

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031723\
 Data File : BF132843.D
 Acq On : 18 Mar 2023 02:20
 Operator : CG\JU
 Sample : 01965-03
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-3

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-BF031623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132843.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.199	439	444	463	rVB	1588454	2025376	39.04%	5.228%
2	5.593	507	511	530	rBV	3838042	4106317	79.16%	10.600%
3	6.593	677	681	695	rBV	3844342	4165821	80.30%	10.754%
4	6.957	740	743	755	rVB	1534362	1274173	24.56%	3.289%
5	7.522	835	839	843	rBV	2798095	2754810	53.10%	7.111%
6	8.240	957	961	965	rBV	1931109	1686176	32.50%	4.353%
7	9.316	1140	1144	1147	rBV	5327410	4705922	90.71%	12.148%
8	9.998	1256	1260	1264	rBV	2330182	1975456	38.08%	5.100%
9	10.710	1378	1381	1385	rBV	426763	366997	7.07%	0.947%
10	10.792	1391	1395	1399	rBV	3253143	3196351	61.61%	8.251%
11	11.492	1510	1514	1518	rBV	2429390	2110085	40.68%	5.447%
12	12.010	1599	1602	1605	rBV3	35913	57953	1.12%	0.150%
13	13.080	1779	1784	1787	rBV	5292770	5187635	100.00%	13.392%
14	13.963	1931	1934	1938	rBV	61555	54031	1.04%	0.139%
15	14.145	1961	1965	1973	rBV	1932541	1757703	33.88%	4.537%
16	14.233	1974	1980	1985	rVV	975227	1094297	21.09%	2.825%
17	14.280	1985	1988	1992	rVB	66698	66901	1.29%	0.173%
18	14.586	2036	2040	2046	rBV	60969	63312	1.22%	0.163%
19	14.980	2103	2107	2113	rVB	481018	520647	10.04%	1.344%
20	15.668	2218	2224	2237	rVB	1033705	1453063	28.01%	3.751%
21	16.110	2294	2299	2306	rVB2	38030	60523	1.17%	0.156%
22	17.268	2491	2496	2508	rVB5	23061	53963	1.04%	0.139%

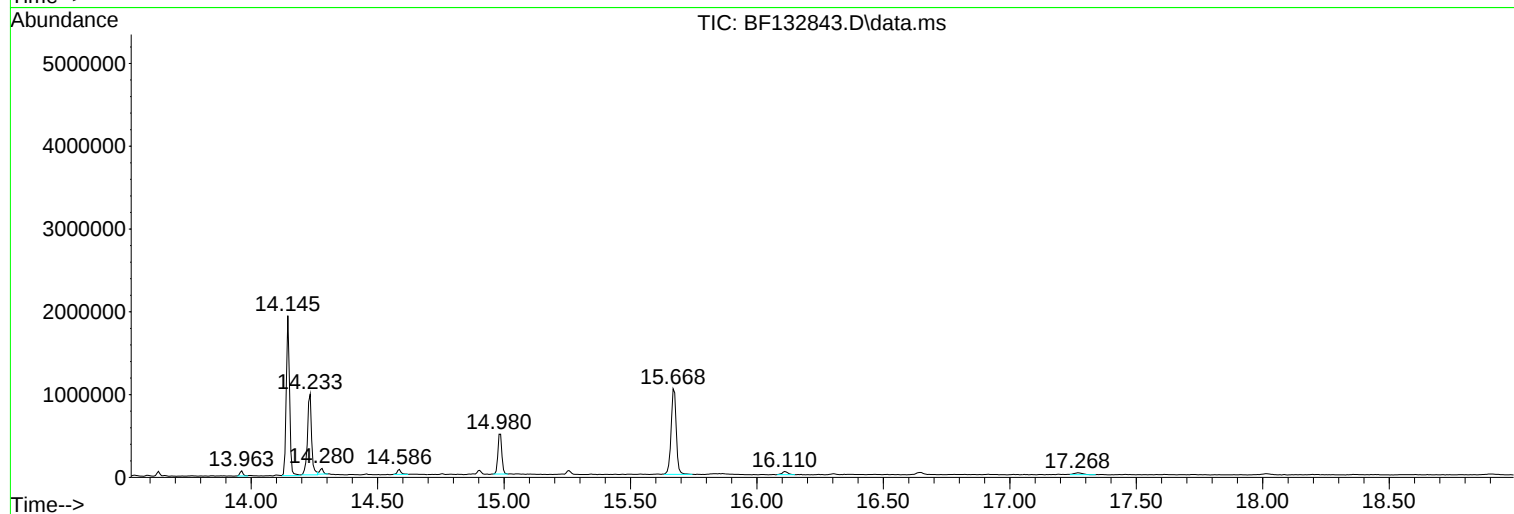
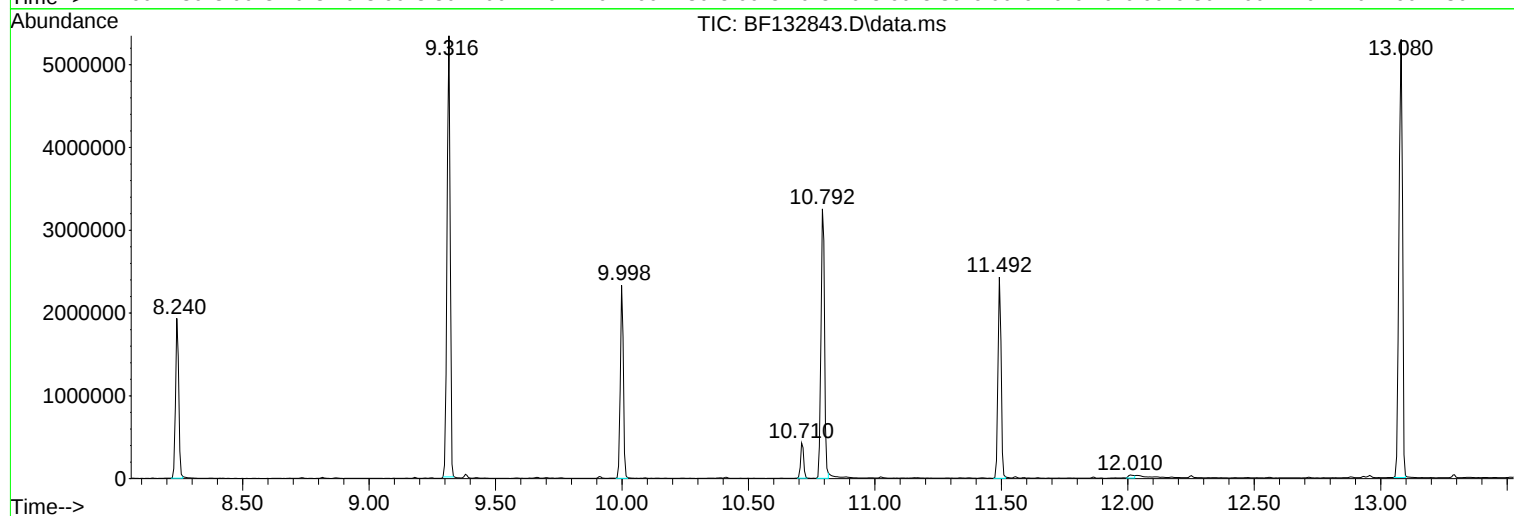
