

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121323\
 Data File : BF136549.D
 Acq On : 13 Dec 2023 21:19
 Operator : CG\JU
 Sample : 05760-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CONCRETE-1

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: BF136549.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.410	390	395	403	rBV	359768	381628	18.75%	3.000%
2	5.039	495	502	505	rBV	1223767	1824814	89.67%	14.347%
3	5.434	565	569	580	rBV	975188	784294	38.54%	6.166%
4	6.433	735	739	742	rBV	1470699	1277804	62.79%	10.046%
5	6.792	797	800	804	rVB	618426	473456	23.27%	3.722%
6	7.357	891	896	898	rBV	1065108	999778	49.13%	7.860%
7	8.069	1013	1017	1021	rBV	747518	621032	30.52%	4.883%
8	9.151	1196	1201	1204	rBV	2384804	2035037	100.00%	16.000%
9	9.827	1312	1316	1330	rBV	811821	656326	32.25%	5.160%
10	10.616	1447	1450	1460	rBV	190626	174370	8.57%	1.371%
11	11.316	1566	1569	1576	rBV	649849	573027	28.16%	4.505%
12	12.915	1837	1841	1844	rBV	1912280	1639220	80.55%	12.888%
13	13.368	1908	1918	1919	rBV8	10024	24969	1.23%	0.196%
