

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021723\
 Data File : BF132462.D
 Acq On : 17 Feb 2023 21:43
 Operator : CG\JU
 Sample : 01595-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S-322-1

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-BF021623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132462.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.266	408	413	424	rVB	2004972	2747079	43.26%	5.712%
2	5.654	473	479	482	rBV	4902470	5420167	85.35%	11.270%
3	6.643	641	647	650	rBV	4882559	5472386	86.17%	11.379%
4	7.019	708	711	715	rBV	1783540	1451906	22.86%	3.019%
5	7.584	802	807	810	rBV	3581628	3599351	56.68%	7.484%
6	8.307	926	930	933	rBV	2338115	1883805	29.66%	3.917%
7	9.384	1107	1113	1116	rBV	6421183	5976529	94.11%	12.427%
8	10.072	1226	1230	1233	rVB	2529146	2178060	34.30%	4.529%
9	10.783	1345	1351	1355	rBV	536518	409926	6.46%	0.852%
10	10.866	1360	1365	1368	rBV	4243878	4138432	65.17%	8.605%
11	11.566	1480	1484	1487	rBV	2730297	2330398	36.70%	4.846%
12	12.077	1567	1571	1576	rBV	517780	554317	8.73%	1.153%
13	12.866	1701	1705	1719	rBV	79363	136945	2.16%	0.285%
14	13.160	1750	1755	1758	rBV	6519717	6350318	100.00%	13.205%
15	14.048	1902	1906	1908	rBV3	77738	102116	1.61%	0.212%
16	14.219	1931	1935	1939	rBV	2148420	1947721	30.67%	4.050%
17	14.307	1944	1950	1957	rBV	1011905	1146972	18.06%	2.385%
18	15.001	2065	2068	2077	rVB3	54389	67452	1.06%	0.140%
19	15.089	2079	2083	2091	rVB	161341	180922	2.85%	0.376%
20	15.777	2194	2200	2212	rVB2	1275227	1789194	28.17%	3.720%
21	16.260	2271	2282	2292	rVB4	54969	141650	2.23%	0.295%
22	16.818	2372	2377	2389	rVB6	29266	66012	1.04%	0.137%

