

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
 Data File : BF133263.D
 Acq On : 05 May 2023 14:31
 Operator : CG\JU
 Sample : 02597-02
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-3-20230503

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-BF042123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133263.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.910	476	480	487	rVB	66740	73438	1.30%	0.241%
2	5.334	548	552	560	rBV	2652753	2309011	40.98%	7.575%
3	6.363	723	727	732	rBV	1598344	1430126	25.38%	4.692%
4	6.722	785	788	792	rBV	1471356	1173184	20.82%	3.849%
5	6.787	795	799	803	rVB	161506	121349	2.15%	0.398%
6	7.292	879	885	888	rBV	3676798	3541715	62.85%	11.619%
7	8.010	1003	1007	1010	rBV	2076276	1569230	27.85%	5.148%
8	8.728	1124	1129	1134	rBV7	37289	88609	1.57%	0.291%
9	9.086	1186	1190	1193	rBV	6057367	5634983	100.00%	18.486%
10	9.422	1244	1247	1250	rBV3	64741	84525	1.50%	0.277%
11	9.516	1259	1263	1267	rBV5	125078	153015	2.72%	0.502%
12	9.757	1301	1304	1307	rBV	1956778	1685120	29.90%	5.528%
13	9.792	1307	1310	1312	rVB	153509	120004	2.13%	0.394%
14	10.475	1424	1426	1428	rBV	146943	102058	1.81%	0.335%
15	10.551	1435	1439	1442	rBV	3298842	3131001	55.56%	10.271%
16	10.575	1442	1443	1447	rVB4	90312	85543	1.52%	0.281%
17	11.239	1553	1556	1560	rBV	1677309	1560657	27.70%	5.120%
18	11.798	1648	1651	1658	rVB2	475439	548547	9.73%	1.800%
19	12.527	1772	1775	1778	rVB	528298	449325	7.97%	1.474%
20	12.574	1781	1783	1786	rVB	213276	183609	3.26%	0.602%
21	12.833	1823	1827	1830	rVB	4301802	4216981	74.84%	13.834%
22	13.739	1979	1981	1985	rVB2	155841	144233	2.56%	0.473%
23	13.880	2001	2005	2008	rVB	1107914	994083	17.64%	3.261%
