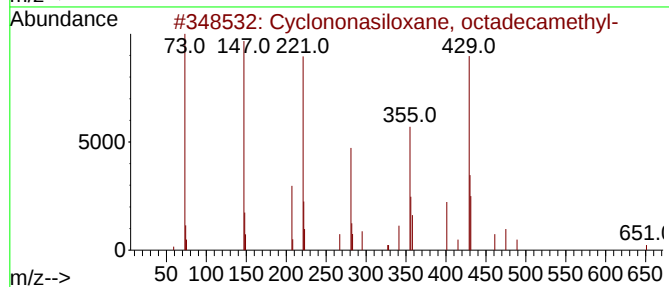
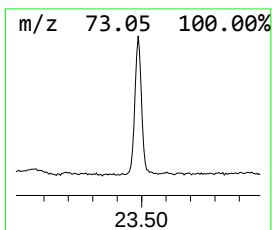
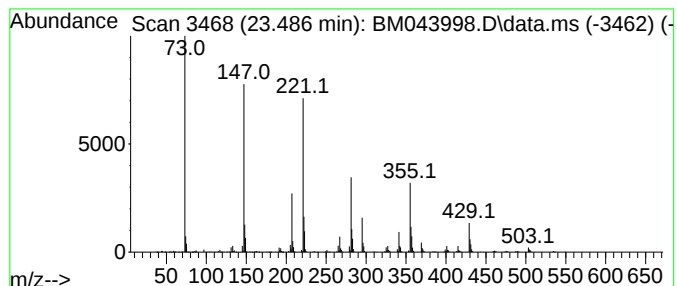
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Peak Number 5 3,6-Dioxa-2,4,5,7-tetrasilaoctane... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
23.486	7.73 ng	2040130	Perylene-d12		23.927	
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	87
3	3,6-Dioxa-2,4,5,7-tetrasilaoctan...		294	C10H30O2Si4	004342-25-0	50
4	Pentasiloxane, dodecamethyl-		384	C12H36O4Si5	000141-63-9	43
5	N-Benzyl-N-ethyl-p-isopropylbenz...		281	C19H23NO	015089-22-2	38



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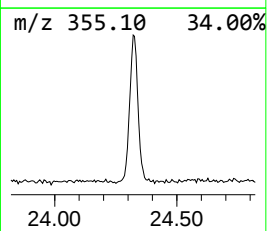
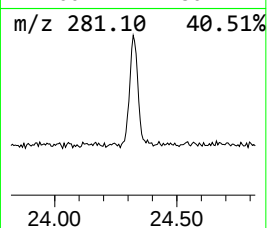
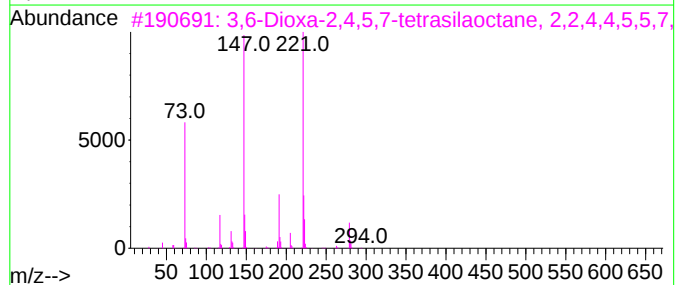
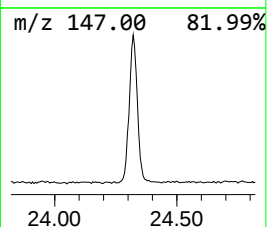
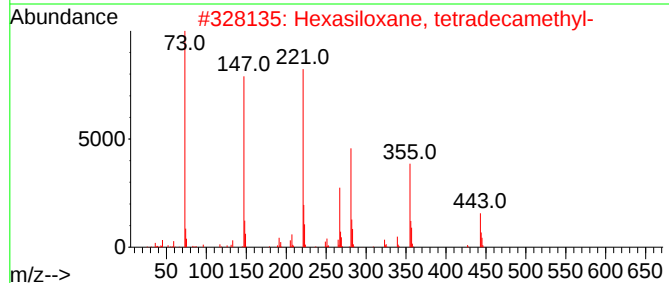
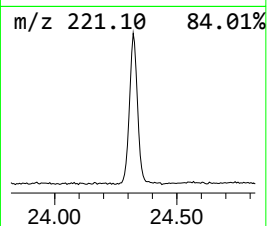
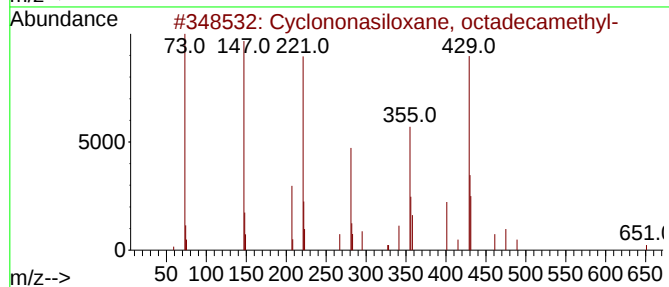
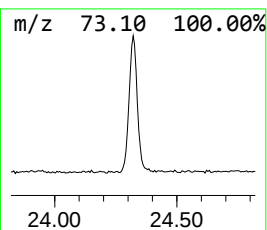
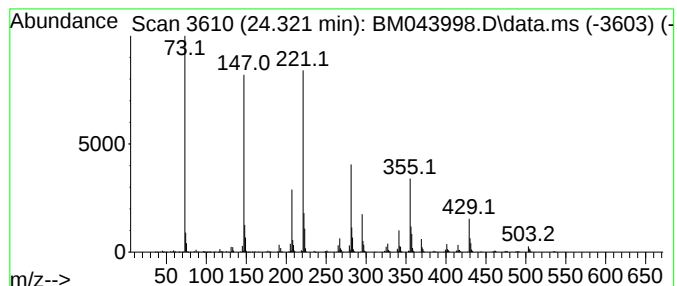
