

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082021\
 Data File : BF125127.D
 Acq On : 20 Aug 2021 10:46
 Operator : JU/CG
 Sample : PB138542BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB138542BL

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-BF081821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125127.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.275	22	32	38	rVB	99738	140818	2.76%	0.422%
2	5.163	519	523	531	rVB	140981	181215	3.55%	0.544%
3	5.545	582	588	591	rBV	4111438	4580875	89.71%	13.743%
4	6.539	751	757	760	rBV	3953593	4485797	87.85%	13.458%
5	6.916	818	821	825	rBV	1104810	960790	18.82%	2.882%
6	7.481	912	917	920	rBV	3016767	2966883	58.10%	8.901%
7	8.198	1035	1039	1043	rBV	1313663	1240696	24.30%	3.722%
8	9.280	1217	1223	1226	rBV	4950365	4960047	97.13%	14.881%
9	9.957	1333	1338	1341	rBV	1670936	1363150	26.70%	4.090%
10	10.745	1467	1472	1475	rBV	3504651	3173316	62.14%	9.520%
11	11.445	1587	1591	1594	rBV	1582577	1372064	26.87%	4.116%
12	13.033	1856	1861	1864	rBV	5257990	5106357	100.00%	15.320%
13	14.086	2036	2040	2043	rBV	1181367	1078415	21.12%	3.235%
14	15.398	2258	2263	2271	rVB2	49733	77760	1.52%	0.233%
15	15.580	2289	2294	2298	rBV	781601	969397	18.98%	2.908%
16	15.915	2344	2351	2358	rBV2	62749	116917	2.29%	0.351%
17	16.068	2371	2377	2383	rBV	49754	76807	1.50%	0.230%
18	16.527	2446	2455	2462	rBV2	56905	126917	2.49%	0.381%
19	16.592	2462	2466	2474	rVB2	42053	73396	1.44%	0.220%
20	17.209	2565	2571	2575	rBV2	25430	51913	1.02%	0.156%
21	17.274	2575	2582	2592	rVB6	41267	124275	2.43%	0.373%
22	18.186	2729	2737	2748	rVB4	34046	104199	2.04%	0.313%

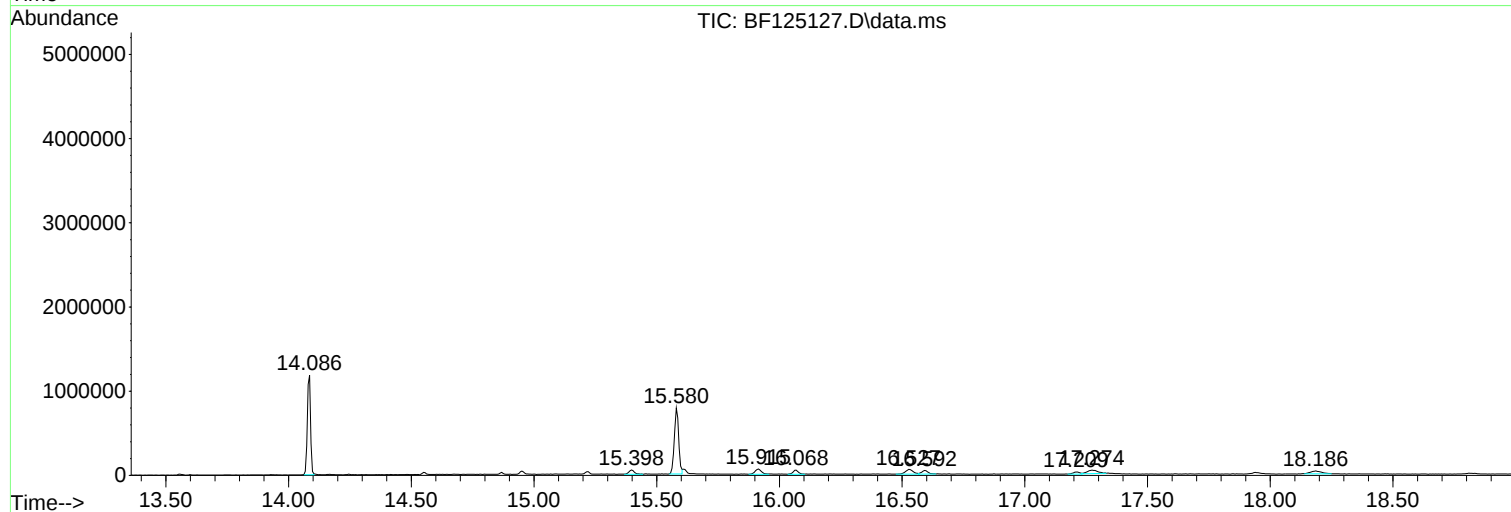
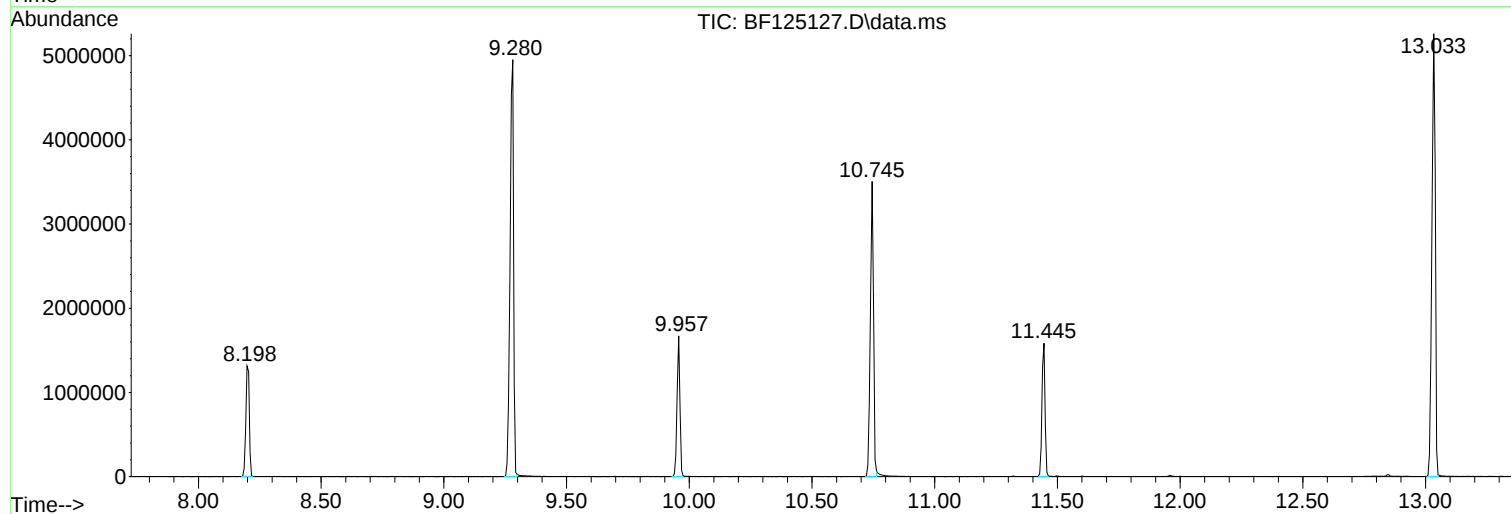
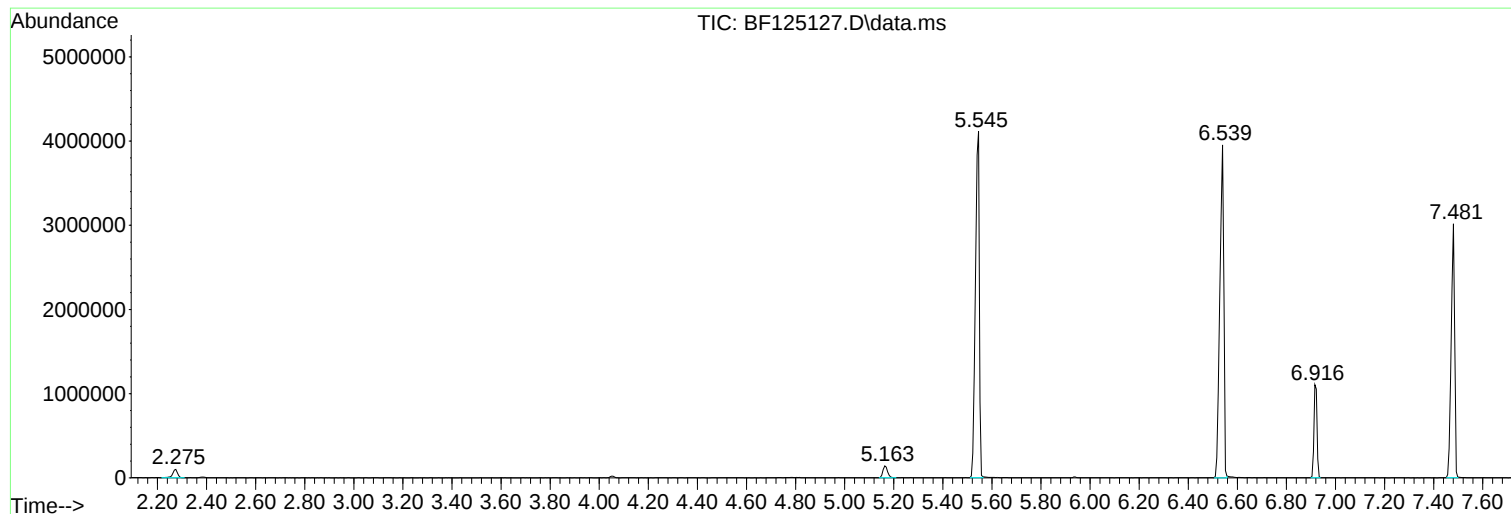
