

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053123\
 Data File : BF133540.D
 Acq On : 31 May 2023 15:41
 Operator : CG\JU
 Sample : 02971-03
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB15

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-BF052523.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133540.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.040	497	502	508	rVB	98189	111792	4.18%	0.527%
2	5.439	565	570	573	rBV	2462839	2272608	85.07%	10.715%
3	6.451	737	742	745	rBV	2301427	2328361	87.16%	10.977%
4	6.828	803	806	810	rBV	864235	723718	27.09%	3.412%
5	7.392	898	902	905	rBV	1731202	1435707	53.74%	6.769%
6	8.116	1021	1025	1028	rBV	1097289	966707	36.19%	4.558%
7	9.192	1204	1208	1211	rBV	3005353	2508631	93.91%	11.827%
8	9.869	1319	1323	1326	rBV	1355273	1053342	39.43%	4.966%
9	10.580	1441	1444	1448	rVB	878297	765358	28.65%	3.608%
10	10.657	1452	1457	1460	rBV	1979587	1732290	64.84%	8.167%
11	10.892	1493	1497	1501	rVB	198631	150754	5.64%	0.711%
12	10.974	1507	1511	1514	rBV	56842	54651	2.05%	0.258%
13	11.269	1558	1561	1565	rBV	49999	38649	1.45%	0.182%
14	11.357	1572	1576	1579	rBV	1333559	1145232	42.87%	5.399%
15	11.580	1610	1614	1617	rBV	26733	34553	1.29%	0.163%
16	11.886	1662	1666	1669	rBV	174468	184109	6.89%	0.868%
17	11.921	1669	1672	1676	rVB	57430	64581	2.42%	0.304%
18	12.563	1775	1781	1784	rBV	58145	69641	2.61%	0.328%
19	12.668	1796	1799	1803	rBV2	41608	41233	1.54%	0.194%
20	12.792	1813	1820	1823	rBV	60988	83461	3.12%	0.393%
21	12.945	1842	1846	1849	rBV	3022655	2671445	100.00%	12.595%
22	13.180	1879	1886	1890	rBV	33378	55503	2.08%	0.262%