24	15.298	2241	2246	2251	rBV	978787	1082214	19.21%	3.550%

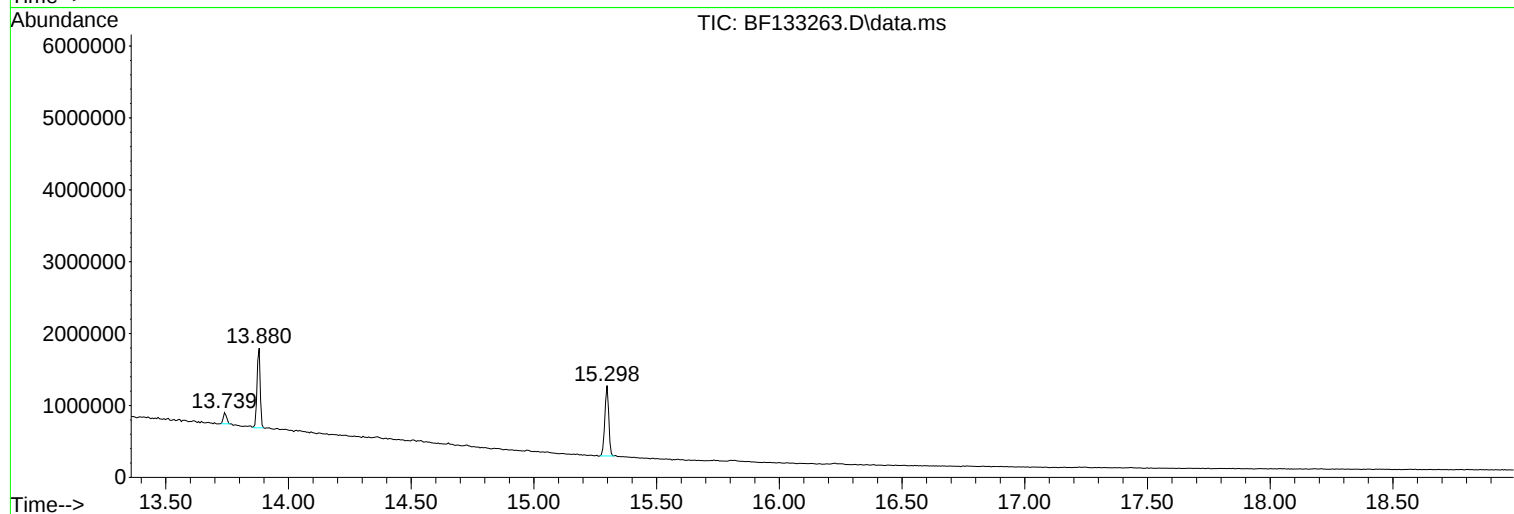
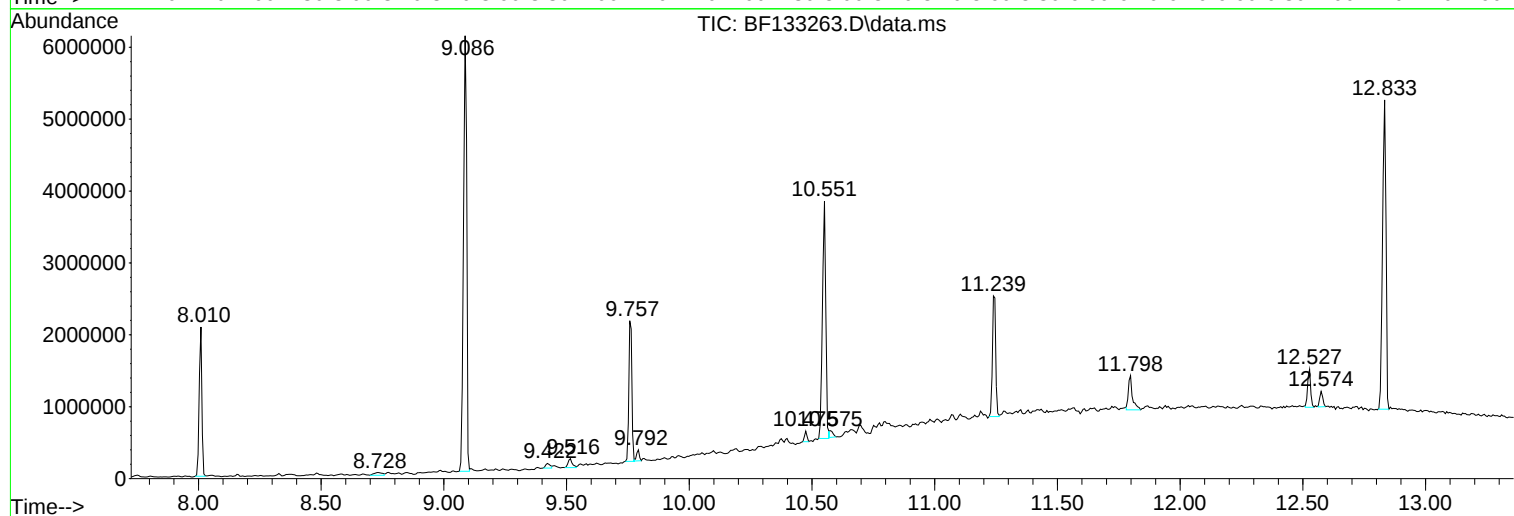
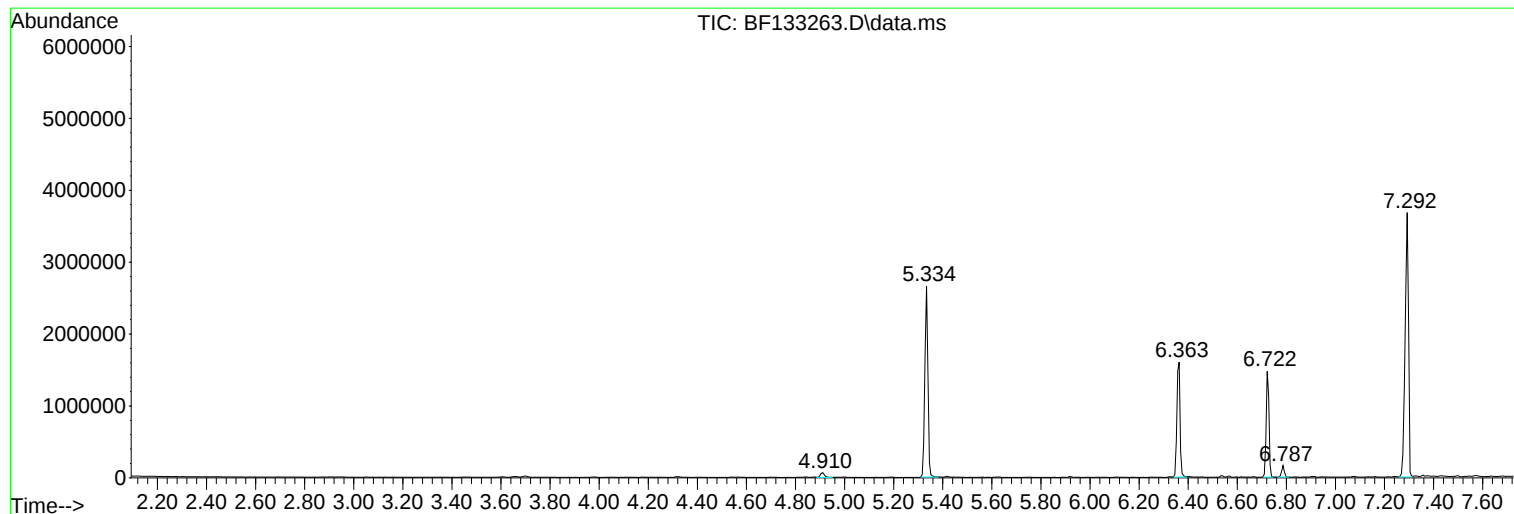
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ClientSampleId :
MW-3-20230503

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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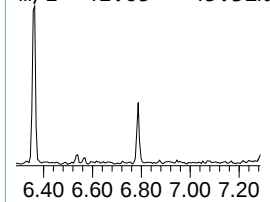
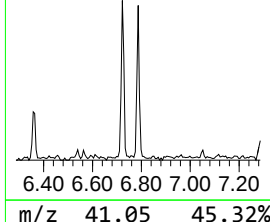
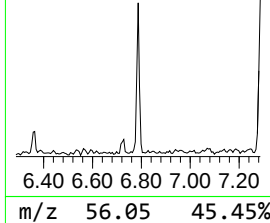
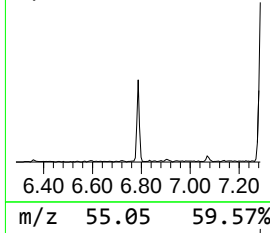
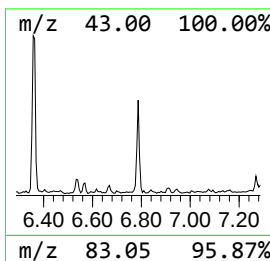
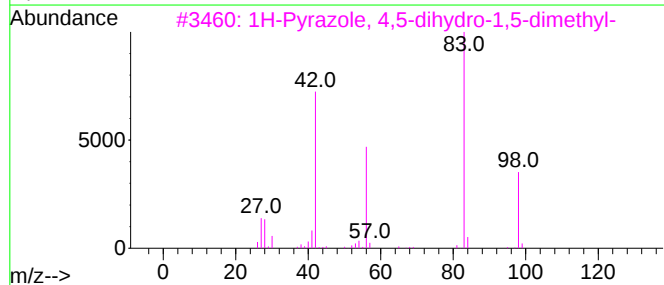
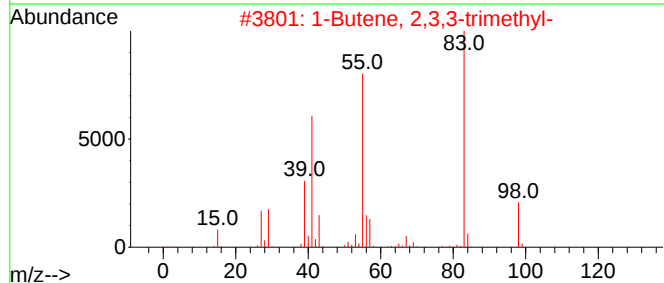
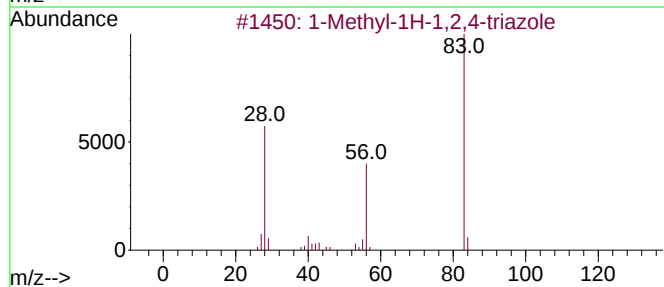
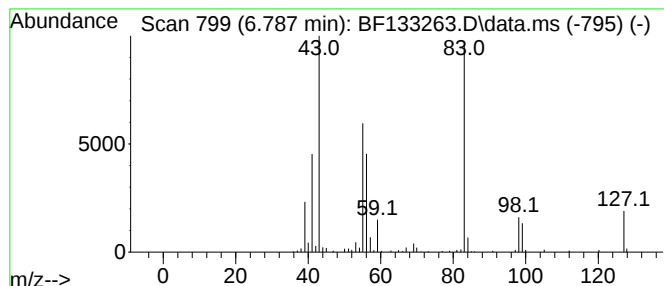
