

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050421\
 Data File : BF123804.D
 Acq On : 4 May 2021 12:49
 Operator : JU/CG
 Sample : PB136145BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB136145BL

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-BF042721.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123804.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	7	14	rVB	404171	491009	5.31%	0.782%
2	2.228	18	24	32	rVB	373033	455274	4.93%	0.725%
3	5.034	497	501	512	rVB	360469	480774	5.20%	0.766%
4	5.434	564	569	572	rBV	8797190	8544731	92.46%	13.607%
5	6.445	735	741	743	rBV	7385732	8590219	92.95%	13.680%
6	6.798	797	801	805	rBV	2167093	1670366	18.07%	2.660%
7	7.363	891	897	900	rBV	5046434	5754893	62.27%	9.165%
8	8.081	1014	1019	1023	rBV	2243228	2159911	23.37%	3.440%
9	9.163	1197	1203	1206	rBV	8871621	8687426	94.00%	13.834%
10	9.839	1313	1318	1321	rBV	2799619	2331398	25.23%	3.713%
11	10.633	1447	1453	1456	rBV	6215338	5846831	63.26%	9.311%
12	11.327	1565	1571	1574	rBV	2961951	2474827	26.78%	3.941%
13	12.921	1835	1842	1845	rBV	9543599	9241908	100.00%	14.717%
14	13.763	1979	1985	1989	rBV	82339	133629	1.45%	0.213%
15	13.804	1989	1992	1994	rVV	116567	135996	1.47%	0.217%
16	13.839	1994	1998	2001	rVB	293920	301861	3.27%	0.481%
17	13.968	2016	2020	2024	rBV	2665164	2218397	24.00%	3.533%
18	14.751	2148	2153	2157	rBV	104708	116980	1.27%	0.186%
19	15.080	2206	2209	2215	rVB	138734	166389	1.80%	0.265%
20	15.427	2262	2268	2271	rBV	1543451	1906626	20.63%	3.036%
21	15.457	2271	2273	2281	rVB	126716	144841	1.57%	0.231%
22	15.886	2342	2346	2352	rBV2	100646	142793	1.55%	0.227%
23	16.386	2425	2431	2436	rBV4	74713	142958	1.55%	0.228%
24	16.762	2484	2495	2508	rBV2	158019	562254	6.08%	0.895%
25	16.962	2525	2529	2538	rVB3	42890	93096	1.01%	0.148%