23	13.421	1920	1927	1931	rBV	111357	107237	4.01%	0.506%
24	13.857	1997	2001	2014	rBV4	97864	251064	9.40%	1.184%
25	13.998	2018	2025	2027	rVV	1121960	1283065	48.03%	6.049%
26	14.021	2027	2029	2035	rVB	152440	130235	4.88%	0.614%
27	14.521	2109	2114	2118	rBV	30675	37570	1.41%	0.177%
28	14.598	2123	2127	2131	rBV	67302	63160	2.36%	0.298%
29	15.027	2195	2200	2202	rBV	36667	49062	1.84%	0.231%
30	15.051	2202	2204	2212	rVB2	31184	37888	1.42%	0.179%
31	15.451	2267	2272	2277	rBV	628017	758716	28.40%	3.577%

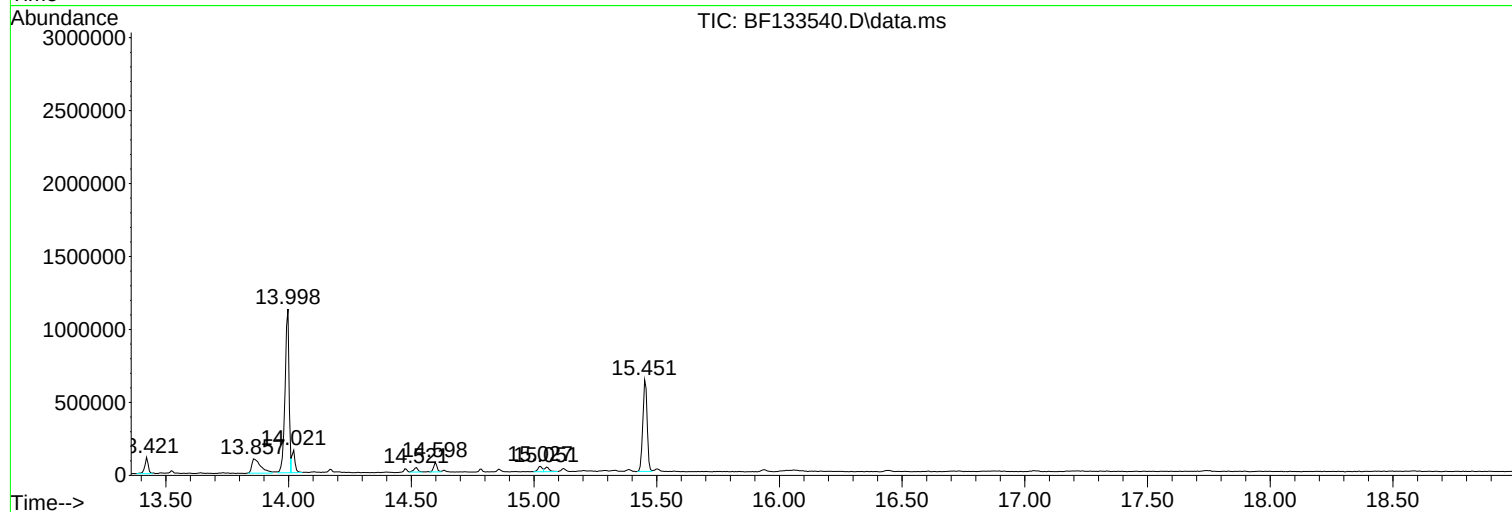
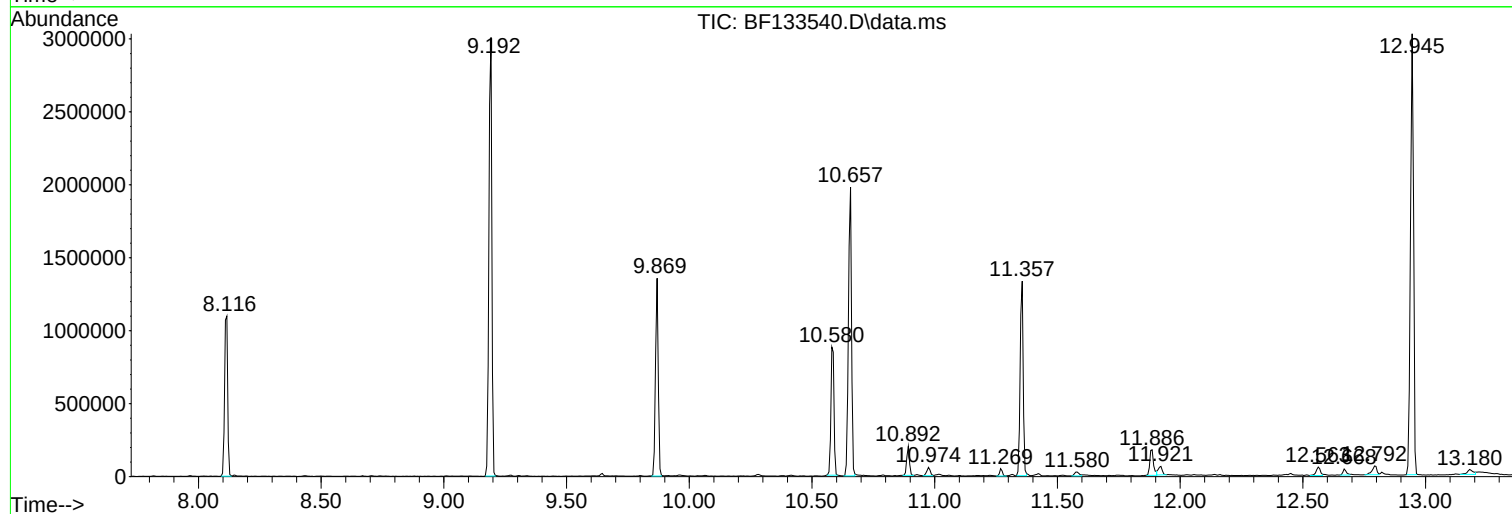
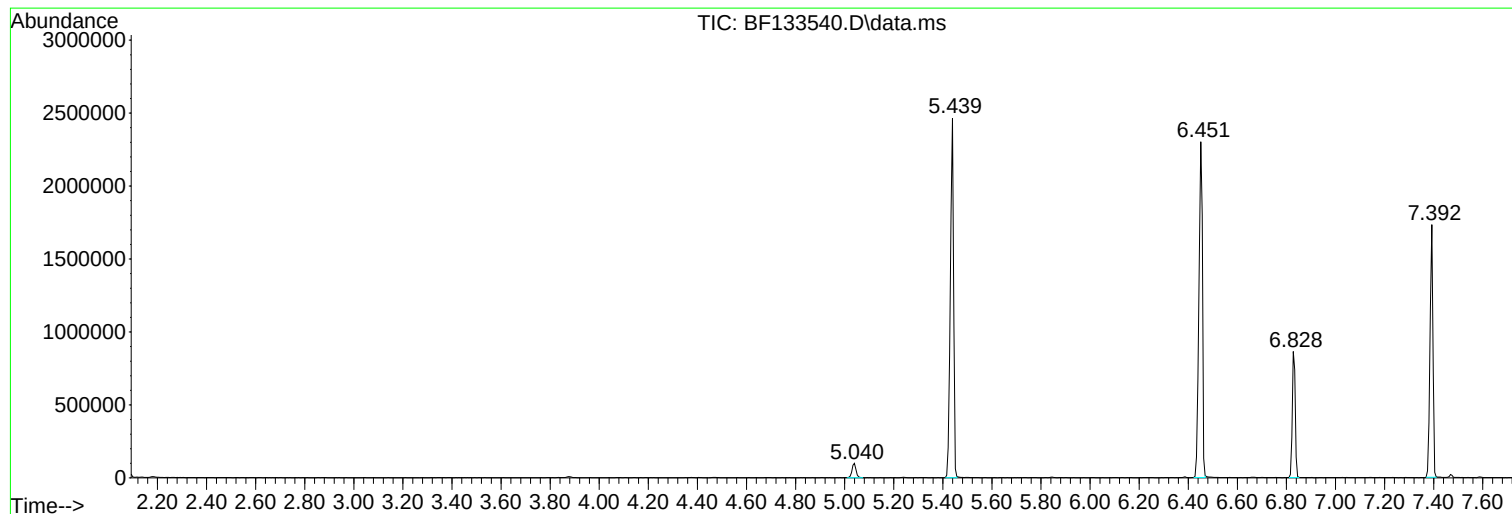
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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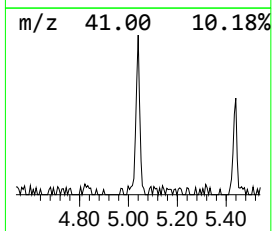
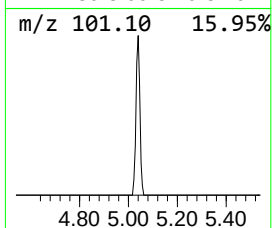
