

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050721\
 Data File : BF123867.D
 Acq On : 7 May 2021 13:02
 Operator : JU/CG
 Sample : PB136202BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB136202BL

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: BF123867.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.404	560	564	579	rBV	6682817	6250971	93.94%	14.354%
2	6.422	732	737	740	rBV	6341116	6237790	93.74%	14.324%
3	6.775	794	797	801	rBV	1513000	1163325	17.48%	2.671%
4	7.345	888	894	897	rBV	3858970	4150413	62.37%	9.531%
5	8.063	1011	1016	1019	rBV	1651161	1490956	22.41%	3.424%
6	9.139	1194	1199	1202	rBV	7020279	6383878	95.94%	14.660%
7	9.816	1309	1314	1317	rBV	2036246	1573335	23.64%	3.613%
8	10.610	1444	1449	1452	rBV	4423460	4198466	63.10%	9.641%
9	11.304	1563	1567	1570	rBV	1944200	1636609	24.60%	3.758%
10	12.892	1832	1837	1840	rBV	7090637	6654058	100.00%	15.280%
11	13.739	1975	1981	1984	rBV	122519	166922	2.51%	0.383%
12	13.780	1984	1988	1990	rVV	154898	201088	3.02%	0.462%
13	13.809	1990	1993	1998	rVB	415159	419382	6.30%	0.963%
14	13.939	2011	2015	2019	rBV	1649203	1374031	20.65%	3.155%
15	14.909	2171	2180	2188	rBV3	42871	151821	2.28%	0.349%
16	15.045	2199	2203	2209	rBV	67811	90112	1.35%	0.207%
17	15.386	2256	2261	2265	rBV	976351	1126326	16.93%	2.586%
18	16.333	2417	2422	2436	rVB4	52956	173940	2.61%	0.399%
19	16.615	2463	2470	2471	rBV4	61982	103805	1.56%	0.238%

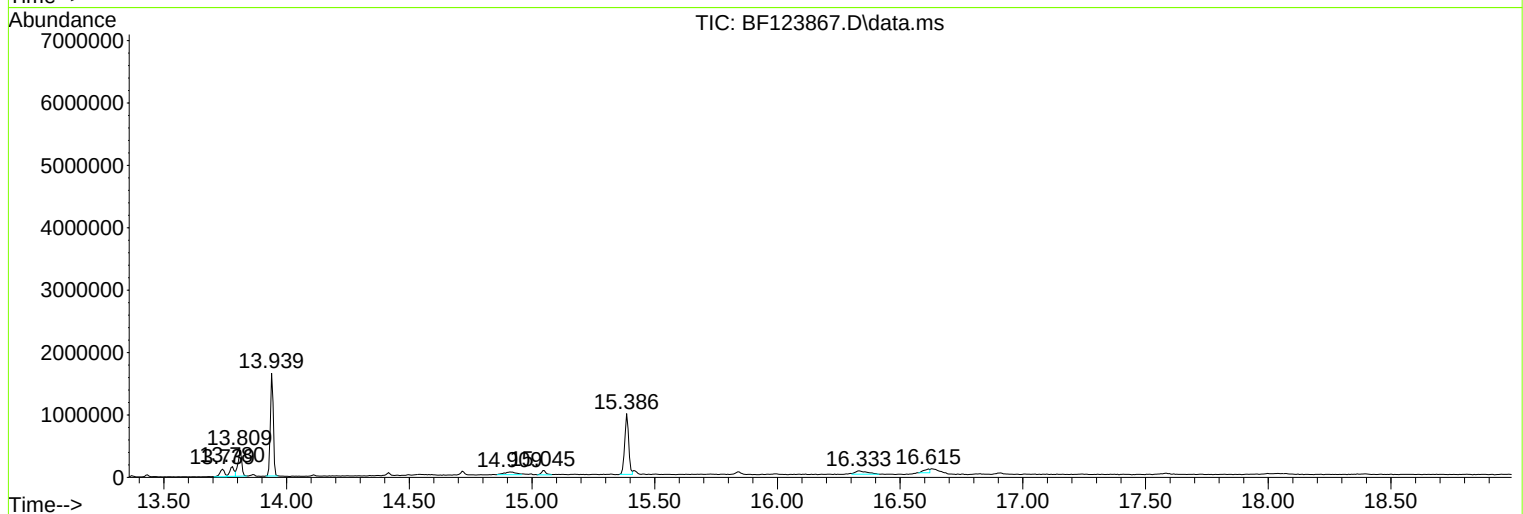
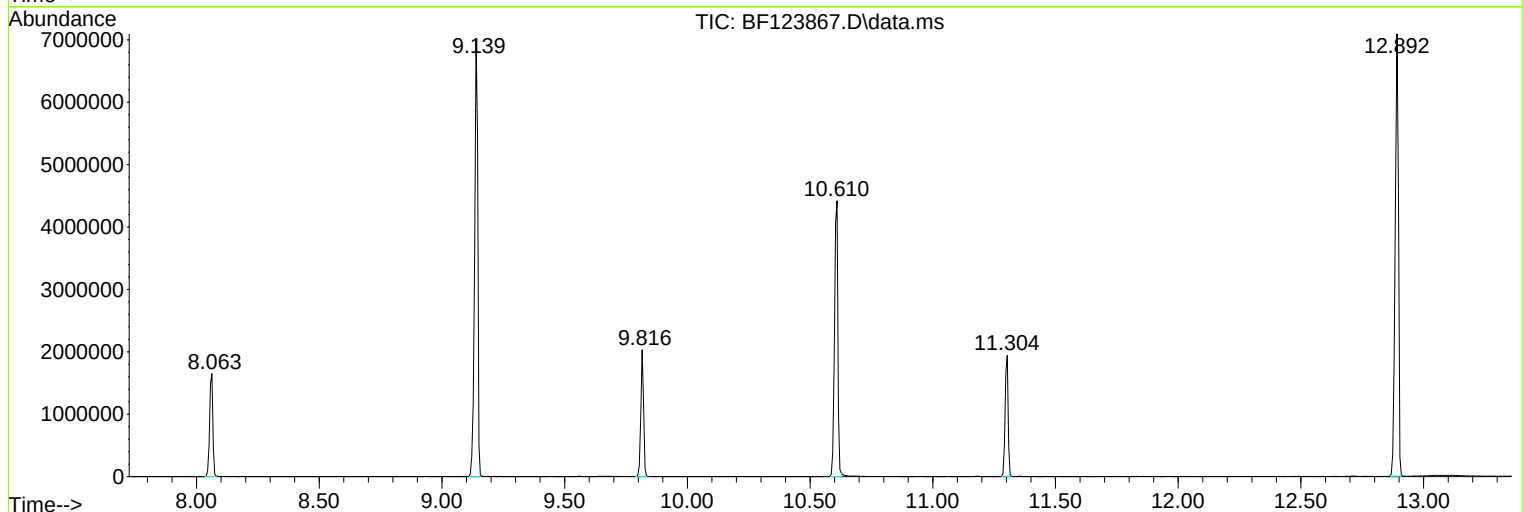
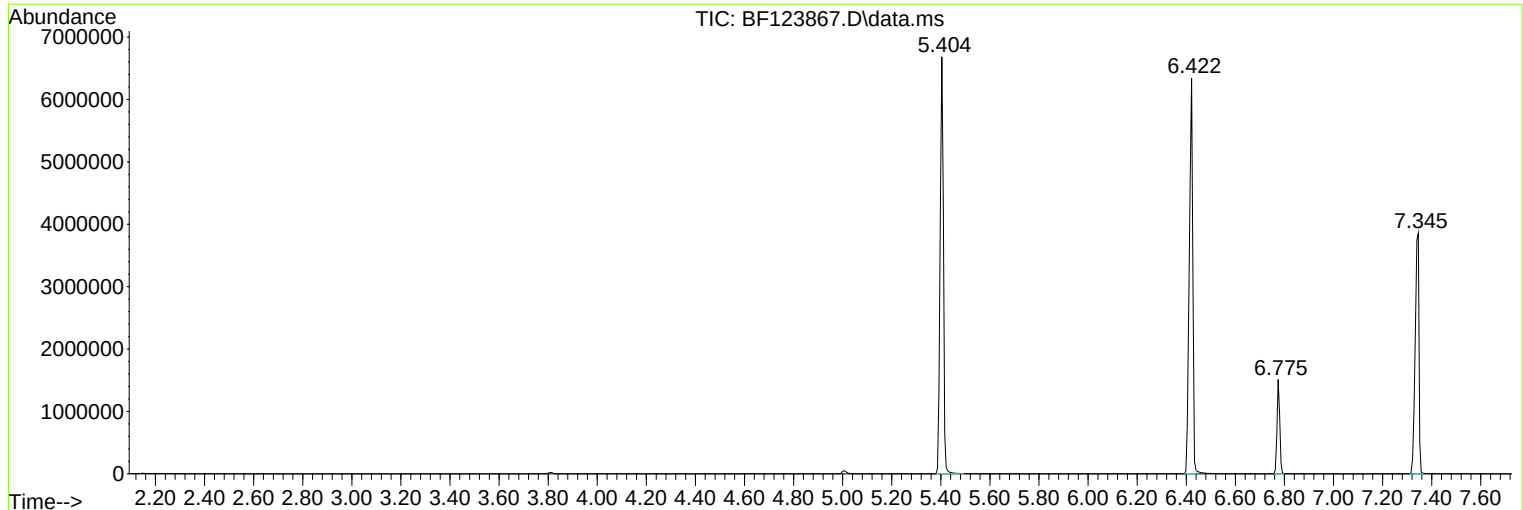
Sum of corrected areas: 43547228

