

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112817\
 Data File : BF100926.D
 Acq On : 28 Nov 2017 11:48
 Operator : SJ/JU
 Sample : PB104515BL
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB104515BL

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:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.093	507	511	519	rBV	77473	99949	4.76%	0.647%
2	5.481	572	577	580	rBV	1514767	1444957	68.80%	9.353%
3	6.487	743	748	751	rBV	1339299	1481337	70.53%	9.588%
4	6.628	767	772	775	rBV	1606916	1537374	73.20%	9.951%
5	6.857	807	811	814	rBV	460777	357866	17.04%	2.316%
6	7.016	833	838	841	rBV	1390793	1244640	59.26%	8.056%
7	7.422	901	907	910	rBV	993708	958540	45.64%	6.204%
8	7.492	916	919	924	rBV	31933	26502	1.26%	0.172%
9	8.139	1024	1029	1032	rVB	531434	468695	22.32%	3.034%
10	9.216	1206	1212	1215	rBV	2048263	1966548	93.63%	12.729%
11	9.245	1215	1217	1220	rVB	84187	63068	3.00%	0.408%
12	9.357	1233	1236	1242	rVB	26827	29631	1.41%	0.192%
13	9.604	1274	1278	1281	rBV	32364	27720	1.32%	0.179%
14	9.892	1323	1327	1333	rBV2	631836	560468	26.68%	3.628%
15	10.280	1386	1393	1396	rBV2	52404	43532	2.07%	0.282%
16	10.604	1445	1448	1454	rVB	39651	35312	1.68%	0.229%
17	10.686	1457	1462	1465	rBV	1226436	1196620	56.97%	7.745%
18	11.380	1576	1580	1583	rBV	754844	612327	29.15%	3.963%
19	12.969	1845	1850	1853	rBV	2212047	2100332	100.00%	13.595%
20	13.851	1996	2000	2002	rBV	65958	76217	3.63%	0.493%
21	13.880	2002	2005	2010	rVB	216994	179857	8.56%	1.164%
22	14.021	2025	2029	2032	rBV	578959	548538	26.12%	3.550%
23	15.486	2273	2278	2289	rBV	294079	389720	18.56%	2.523%

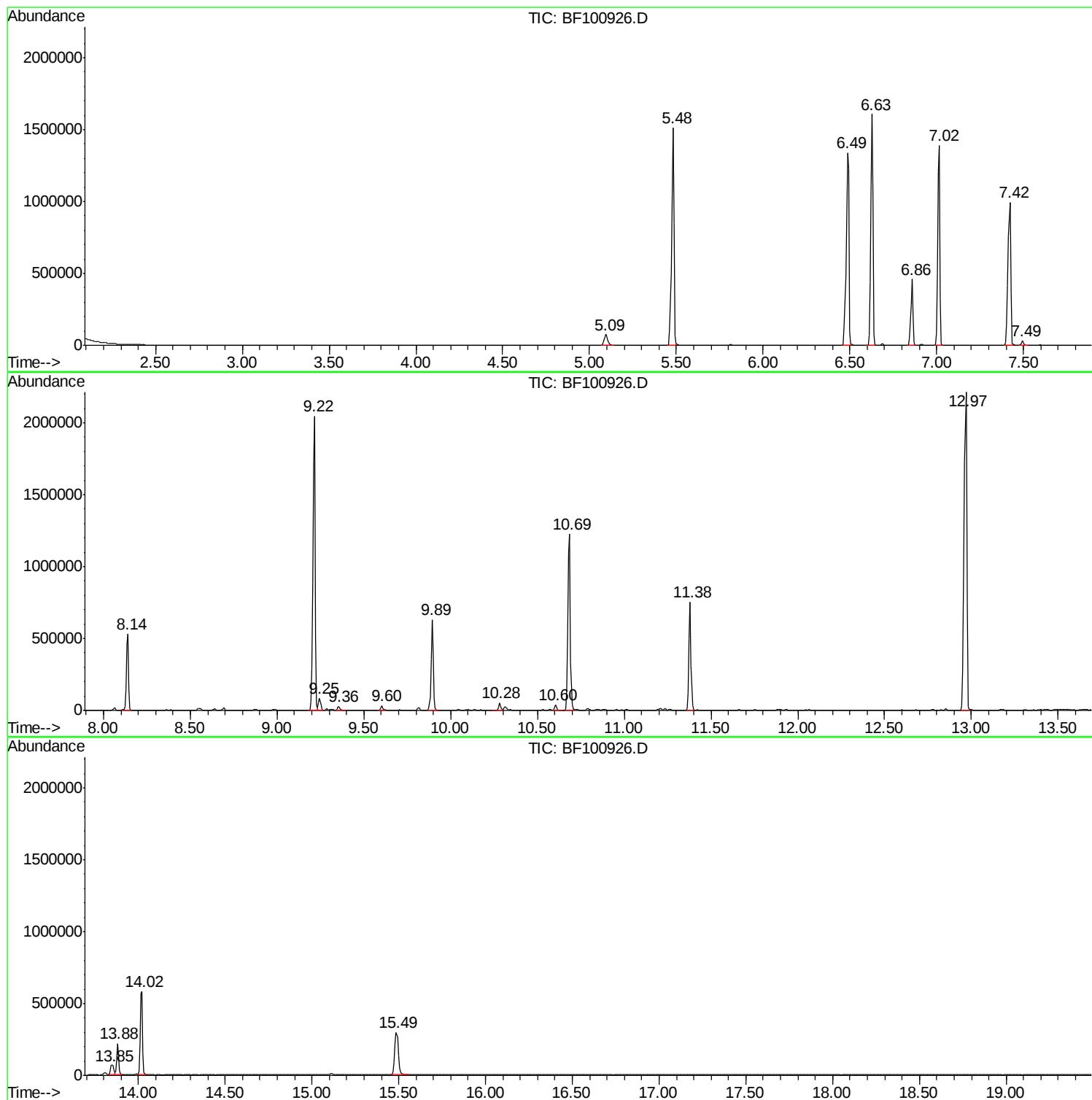
Sum of corrected areas: 15449750

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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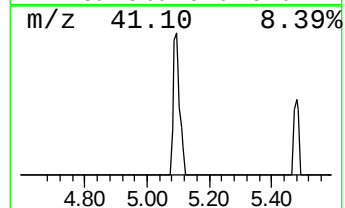
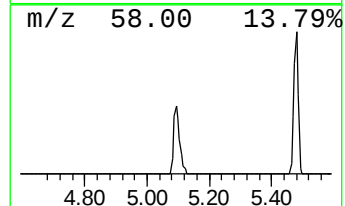
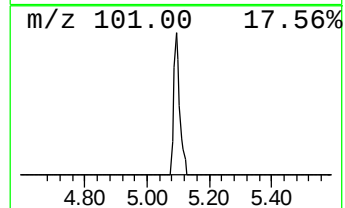
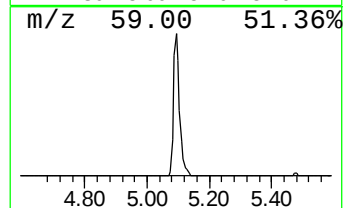
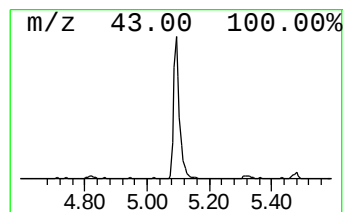