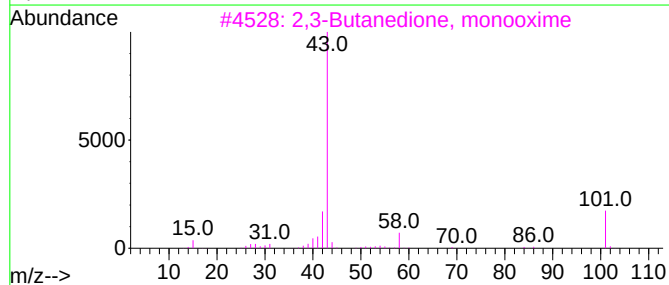
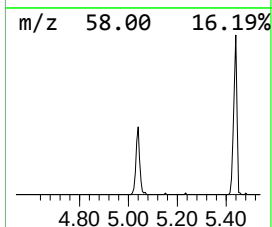
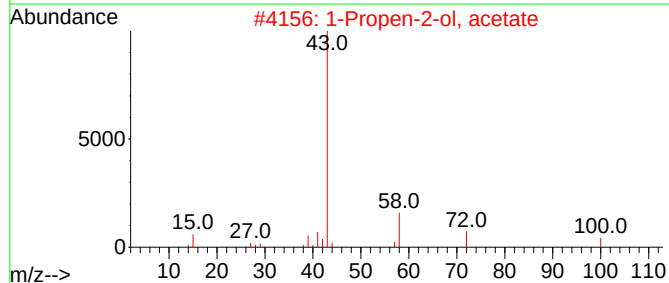
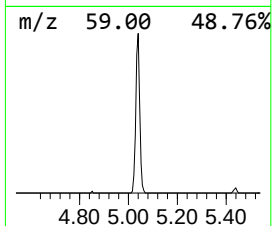
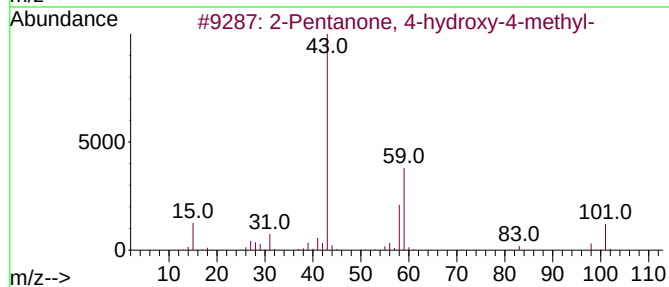
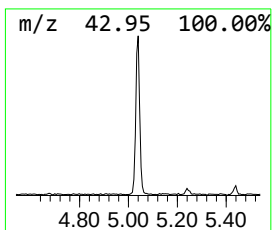
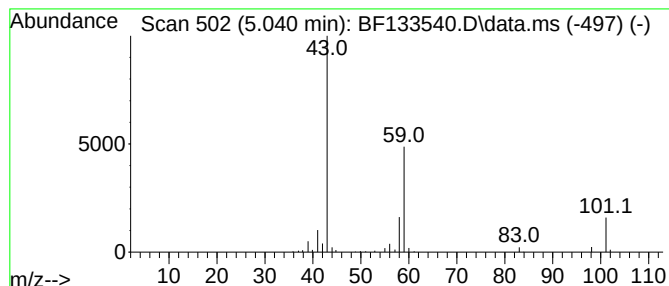
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	3.09 ng	111792	1,4-Dichlorobenzene-d4	6.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
4	Allyl acetate	100	C5H8O2	000591-87-7	9		
5	Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	7		



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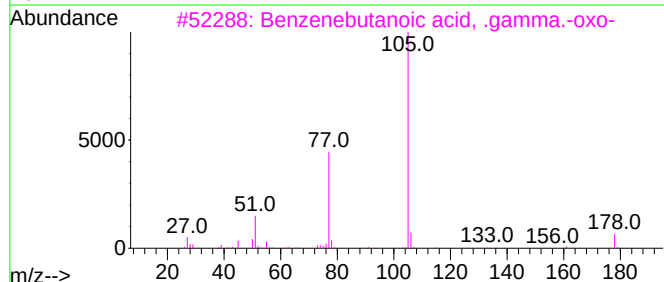
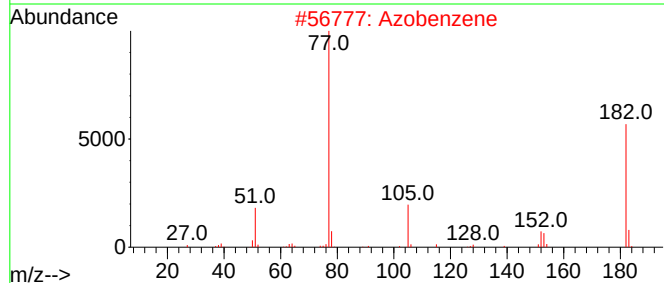
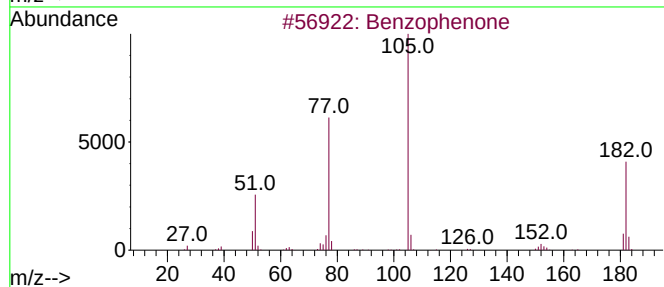
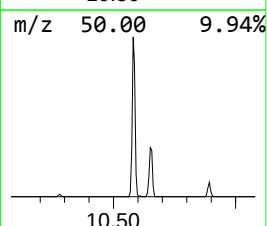
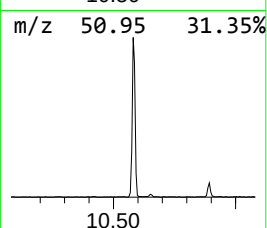