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1-Methyl-1H-1,2,4-triazole Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.787	2.07 ng	121349	1,4-Dichlorobenzene-d4	6.722

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Methyl-1H-1,2,4-triazole	83	C3H5N3	006086-21-1	50
2			1-Butene, 2,3,3-trimethyl-	98	C7H14	000594-56-9	49
3			1H-Pyrazole, 4,5-dihydro-1,5-dim...	98	C5H10N2	005775-96-2	43
4			1-Heptanol, 2,4-dimethyl-,	144	C9H20O	098982-97-9	38
5			2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	37



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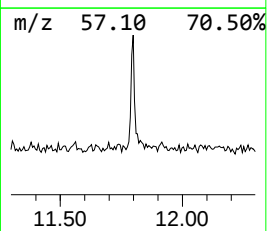
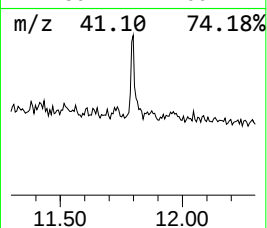
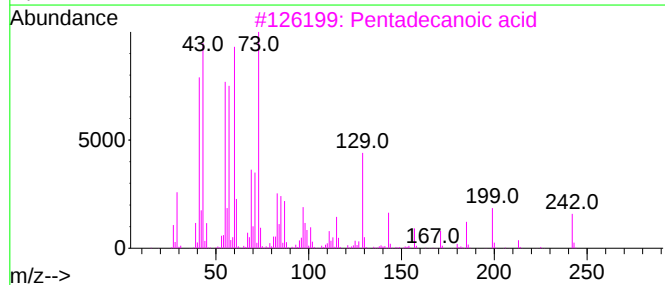
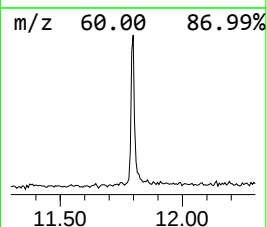
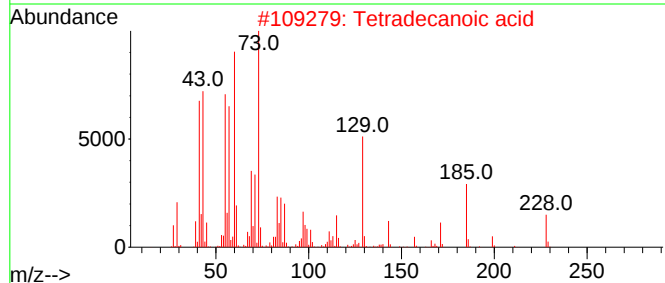
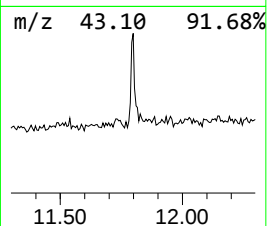
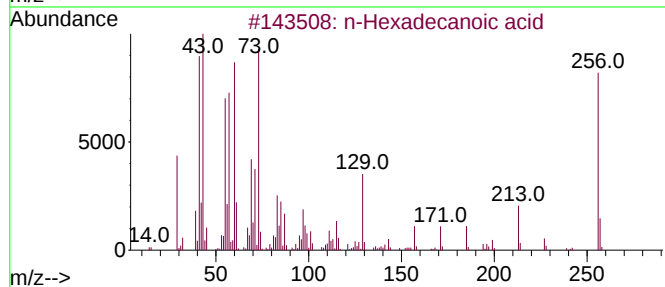