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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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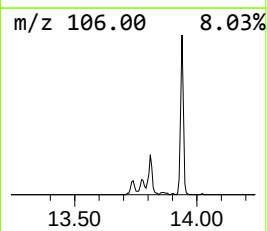
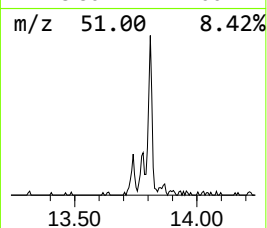
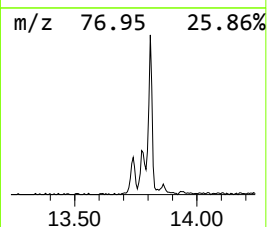
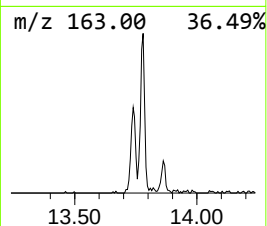
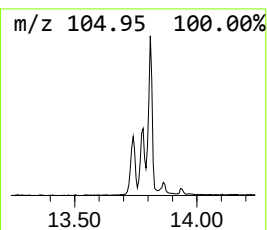
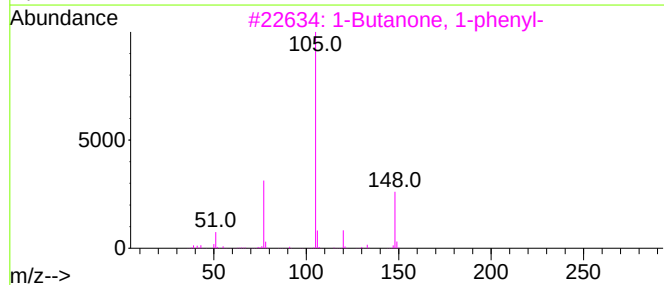
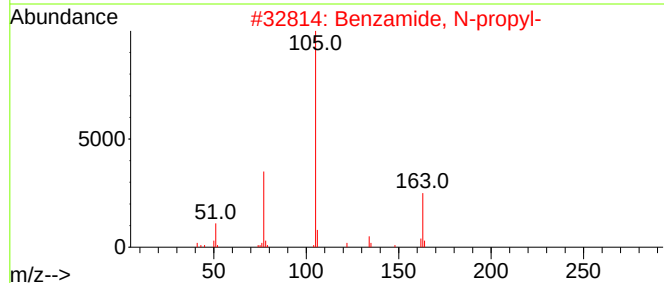
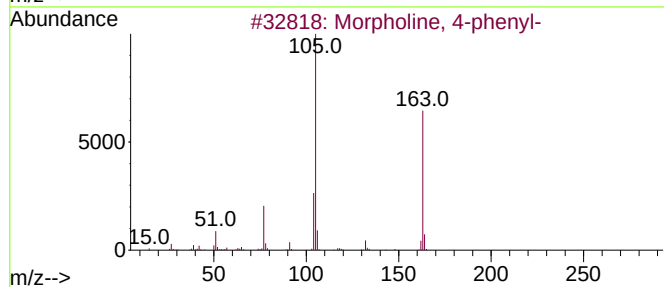
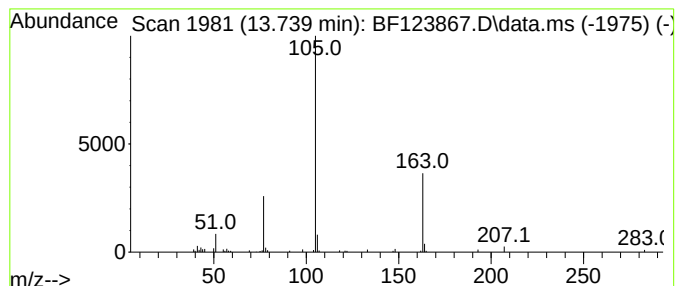
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Morpholine, 4-phenyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.739	2.43 ng	166922	Chrysene-d12	13.939

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	72
2		Benzamide, N-propyl-	163	C10H13NO	010546-70-0	72