14	13.968	2016	2020	2028	rVB	512802	461458	22.68%	3.628%
15	14.451	2098	2102	2107	rBV3	32476	37562	1.85%	0.295%
16	14.833	2163	2167	2174	rBV2	49669	65495	3.22%	0.515%
17	15.104	2210	2213	2218	rBV3	23006	47693	2.34%	0.375%
18	15.274	2238	2242	2247	rVB4	41307	66924	3.29%	0.526%
19	15.451	2267	2272	2277	rBV	374540	464078	22.80%	3.649%
20	15.780	2323	2328	2335	rBV2	28794	58583	2.88%	0.461%
21	16.392	2427	2432	2440	rBV7	23227	51523	2.53%	0.405%

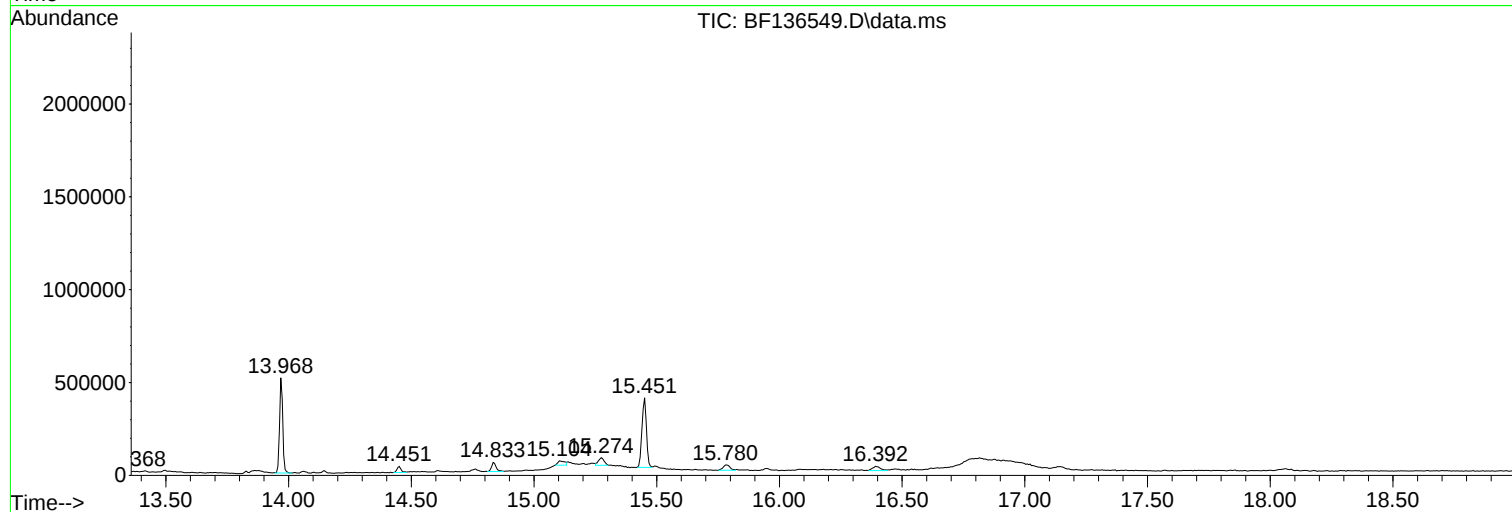
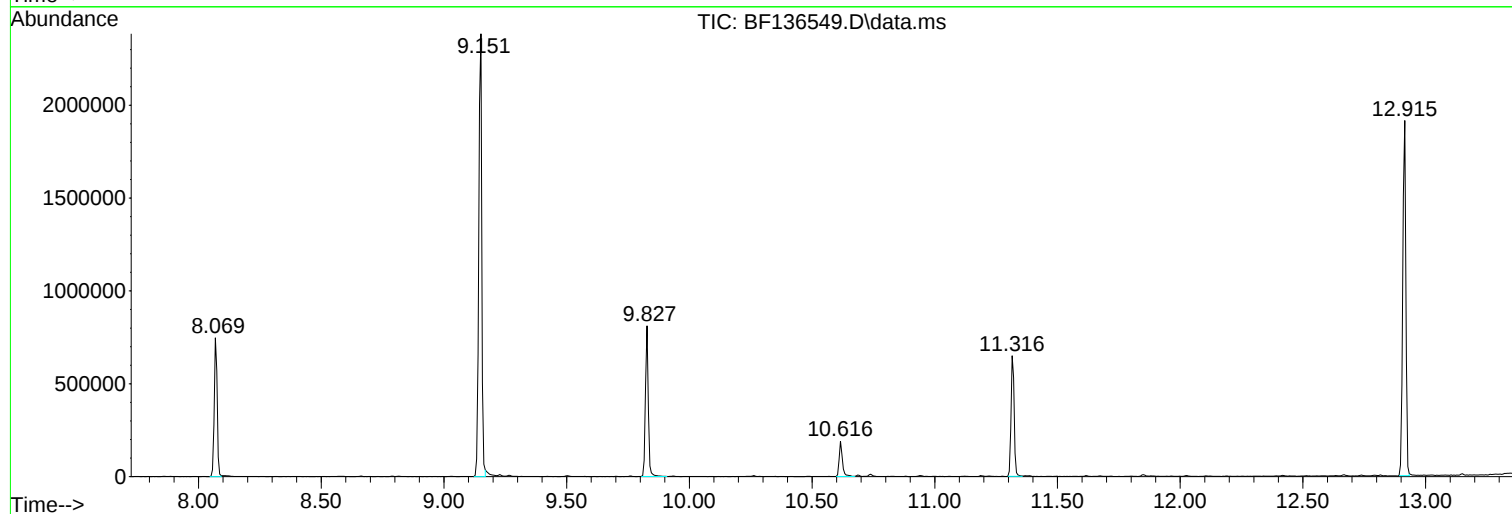
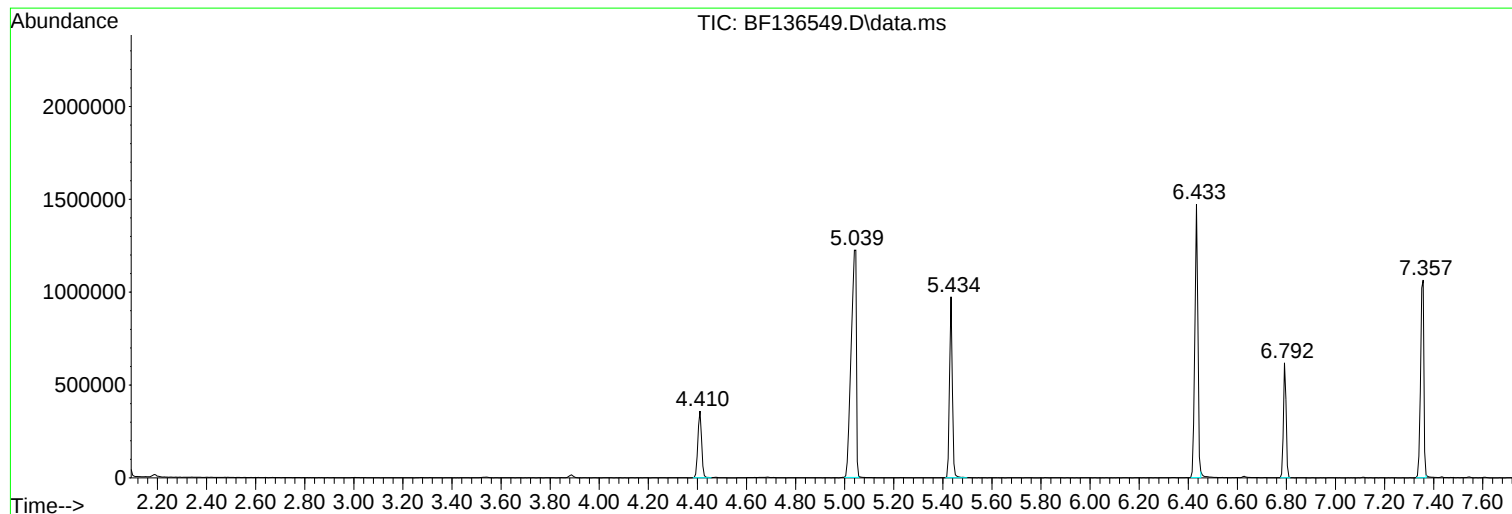
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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ClientSampleId :
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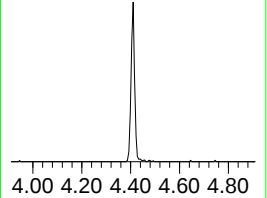
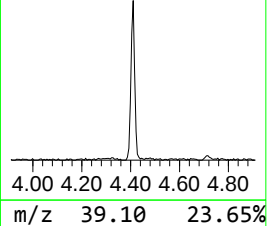
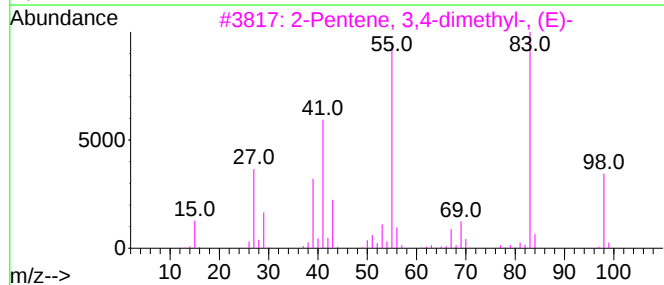
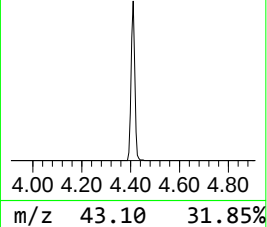
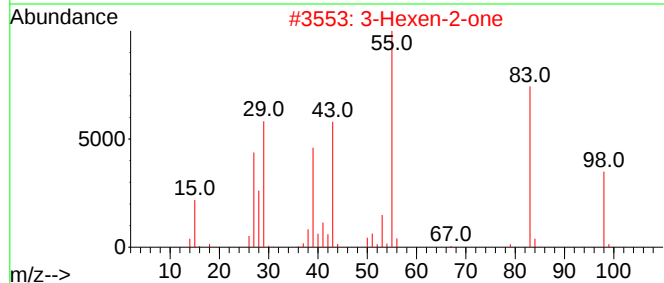
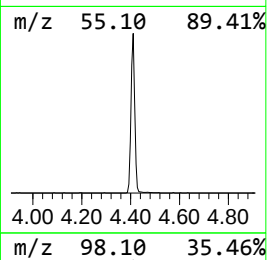
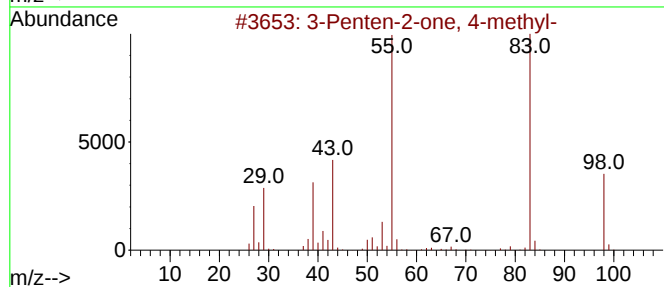