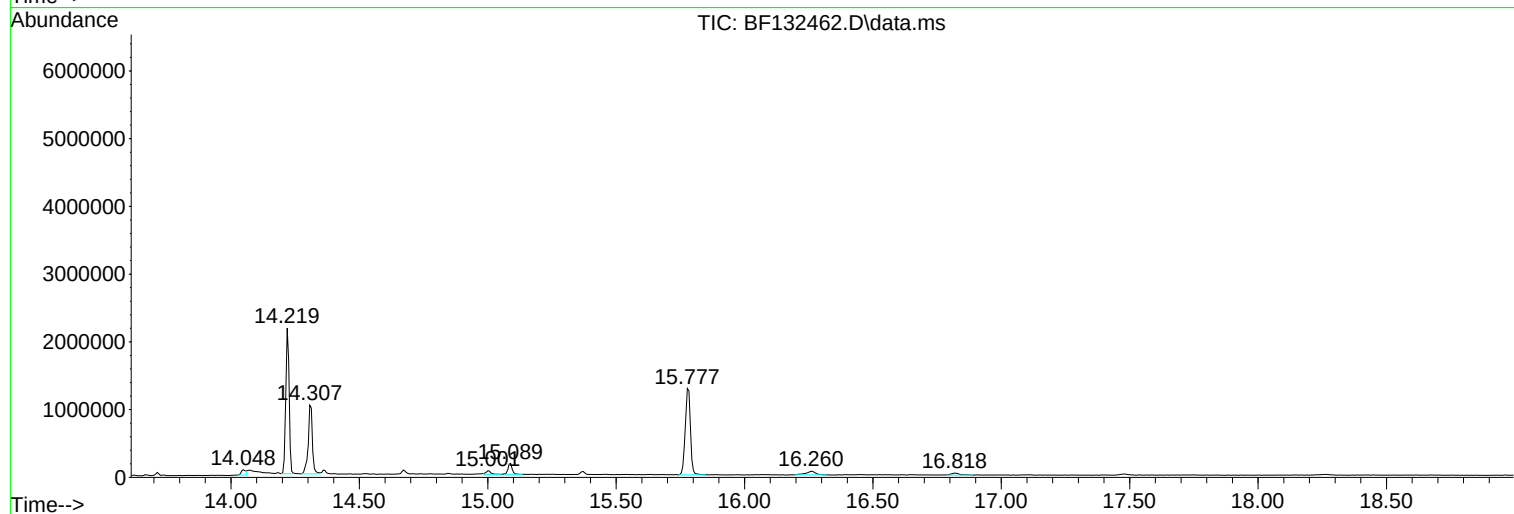
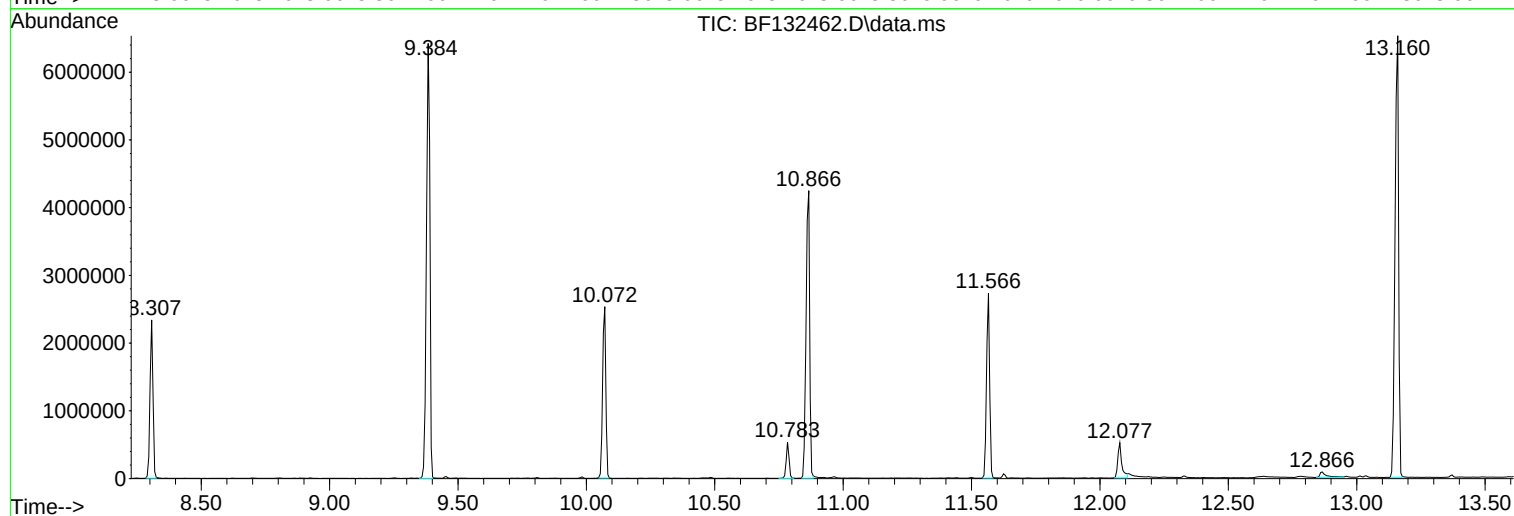
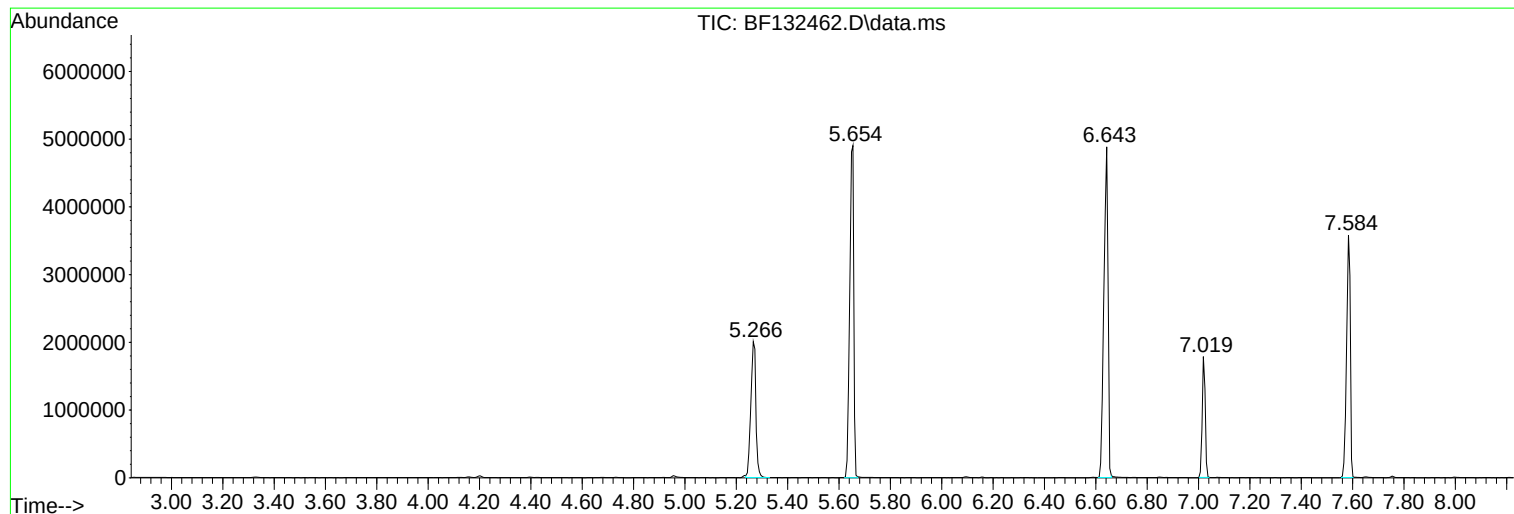
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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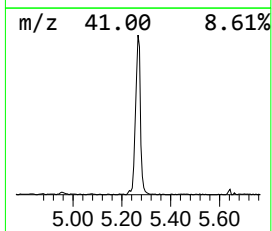
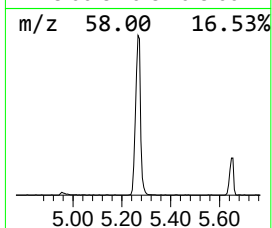
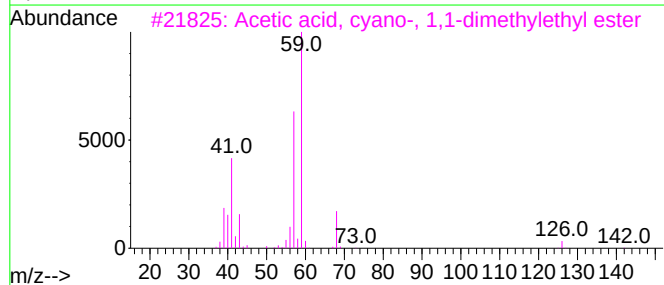
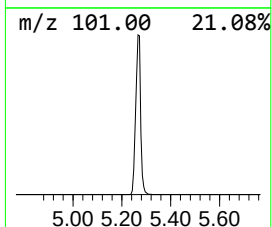
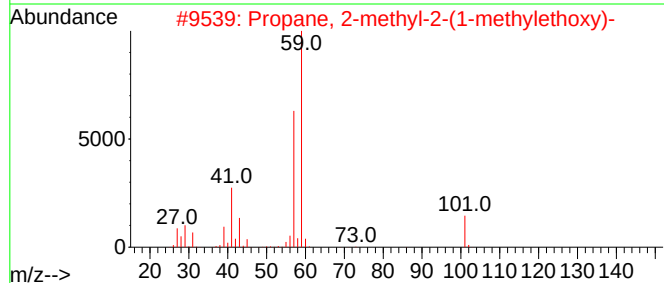
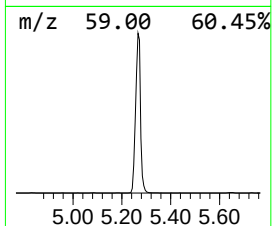
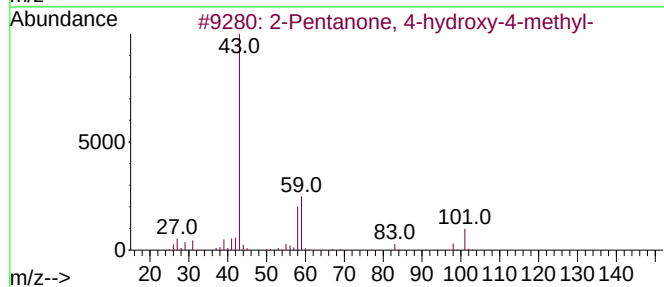
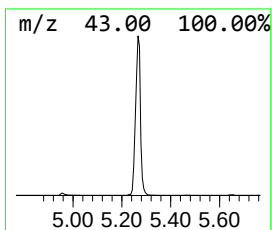
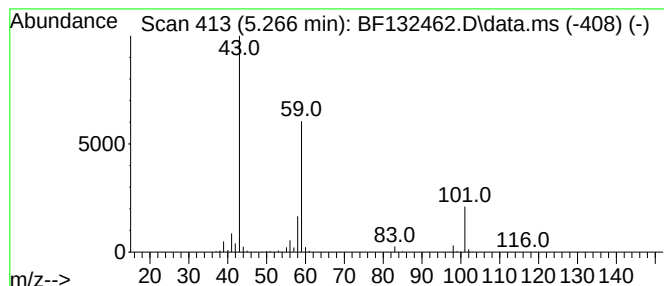
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.266	37.84 ng	2747080	1,4-Dichlorobenzene-d4	7.019	