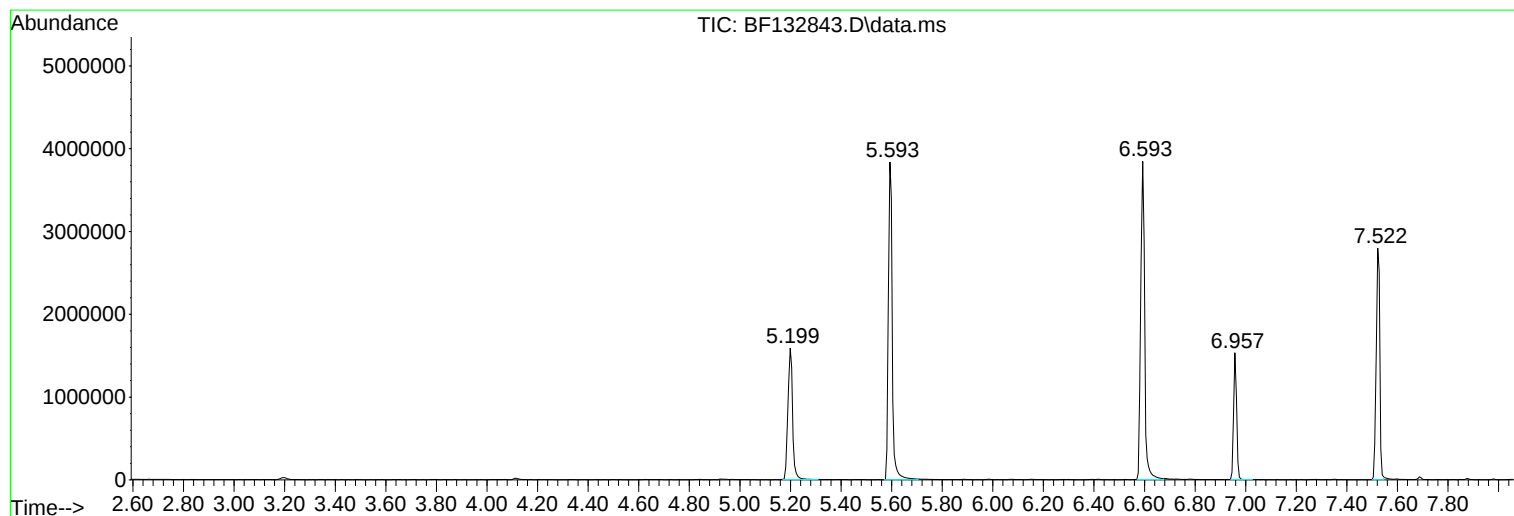
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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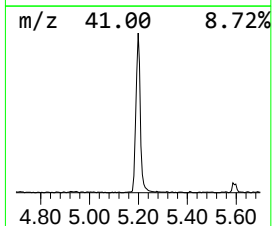
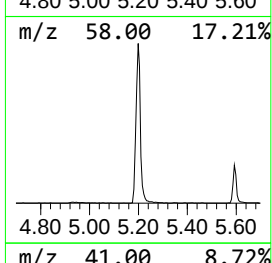
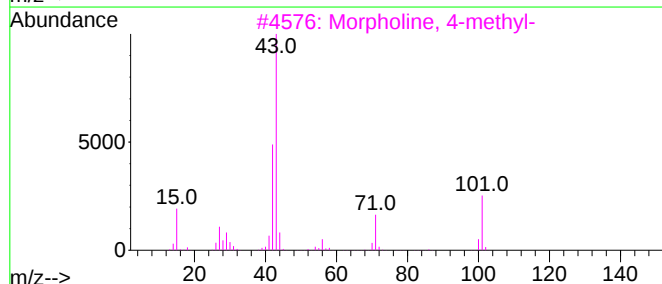
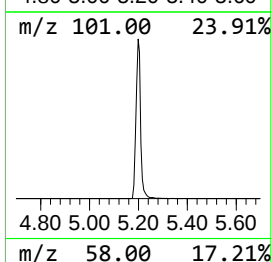
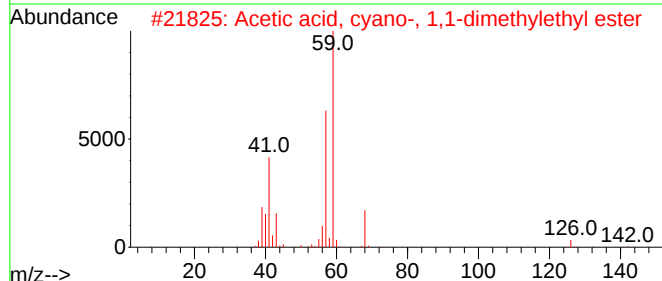
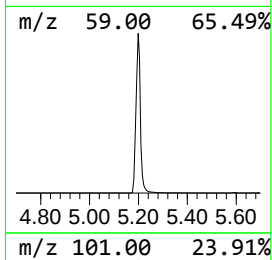
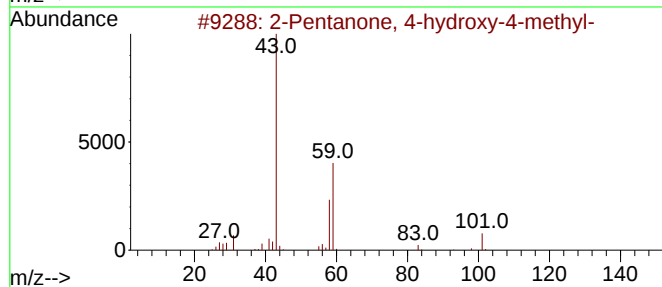
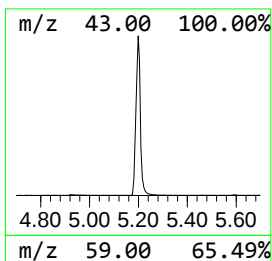
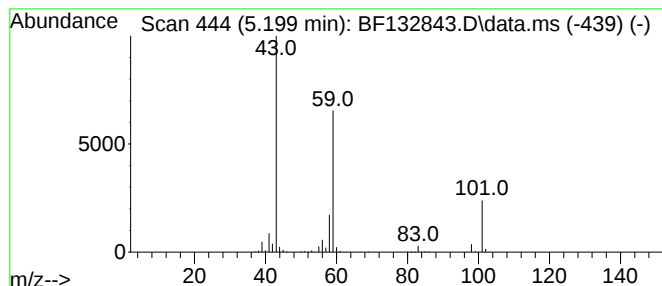
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.199	31.79 ng	2025380	1,4-Dichlorobenzene-d4	6.957

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	17		
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9		



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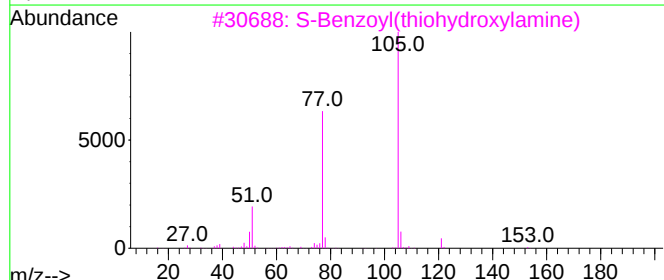