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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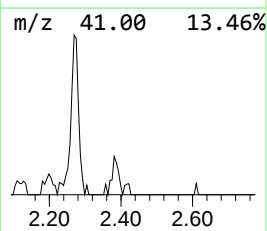
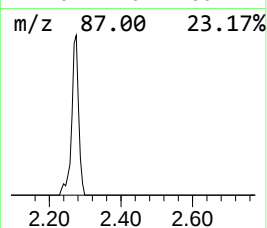
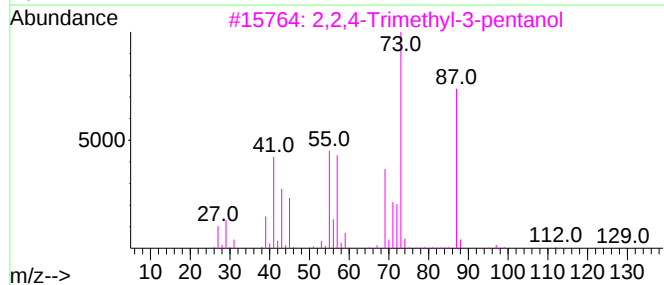
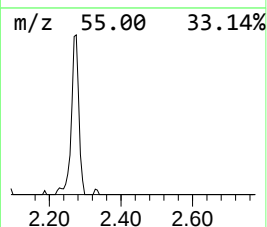
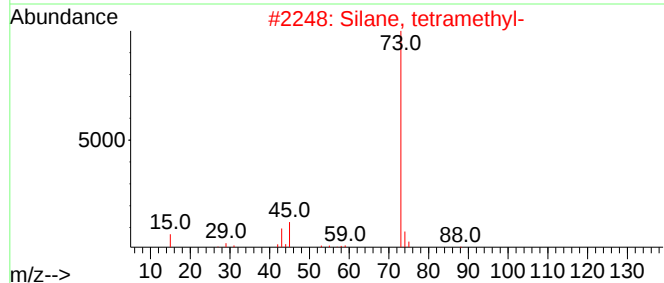
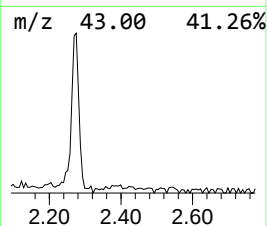
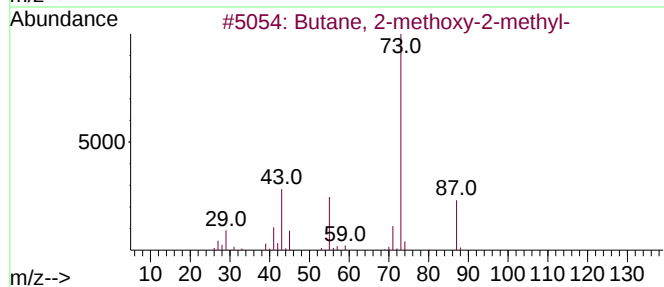
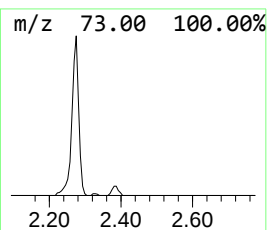
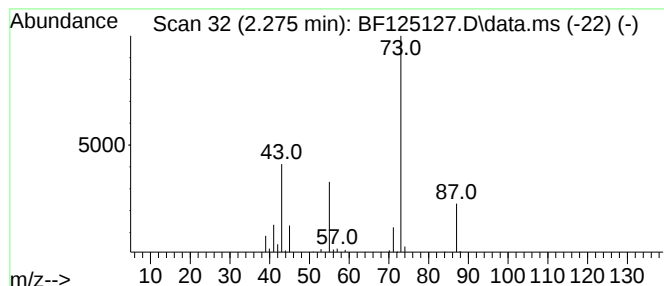
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.275	2.93 ng	140818	1,4-Dichlorobenzene-d4	6.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	28
5			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25



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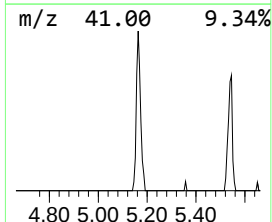
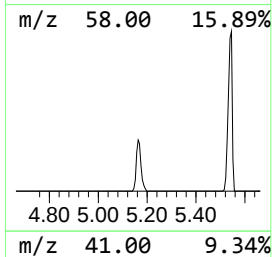
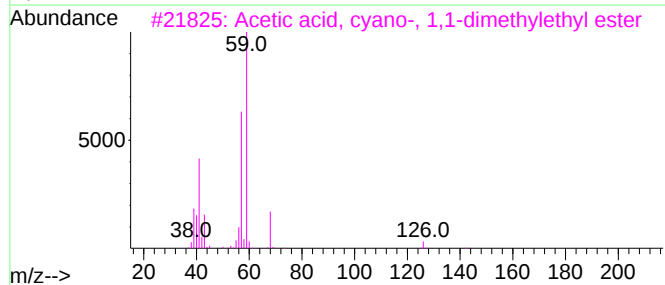
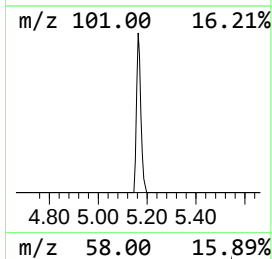
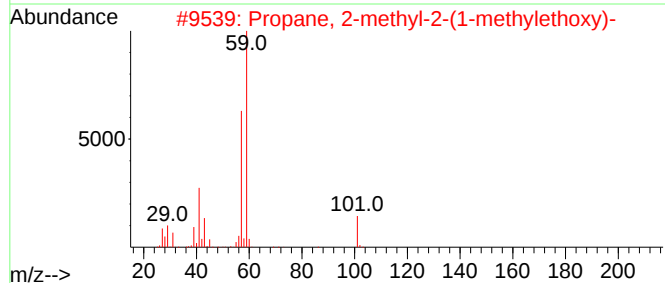