3		1-Butanone, 1-phenyl-	148	C10H12O	000495-40-9	47
4		Benzoic acid, 2-propenyl ester	162	C10H10O2	000583-04-0	43
5		1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	43



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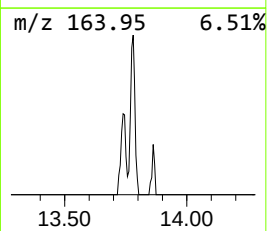
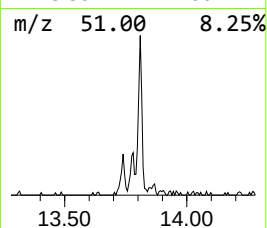
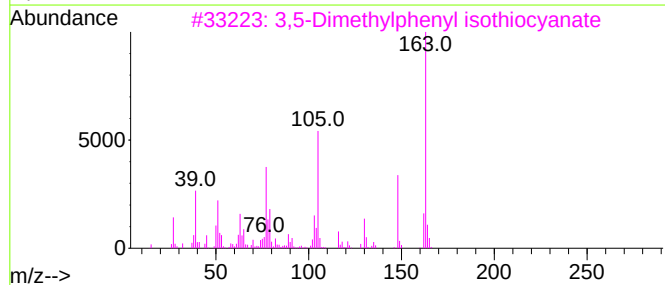
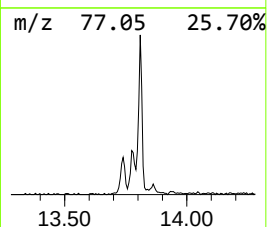
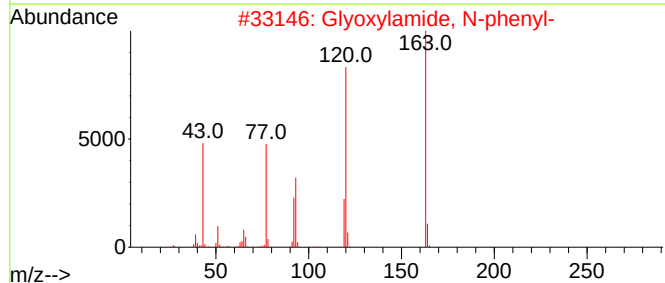
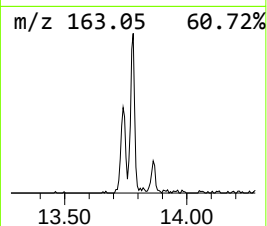
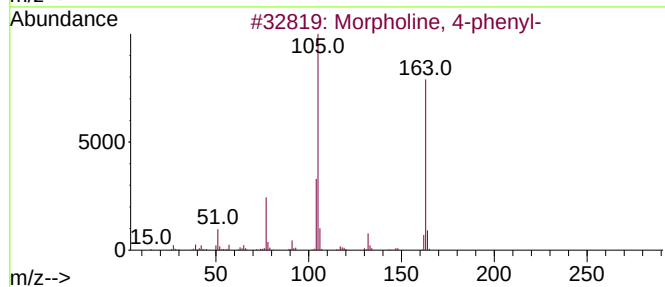
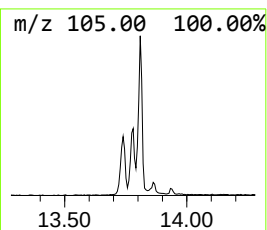
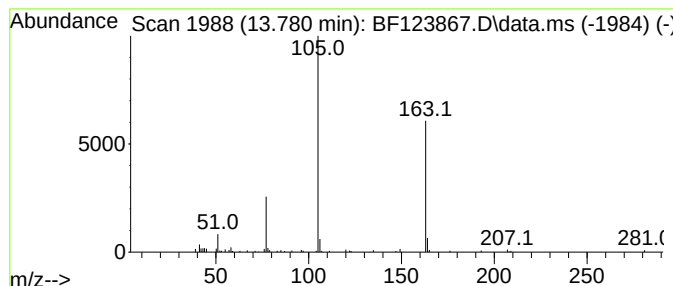
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Peak Number 2 unknown13.78 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.780	2.93 ng	201088	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	50