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown24.321 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.321	9.36 ng	2470350	Perylene-d12	23.927

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	72
3			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	50
4			Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	38
5			1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM020624\
Data File : BM043998.D
Acq On : 06 Feb 2024 18:53
Operator : MA/JU
Sample : PB158215BL
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB158215BL

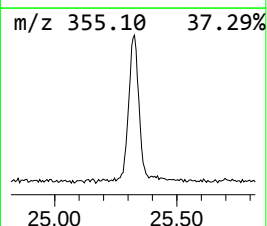
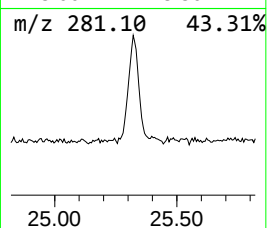
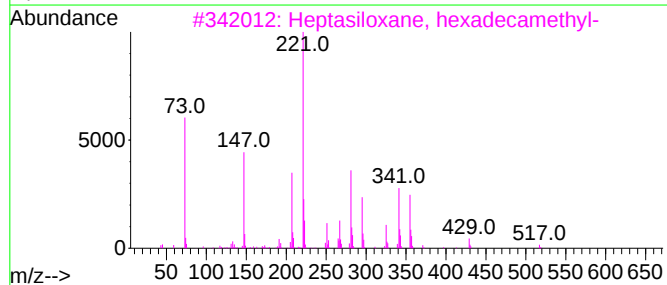
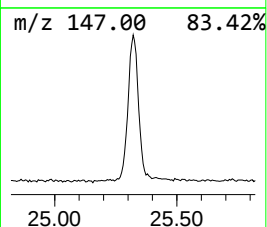
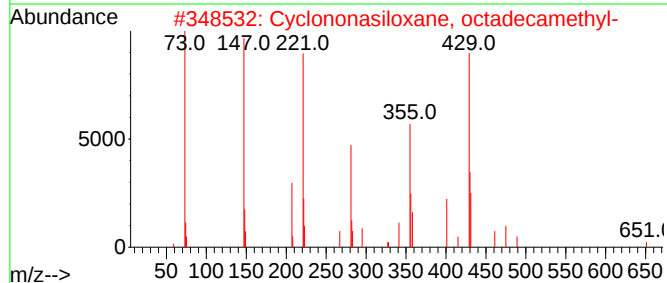
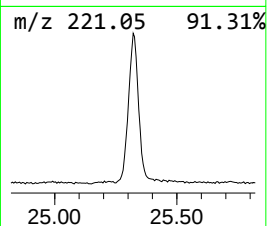
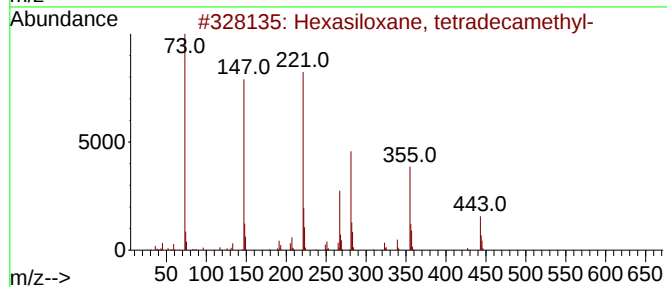
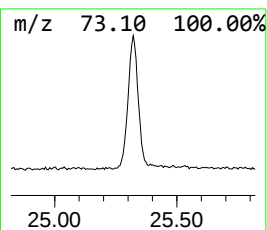
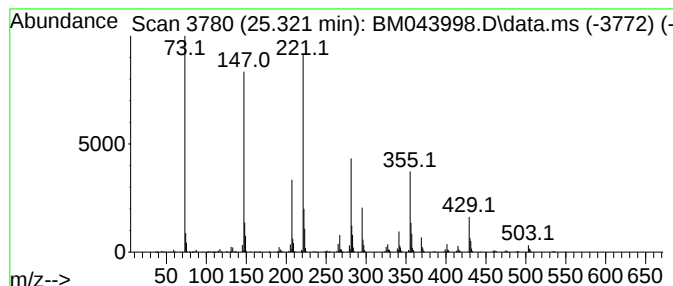
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptasiloxane, hexadecamethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.321	9.97 ng	2632420	Perylene-d12	23.927