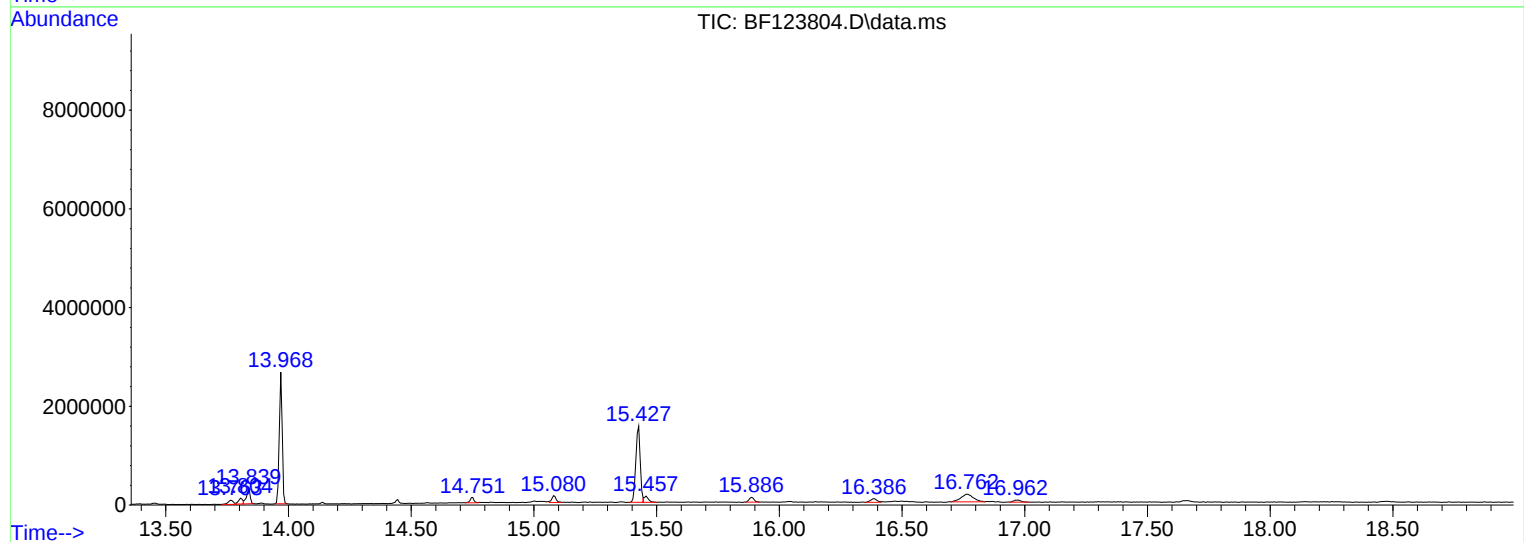
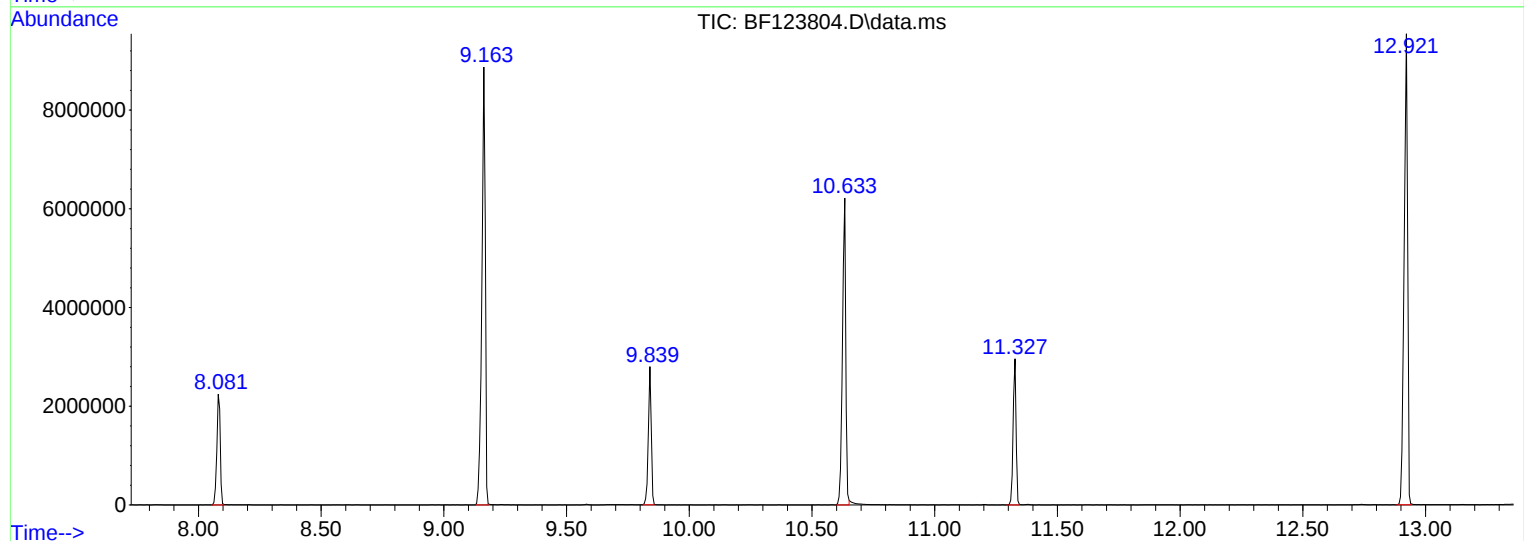
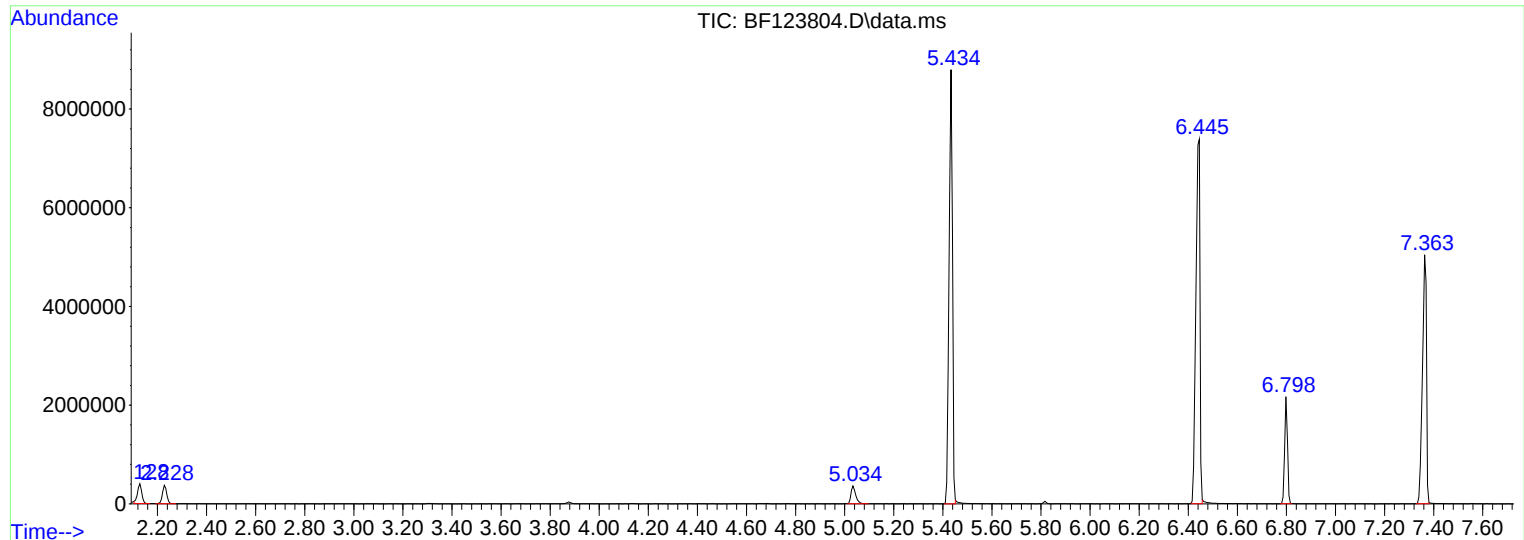
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ClientSampleId :
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Quant Title :

