

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011022\
 Data File : BF126575.D
 Acq On : 10 Jan 2022 19:16
 Operator : JU/CG
 Sample : N1054-17
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20220024-CAPE-6-MODIFIED-ELUTRIATE

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-BF122921.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126575.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	10	14	19	rVB2	27754	35961	1.08%	0.201%
2	4.987	489	493	502	rVB	88229	112565	3.37%	0.629%
3	5.393	557	562	565	rBV	2107744	2068528	61.98%	11.562%
4	6.404	729	734	737	rBV	1908771	1834864	54.98%	10.256%
5	6.769	792	796	799	rBV	597514	497527	14.91%	2.781%
6	7.334	886	892	895	rBV	1861475	2169867	65.01%	12.129%
7	7.957	994	998	1006	rBV	81075	79607	2.39%	0.445%
8	8.051	1009	1014	1017	rBV	802550	704254	21.10%	3.937%
9	9.134	1192	1198	1201	rBV	3164813	3337569	100.00%	18.656%
10	9.810	1307	1313	1316	rBV	791463	730121	21.88%	4.081%
11	10.604	1442	1448	1451	rBV	1930474	2060226	61.73%	11.516%
12	11.292	1561	1565	1569	rVB	802785	670387	20.09%	3.747%
13	11.833	1653	1657	1674	rBV2	52245	77527	2.32%	0.433%
14	12.886	1831	1836	1840	rBV	2276384	2439291	73.09%	13.635%
15	13.792	1984	1990	2001	rBV2	70270	123409	3.70%	0.690%
16	13.933	2011	2014	2018	rVB	465492	429456	12.87%	2.401%
17	14.033	2027	2031	2037	rBV	71369	69378	2.08%	0.388%
18	15.380	2255	2260	2264	rBV	406242	449708	13.47%	2.514%

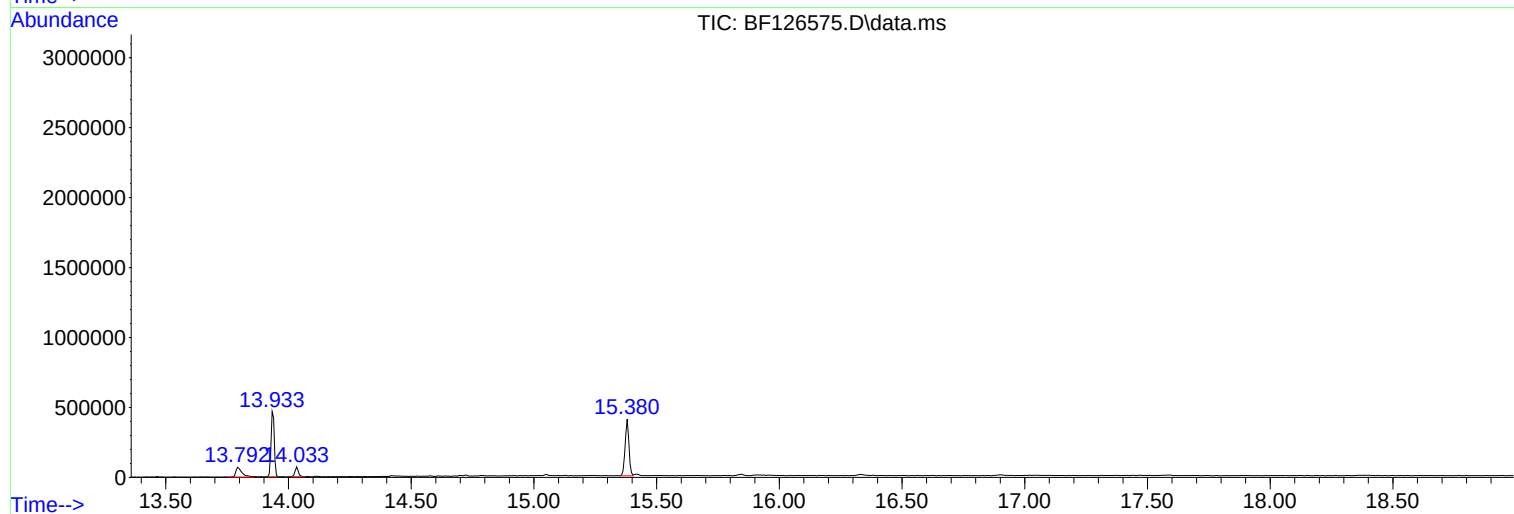
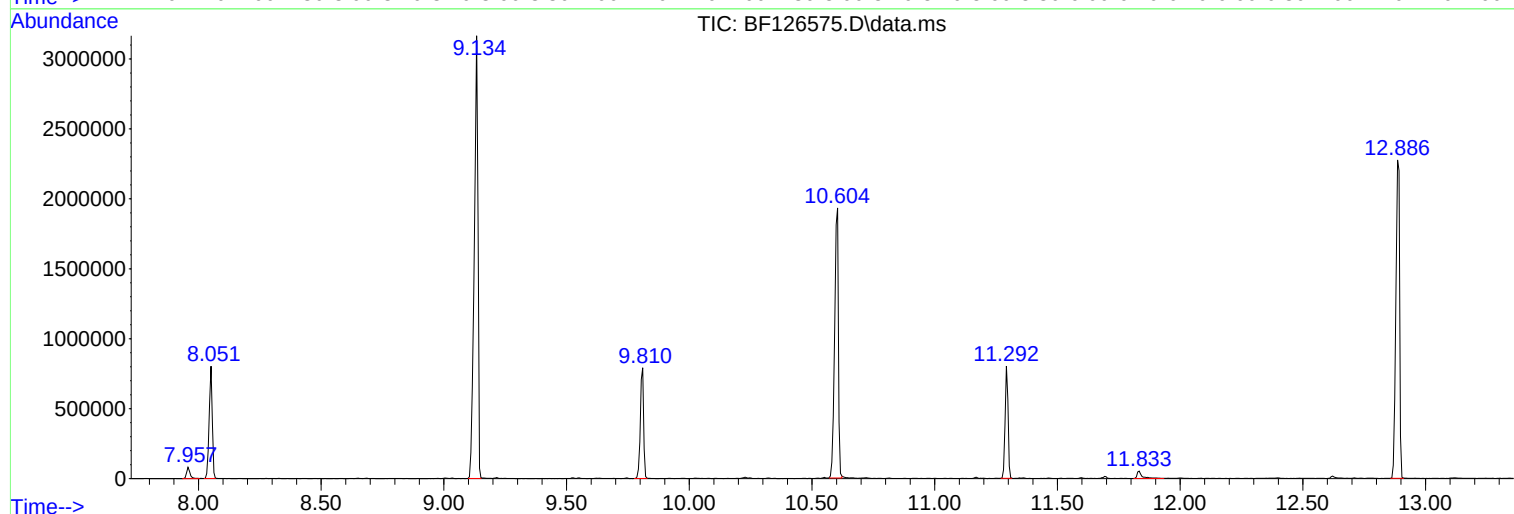
