

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031822\
 Data File : BF127395.D
 Acq On : 18 Mar 2022 16:51
 Operator : CG\JU
 Sample : N1709-02
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PPSP-B18-26.0-26.5

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-BF031022.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127395.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.081	472	475	485	rVB	25771	32450	1.36%	0.203%
2	5.481	539	543	560	rBV	1683524	1696192	71.26%	10.618%
3	6.492	710	715	732	rBV	1820385	1823727	76.62%	11.417%
4	6.857	773	777	780	rBV	552413	465752	19.57%	2.916%
5	7.422	869	873	876	rBV	1416501	1193135	50.13%	7.469%
6	8.039	975	978	991	rBV	127471	209877	8.82%	1.314%
7	8.139	991	995	998	rVV	780093	605079	25.42%	3.788%
8	9.216	1173	1178	1181	rBV	2450220	2116503	88.92%	13.249%
9	9.322	1192	1196	1205	rBV	290256	283649	11.92%	1.776%
10	9.898	1290	1294	1297	rBV	830363	747241	31.39%	4.678%
11	10.686	1424	1428	1432	rBV	1426547	1392728	58.51%	8.718%
12	11.227	1513	1520	1524	rBV3	21242	33771	1.42%	0.211%
13	11.327	1534	1537	1541	rVB	40468	33429	1.40%	0.209%
14	11.386	1543	1547	1551	rBV	970606	817970	34.37%	5.120%
15	11.545	1570	1574	1578	rBV	30772	29617	1.24%	0.185%
16	11.769	1609	1612	1615	rVB	92292	78014	3.28%	0.488%
17	11.904	1631	1635	1639	rBV3	38278	50285	2.11%	0.315%
18	11.939	1639	1641	1647	rVB	43988	39182	1.65%	0.245%
19	12.151	1674	1677	1680	rVB2	45980	34305	1.44%	0.215%
20	12.474	1725	1732	1735	rBV	231075	205284	8.62%	1.285%
21	12.557	1744	1746	1751	rVB	105862	95800	4.02%	0.600%
22	12.974	1812	1817	1820	rBV	2689550	2380148	100.00%	14.900%
23	13.410	1885	1891	1894	rBV2	61978	70028	2.94%	0.438%
24	13.951	1974	1983	1988	rBV10	15640	53551	2.25%	0.335%
25	14.033	1993	1997	2001	rVB	740817	639107	26.85%	4.001%