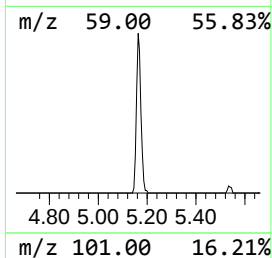
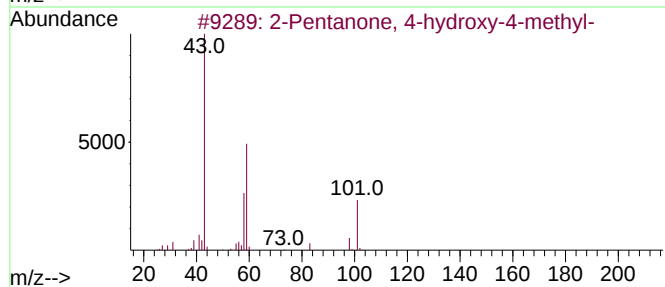
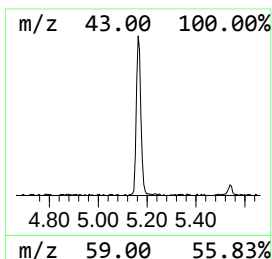
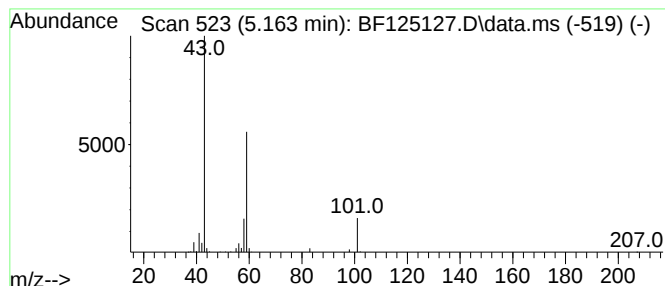
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.163	3.77 ng	181215	1,4-Dichlorobenzene-d4	6.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4			3-Octanol	130	C8H18O	000589-98-0	28
5			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28



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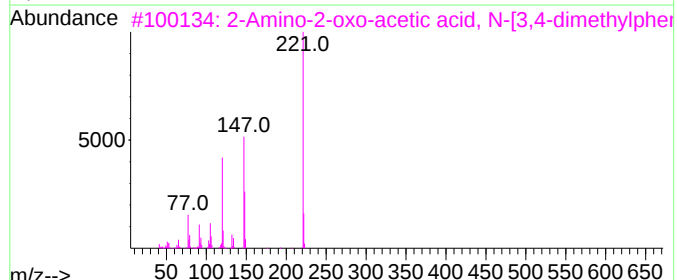
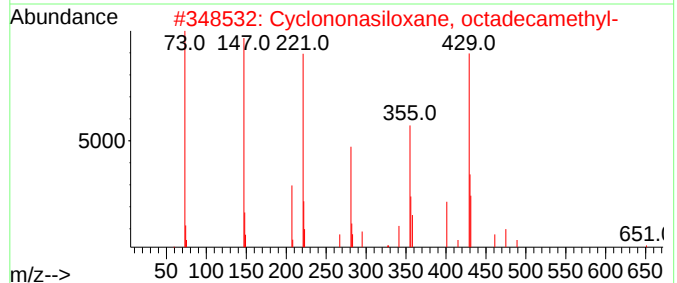
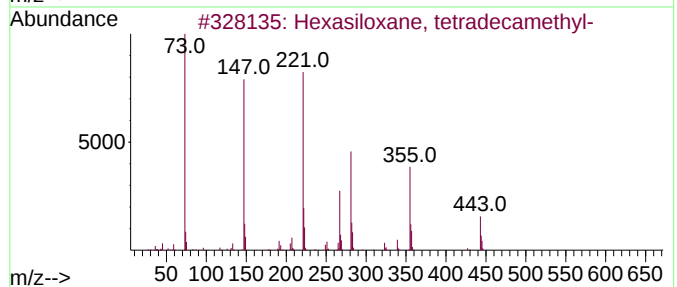
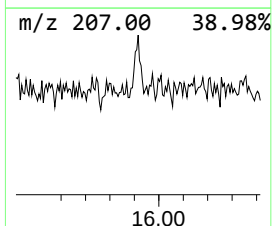
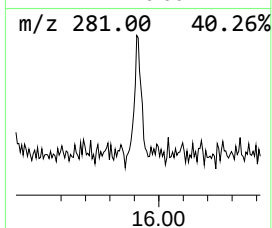
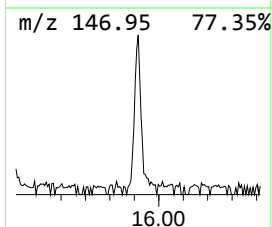
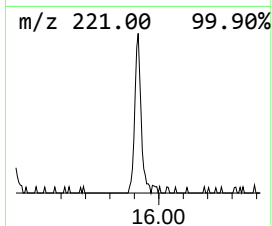
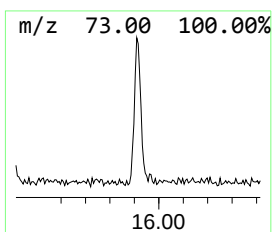
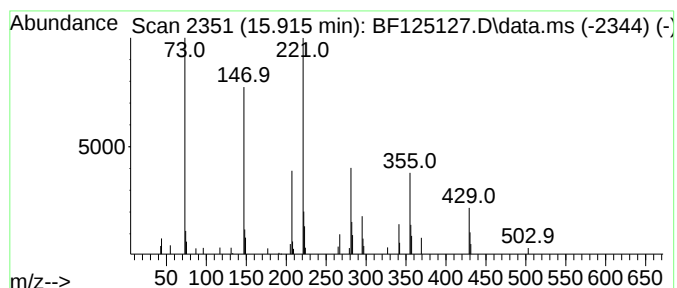