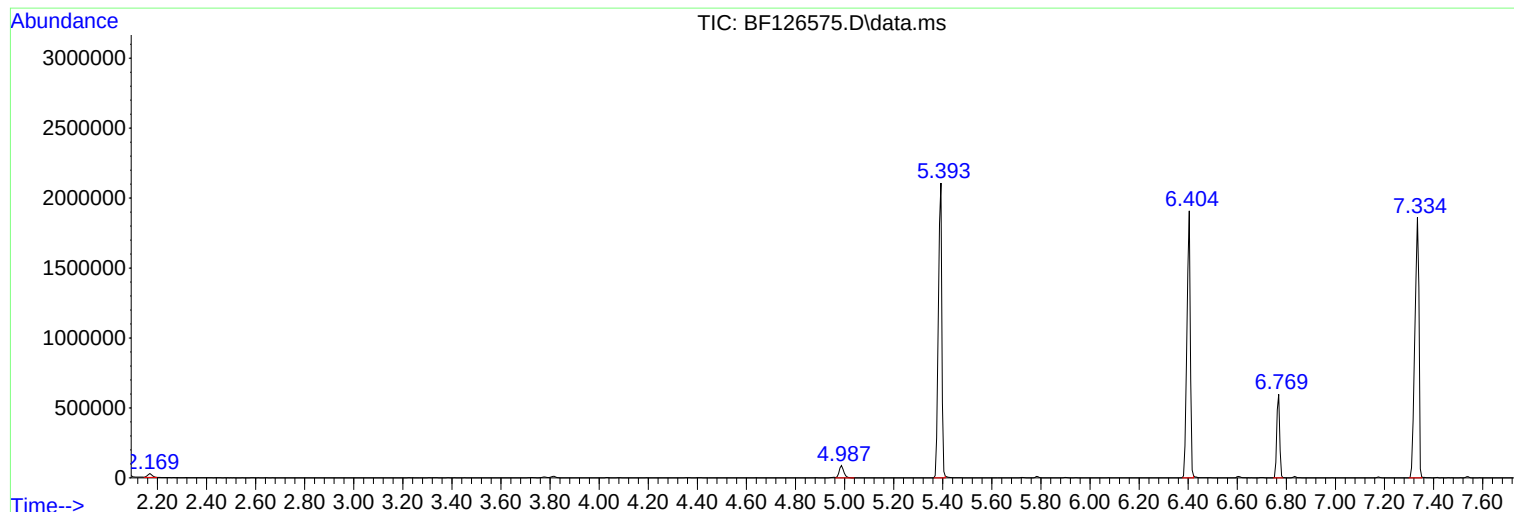
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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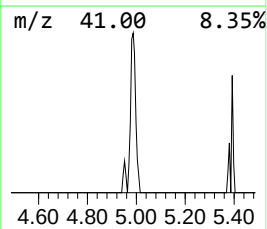
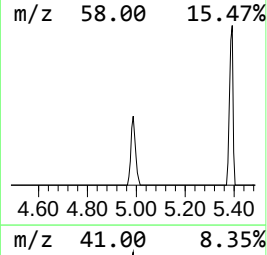
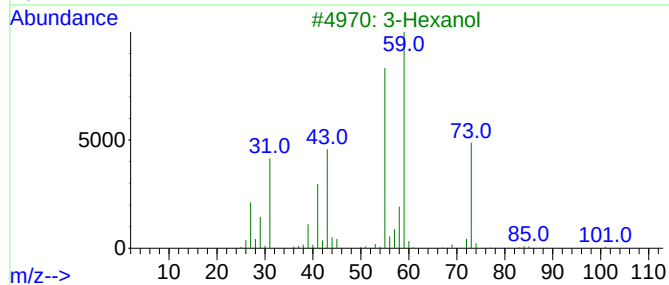
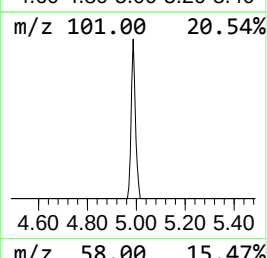
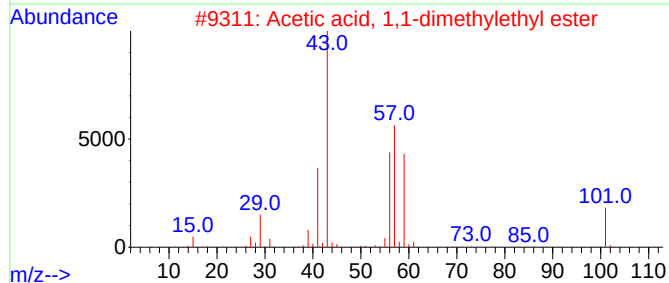
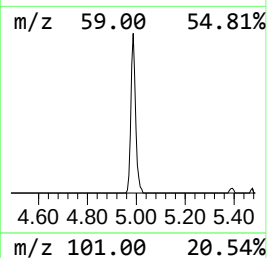
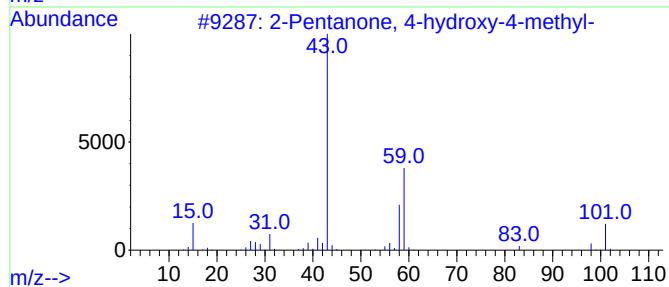
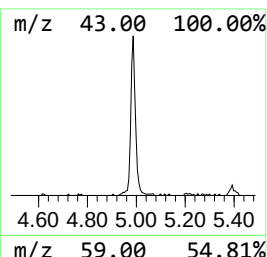
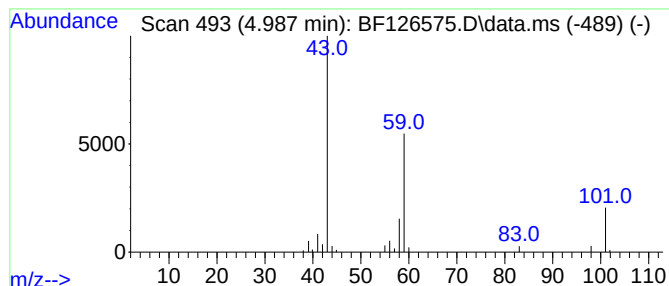
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.987	4.52 ng	112565	1,4-Dichlorobenzene-d4	6.769

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	39		
