

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
 Data File : BF133163.D
 Acq On : 01 May 2023 19:09
 Operator : CG\JU
 Sample : 02558-06
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P001-SS013-0006-01

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: BF133163.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.710	266	276	281	rBV	25170	41908	1.21%	0.150%
2	4.910	474	480	489	rBV	86316	129539	3.75%	0.462%
3	5.340	548	553	556	rBV	3056721	2896601	83.91%	10.341%
4	6.363	723	727	730	rBV	2998073	3059641	88.63%	10.923%
5	6.728	785	789	792	rBV	1600476	1212155	35.11%	4.327%
6	7.292	880	885	888	rBV	2340077	1998612	57.90%	7.135%
7	8.010	1004	1007	1011	rBV	1971067	1675894	48.55%	5.983%
8	9.086	1186	1190	1193	rBV	4163073	3451973	100.00%	12.323%
9	9.175	1200	1205	1209	rBV5	28598	41898	1.21%	0.150%
10	9.510	1259	1262	1270	rVB	571350	507126	14.69%	1.810%
11	9.763	1301	1305	1308	rBV	2466518	1887655	54.68%	6.739%
12	10.475	1423	1426	1430	rBV	323867	242111	7.01%	0.864%
13	10.551	1435	1439	1442	rBV	2292070	1974585	57.20%	7.049%
14	11.245	1553	1557	1560	rBV	2339508	1876356	54.36%	6.698%
15	11.780	1645	1648	1656	rBV2	378393	409839	11.87%	1.463%
16	12.451	1759	1762	1765	rBV2	67768	66433	1.92%	0.237%
17	12.569	1779	1782	1787	rBV4	119299	139160	4.03%	0.497%
18	12.833	1823	1827	1830	rBV	3381549	2926430	84.78%	10.447%
19	13.074	1866	1868	1871	rBV	71675	69876	2.02%	0.249%
20	13.745	1980	1982	1984	rBV	89323	78596	2.28%	0.281%
21	13.880	2001	2005	2009	rVB2	1501892	1389041	40.24%	4.959%
22	14.368	2086	2088	2092	rBV	94238	76304	2.21%	0.272%
23	14.804	2159	2162	2167	rVB3	171937	172557	5.00%	0.616%
24	15.304	2243	2247	2252	rVB	941921	1055428	30.57%	3.768%
25	15.539	2283	2287	2294	rVB2	163609	240265	6.96%	0.858%
26	15.763	2321	2325	2331	rBV	170542	243558	7.06%	0.869%
27	16.510	2449	2452	2459	rVB3	88851	148313	4.30%	0.529%