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexasiloxane, tetradecamethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.915	2.41 ng	116917	Perylene-d12	15.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	76
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	64
3			2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	37
4			3,6-Dioxo-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	37
5			Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	27



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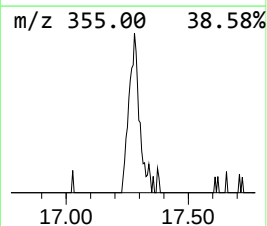
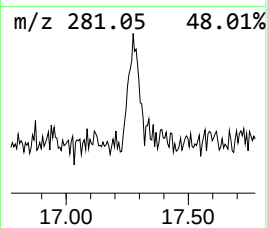
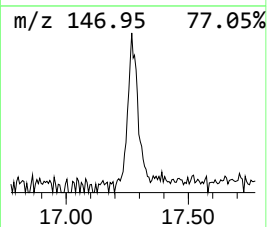
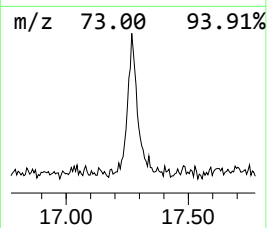
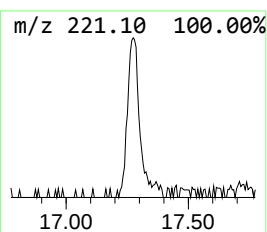
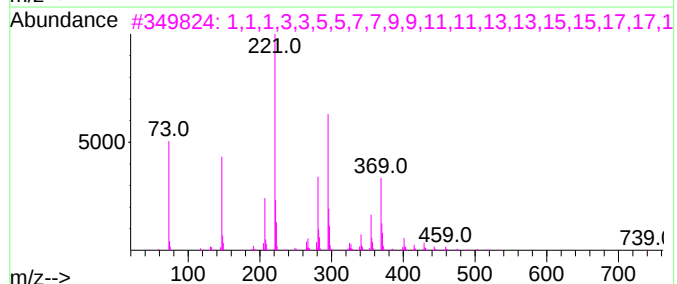
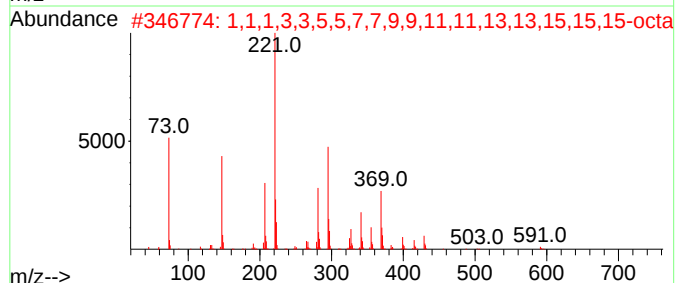
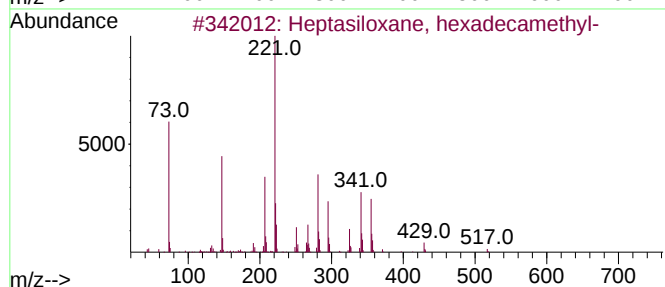
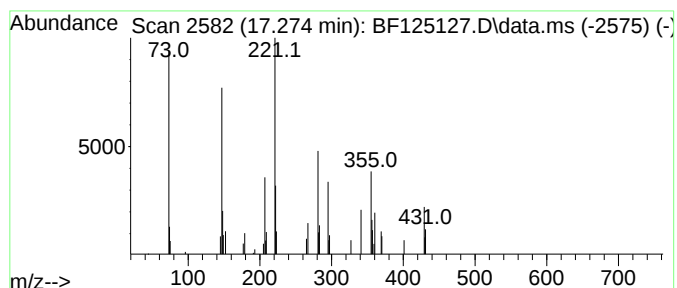