3	3-Hexanol	102	C6H14O	000623-37-0	28		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		



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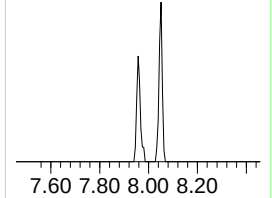
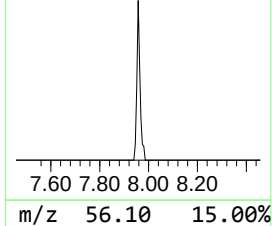
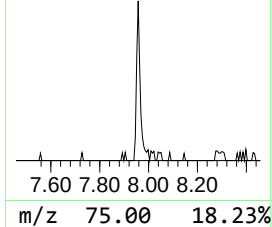
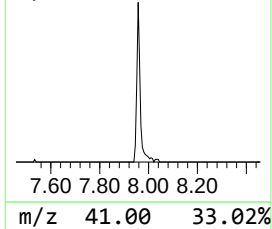
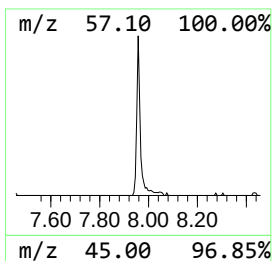
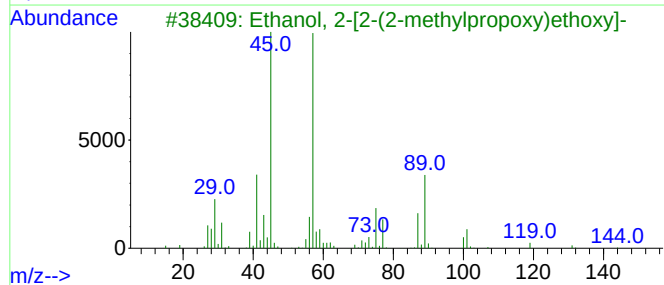
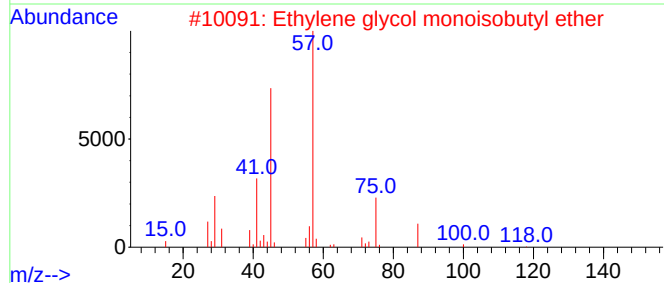
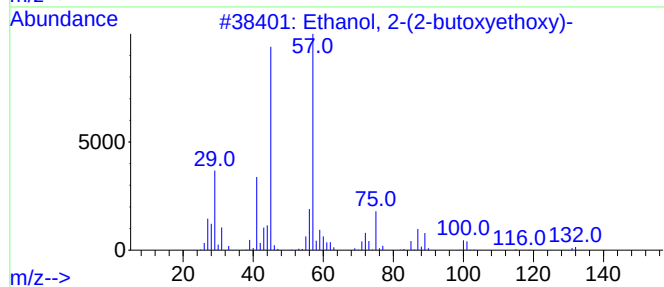
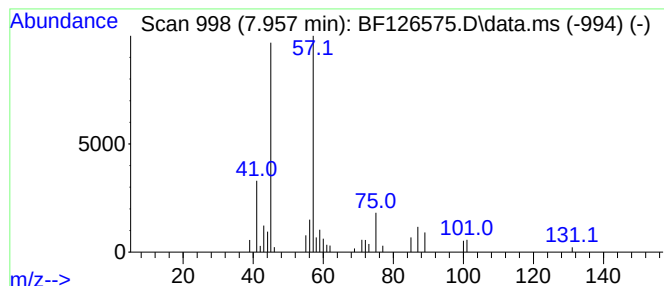
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.957	2.26 ng	79607	Naphthalene-d8	8.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
3			Ethanol, 2-[2-(2-methylpropoxy)ethoxy]-	162	C8H18O3	018912-80-6	56
4			Pentaethylene glycol	238	C10H22O6	004792-15-8	50