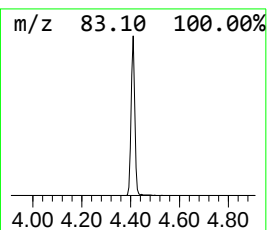
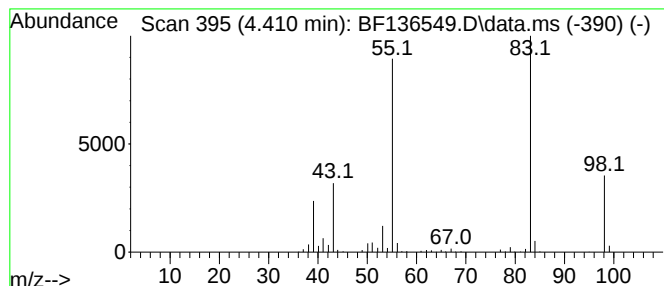
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.410	16.12 ng	381628	1,4-Dichlorobenzene-d4	6.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
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			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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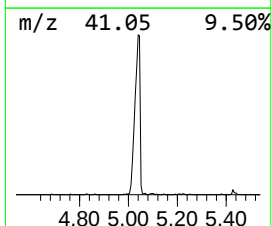
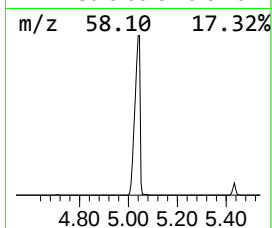
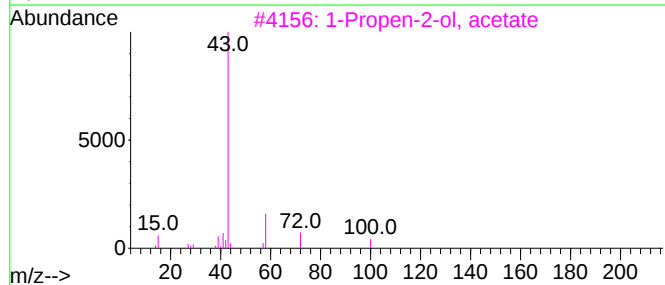
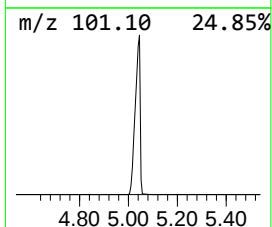
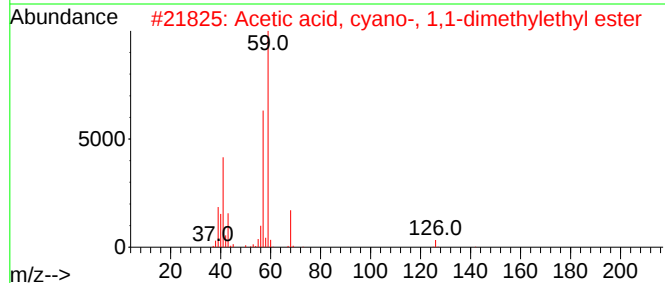
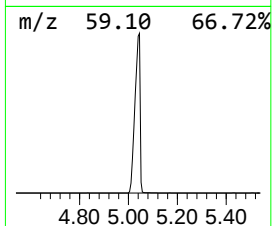
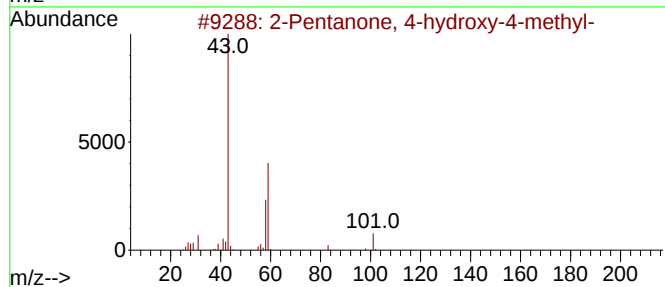
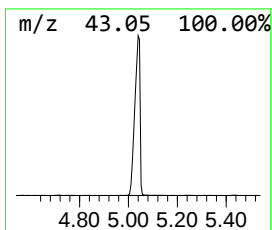
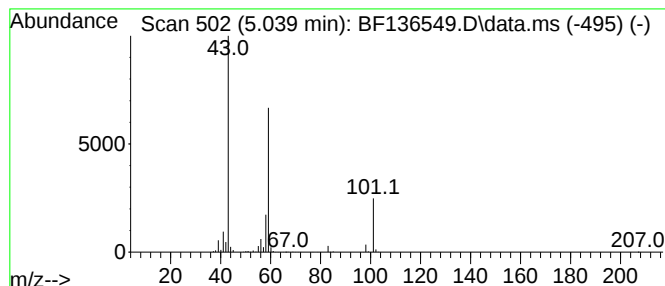
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.039	77.08 ng	1824810	1,4-Dichlorobenzene-d4	6.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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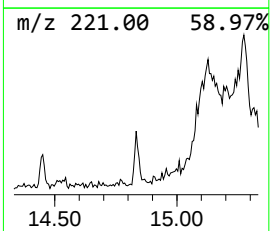
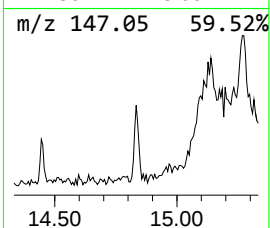