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



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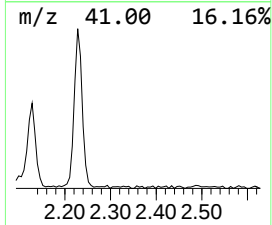
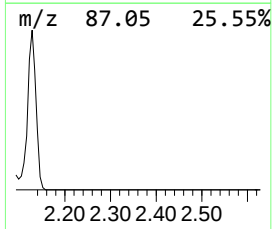
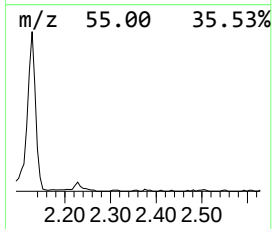
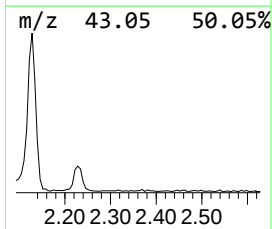
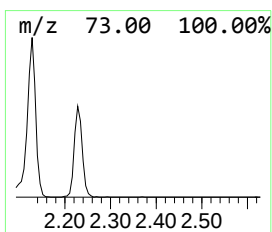
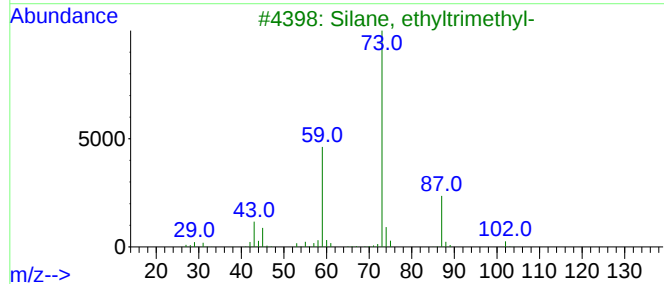
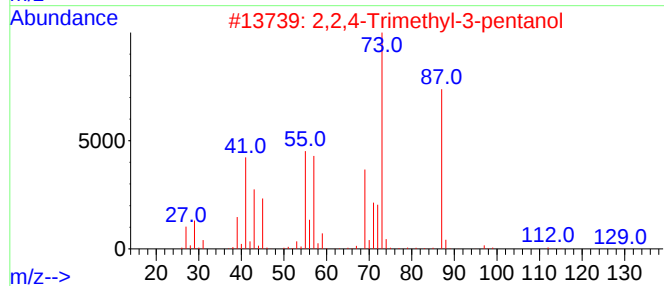
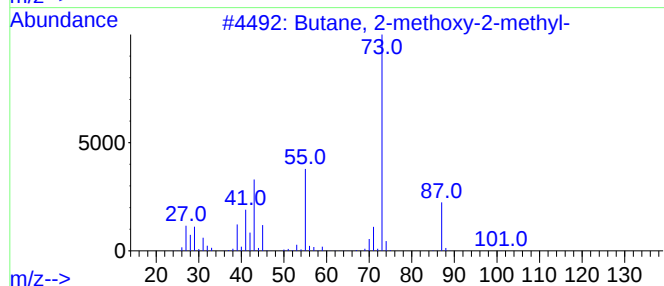
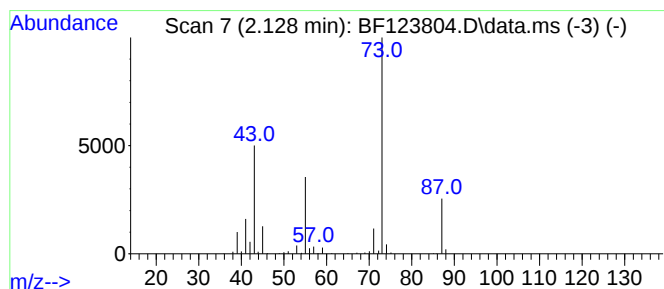
Quant Title :

TIC Library : C:\DATABASE\NIST11.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.
2.128	5.88 ng	491009	1,4-Dichlorobenzene-d4	6.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	36
4			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	23