26	14.127	2008	2013	2017	rBV2	31216	42955	1.80%	0.269%
27	15.127	2179	2183	2187	rBV2	28268	35395	1.49%	0.222%
28	15.515	2244	2249	2258	rVB2	485920	623798	26.21%	3.905%
29	15.945	2318	2322	2327	rVB2	35550	54505	2.29%	0.341%
30	16.457	2404	2409	2417	rVB2	27753	50768	2.13%	0.318%
31	17.051	2506	2510	2517	rVB6	19973	40228	1.69%	0.252%

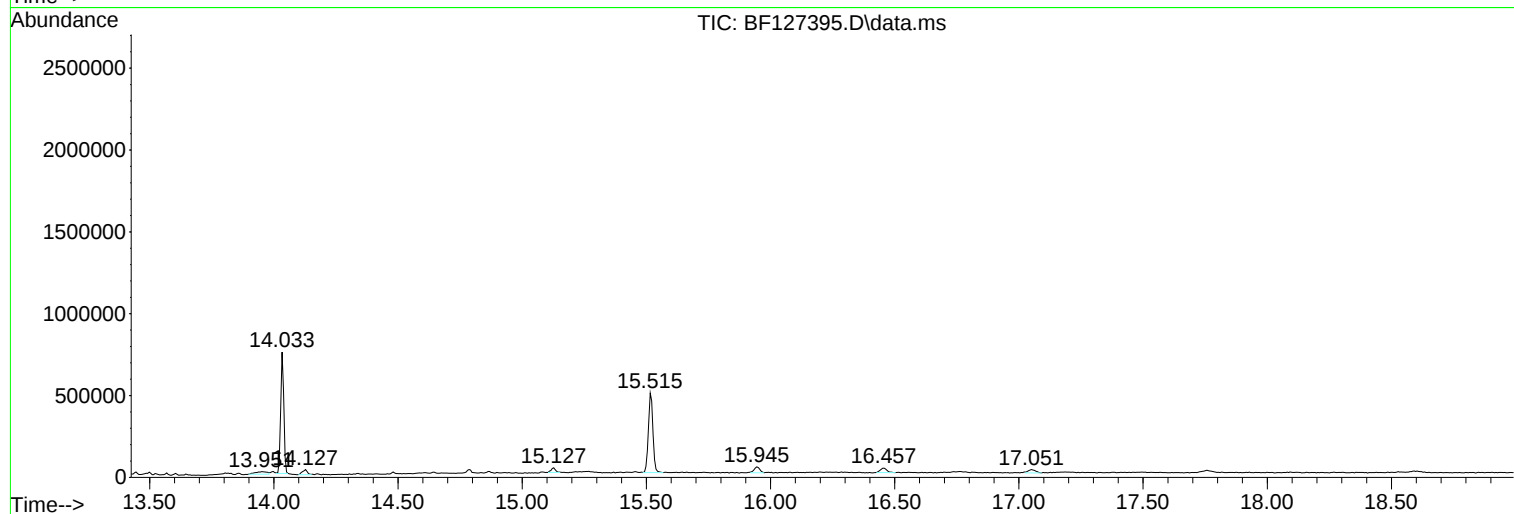
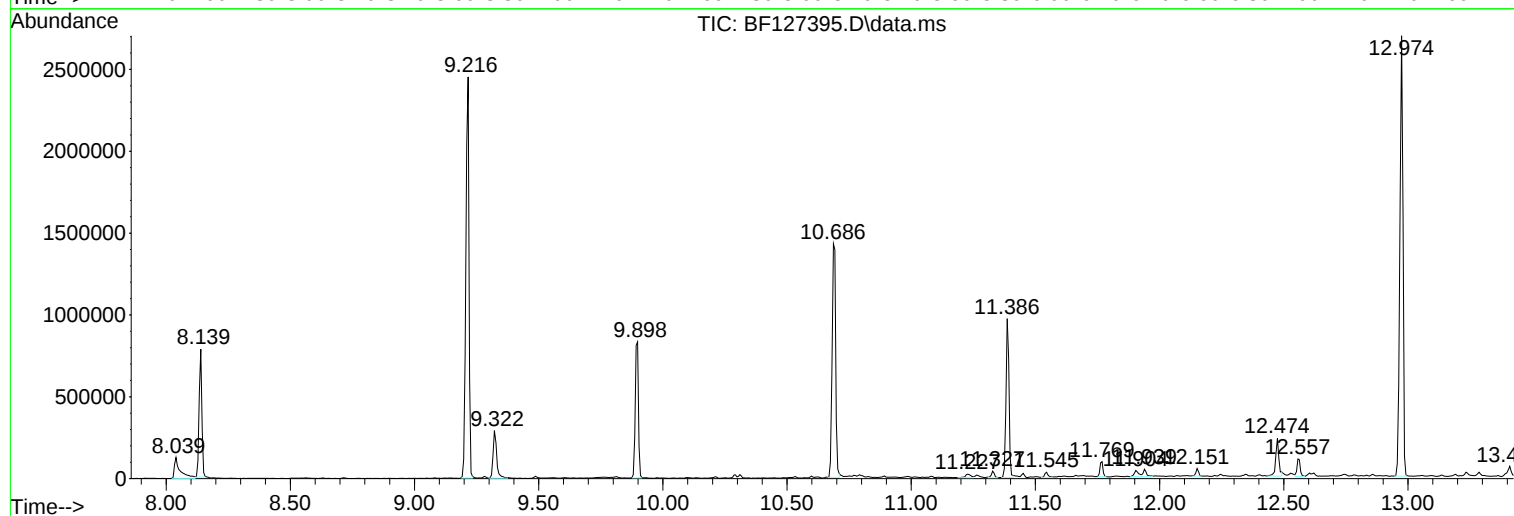
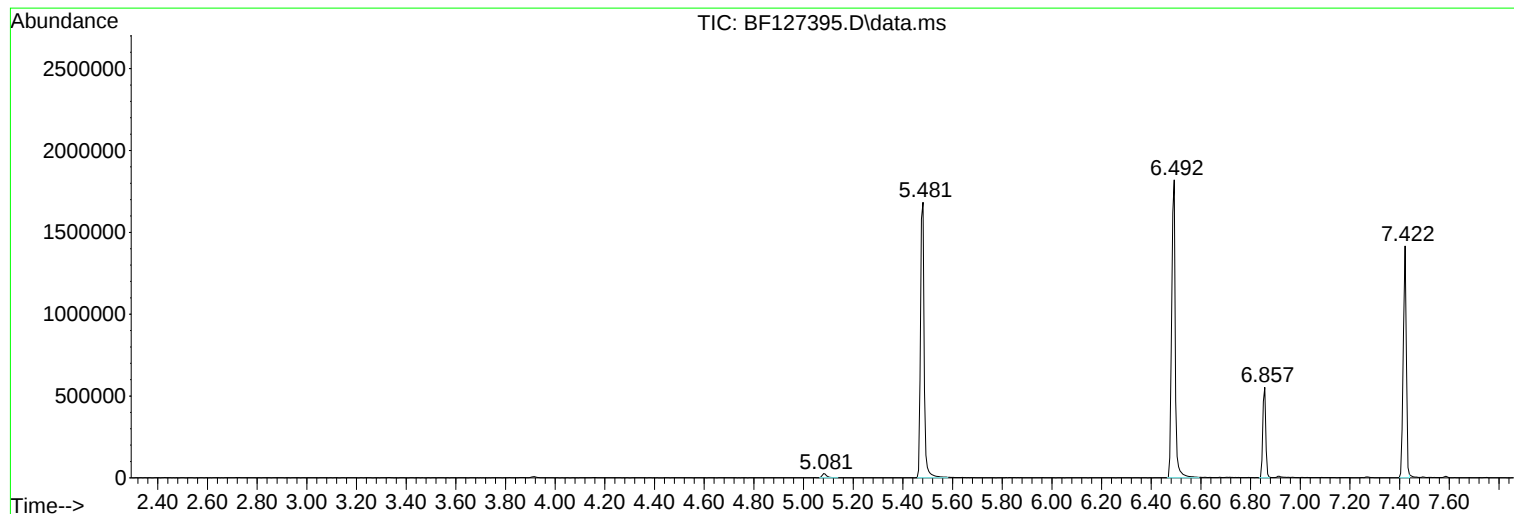
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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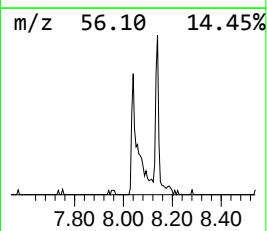
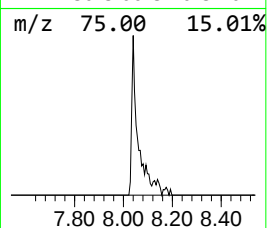
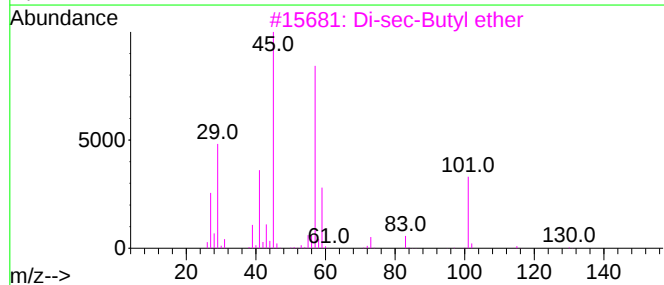
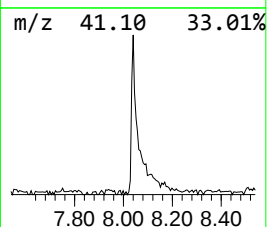
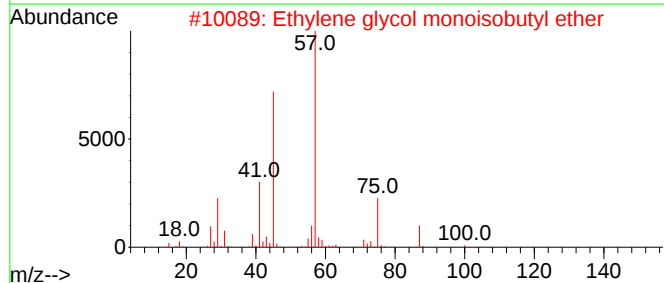
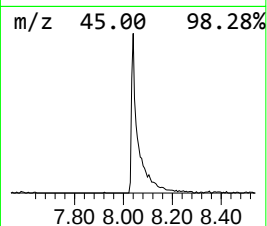
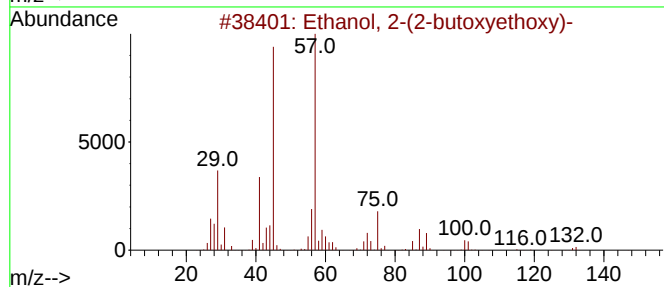