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	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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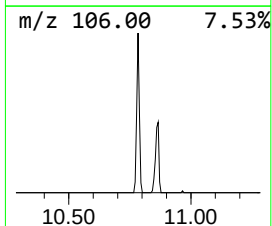
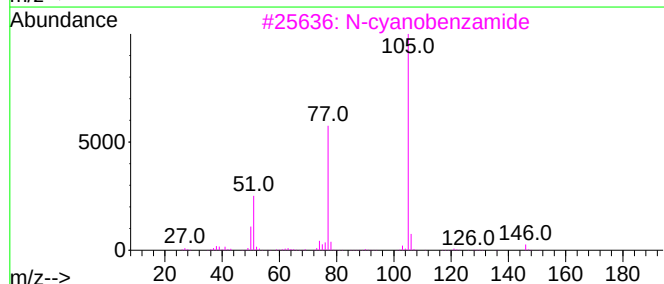
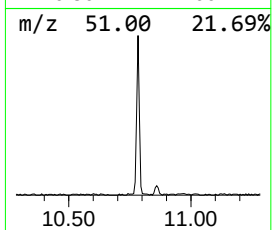
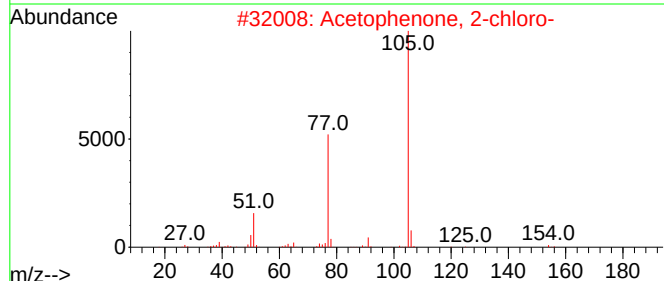
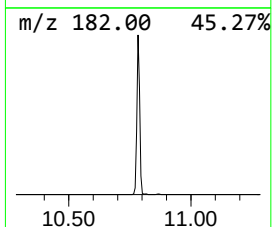
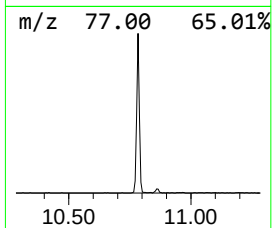
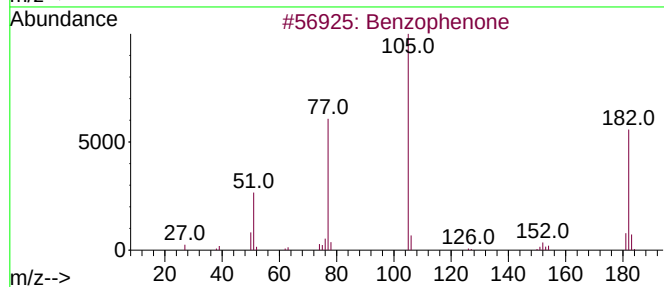
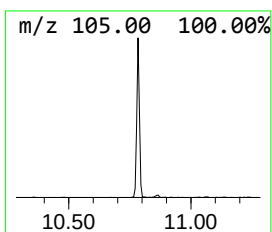
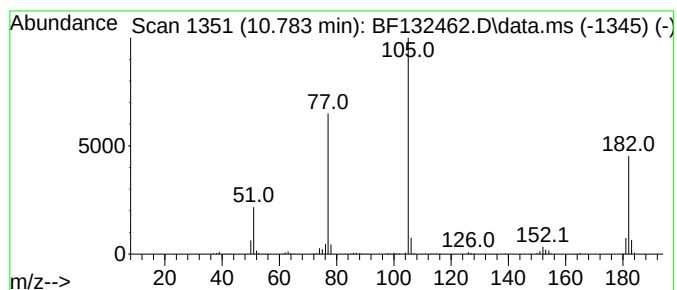
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.784	3.76 ng	409926	Acenaphthene-d10	10.072

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3			N-cyanobenzamide	146	C8H6N2O	015150-25-1	47
4			Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	47
5			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47