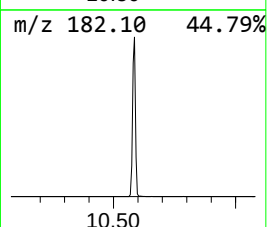
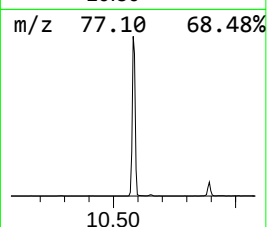
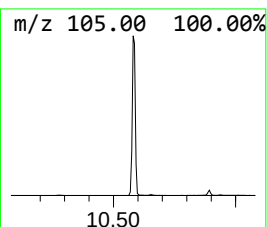
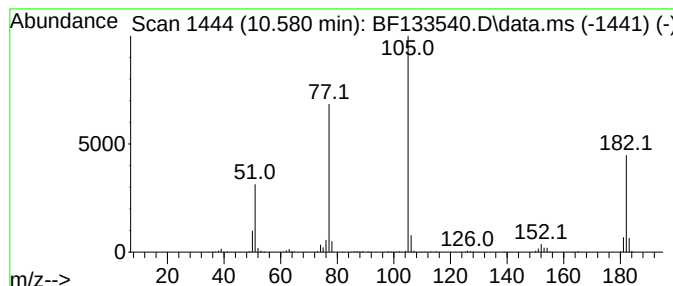
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.580	14.53 ng	765358	Acenaphthene-d10	9.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Azobenzene	182	C12H10N2	000103-33-3	53
3			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	50
4			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	50
5			5-Oxo-5-phenylpentanenitrile	173	C11H11NO	1000486-83-7	50



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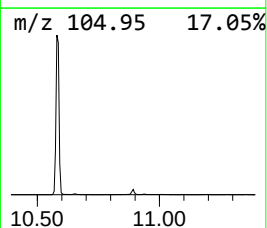
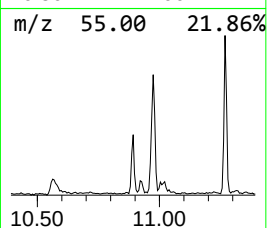
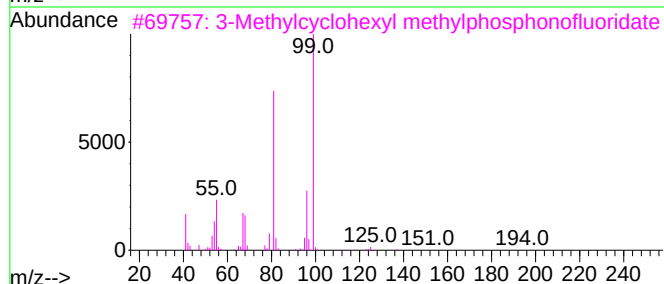
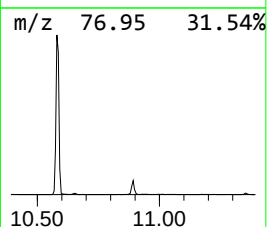
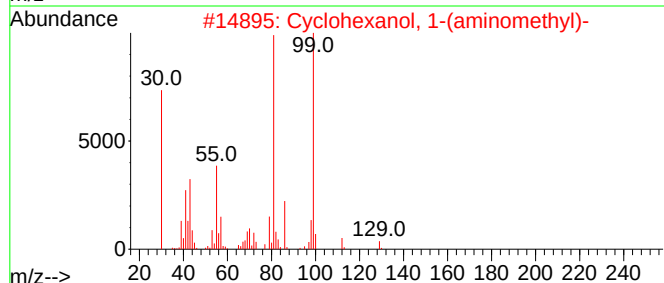