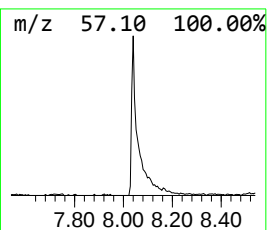
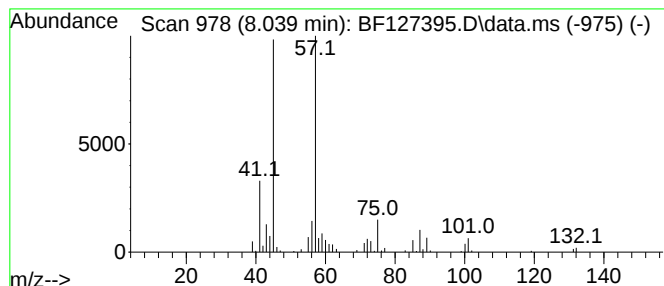
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031022.M
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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.039	6.94 ng	209877	Naphthalene-d8	8.139

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			Di-sec-Butyl ether	130	C8H18O	006863-58-7	59
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	52



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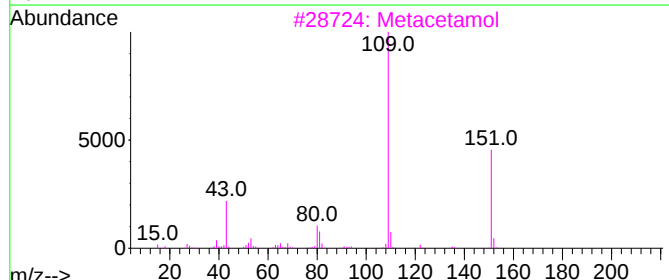
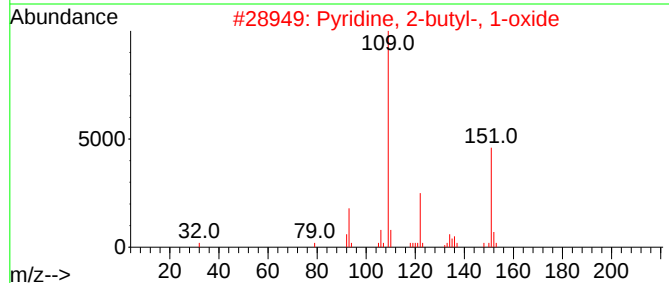
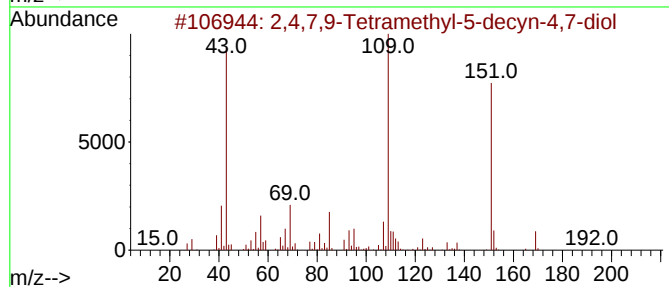
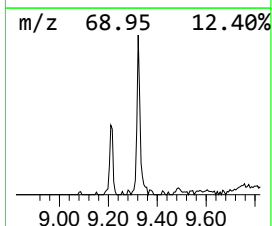
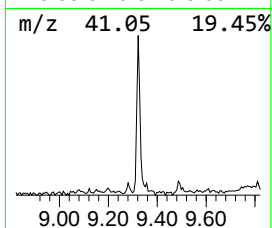
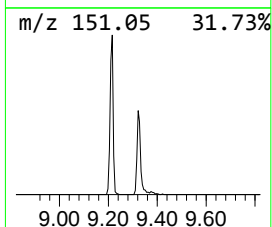
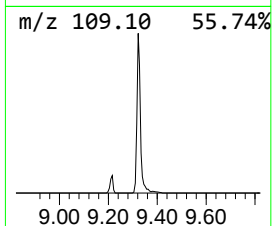
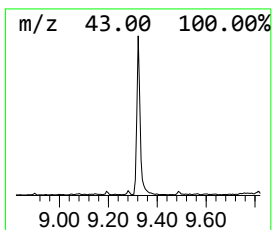
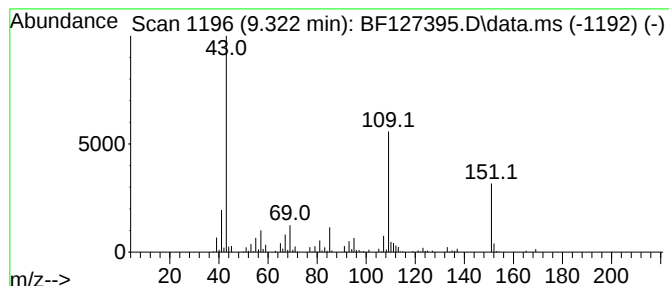