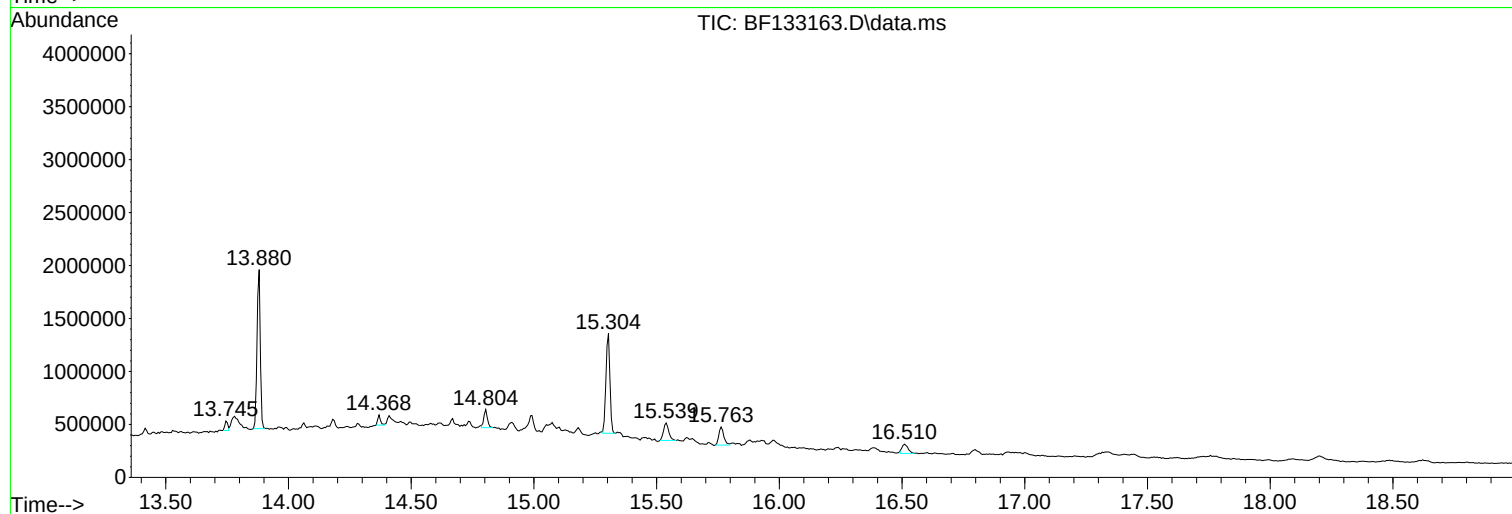
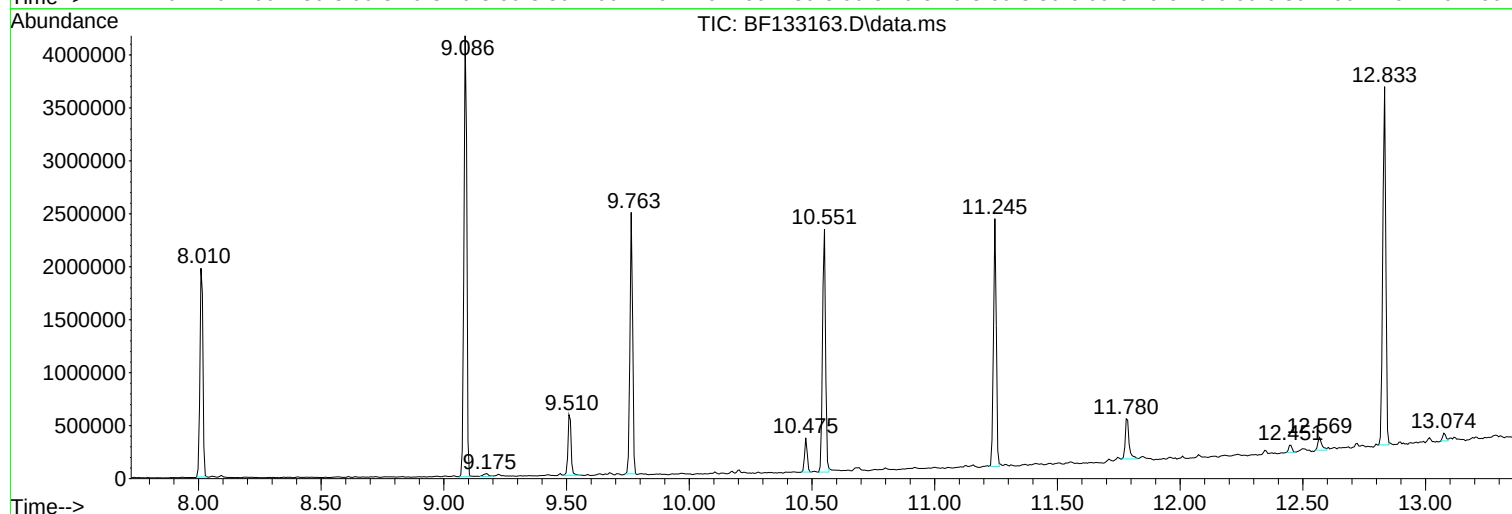
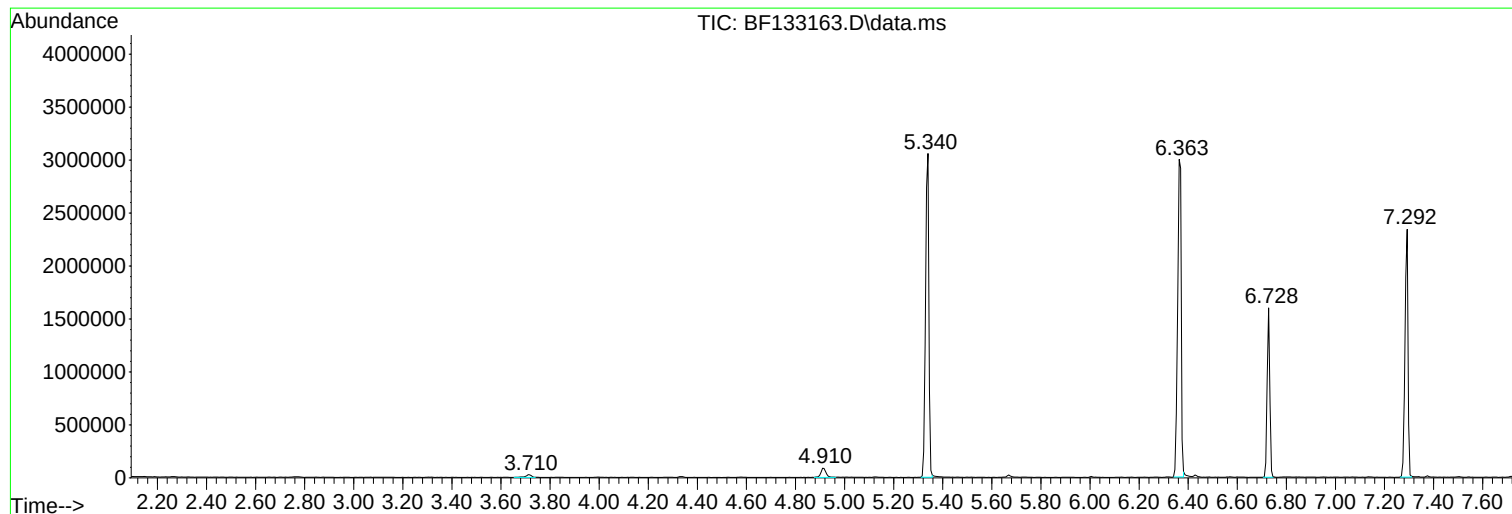
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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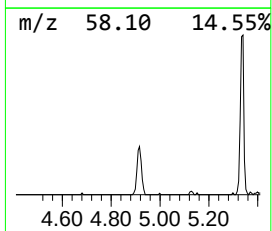
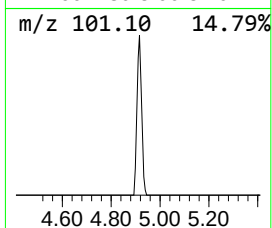
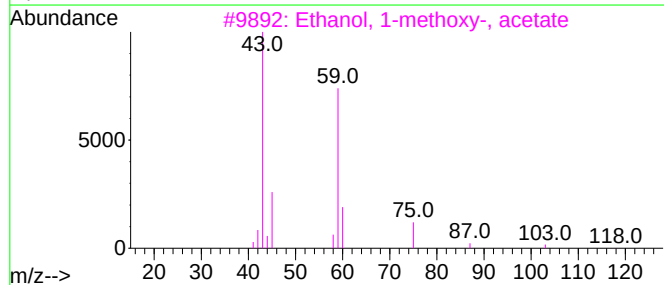
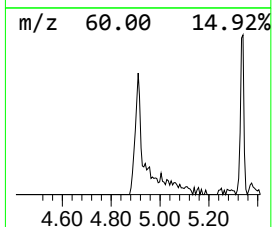
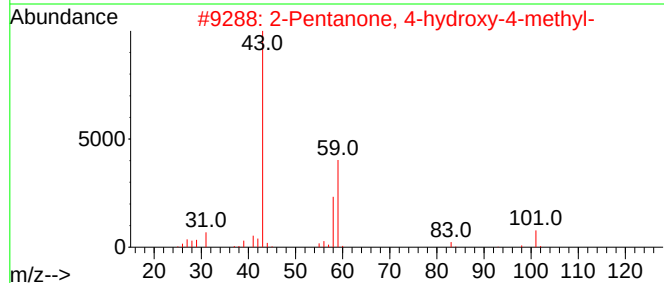
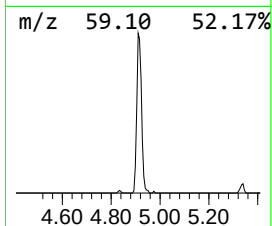
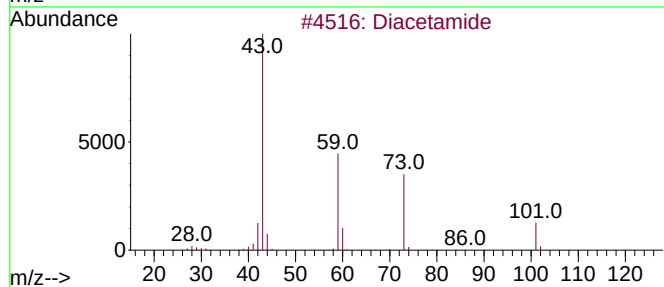
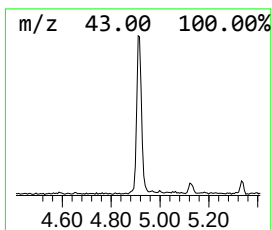
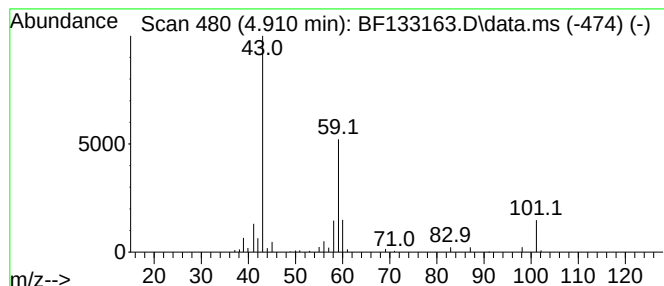
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TIC Library : C:\Database\NIST20.L
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Peak Number 1 Diacetamide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.910	2.14 ng	129539	1,4-Dichlorobenzene-d4	6.728