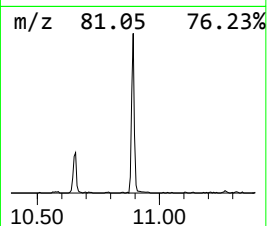
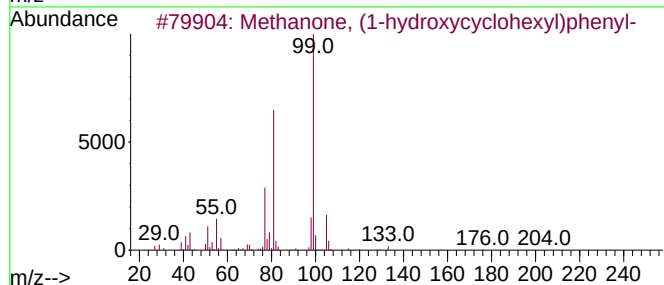
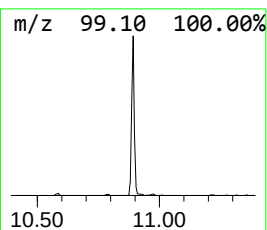
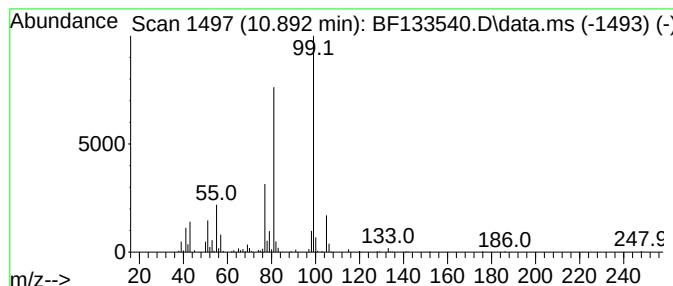
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Methanone, (1-hydroxycyclohexyl) Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.892	2.63 ng	150754	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	91
2			Cyclohexanol, 1-(aminomethyl)-	129	C7H15NO	004000-72-0	64
3			3-Methylcyclohexyl methylphospho...	194	C8H16FO2P	113548-86-0	59
4			1-Hydroxycyclohexanecarboxylic acid	144	C7H12O3	001123-28-0	59
5			2-Methylcyclosarin	194	C8H16FO2P	085473-32-1	38



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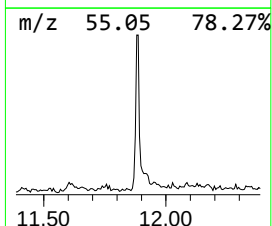
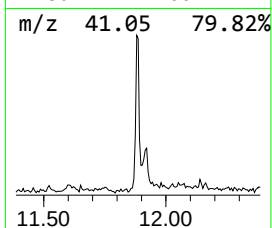
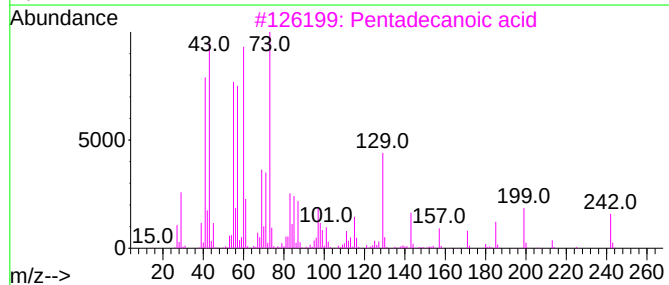