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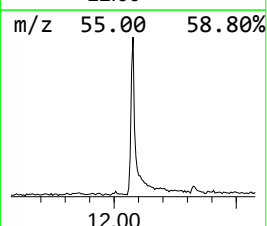
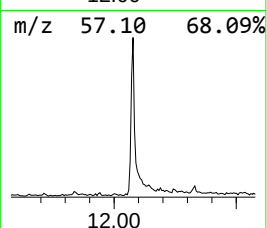
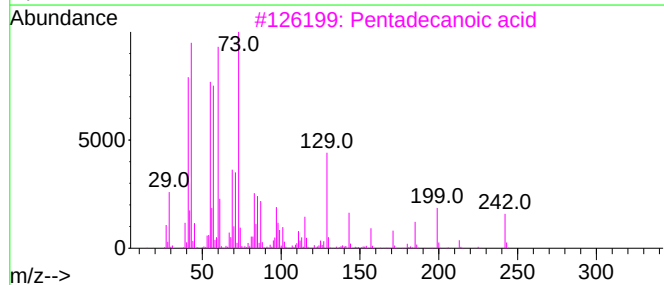
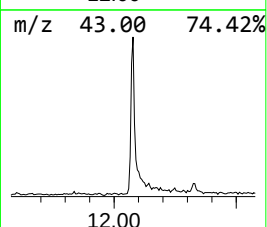
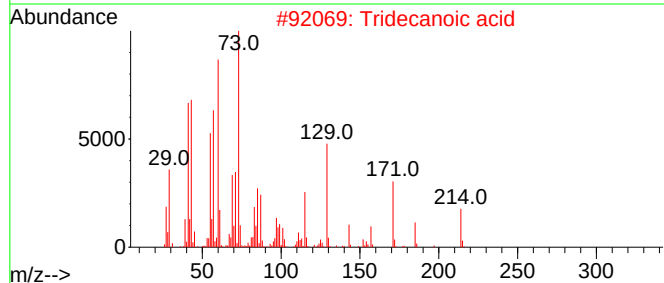
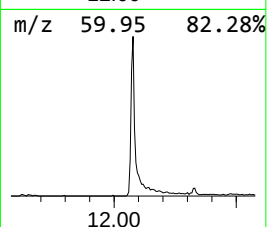
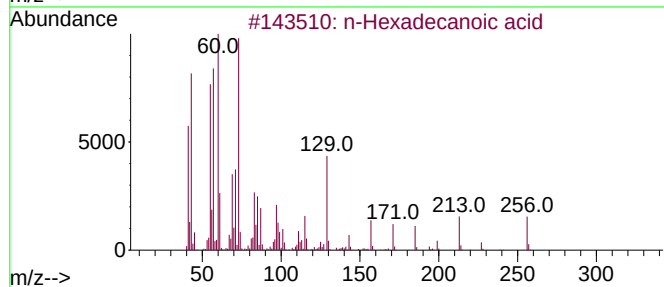
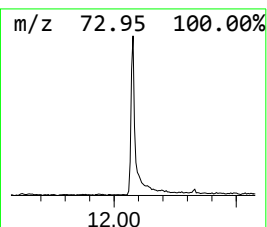
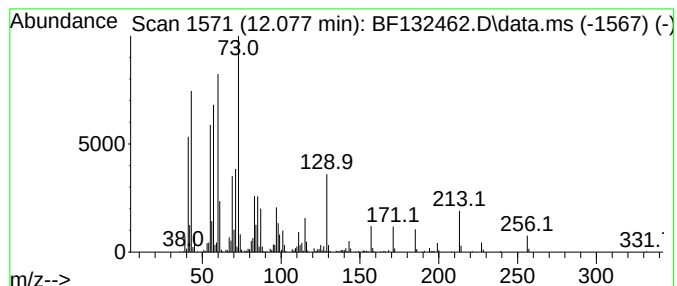
Instrument :
BNA_F
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.078	4.76 ng	554317	Phenanthrene-d10	11.566	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Octadecanoic acid	284	C18H36O2	000057-11-4	62



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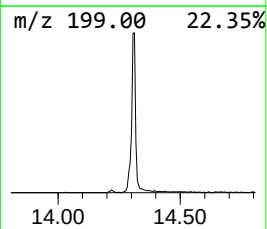
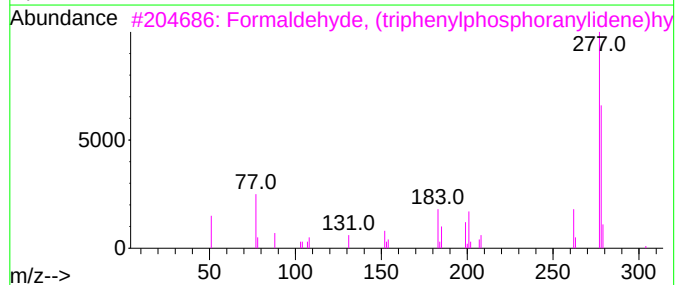
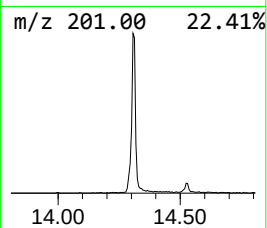