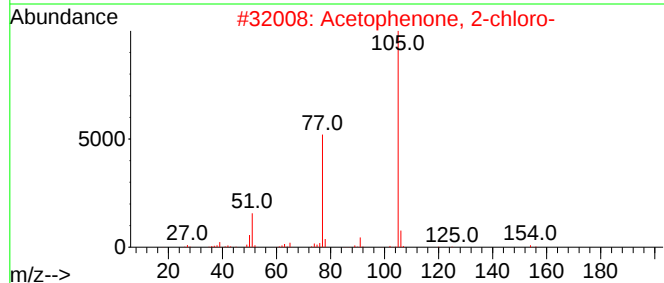
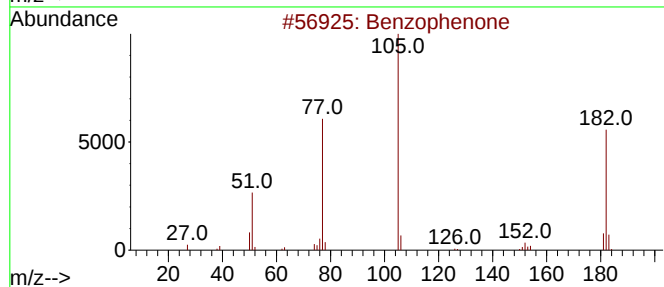
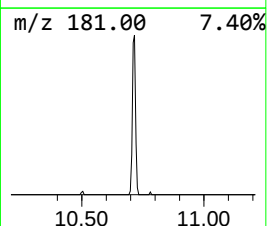
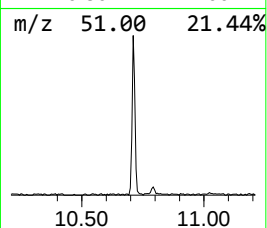
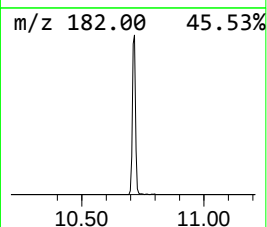
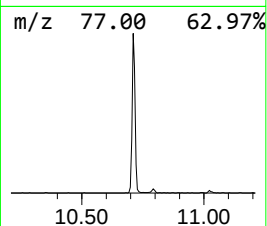
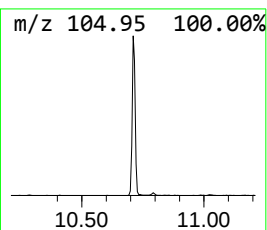
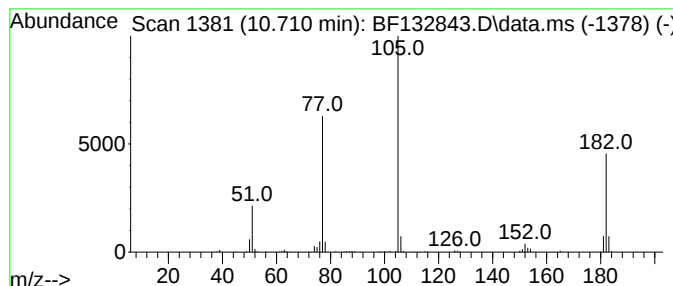
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Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.710	3.72 ng	366997	Acenaphthene-d10	9.998

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			S-Benzoyl(thiohydroxylamine)	153	C7H7NOS	025740-80-1	47
4			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
5			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47



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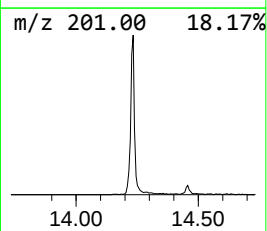
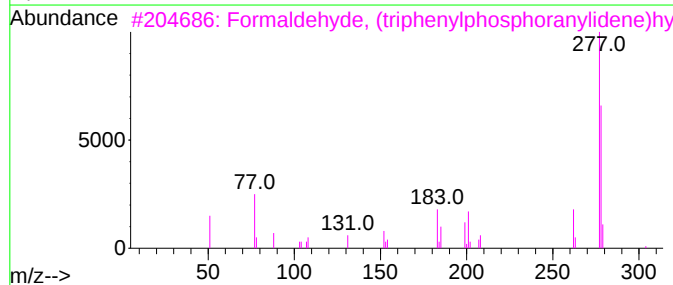