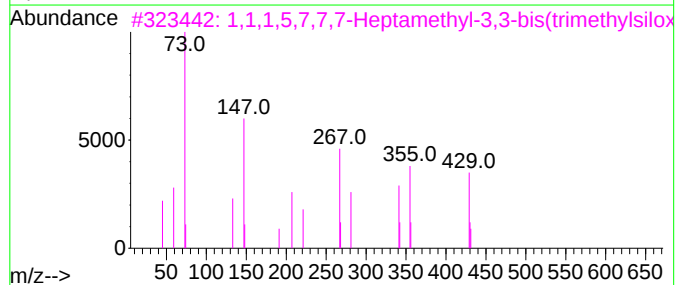
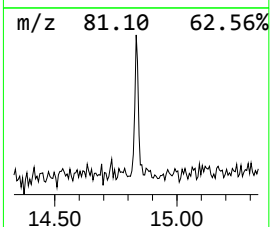
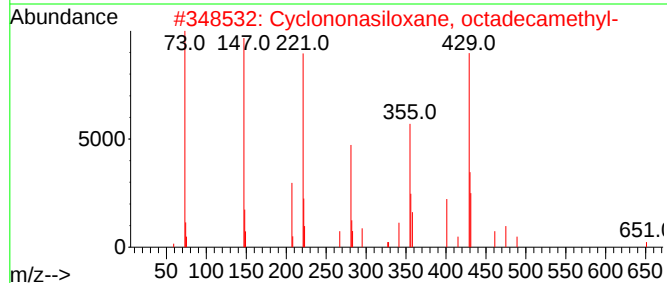
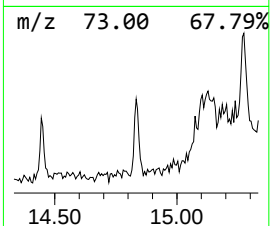
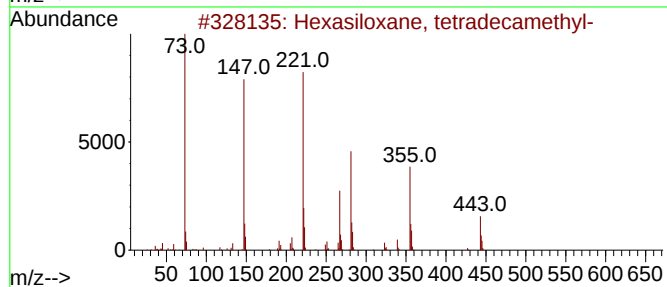
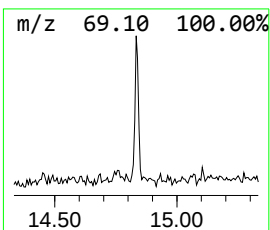
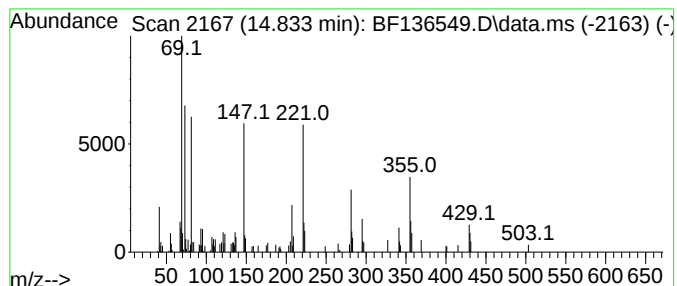
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 unknown14.833 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.833	2.82 ng	65495	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	49
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	37
3			1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	25
4			1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	606	C18H54O7Si8	000556-69-4	16
5			1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	680	C20H60O8Si9	002652-13-3	16



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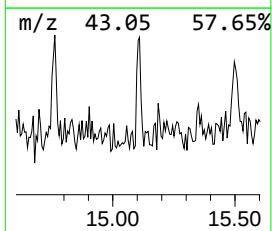
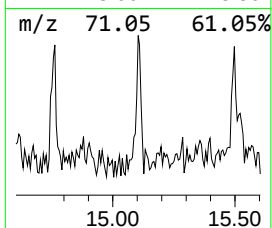
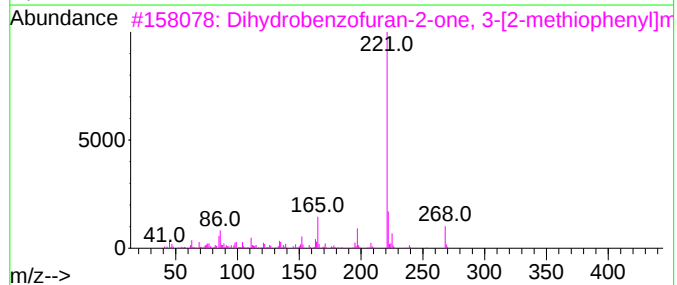
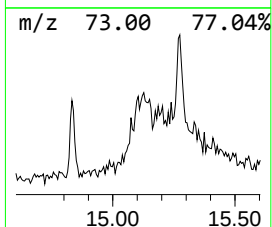
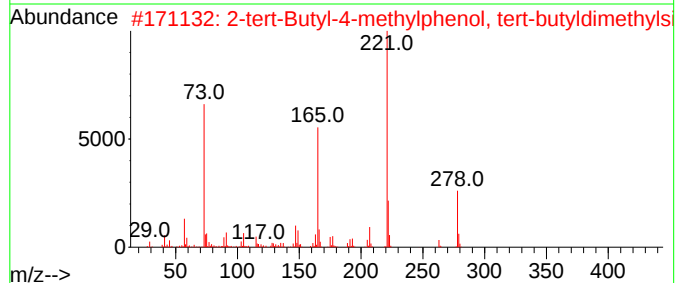