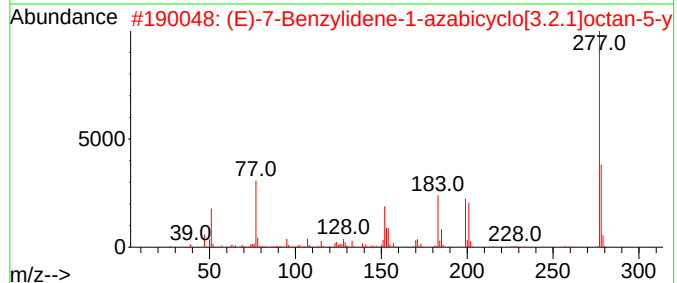
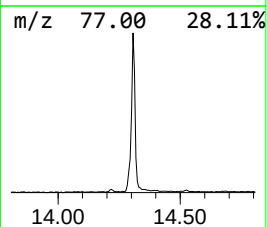
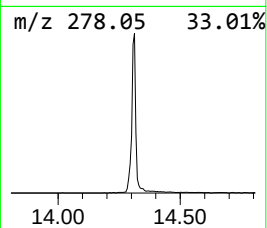
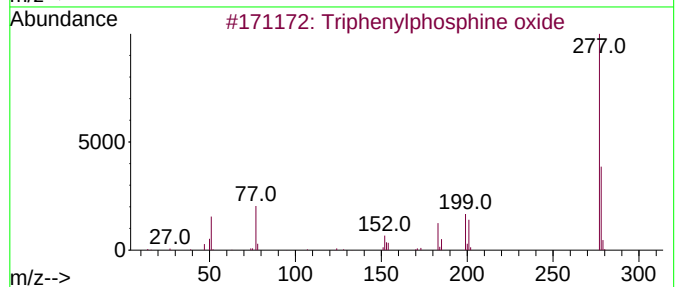
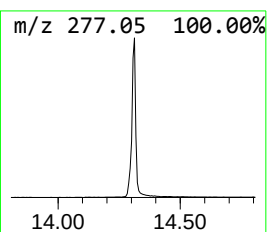
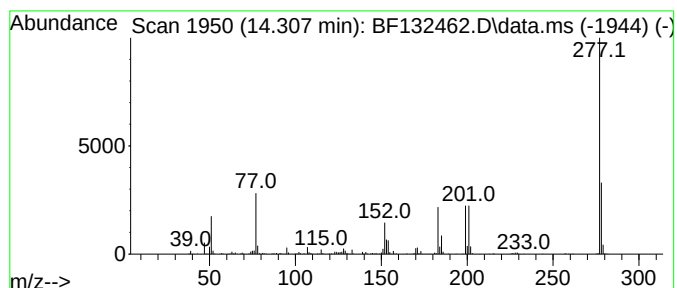
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.307	11.78 ng	1146970	Chrysene-d12	14.219

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45
4			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	43
5			4-Nitro-4'-methyldiphenylsulfone	277	C13H11NO4S	004094-37-5	38



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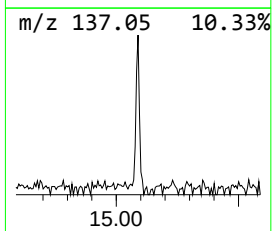
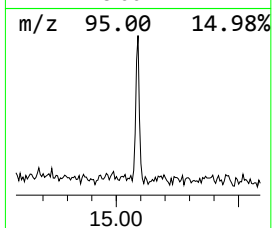
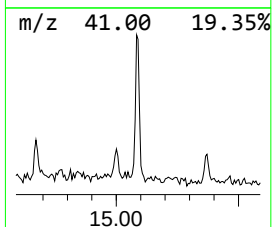
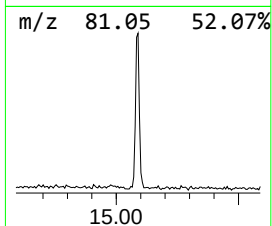
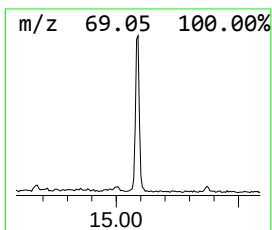
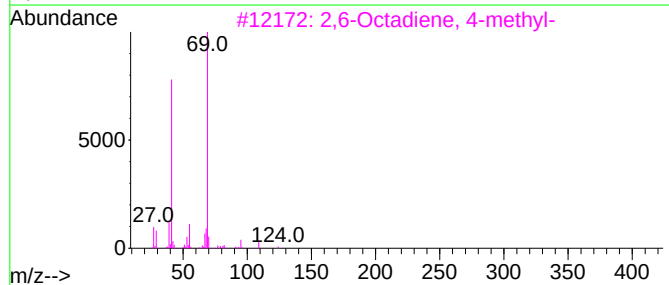