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	80
3			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	78
4			Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	27
5			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM020624\
Data File : BM043998.D
Acq On : 06 Feb 2024 18:53
Operator : MA/JU
Sample : PB158215BL
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB158215BL

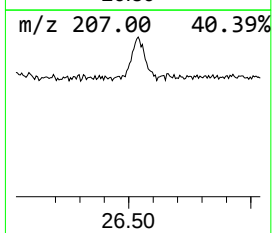
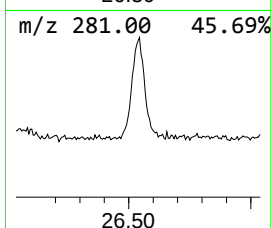
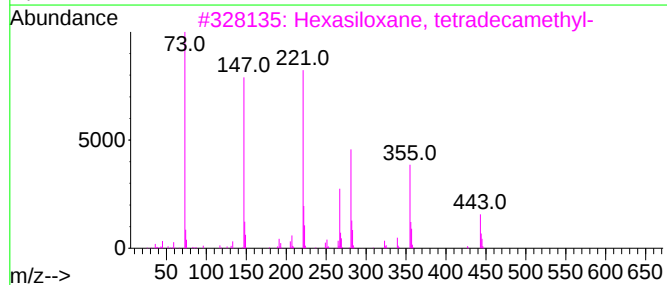
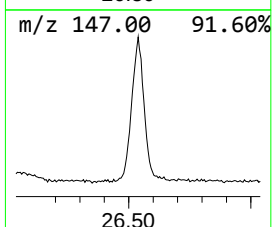
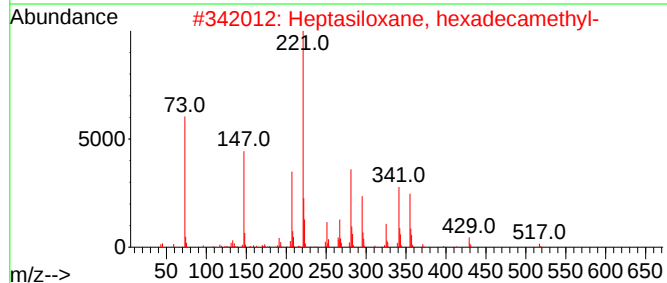
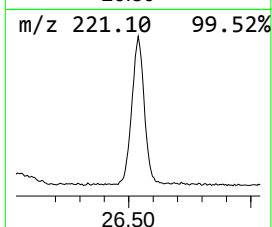
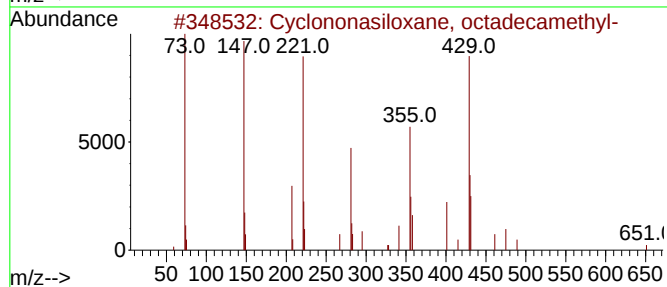
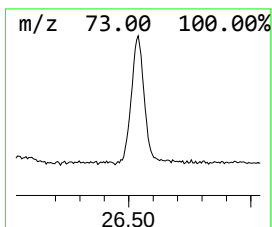
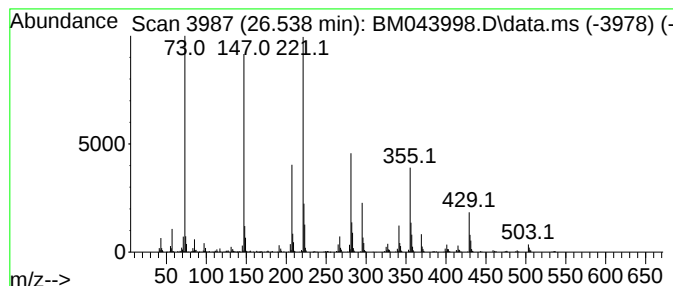
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown26.538 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.538	11.31 ng	2986210	Perylene-d12	23.927