2			Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	47
3			3,5-Dimethylphenyl isothiocyanate	163	C9H9NS	040046-30-8	40
4			.delta.2-1,3,4-Oxadiazolin-5-one...	163	C7H5N3O2	002845-82-1	38
5			Imidazole, 2-fluoro-1-tribenzoyl...	530	C29H23FN2O7	1000129-58-6	27



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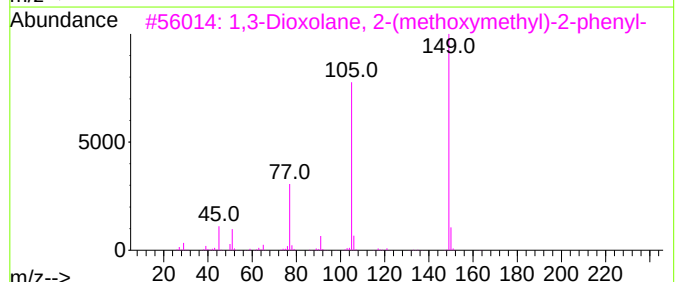
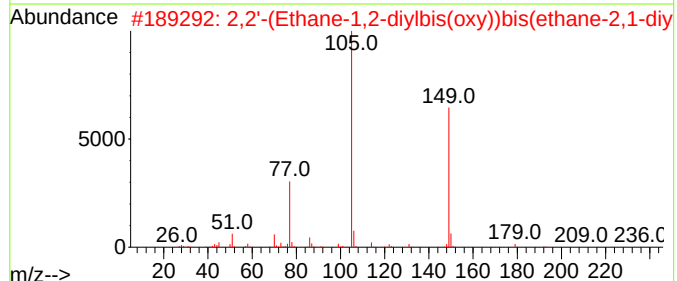
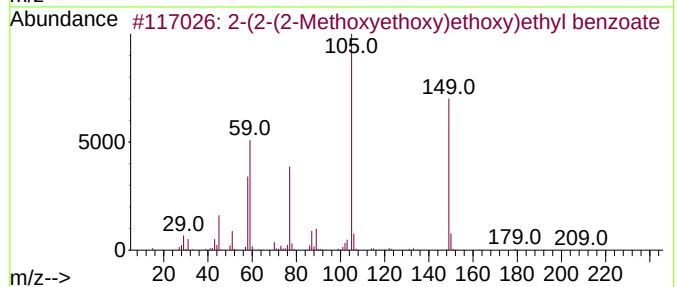
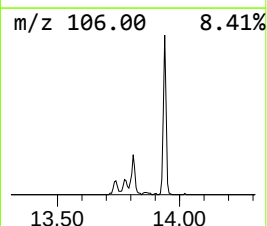
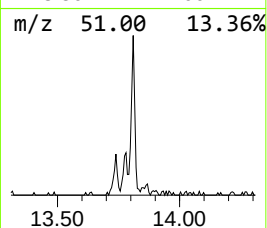
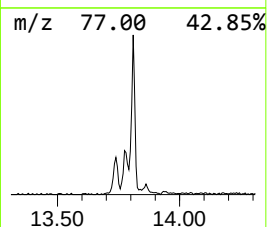
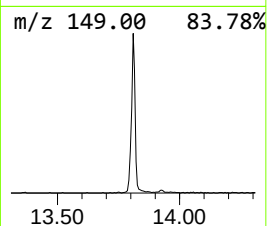
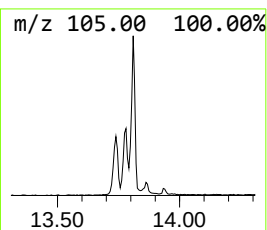
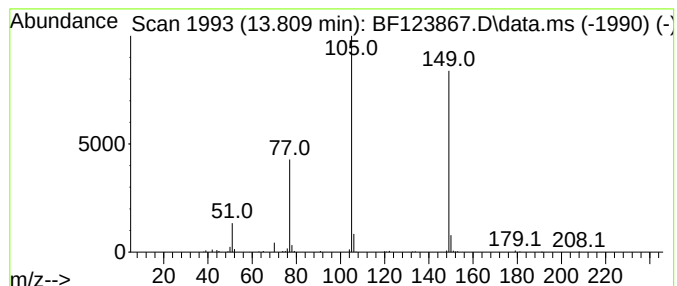