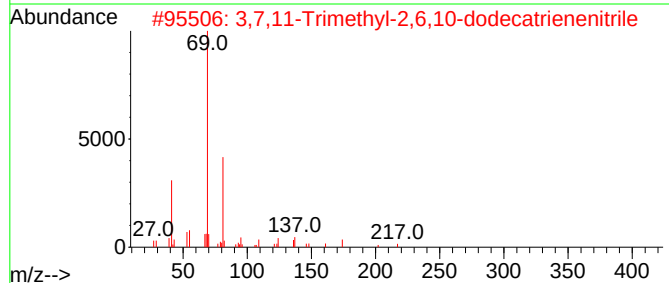
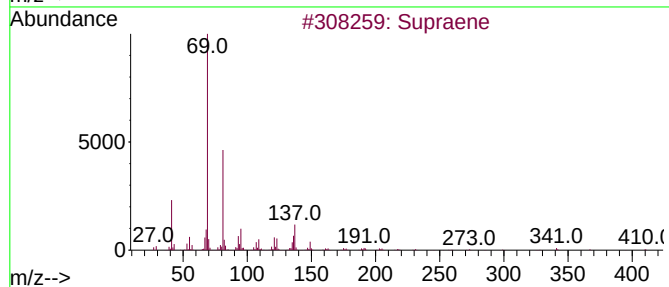
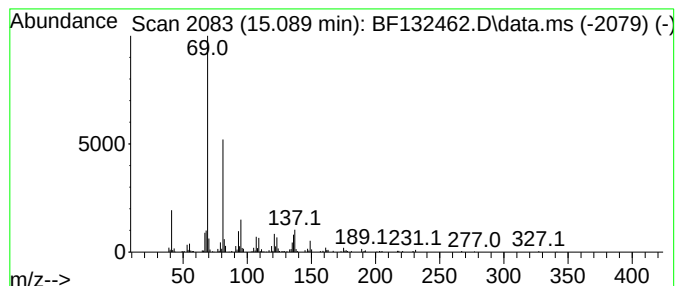
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Peak Number 5 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.089	2.02 ng	180922	Perylene-d12	15.777

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	64
3			2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	50
4			1,5-Heptadiene, 3,4-dimethyl-	124	C9H16	1000061-77-9	50
5			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.266	37.8	ng	2747080	1	7.019	1451910	20.0
Benzophenone	10.784	3.8	ng	409926	3	10.072	2178060	20.0
n-Hexadecanoic ...	12.078	4.8	ng	554317	4	11.566	2330400	20.0
Triphenylphosph...	14.307	11.8	ng	1146970	5	14.219	1947720	20.0
Supraene	15.089	2.0	ng	180922	6	15.777	1789190	20.0