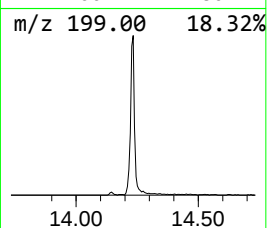
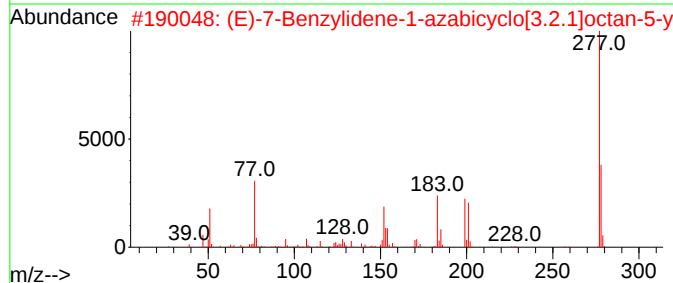
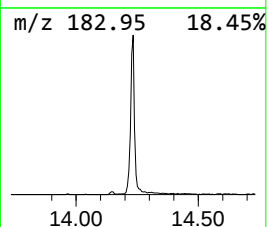
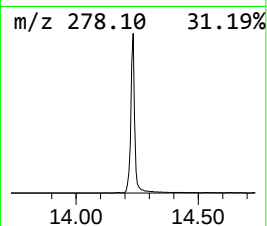
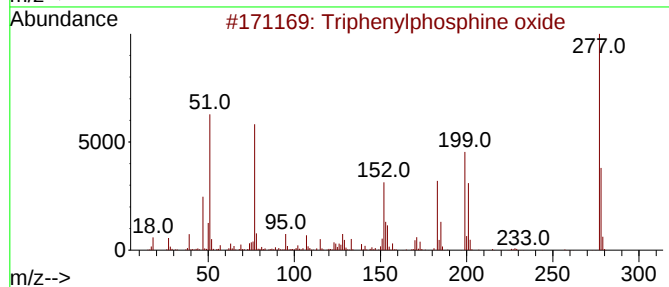
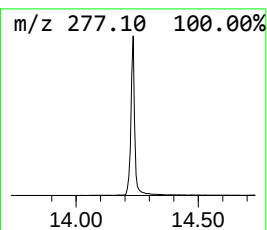
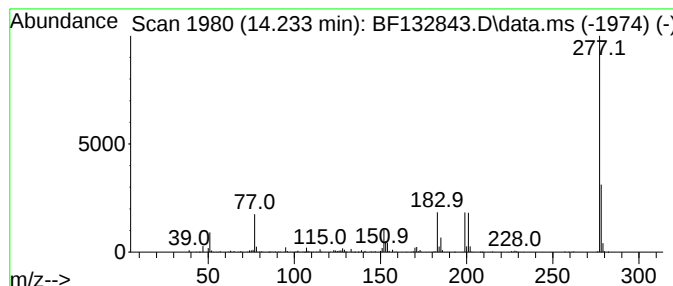
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Peak Number 3 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.233	12.45 ng	1094300	Chrysene-d12	14.145

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	28
4			5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	28
5			5-quinolinol, 8-[2-(3,5-dimethyl...	277	C17H15N3O	1000397-10-2	9



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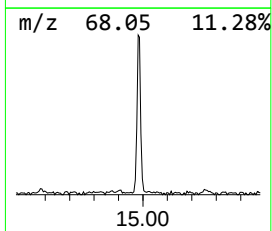
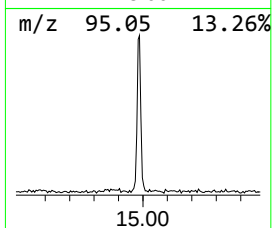
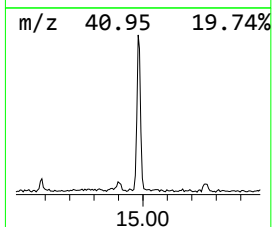
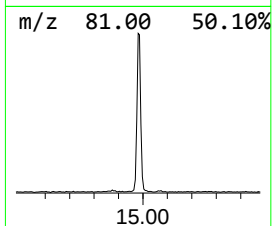