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-(2-(2-Methoxyethoxy)ethox... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.810	6.10 ng	419382	Chrysene-d12	13.939	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	83
2	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	83
3	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	72
4	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	64
5	1-Propanone, 1-phenyl-	134	C9H10O	000093-55-0	35



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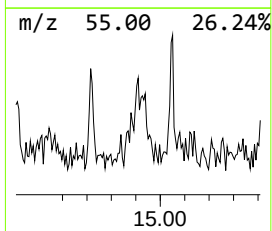
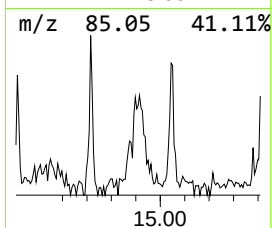
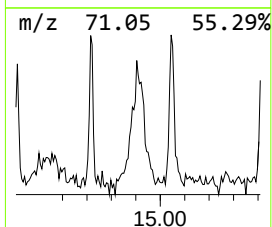
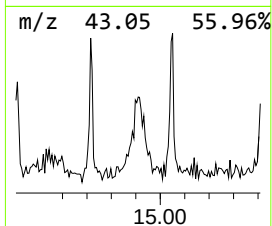
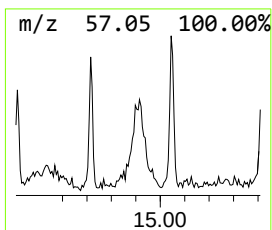
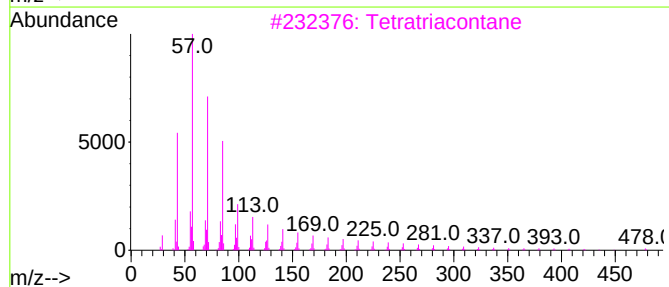
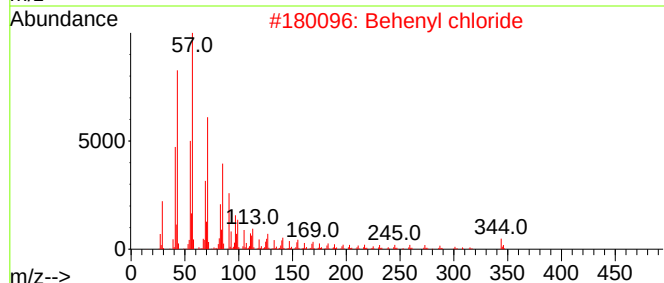