5			Ethanol, 2-[2-(2-butoxyethoxy)ethoxy]-	206	C10H22O4	000143-22-6	45



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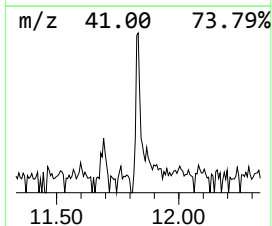
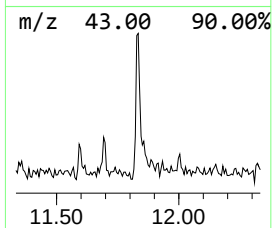
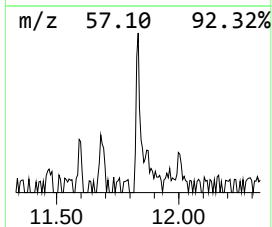
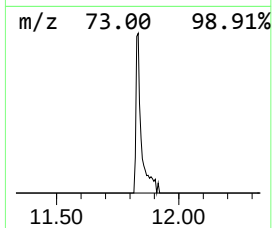
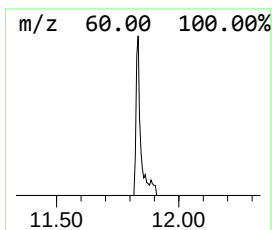
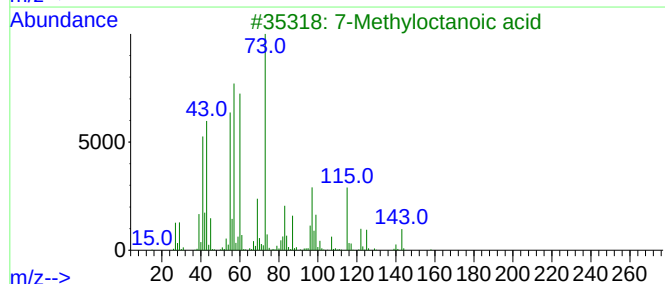
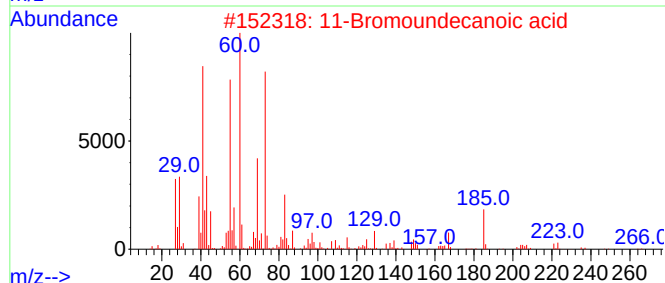
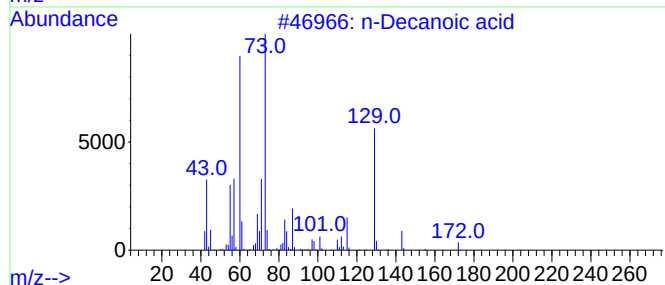
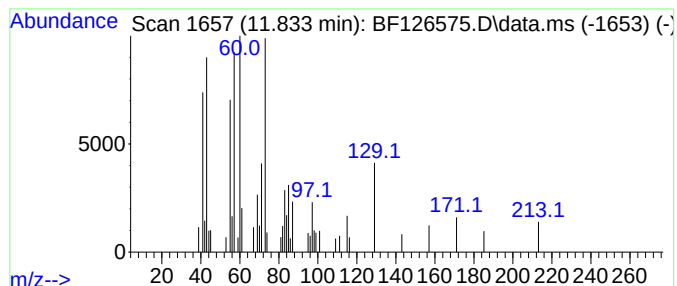
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Decanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.833	2.31 ng	77527	Phenanthrene-d10	11.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Decanoic acid	172	C10H20O2	000334-48-5	64