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.322	7.59 ng	283649	Acenaphthene-d10	9.898

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	58	
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	53	
3	Metacetamol	151	C8H9NO2	000621-42-1	49	
4	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	47	
5	(-)-10-Camphorsulfonyl chloride	250	C10H15ClO3S	039262-22-1	42	



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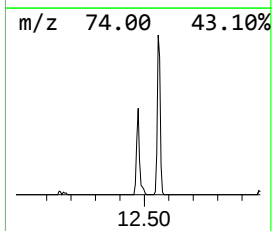
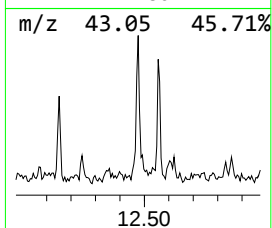
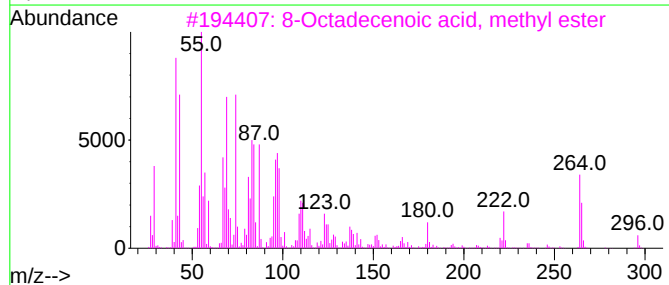
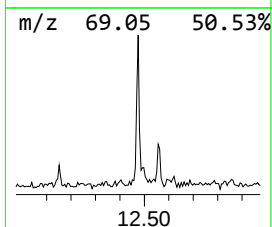
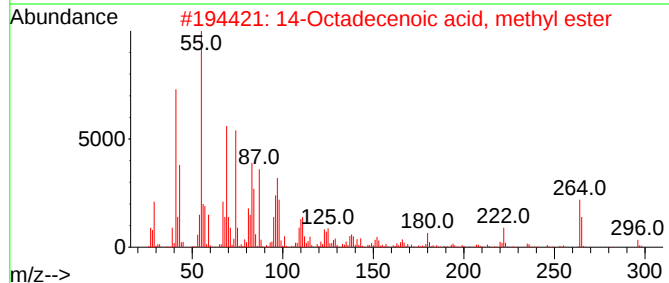
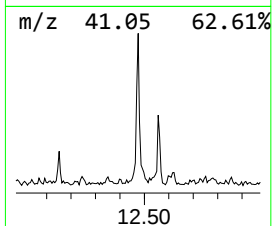
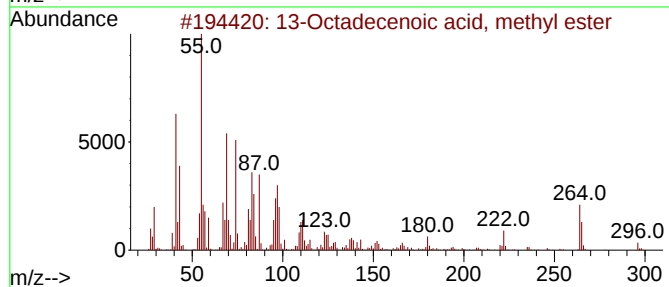
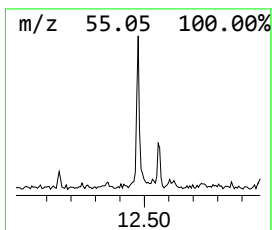
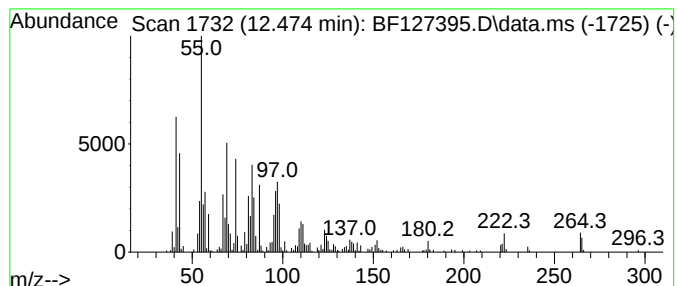