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diacetamide	101	C4H7NO2	000625-77-4	59
2			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	36
3			Ethanol, 1-methoxy-, acetate	118	C5H10O3	004382-77-8	36
4			n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
5			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9



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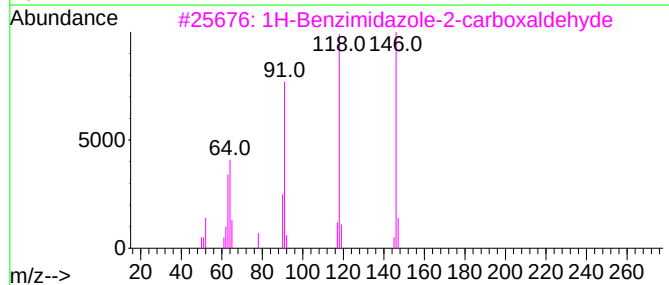
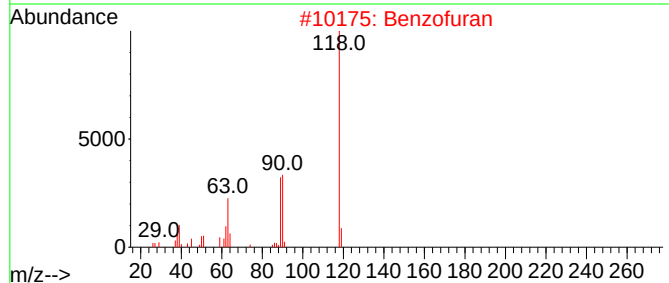
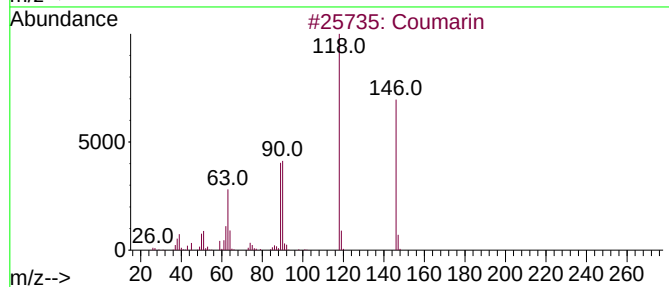
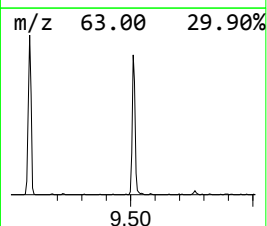
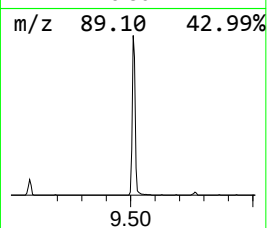
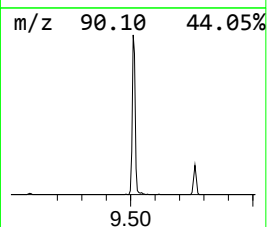
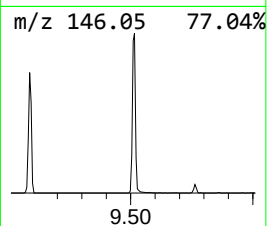
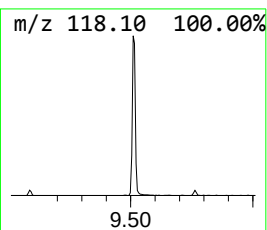
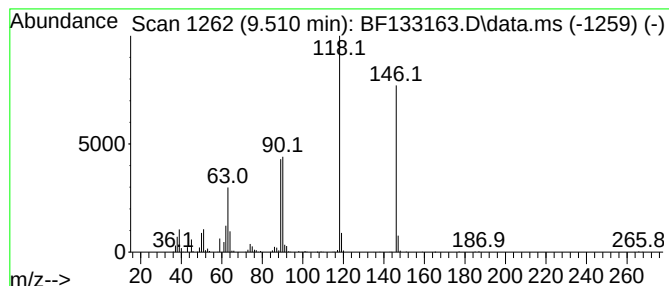
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Peak Number 2 Coumarin Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.510	5.37 ng	507126	Acenaphthene-d10	9.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Coumarin	146	C9H6O2	000091-64-5	98
2			Benzofuran	118	C8H6O	000271-89-6	96
3			1H-Benzimidazole-2-carboxaldehyde	146	C8H6N2O	003314-30-5	64
4			2H-1-Benzopyran-3-carboxaldehyde...	174	C10H6O3	095306-75-5	59
5			2(1H)-Quinoxalinone	146	C8H6N2O	001196-57-2	58