2			11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	38
3			7-Methyloctanoic acid	158	C9H18O2	000693-19-6	14
4			Methyl-.alpha.-d-ribofuranoside	164	C6H12O5	1000129-83-1	14
5			Octane, 3,4,5,6-tetramethyl-	170	C12H26	062185-21-1	10



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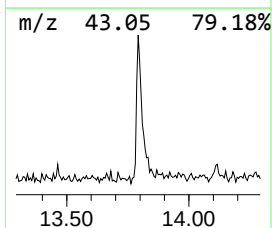
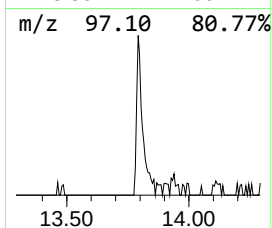
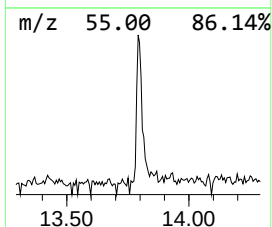
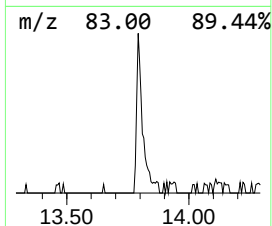
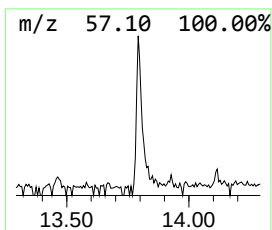
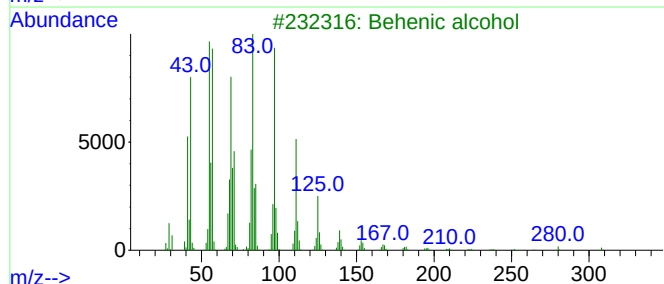
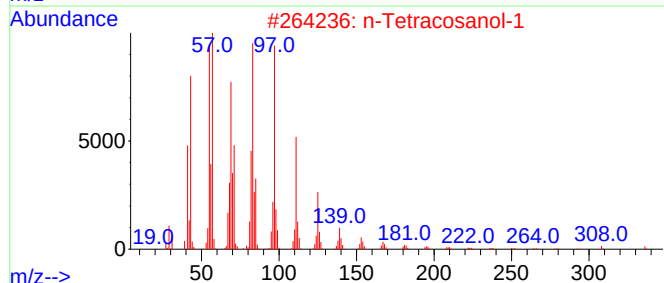
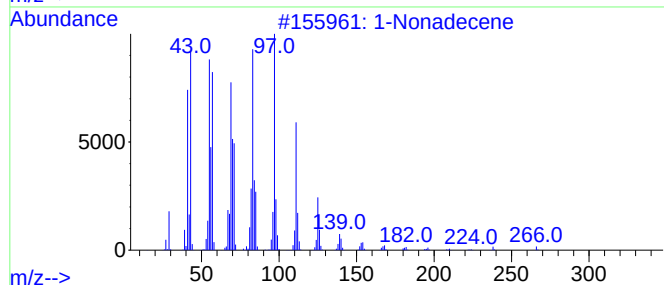
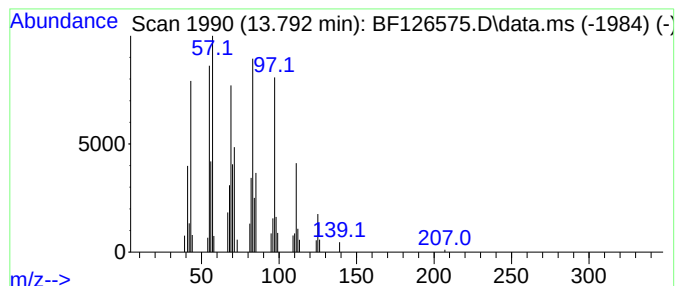