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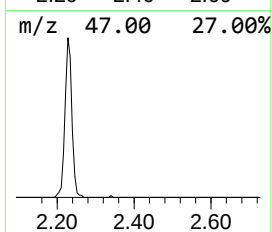
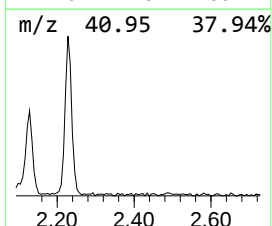
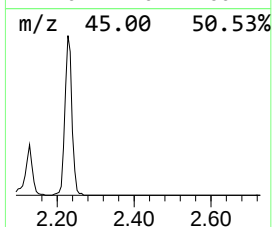
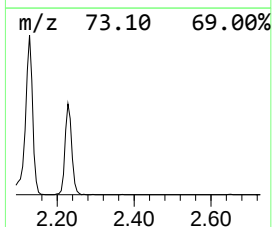
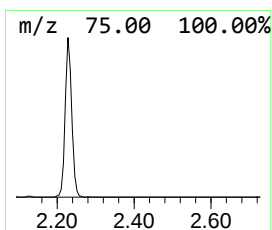
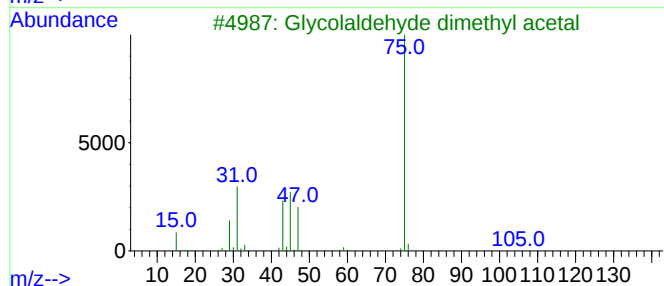
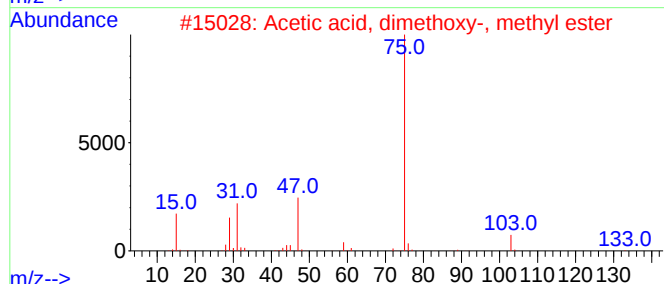
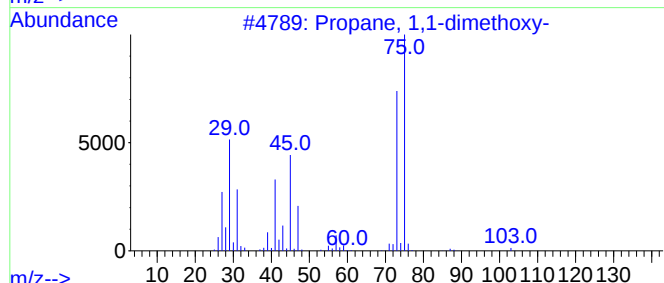
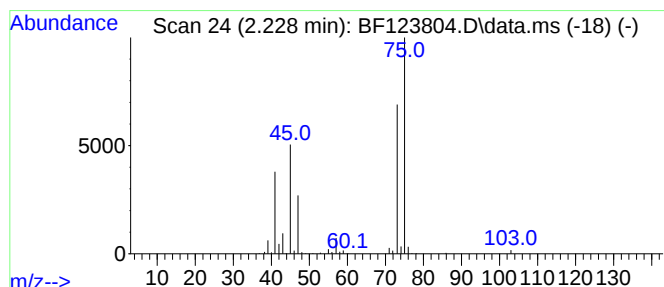
Quant Title :

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

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.228	5.45 ng	455274	1,4-Dichlorobenzene-d4	6.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2			Acetic acid, dimethoxy-, methyl ...	134	C5H10O4	000089-91-8	40
3			Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	38
4			Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	33
5			Methane, trimethoxy-	106	C4H10O3	000149-73-5	33