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 13-Octadecenoic acid, methyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.474	5.02 ng	205284	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
2			14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	97
3			8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	97
4			16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	95
5			7-Octadecenoic acid, methyl ester	296	C19H36O2	057396-98-2	95



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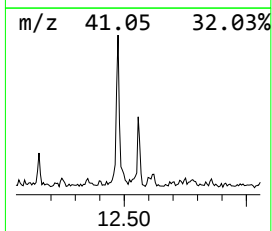
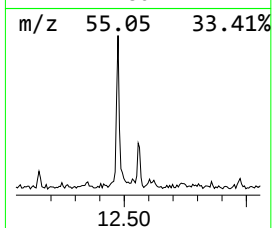
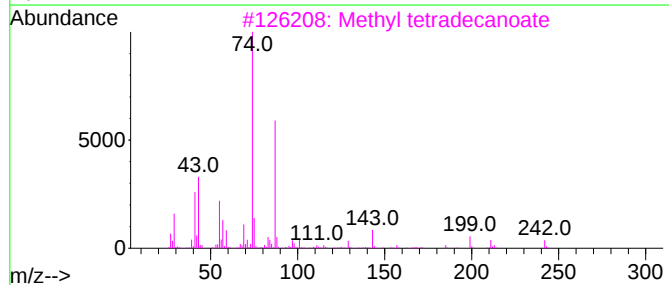
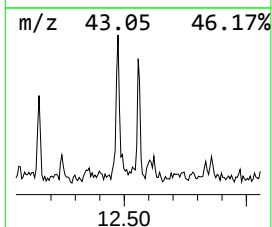
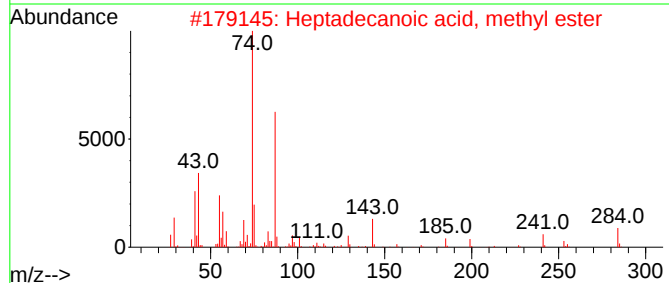
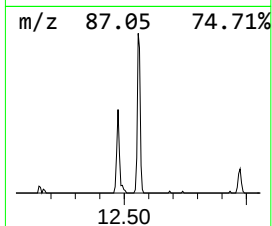
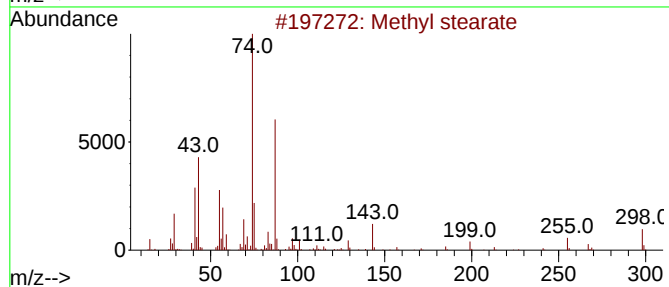
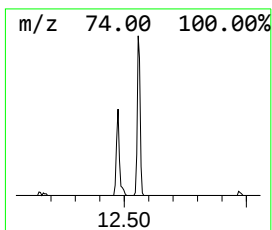
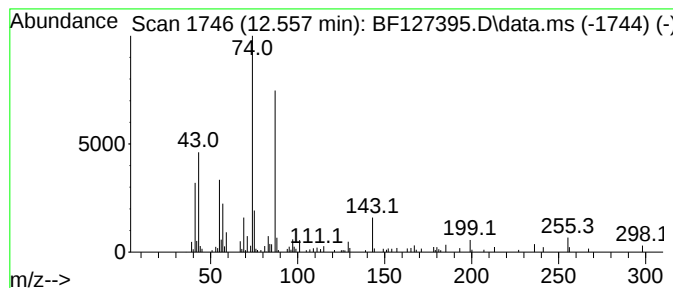