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Peak Number 4 1-Nonadecene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.792	5.75 ng	123409	Chrysene-d12	13.933	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	91
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3	Behenic alcohol	326	C22H46O	000661-19-8	91
4	1-Heneicosanol	312	C21H44O	015594-90-8	91
5	1-Hexacosene	364	C26H52	018835-33-1	91



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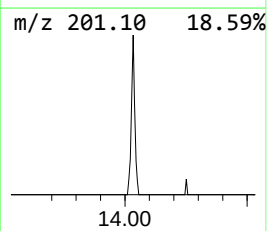
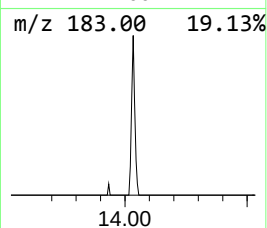
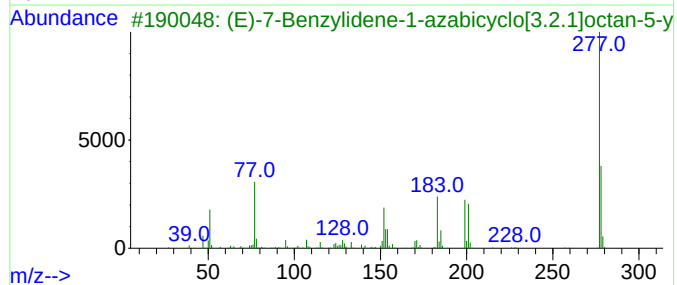
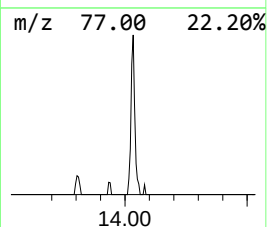
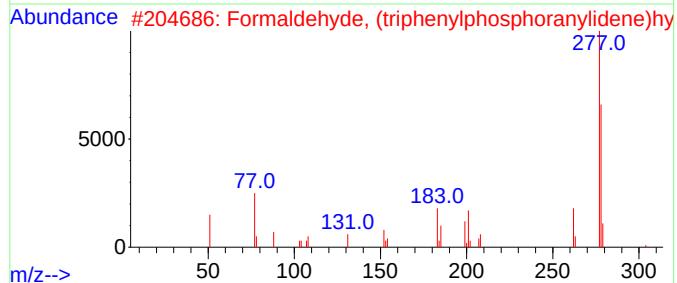
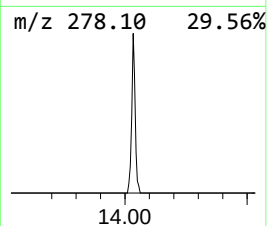
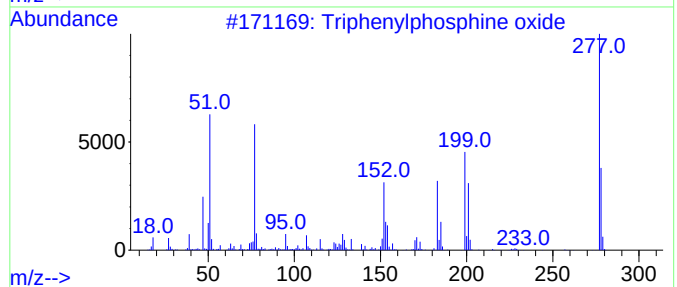