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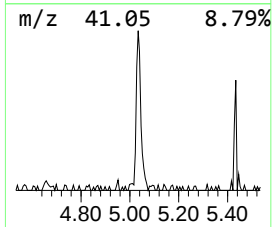
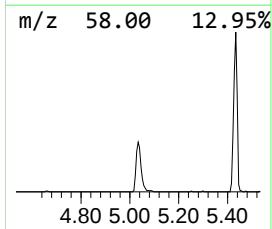
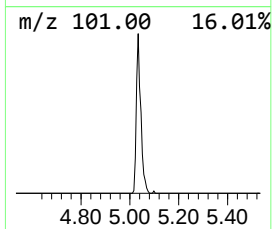
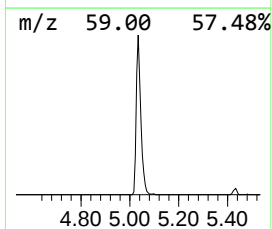
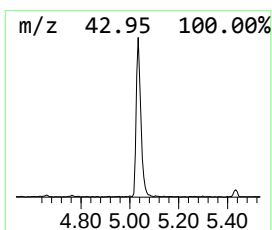
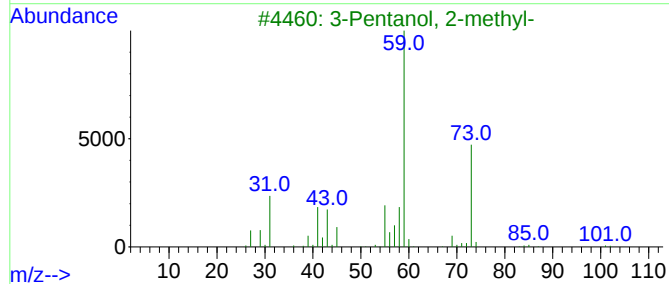
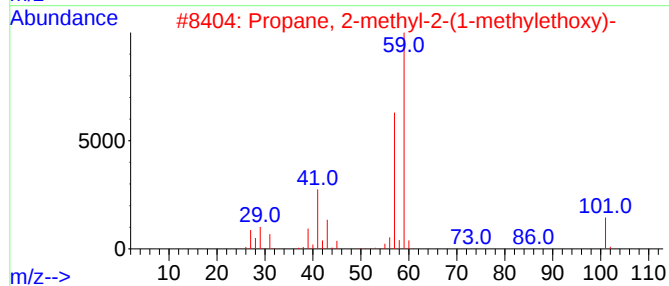
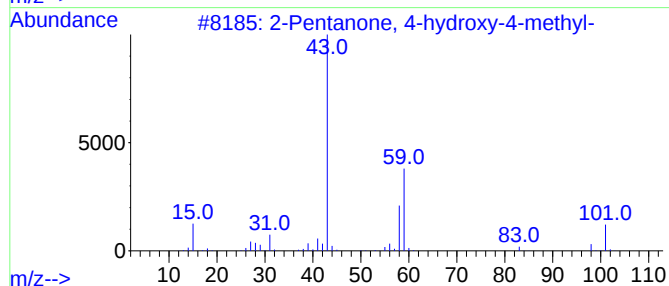
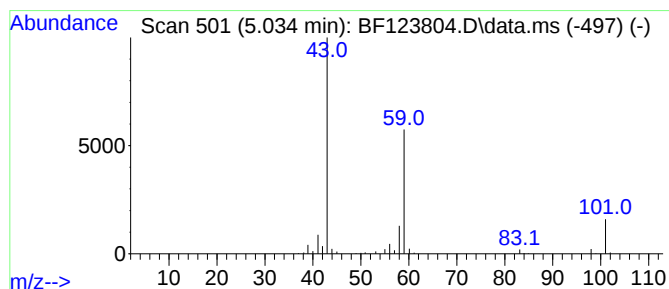
Quant Title :

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.034	5.76 ng	480774	1,4-Dichlorobenzene-d4	6.798

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42	
3	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	40	
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33	
5	Pentane, 2-methoxy-	102	C6H14O	006795-88-6	32	