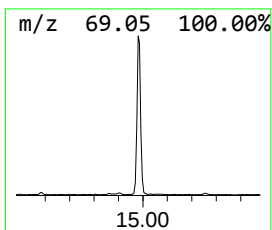
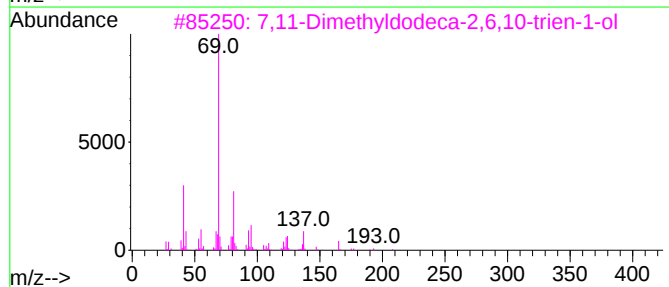
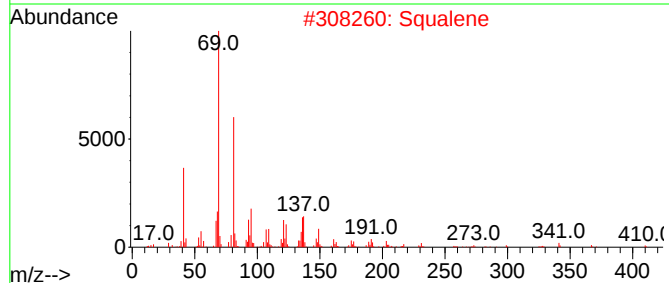
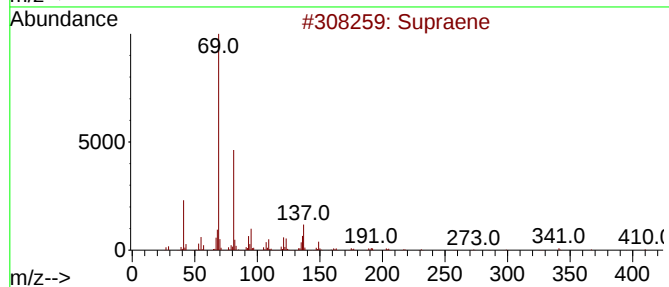
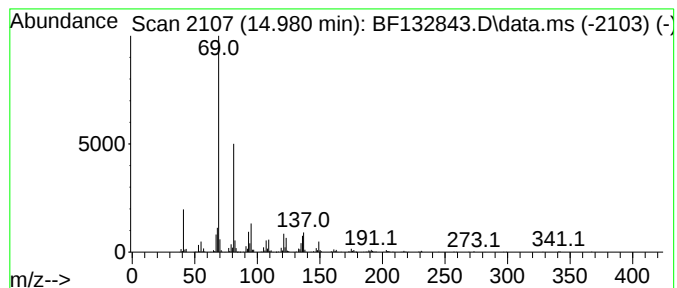
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Peak Number 4 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.980	7.17 ng	520647	Perylene-d12	15.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			Squalene	410	C30H50	000111-02-4	91
3			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4			2,6,10,14-Hexadecatetraen-1-ol, ...	332	C22H36O2	061691-98-3	72
5			2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.199	31.8	ng	2025380	1	6.957	1274170	20.0
Benzophenone	10.710	3.7	ng	366997	3	9.998	1975460	20.0
Triphenylphosph...	14.233	12.4	ng	1094300	5	14.145	1757700	20.0
Supraene	14.980	7.2	ng	520647	6	15.669	1453060	20.0