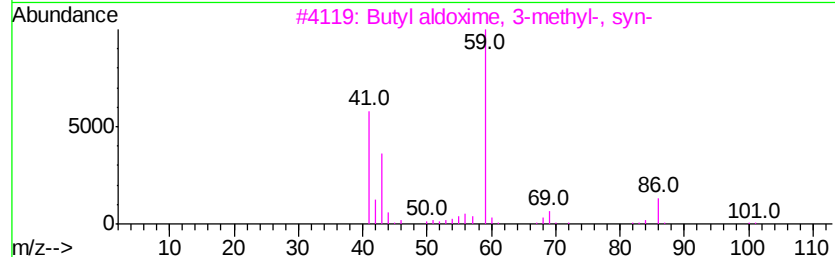
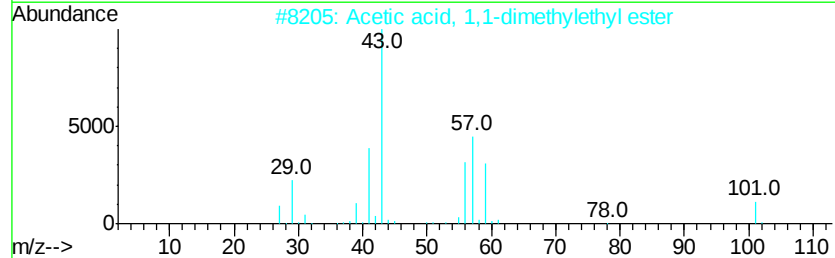
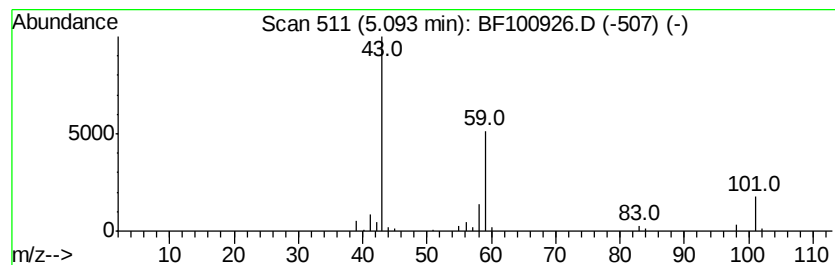
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	5.59 ng	99949	1,4-Dichlorobenzene-d4	6.86

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25
3			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
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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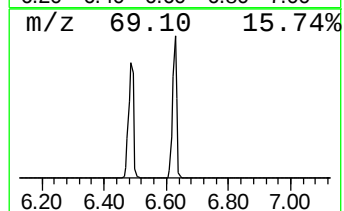
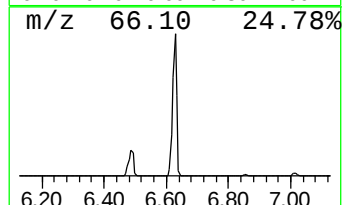
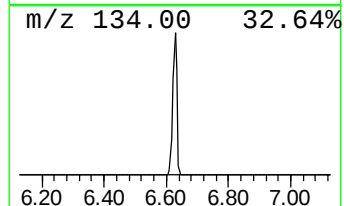
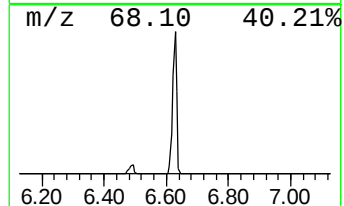
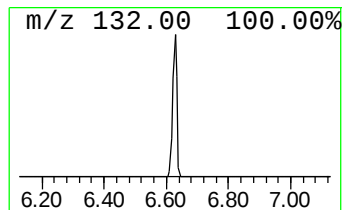
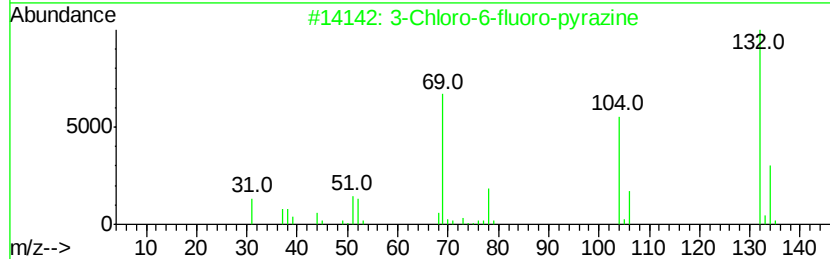
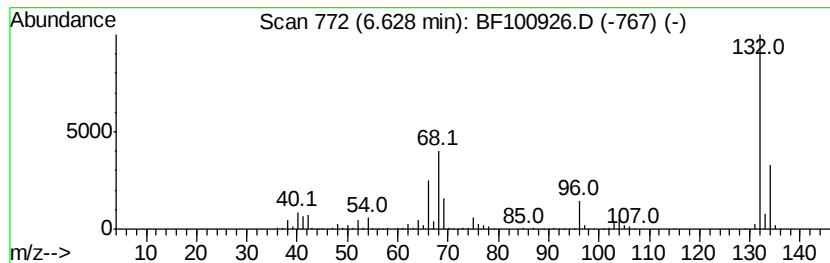
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	85.92 ng	1537370	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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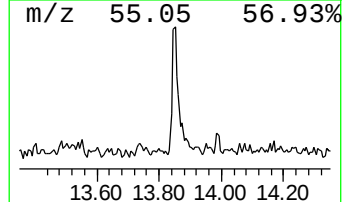
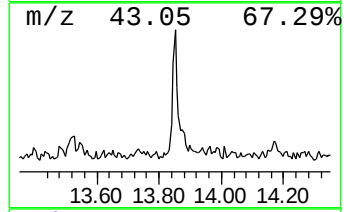