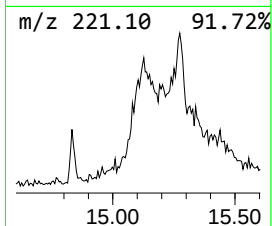
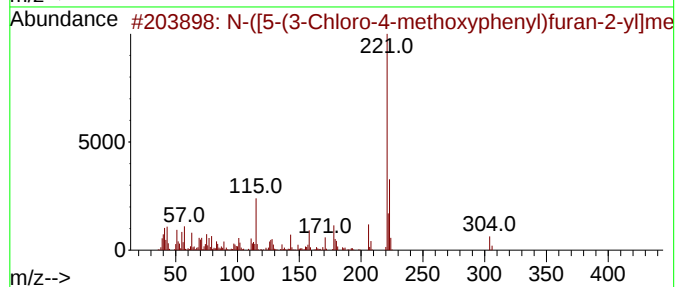
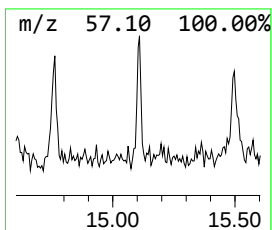
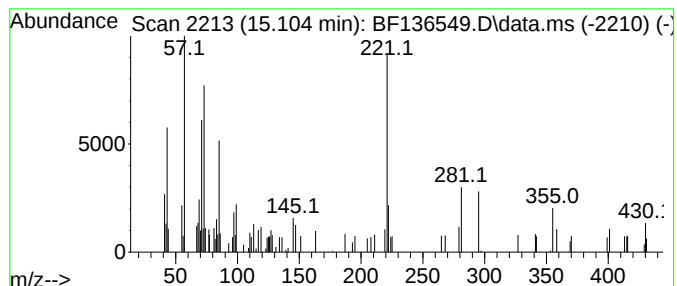
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown15.104 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.104	2.06 ng	47693	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-([5-(3-Chloro-4-methoxyphenyl)]...	304	C14H13ClN4O2	1000386-83-2	27
2			2-tert-Butyl-4-methylphenol, ter...	278	C17H30OSi	174362-55-1	27
3			Dihydrobenzofuran-2-one, 3-[2-me...	268	C16H12O2S	1000132-67-5	27
4			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	25
5			2-(Trifluoromethyl)-7H-1,3,4-thi...	221	C6H2F3N3OS	094605-13-7	22



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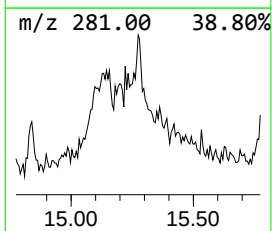
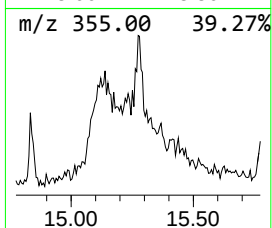
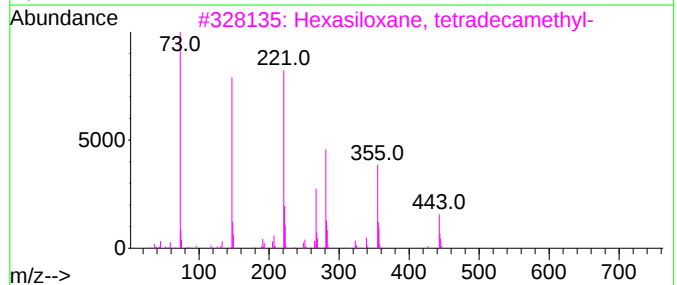
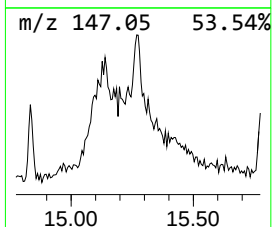
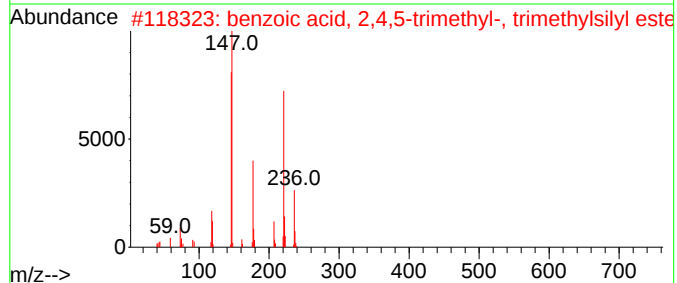
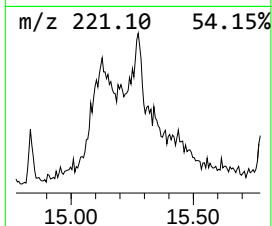
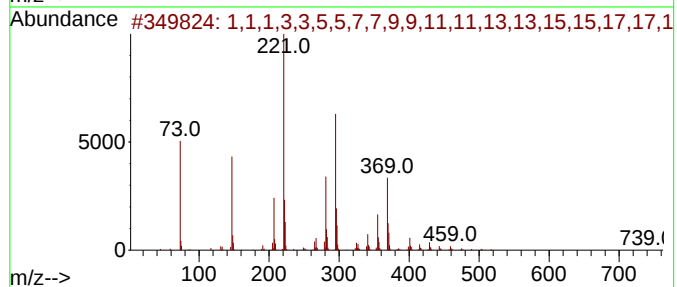