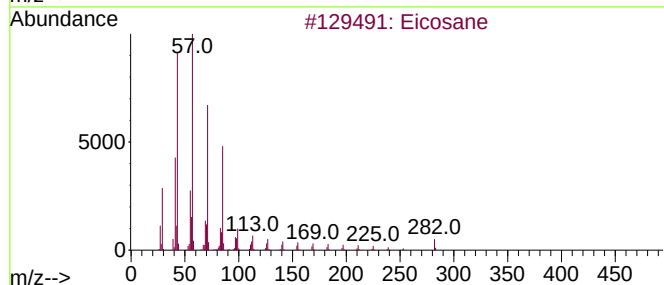
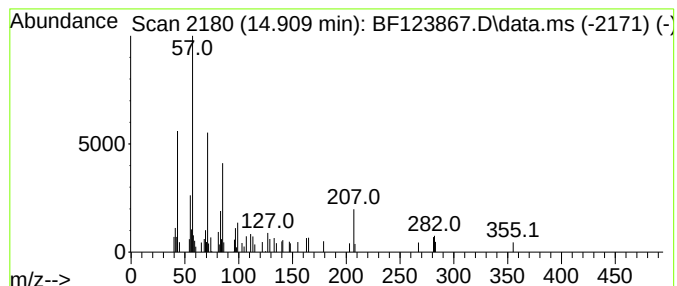
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Peak Number 4 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.909	2.70 ng	151821	Perylene-d12	15.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	83
2			Behenyl chloride	344	C22H45Cl	042217-03-8	64
3			Tetratriacontane	479	C34H70	014167-59-0	59
4			Tricosane	324	C23H48	000638-67-5	59
5			Hexacosane	366	C26H54	000630-01-3	59



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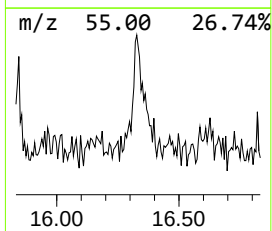
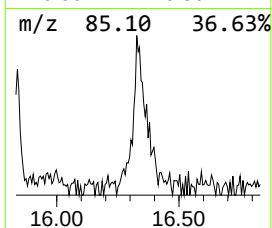
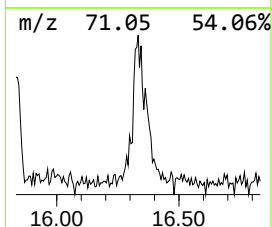
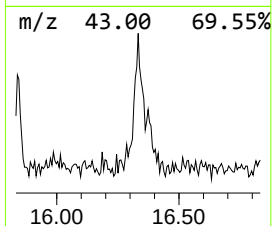
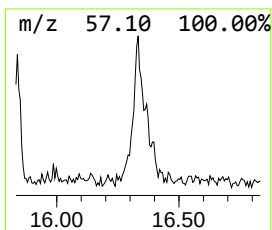
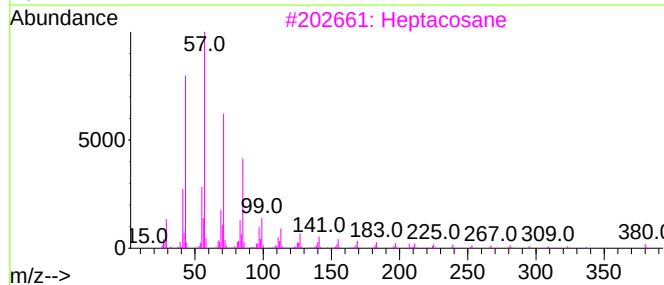