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	87
2			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	78
3			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	76
4			3,6-Dioxo-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	55
5			Cyclodecasiloxane, eicosamethyl-	740	C20H60O10Si10	018772-36-6	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM020624\
Data File : BM043998.D
Acq On : 06 Feb 2024 18:53
Operator : MA/JU
Sample : PB158215BL
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB158215BL

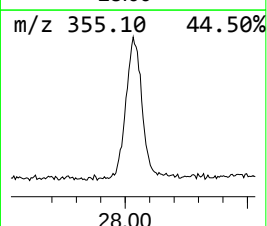
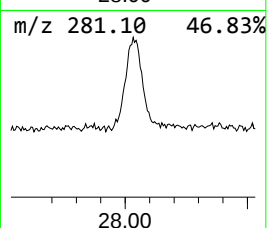
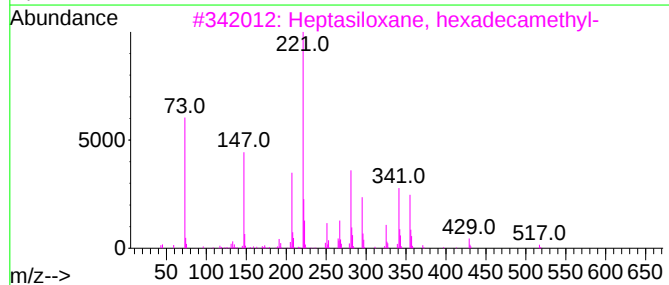
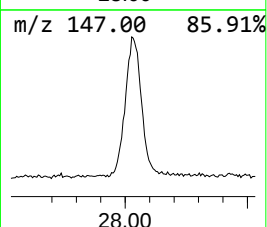
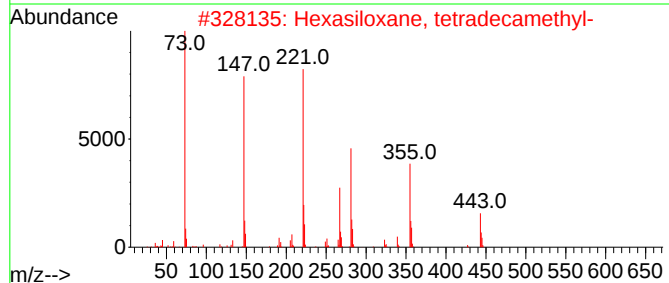
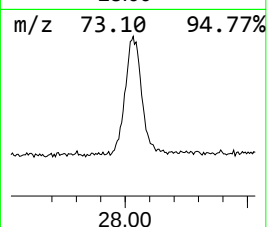
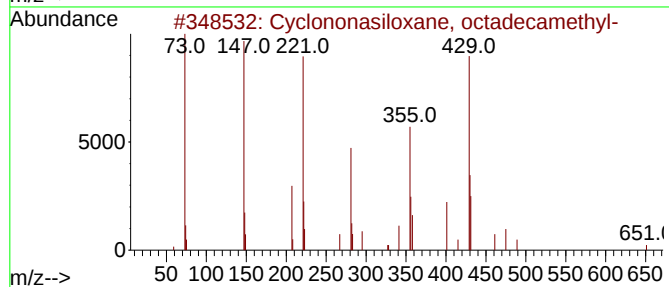
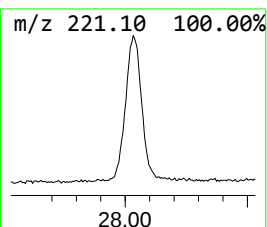
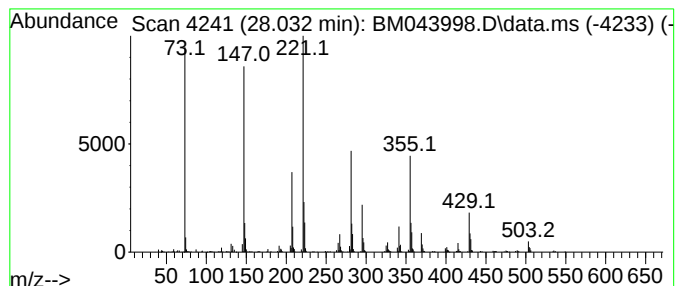
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown28.032 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.032	9.88 ng	2608840	Perylene-d12	23.927

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	87
3			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	64
4			3,6-Dioxo-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	60
5			Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM020624\
Data File : BM043998.D
Acq On : 06 Feb 2024 18:53
Operator : MA/JU
Sample : PB158215BL
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020524.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,...	4.428	6.4	ng	357396	1	7.922	1120600	20.0
2-Pentanone, 4-...	5.034	29.7	ng	1663680	1	7.922	1120600	20.0
Cyclononasiloxa...	22.139	3.7	ng	870456	5	21.515	4667260	20.0
Hexasiloxane, t...	22.774	5.2	ng	1364840	6	23.927	5279370	20.0
3,6-Dioxa-2,4,5...	23.486	7.7	ng	2040130	6	23.927	5279370	20.0
unknown24.321	24.321	9.4	ng	2470350	6	23.927	5279370	20.0
Heptasiloxane, ...	25.321	10.0	ng	2632420	6	23.927	5279370	20.0
unknown26.538	26.538	11.3	ng	2986210	6	23.927	5279370	20.0
unknown28.032	28.032	9.9	ng	2608840	6	23.927	5279370	20.0