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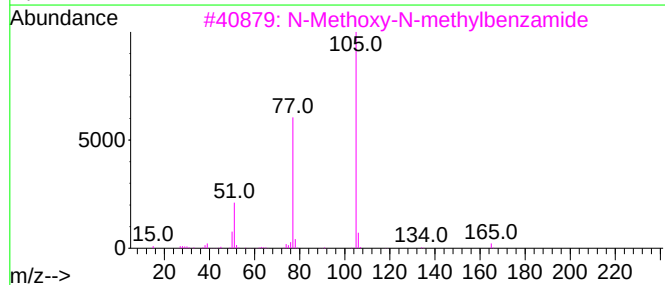
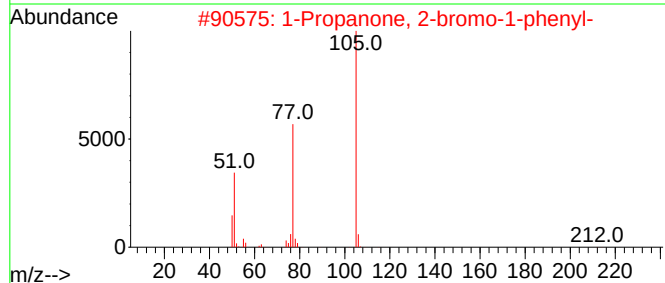
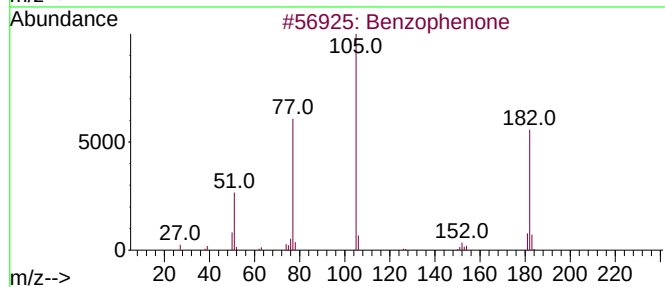
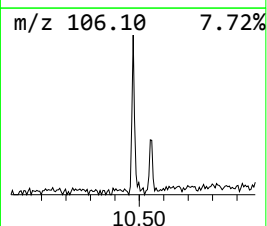
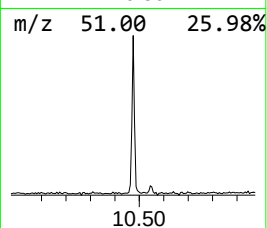
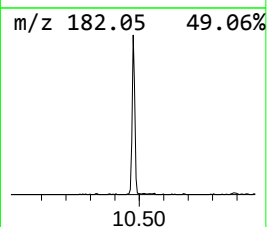
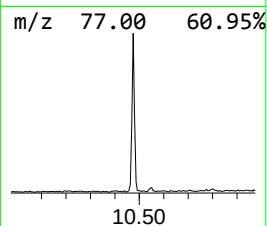
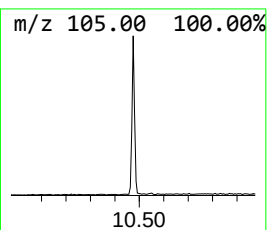
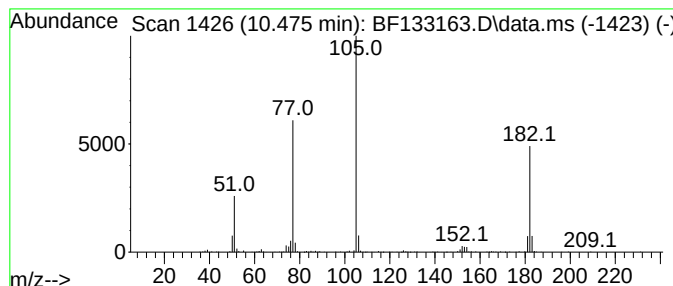
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Peak Number 3 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.475	2.57 ng	242111	Acenaphthene-d10	9.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
3			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
4			1-Butanone, 1-phenyl-	148	C10H12O	000495-40-9	47
5			N-Methylbenzamide, N-chlorodiflu...	247	C10H8ClF2NO2	1000446-98-2	47