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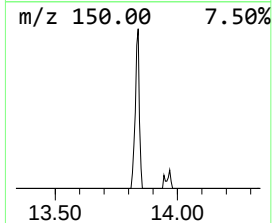
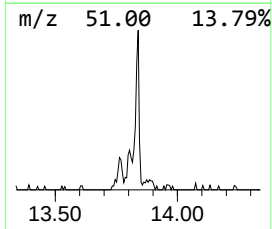
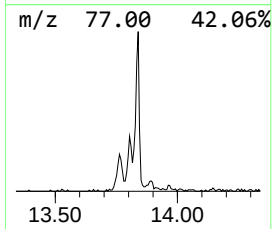
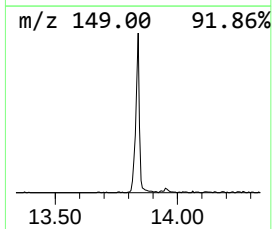
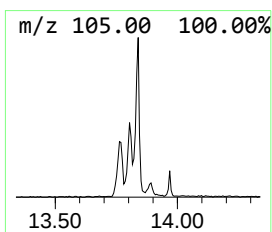
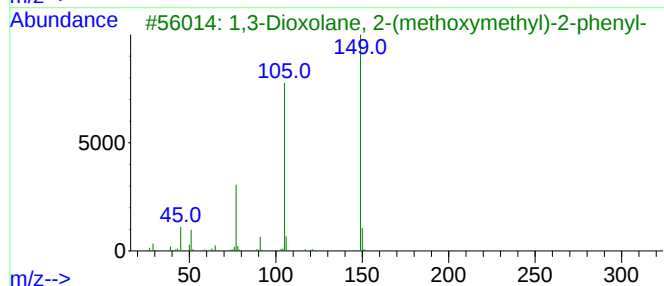
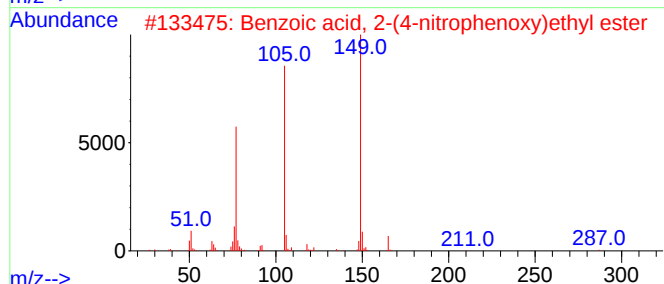
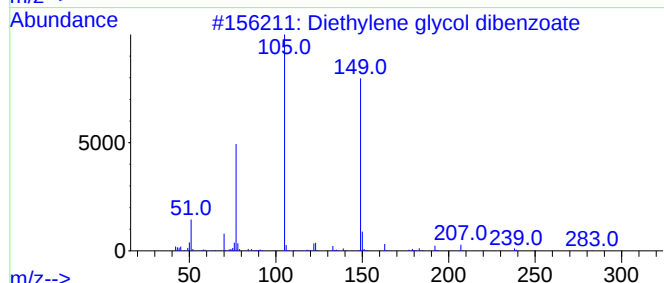
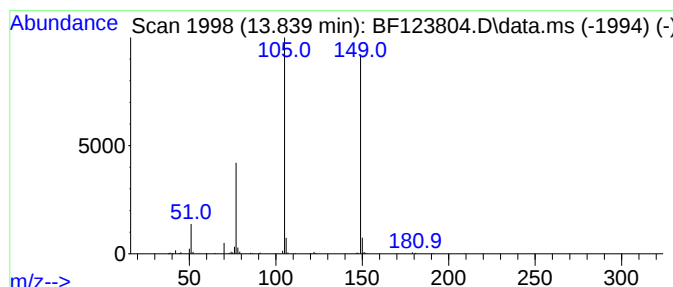
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Diethylene glycol dibenzoate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.839	2.72 ng	301861	Chrysene-d12	13.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	74
2			Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	72
3			1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	59
4			2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	43
5			2,3-Dimethyl-4a,8a-diphenyl-hexa...	326	C20H22O4	1000297-07-0	37