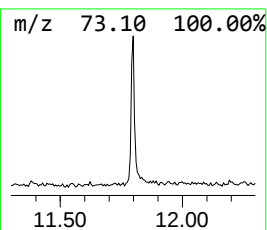
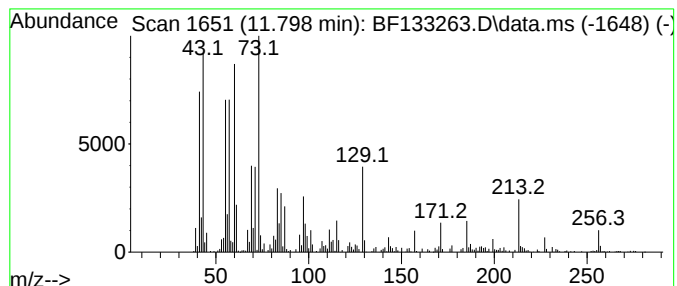
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.798	7.03 ng	548547	Phenanthrene-d10	11.239

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tridecanoic acid	214	C13H26O2	000638-53-9	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	76



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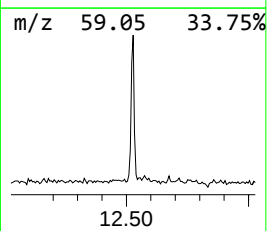
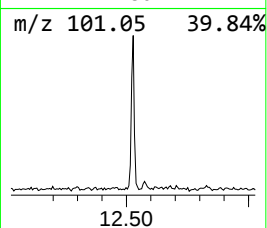
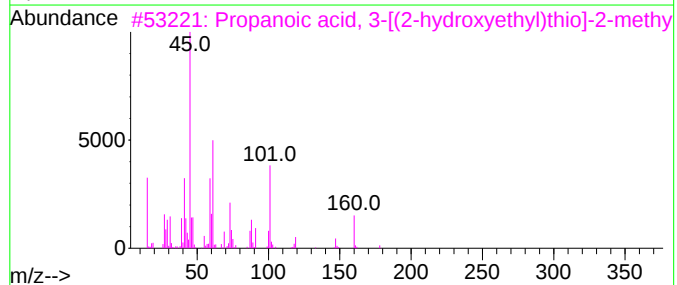
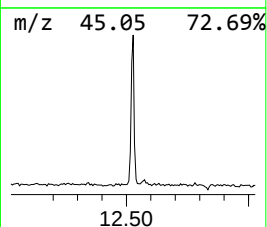
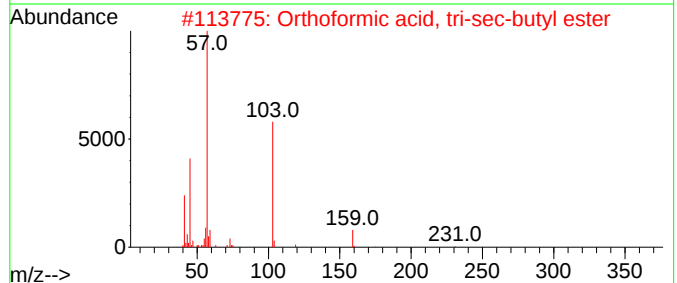
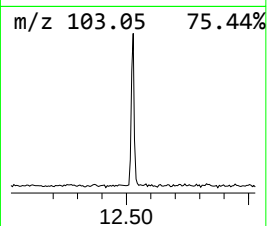
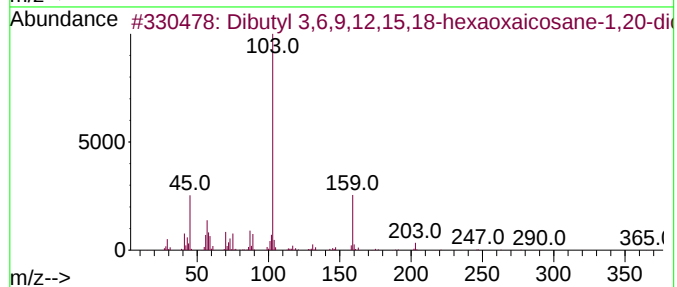
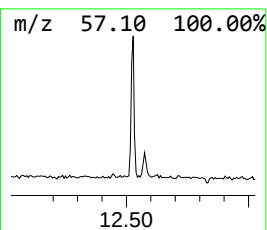
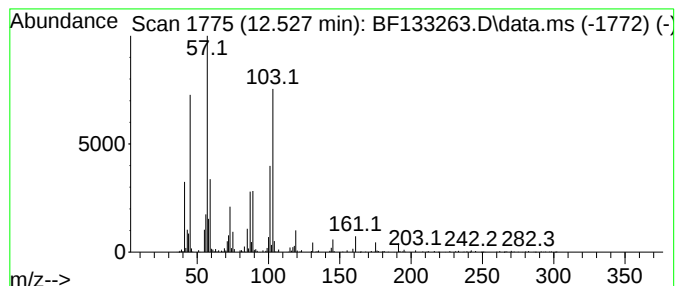
Instrument :
BNA_F
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MW-3-20230503