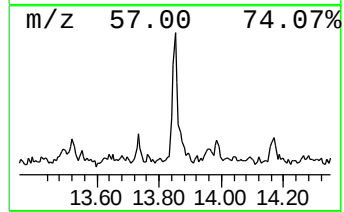
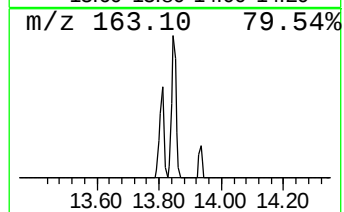
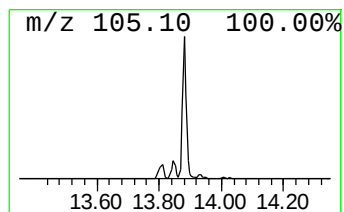
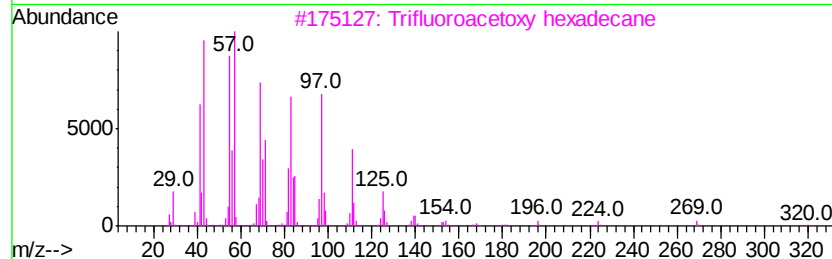
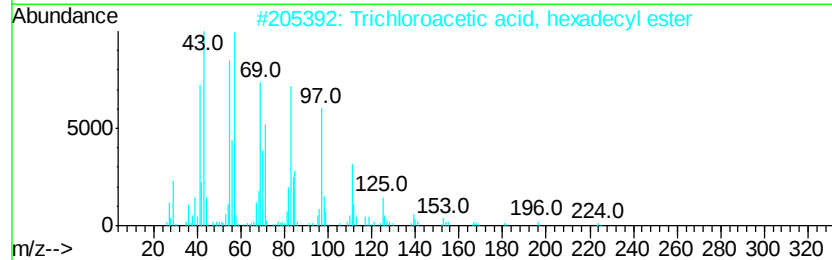
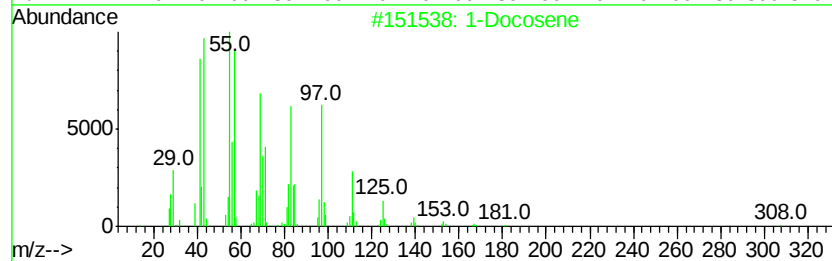
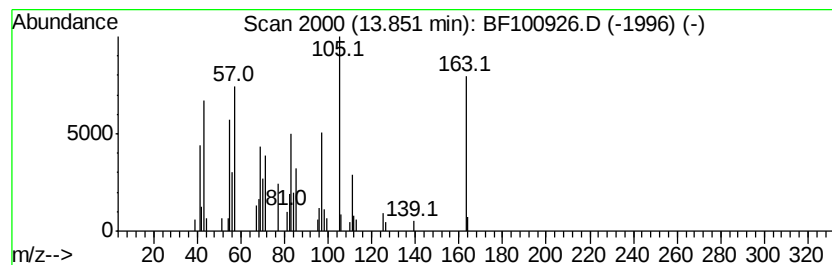
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Peak Number 4 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	2.78 ng	76217	Chrysene-d12	14.02
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Docosene		308 C22H44	001599-67-3 60
2	Trichloroacetic acid, hexadecyl ...		386 C18H33Cl3O2	074339-54-1 60
3	Trifluoroacetoxy hexadecane		338 C18H33F3O2	006222-03-3 55
4	Octadecyl trifluoroacetate		366 C20H37F3O2	079392-43-1 53
5	Tricosyl trifluoroacetate		436 C25H47F3O2	1000351-75-1 53



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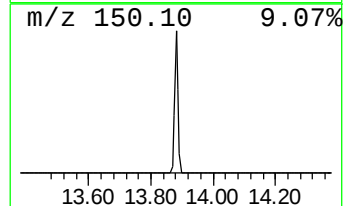
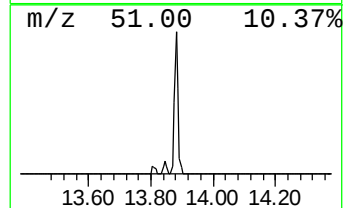
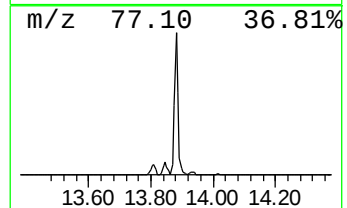