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Peak Number 4 Methyl stearate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.557	2.34 ng	95800	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	95
2			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	90
3			Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
4			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	87
5			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	87



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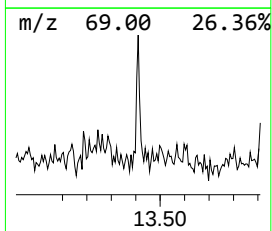
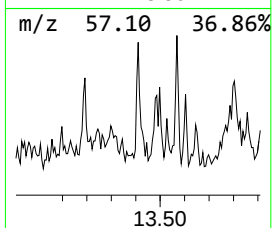
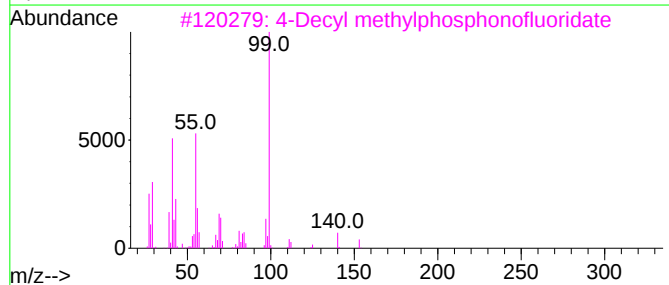
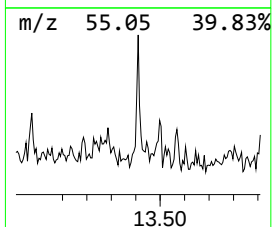
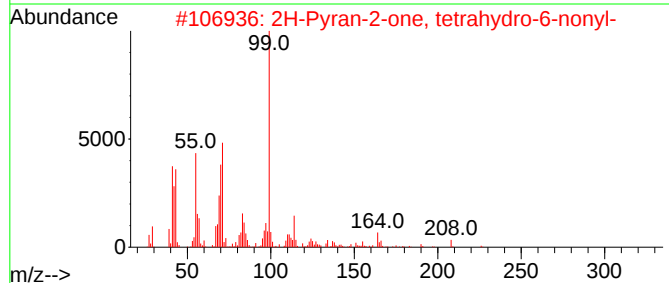
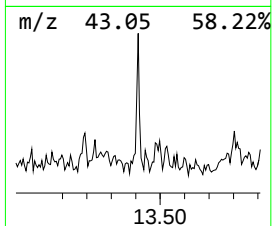
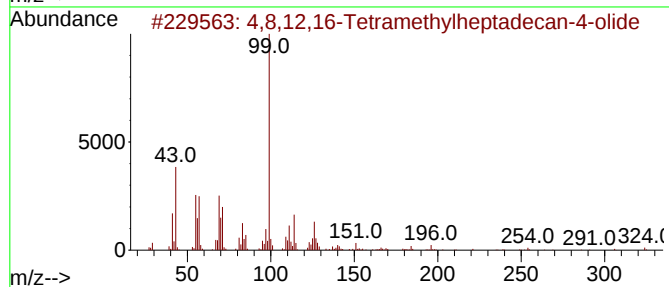
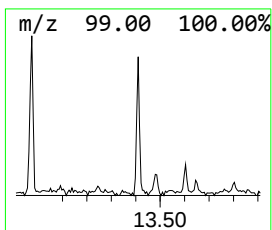
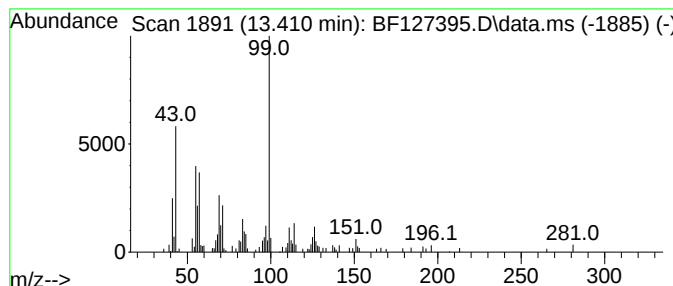
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 4,8,12,16-Tetramethylheptad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.410	2.19 ng	70028	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,8,12,16-Tetramethylheptadecan-...	324	C21H40O2	096168-15-9	74		
2	2H-Pyran-2-one, tetrahydro-6-nonyl-	226	C14H26O2	002721-22-4	52		
3	4-Decyl methylphosphonofluoridate	238	C11H24F02P	1000216-71-5	47		
4	2(3H)-Furanone, 5-butyldihydro-4...	156	C9H16O2	039212-23-2	47		
5	1,1'-Ethane-1,2-diylpiperazine	198	C10H22N4	019479-83-5	47		



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BNA_F
ClientSampleId :
PPSP-B18-26.0-26.5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol, 2-(2-b...	8.039	6.9	ng	209877	2	8.139	605079	20.0
2,4,7,9-Tetrame...	9.322	7.6	ng	283649	3	9.898	747241	20.0
13-Octadecenoic...	12.474	5.0	ng	205284	4	11.386	817970	20.0
Methyl stearate	12.557	2.3	ng	95800	4	11.386	817970	20.0
4,8,12,16-Tetra...	13.410	2.2	ng	70028	5	14.033	639107	20.0