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown12.527 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.527	5.76 ng	449325	Phenanthrene-d10	11.239	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibutyl 3,6,9,12,15,18-hexaoxaic...	466	C22H42O10	1000366-80-0	37
2	Orthoformic acid, tri-sec-butyl ...	232	C13H28O3	016754-48-6	37
3	Propanoic acid, 3-[(2-hydroxyeth...	178	C7H14O3S	085099-03-2	35
4	Dimethyl diglycolcarbonate	222	C8H14O7	087292-23-7	32
5	1,4,7,10,13,16-Hexaoxacyclooctad...	264	C12H24O6	017455-13-9	27



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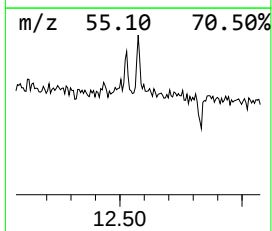
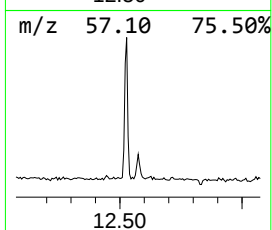
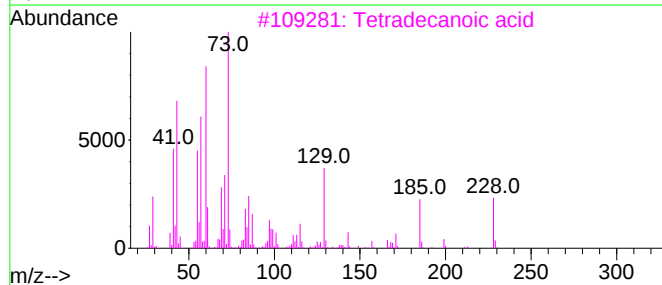
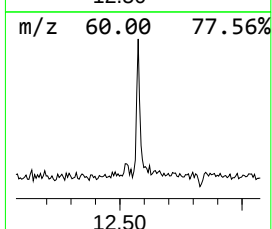
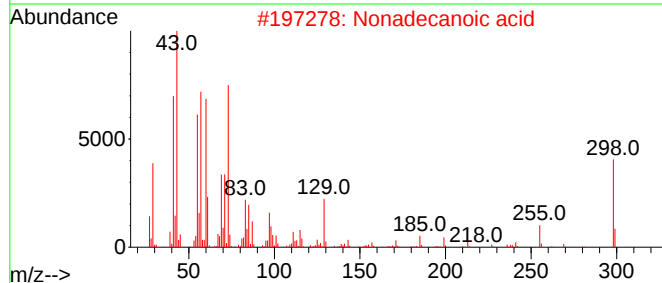