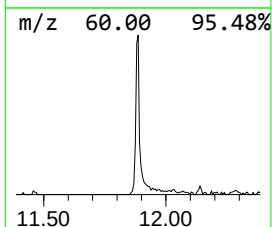
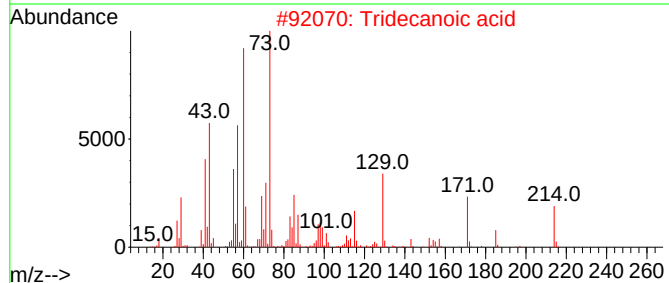
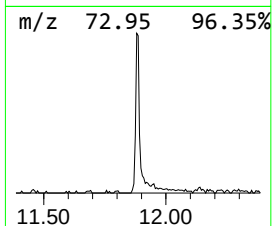
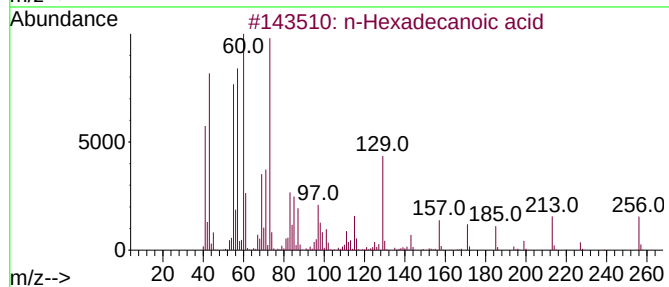
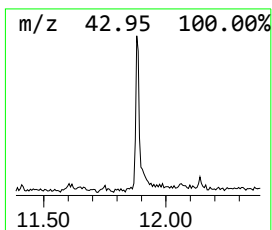
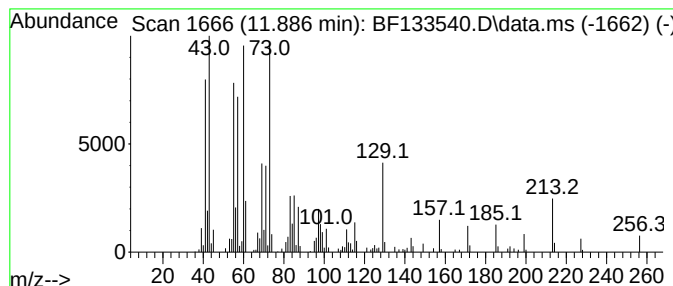
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	3.22 ng	184109	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5			n-Decanoic acid	172	C10H20O2	000334-48-5	76



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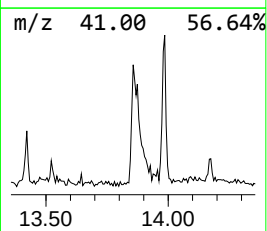
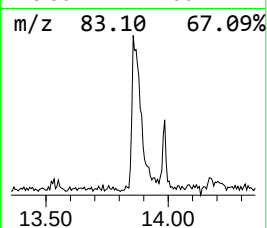
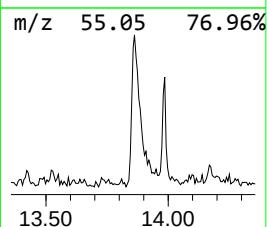
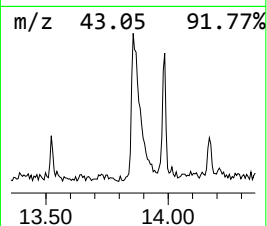
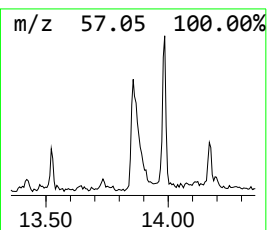
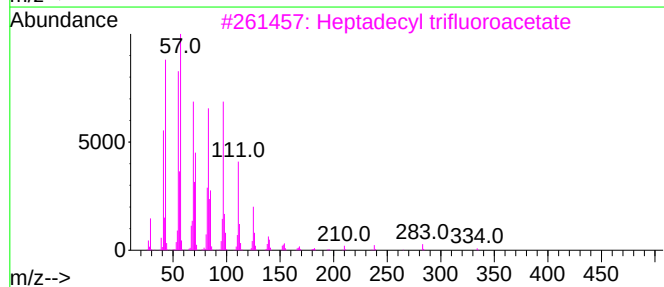
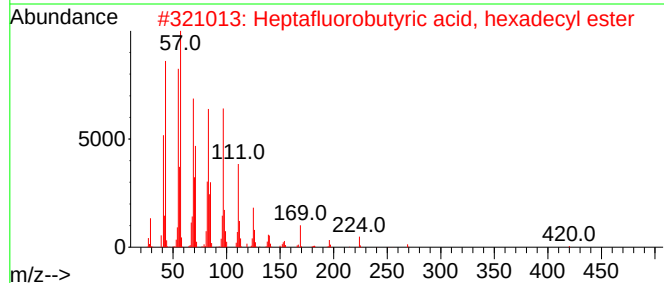
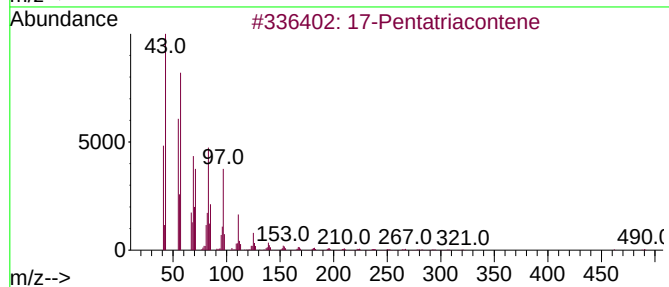