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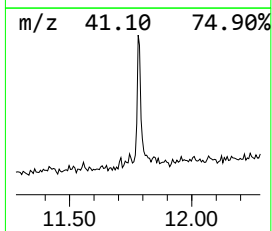
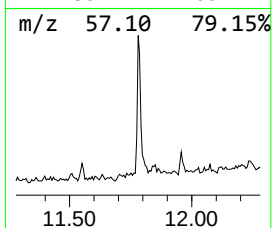
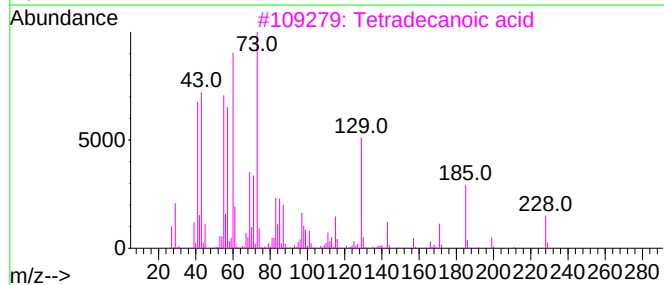
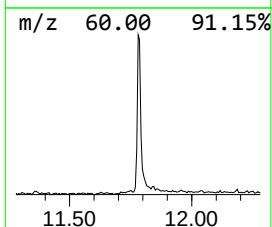
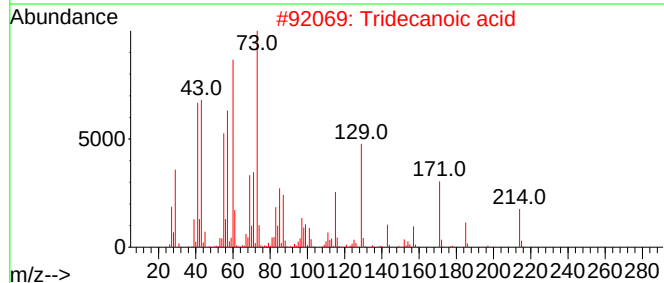
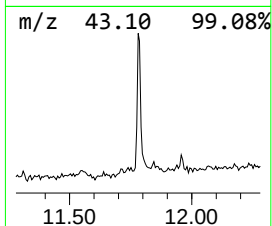
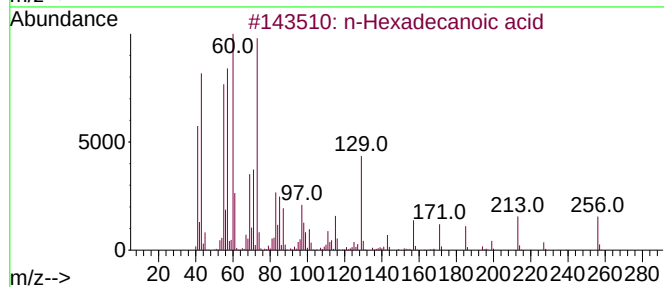
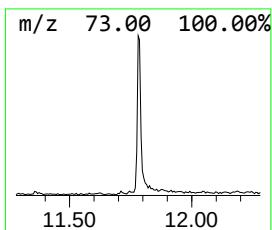
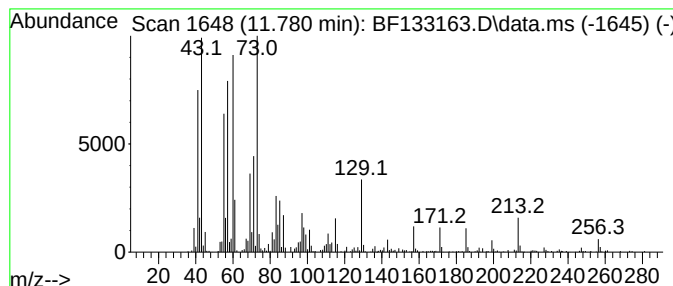
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.780	4.37 ng	409839	Phenanthrene-d10	11.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	96
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			Dodecanoic acid	200	C12H24O2	000143-07-7	68



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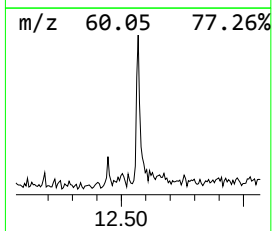
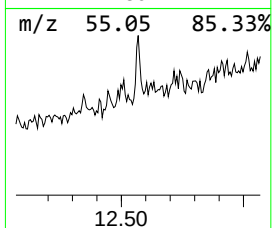
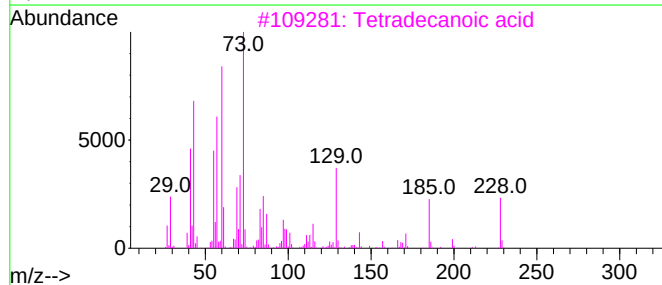
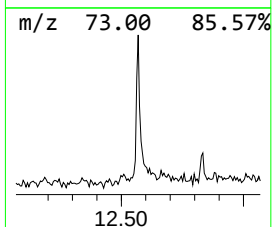
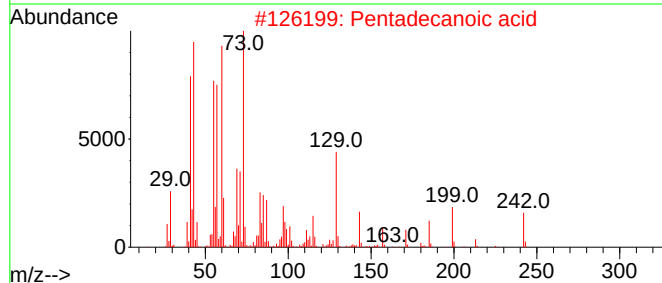
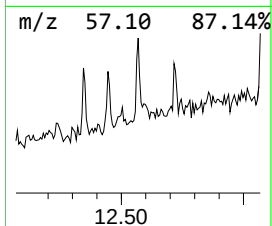
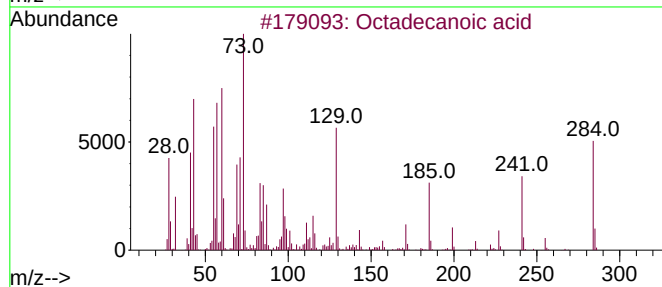
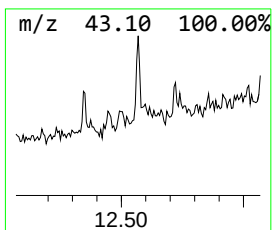
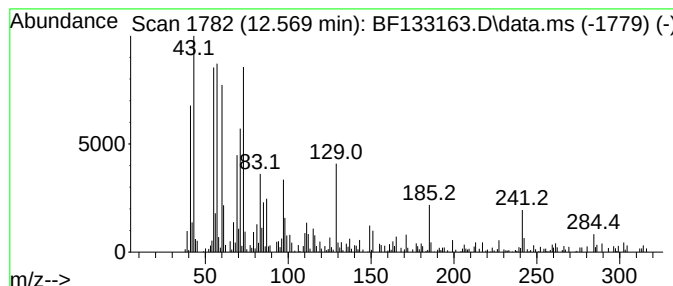
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Peak Number 5 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.569	2.00 ng	139160	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	97
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	70
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	53