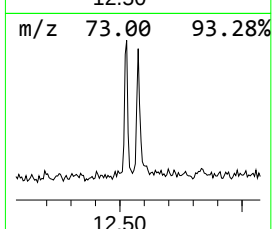
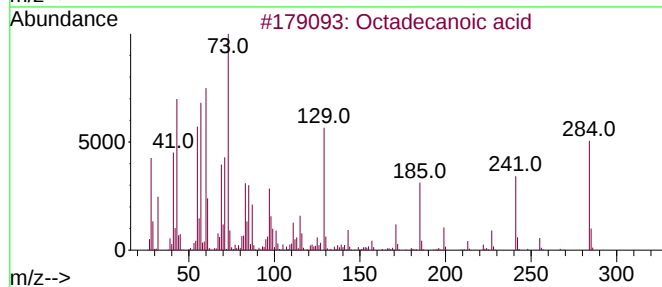
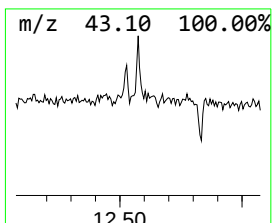
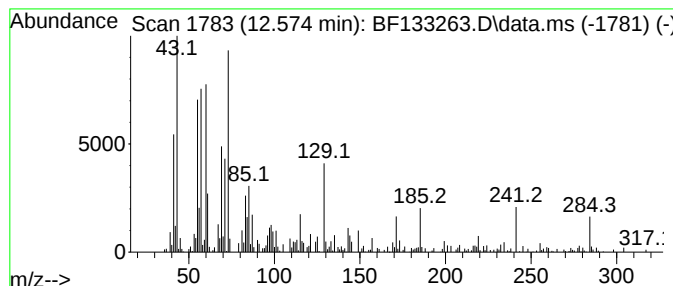
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.575	3.69 ng	183609	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	94
2			Nonadecanoic acid	298	C19H38O2	000646-30-0	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			n-Decanoic acid	172	C10H20O2	000334-48-5	70
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



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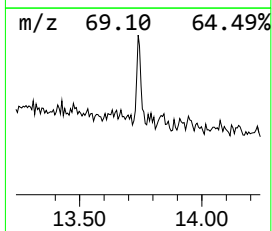
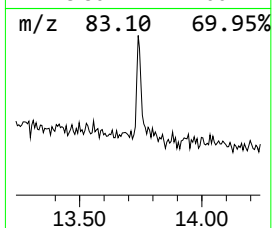
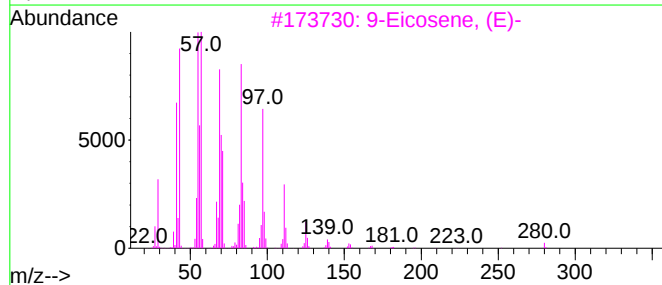
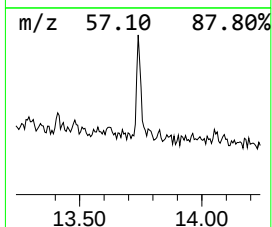
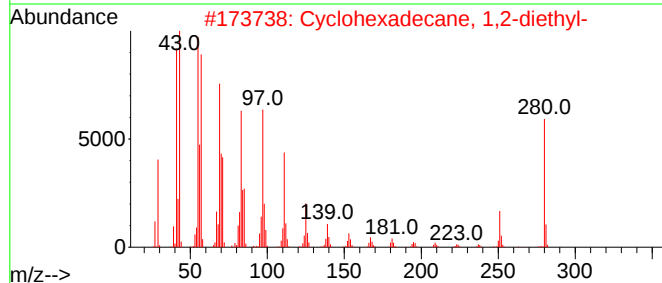
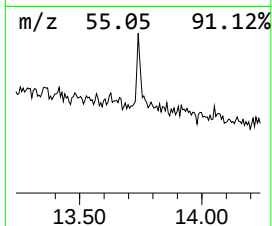
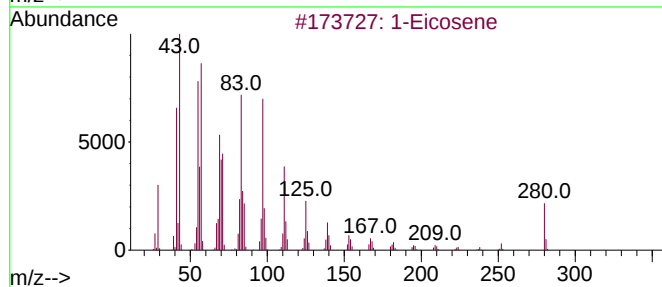