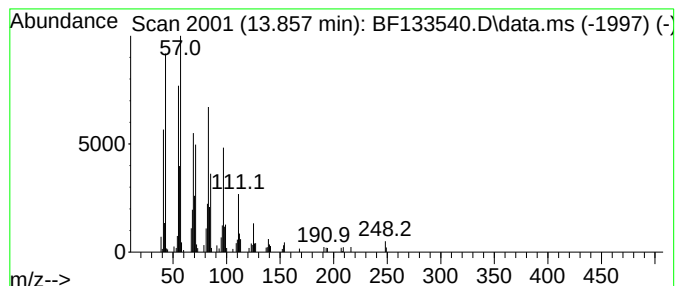
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Peak Number 5 17-Pentatriacontene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	3.91 ng	251064	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17-Pentatriacontene	491	C35H70	006971-40-0	90
2			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	90
3			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	90
4			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	90
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.040	3.1	ng	111792	1	6.828	723718	20.0
Benzophenone	10.580	14.5	ng	765358	3	9.869	1053340	20.0
Methanone, (1-h...	10.892	2.6	ng	150754	4	11.357	1145230	20.0
n-Hexadecanoic ...	11.886	3.2	ng	184109	4	11.357	1145230	20.0
17-Pentatriacon...	13.857	3.9	ng	251064	5	13.998	1283070	20.0