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown17.274 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.274	2.56 ng	124275	Perylene-d12	15.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	43
2			1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	606	C18H54O7Si8	000556-69-4	42
3			1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	754	C22H66O9Si10	000556-70-7	40
4			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	38
5			Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	22



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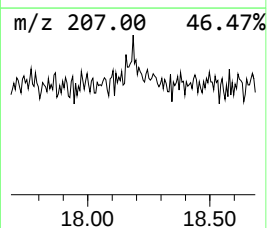
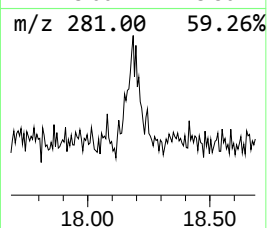
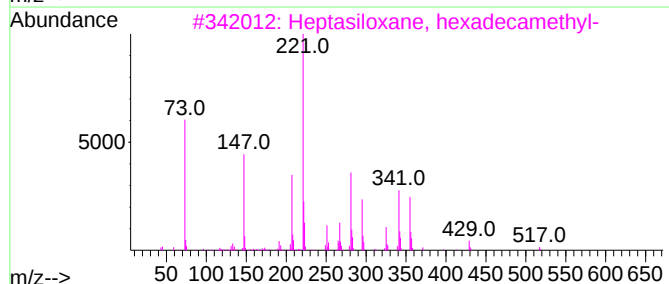
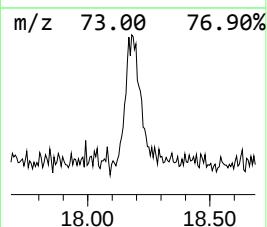
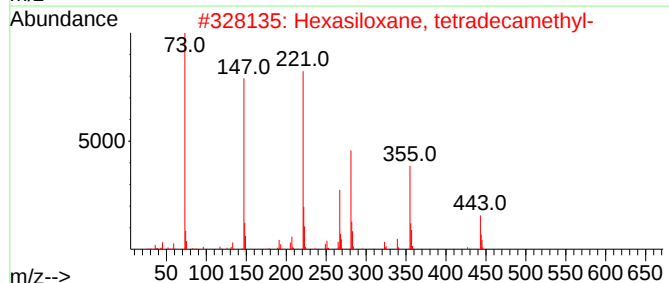
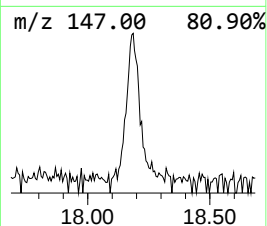
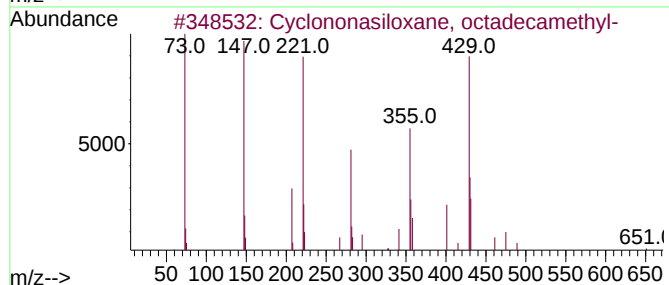
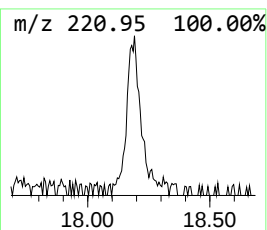
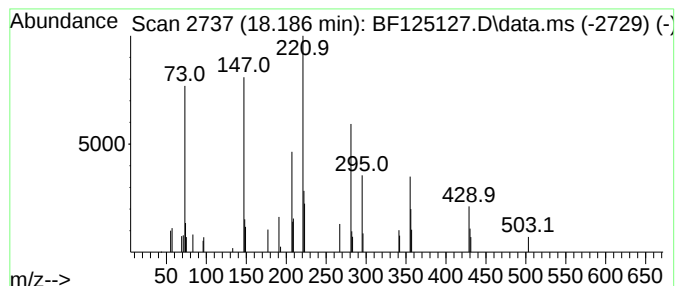
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TIC Library : C:\Database\NIST20.L
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Peak Number 6 Cyclononasiloxane, octadeca... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.186	2.15 ng	104199	Perylene-d12	15.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	80
2			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	50
3			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	50
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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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.275	2.9	ng	140818	1	6.922	960790	20.0
2-Pentanone, 4-...	5.163	3.8	ng	181215	1	6.922	960790	20.0
Hexasiloxane, t...	15.915	2.4	ng	116917	6	15.580	969397	20.0
unknown17.274	17.274	2.6	ng	124275	6	15.580	969397	20.0
Cyclononasiloxa...	18.186	2.1	ng	104199	6	15.580	969397	20.0