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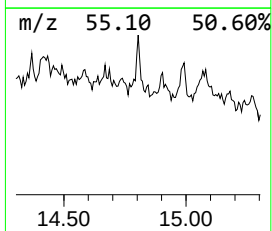
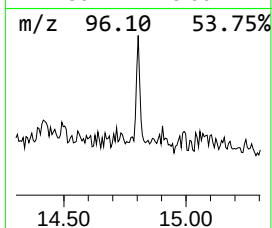
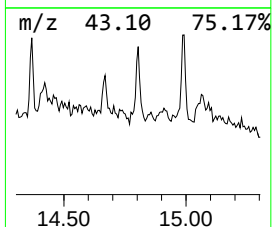
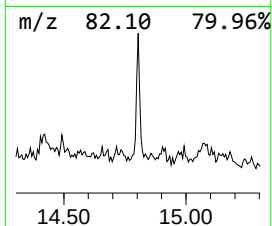
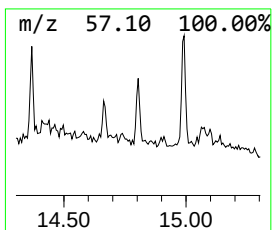
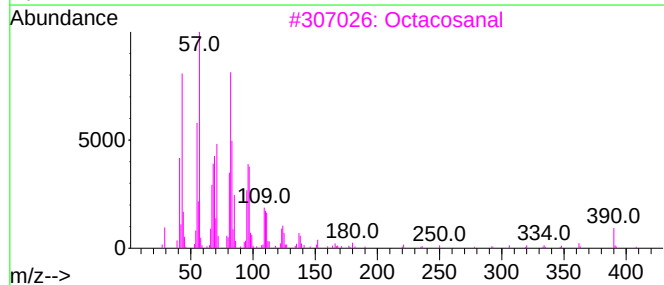
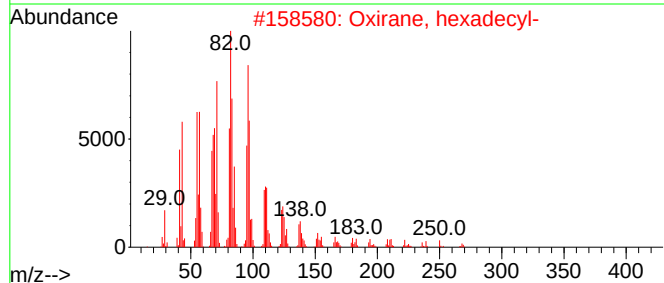
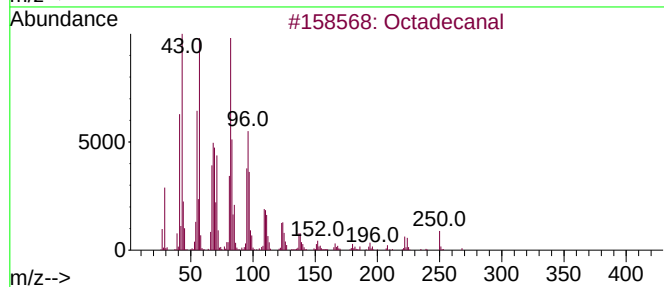
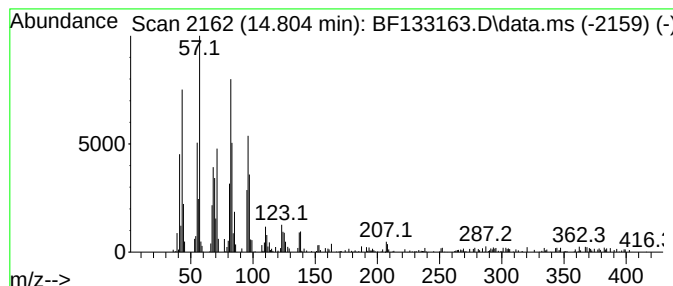
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.804	3.27 ng	172557	Perylene-d12	15.304

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanal	268	C18H36O	000638-66-4	91
2		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	86
3		Octacosanal	408	C28H56O	022725-64-0	72
4		1,19-Eicosadiene	278	C20H38	014811-95-1	72
5		Z-2-Octadecen-1-ol	268	C18H36O	1000131-11-0	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133163.D
Acq On : 01 May 2023 19:09
Operator : CG\JU
Sample : 02558-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P001-SS013-0006-01