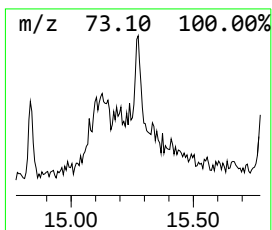
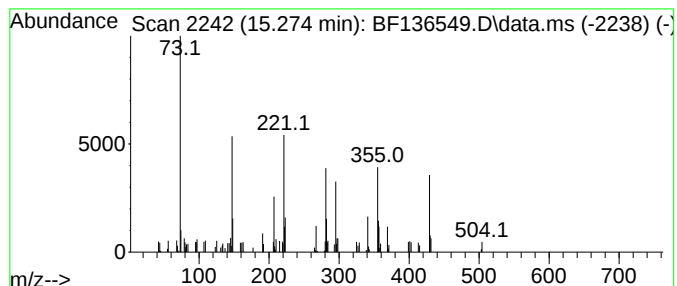
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown15.274 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.274	2.88 ng	66924	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	754	C22H66O9Si10	000556-70-7	35		
2	benzoic acid, 2,4,5-trimethyl-, ...	236	C13H20O2Si	1000396-43-7	22		
3	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	22		
4	1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	16		
5	1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	606	C18H54O7Si8	000556-69-4	14		



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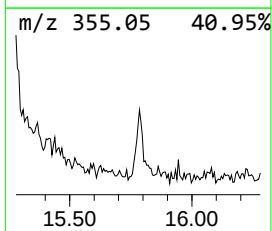
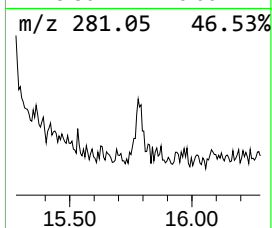
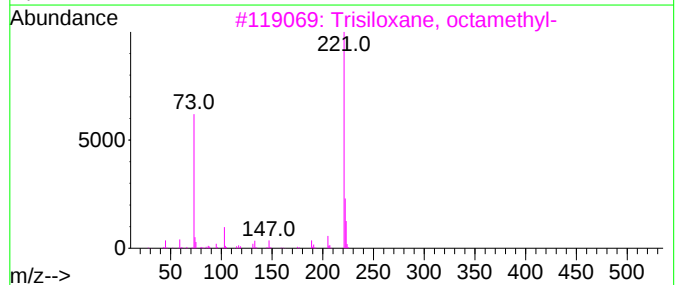
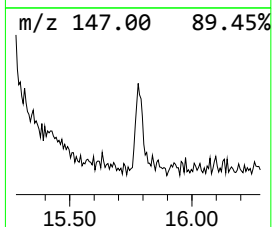
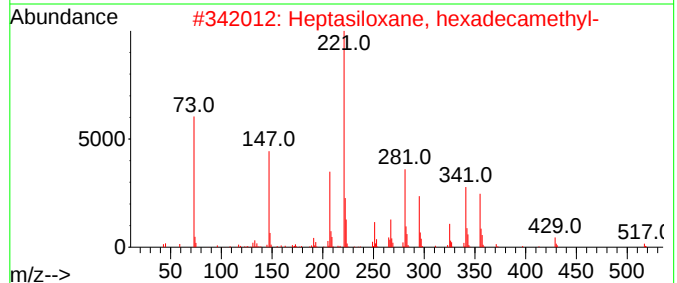
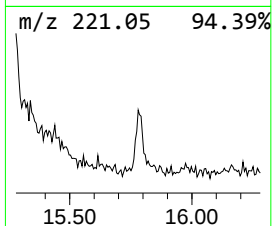
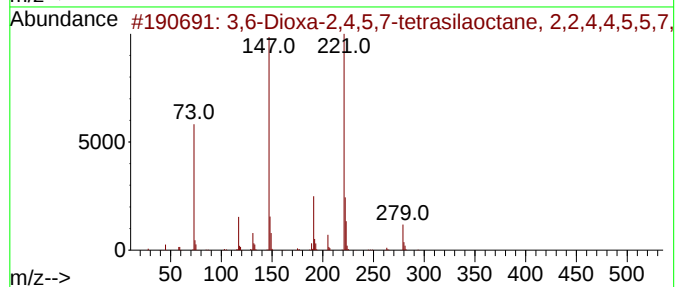
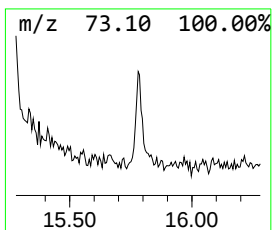
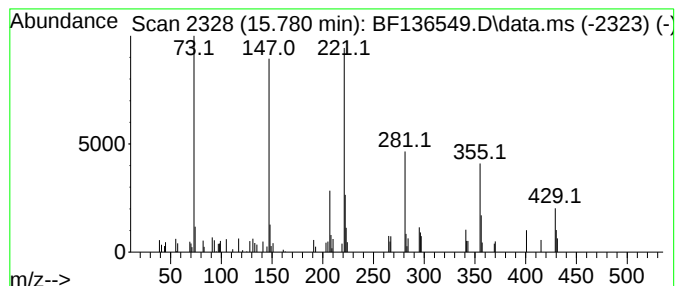