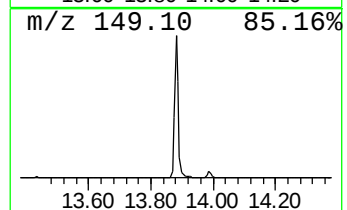
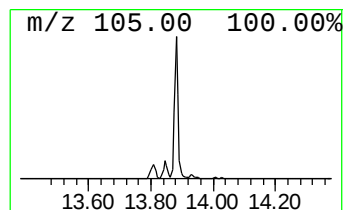
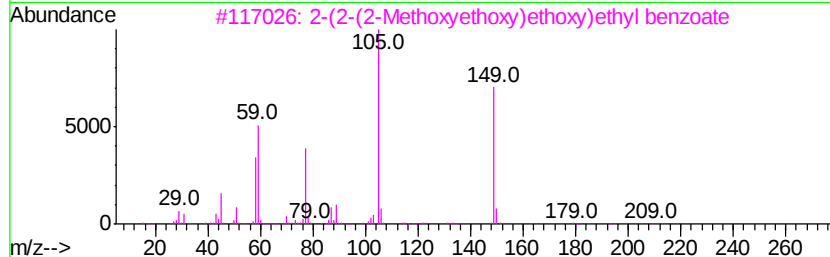
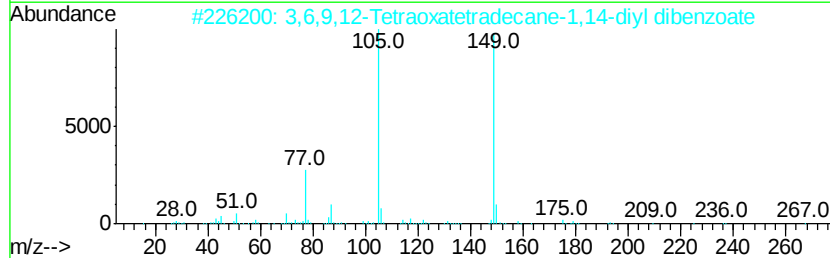
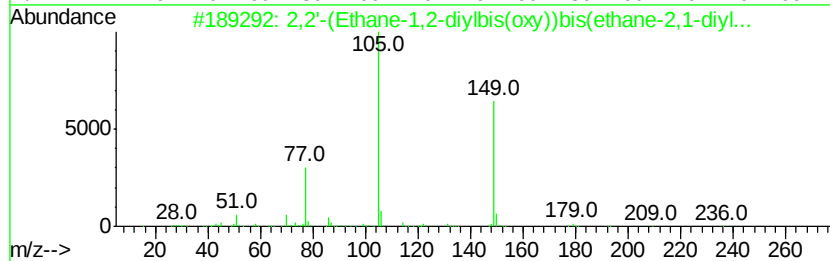
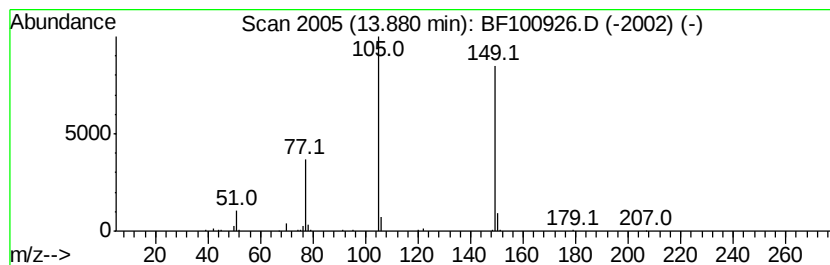
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2,2'-(Ethane-1,2-diylbis(ox... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	6.56 ng	179857	Chrysene-d12	14.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,2'-(Ethane-1,2-diylbis(oxv))bi...	358	C20H22O6	1000366-99-4	78
2		3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	74
3		2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	74
4		2,5,8,11-Tetraoxatridecan-13-yl ...	312	C16H24O6	1000366-96-7	72
5		1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.09	5.6	ng	99949	1	6.86	357866	20.0
unknown6.63	6.63	85.9	ng	1537370	1	6.86	357866	20.0
1-Docosene	13.85	2.8	ng	76217	5	14.02	548538	20.0
2,2'-(Ethane-1,2-...	13.88	6.6	ng	179857	5	14.02	548538	20.0