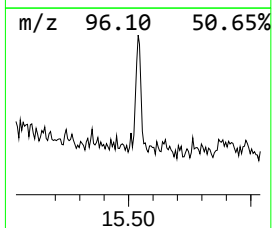
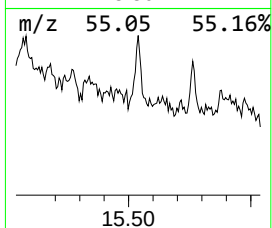
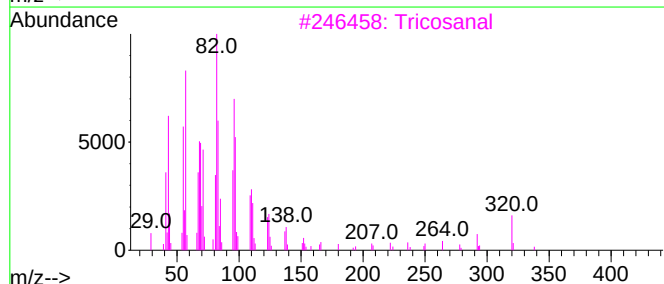
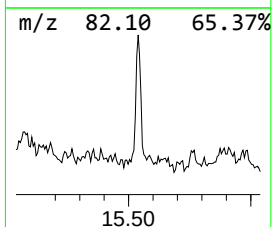
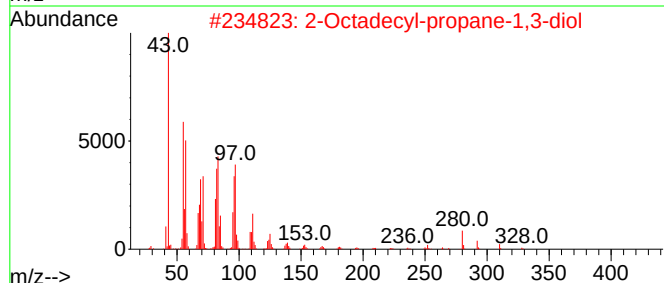
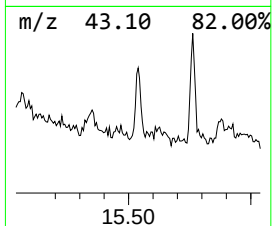
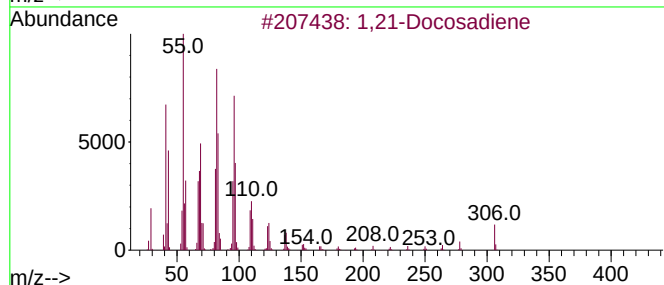
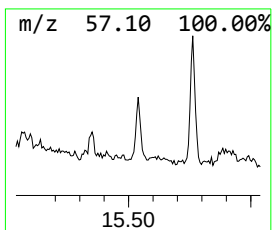
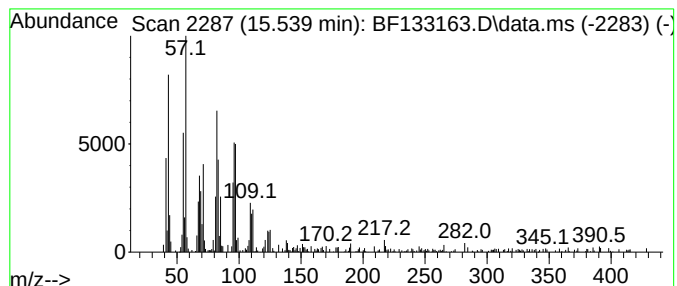
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1,21-Docosadiene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.539	4.55 ng	240265	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,21-Docosadiene			306	C22H42	053057-53-7	90
2	2-Octadecyl-propane-1,3-diol			328	C21H44O2	005337-61-1	89
3	Tricosanal			338	C23H46O	072934-02-2	76
4	Octacosanal			408	C28H56O	022725-64-0	76
5	Docosanal			324	C22H44O	057402-36-5	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133163.D
Acq On : 01 May 2023 19:09
Operator : CG\JU
Sample : 02558-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P001-SS013-0006-01

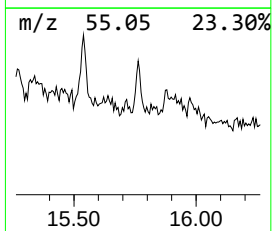
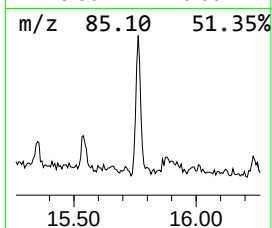
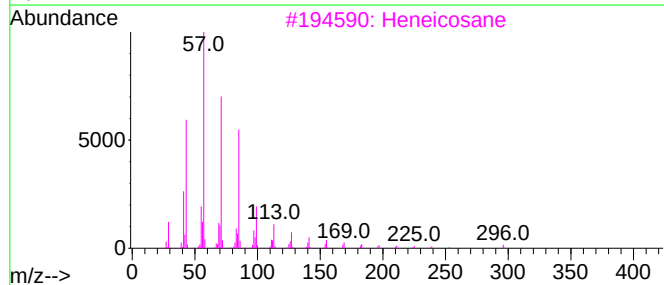
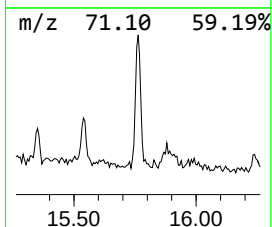
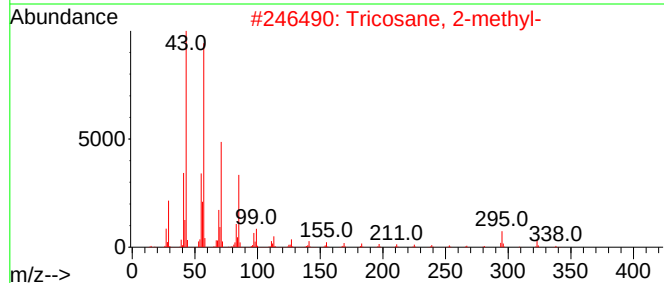
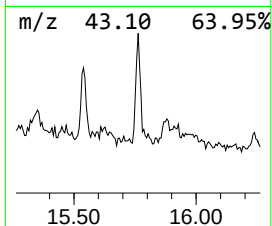
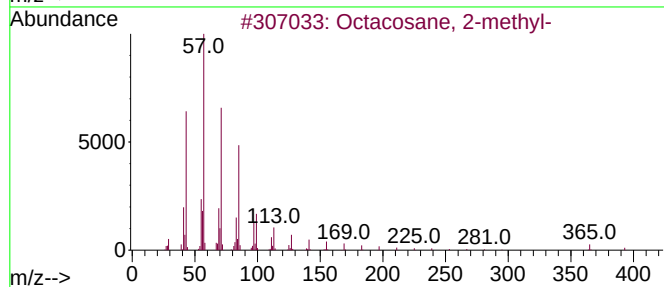
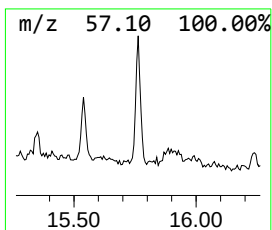
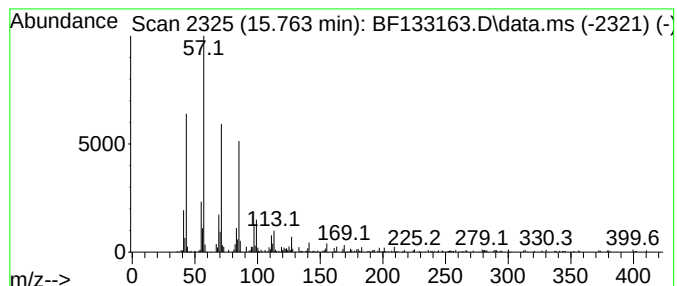
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octacosane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.762	4.62 ng	243558	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
2			Tricosane, 2-methyl-	338	C24H50	001928-30-9	89
3			Heneicosane	296	C21H44	000629-94-7	87
4			Docosane	310	C22H46	000629-97-0	87
5			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133163.D
Acq On : 01 May 2023 19:09
Operator : CG\JU
Sample : 02558-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P001-SS013-0006-01