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown15.780 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.780	2.52 ng	58583	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	37
2			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	33
3			Trisiloxane, octamethyl-	236	C8H24O2Si3	000107-51-7	22
4			benzenamine, N-[bis(2,4,6-trimet...	341	C24H28BN	1000398-20-2	14
5			3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121323\
Data File : BF136549.D
Acq On : 13 Dec 2023 21:19
Operator : CG\JU
Sample : 05760-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONCRETE-1

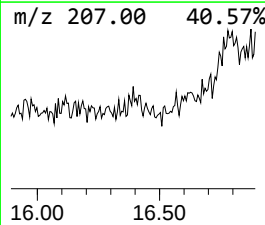
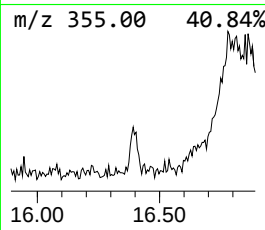
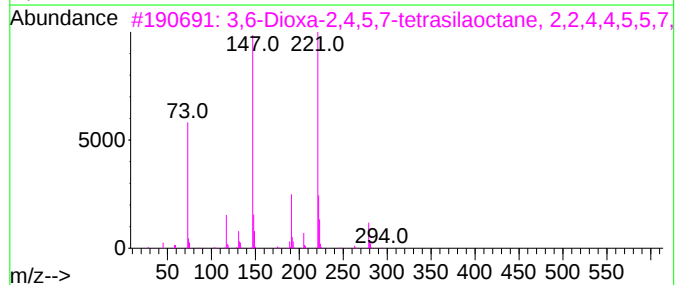
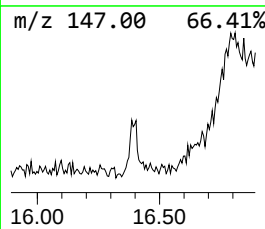
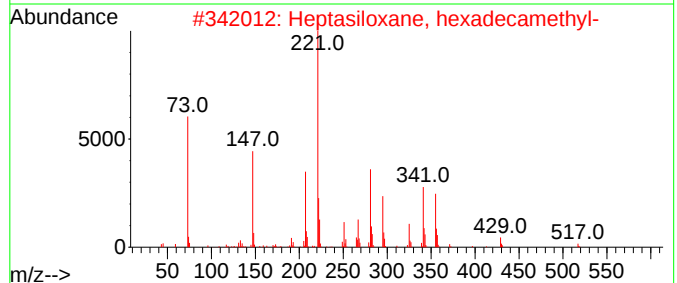
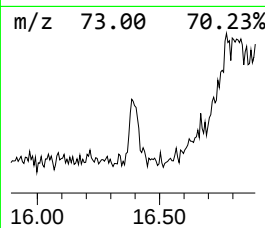
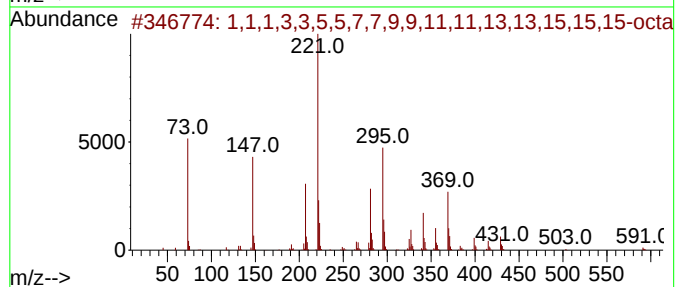
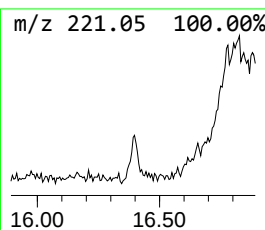
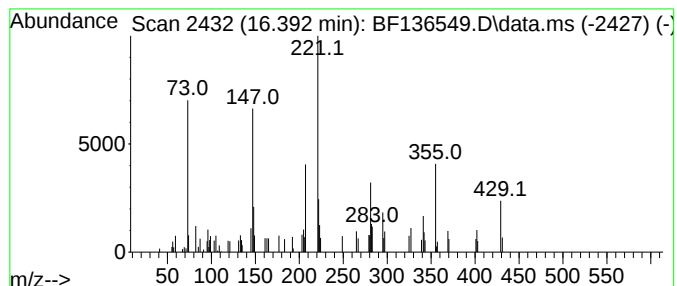
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown16.392 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.392	2.22 ng	51523	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	606	C18H5407Si8	000556-69-4	45		
2	Heptasiloxane, hexadecamethyl-	532	C16H4806Si7	000541-01-5	42		
3	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H3002Si4	004342-25-0	38		
4	1-(2-Hydroxy-5-methylphenyl)prop...	236	C13H2002Si	1000506-71-9	38		
5	Turmeronol A, TMS	304	C18H2802Si	1000495-94-9	38		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121323\
Data File : BF136549.D
Acq On : 13 Dec 2023 21:19
Operator : CG\JU
Sample : 05760-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONCRETE-1

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one,...	4.410	16.1	ng	381628	1	6.792	473456	20.0
2-Pentanone, 4-...	5.039	77.1	ng	1824810	1	6.792	473456	20.0
unknown14.833	14.833	2.8	ng	65495	6	15.451	464078	20.0
unknown15.104	15.104	2.1	ng	47693	6	15.451	464078	20.0
unknown15.274	15.274	2.9	ng	66924	6	15.451	464078	20.0
unknown15.780	15.780	2.5	ng	58583	6	15.451	464078	20.0
unknown16.392	16.392	2.2	ng	51523	6	15.451	464078	20.0