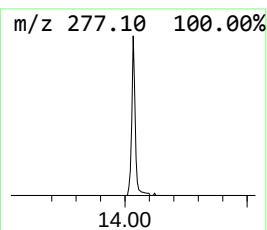
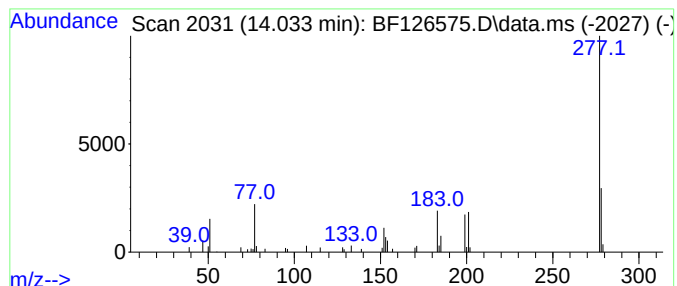
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.033	3.23 ng	69378	Chrysene-d12	13.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	91
2			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	72
3			(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	58
4			2-Propenoic acid, 2-cyano-3-(3-p...	277	C18H15NO2	1000080-00-3	50
5			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.987	4.5	ng	112565	1	6.769	497527	20.0
Ethanol, 2-(2-b...	7.957	2.3	ng	79607	2	8.051	704254	20.0
n-Decanoic acid	11.833	2.3	ng	77527	4	11.292	670387	20.0
1-Nonadecene	13.792	5.8	ng	123409	5	13.933	429456	20.0
Triphenylphosph...	14.033	3.2	ng	69378	5	13.933	429456	20.0