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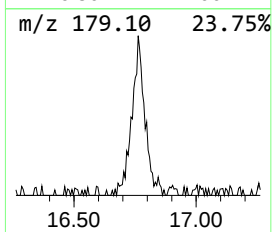
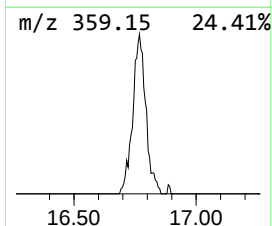
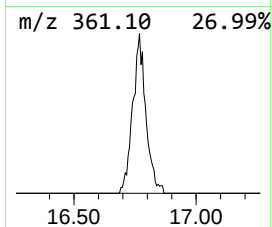
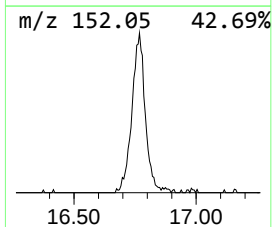
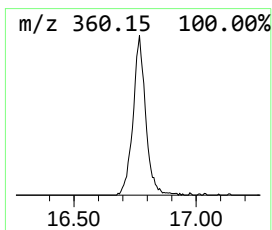
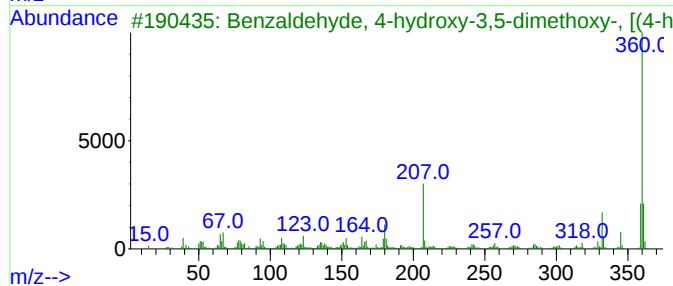
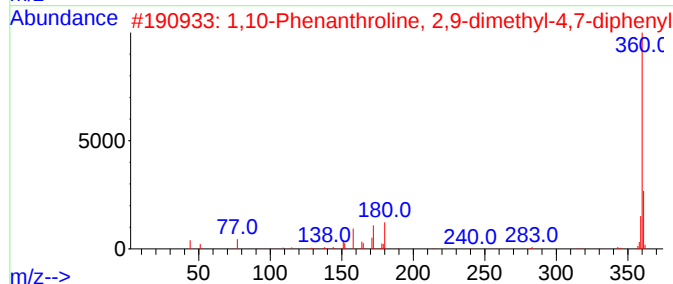
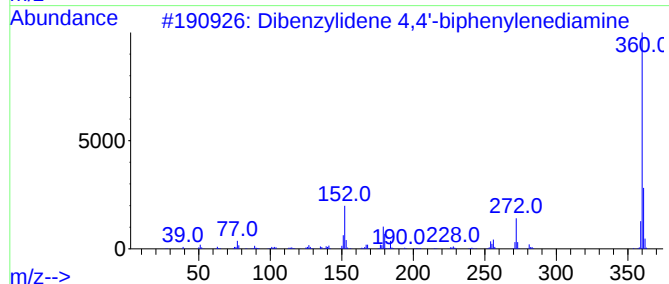
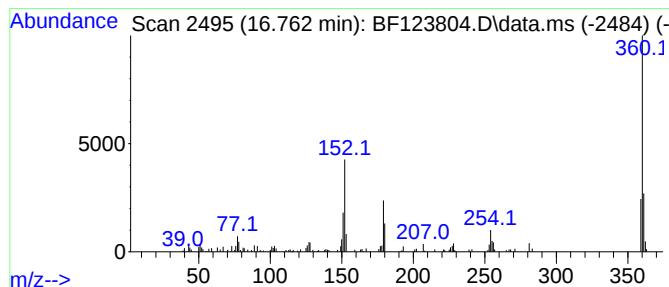
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Dibenzylidene 4,4'-biphenyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.762	5.90 ng	562254	Perylene-d12	15.427

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dibenzylidene 4,4'-biphenylenedi...	360	C26H20N2	006311-48-4	87
2		1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	47
3		Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	47
4		N,N'-di-2-Naphthyl-p-phenylenedi...	360	C26H20N2	000093-46-9	46
5		Ethene, 1-(anthracen-9-yl)-2-(4-...	360	C27H20O	1000163-55-1	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.128	5.9	ng	491009	1	6.798	1670370	20.0
Propane, 1,1-di...	2.228	5.5	ng	455274	1	6.798	1670370	20.0
2-Pentanone, 4-...	5.034	5.8	ng	480774	1	6.798	1670370	20.0
Diethylene glyc...	13.839	2.7	ng	301861	5	13.969	2218400	20.0
Dibenzylidene 4...	16.762	5.9	ng	562254	6	15.427	1906630	20.0