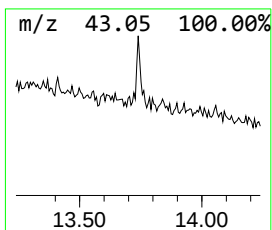
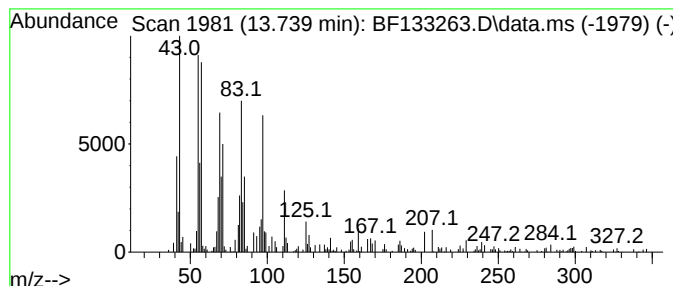
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Eicosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.739	2.90 ng	144233	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Eicosene	280	C20H40	003452-07-1	91
2			Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	90
3			9-Eicosene, (E)-	280	C20H40	074685-29-3	89
4			1-Hexacosene	364	C26H52	018835-33-1	87
5			2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Methyl-1H-1,2...	6.787	2.1	ng	121349	1	6.722	1173180	20.0
n-Hexadecanoic ...	11.798	7.0	ng	548547	4	11.239	1560660	20.0
unknown12.527	12.527	5.8	ng	449325	4	11.239	1560660	20.0
Octadecanoic acid	12.575	3.7	ng	183609	5	13.880	994083	20.0
1-Eicosene	13.739	2.9	ng	144233	5	13.880	994083	20.0