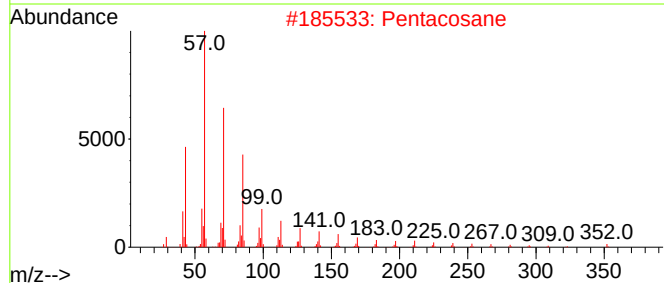
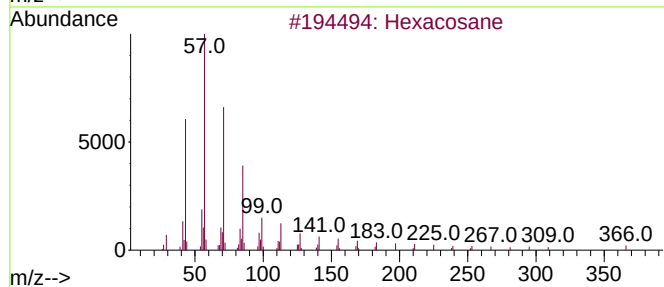
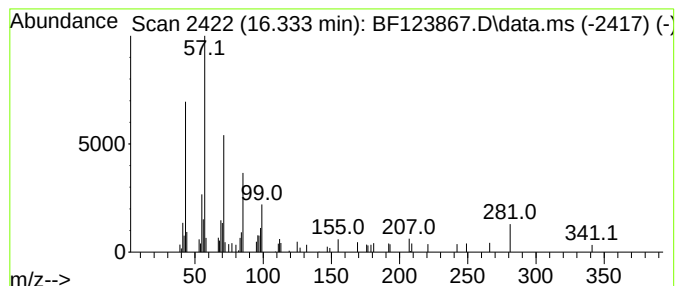
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.333	3.09 ng	173940	Perylene-d12	15.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	64
2			Pentacosane	352	C25H52	000629-99-2	64
3			Heptacosane	380	C27H56	000593-49-7	59
4			10-Methylnonadecane	282	C20H42	056862-62-5	53
5			Eicosane, 10-methyl-	296	C21H44	054833-23-7	53



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Morpholine, 4-p...	13.739	2.4	ng	166922	5	13.939	1374030	20.0
unknown13.78	13.780	2.9	ng	201088	5	13.939	1374030	20.0
2-(2-(2-Methoxy...	13.810	6.1	ng	419382	5	13.939	1374030	20.0
Eicosane	14.909	2.7	ng	151821	6	15.386	1126330	20.0
Hexacosane	16.333	3.1	ng	173940	6	15.386	1126330	20.0