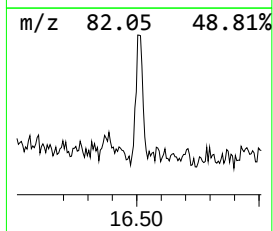
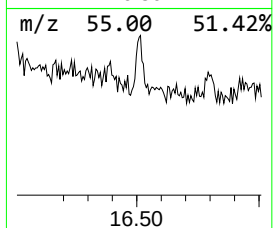
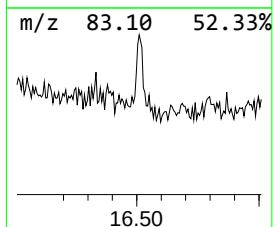
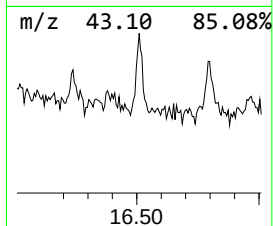
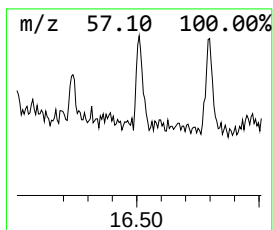
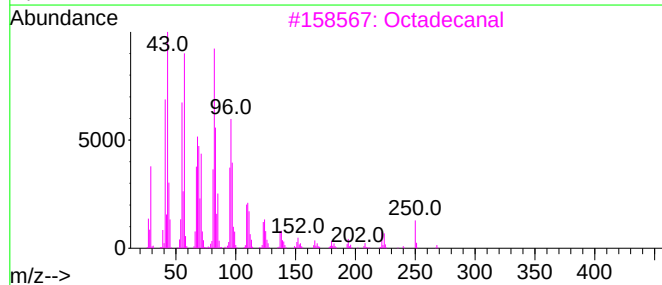
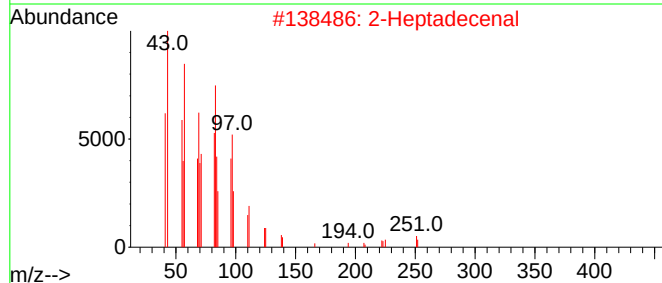
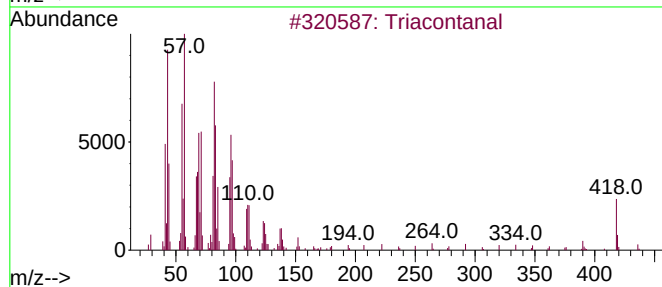
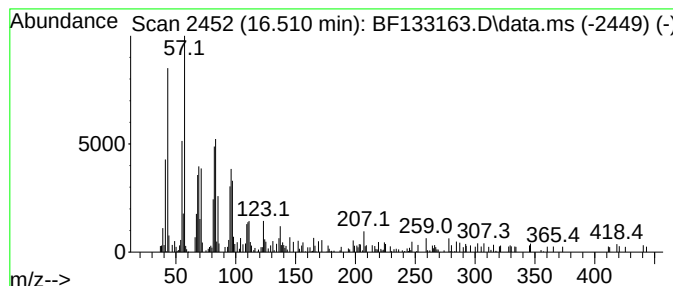
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Triacontanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.509	2.81 ng	148313	Perylene-d12	15.304

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Triacontanal	436	C30H60O	022725-63-9	91
2		2-Heptadecenal	252	C17H32O	1000143-48-6	90
3		Octadecanal	268	C18H36O	000638-66-4	86
4		2-Octadecyl-propane-1,3-diol	328	C21H44O2	005337-61-1	64
5		1,19-Eicosadiene	278	C20H38	014811-95-1	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133163.D
Acq On : 01 May 2023 19:09
Operator : CG\JU
Sample : 02558-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P001-SS013-0006-01

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Diacetamide	4.910	2.1	ng	129539	1	6.728	1212160	20.0
Coumarin	9.510	5.4	ng	507126	3	9.763	1887660	20.0
Benzophenone	10.475	2.6	ng	242111	3	9.763	1887660	20.0
n-Hexadecanoic ...	11.780	4.4	ng	409839	4	11.245	1876360	20.0
Octadecanoic acid	12.569	2.0	ng	139160	5	13.880	1389040	20.0
Octadecanal	14.804	3.3	ng	172557	6	15.304	1055430	20.0
1,21-Docosadiene	15.539	4.5	ng	240265	6	15.304	1055430	20.0
Octacosane, 2-m...	15.762	4.6	ng	243558	6	15.304	1055430	20.0
Triacontanal	16.509	2.8	ng	148313	6	15.304	1055430	20.0