

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072823\
 Data File : BF134526.D
 Acq On : 28 Jul 2023 21:06
 Operator : CG\JU
 Sample : 03742-08
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DUP-04

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-BF072423.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134526.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	14	rVB	529205	553947	42.12%	6.103%
2	5.075	505	508	515	rBV	47069	59278	4.51%	0.653%
3	5.475	572	576	592	rBV	1074439	1071415	81.47%	11.804%
4	6.475	742	746	753	rBV	1251443	1109019	84.33%	12.219%
5	6.828	803	806	815	rBV	463038	434913	33.07%	4.792%
6	7.392	898	902	913	rBV	764119	660590	50.23%	7.278%
7	8.110	1020	1024	1032	rBV	638876	536754	40.82%	5.914%
8	9.186	1202	1207	1210	rBV	1549428	1315063	100.00%	14.489%
9	9.298	1222	1226	1229	rBV	16335	14738	1.12%	0.162%
10	9.863	1319	1322	1326	rBV	621277	519863	39.53%	5.728%
11	10.657	1454	1457	1467	rBV	642197	578194	43.97%	6.370%
12	11.357	1573	1576	1583	rBV	443009	411244	31.27%	4.531%
13	11.886	1663	1666	1676	rVB	100700	107859	8.20%	1.188%
14	12.616	1783	1790	1796	rBV6	25028	38097	2.90%	0.420%
15	12.680	1796	1801	1809	rBV6	22982	41017	3.12%	0.452%
16	12.951	1843	1847	1851	rBV	986910	854910	65.01%	9.419%
17	13.857	1997	2001	2010	rBV4	41649	73416	5.58%	0.809%
18	14.021	2025	2029	2032	rBV	324067	318704	24.23%	3.511%
19	14.474	2104	2106	2108	rBV3	19056	17127	1.30%	0.189%
20	14.939	2183	2185	2190	rVB4	28297	27835	2.12%	0.307%
21	15.133	2216	2218	2222	rVB4	22467	21696	1.65%	0.239%
22	15.515	2279	2283	2290	rVB	203978	277697	21.12%	3.060%
23	15.739	2317	2321	2324	rVB5	24071	32969	2.51%	0.363%

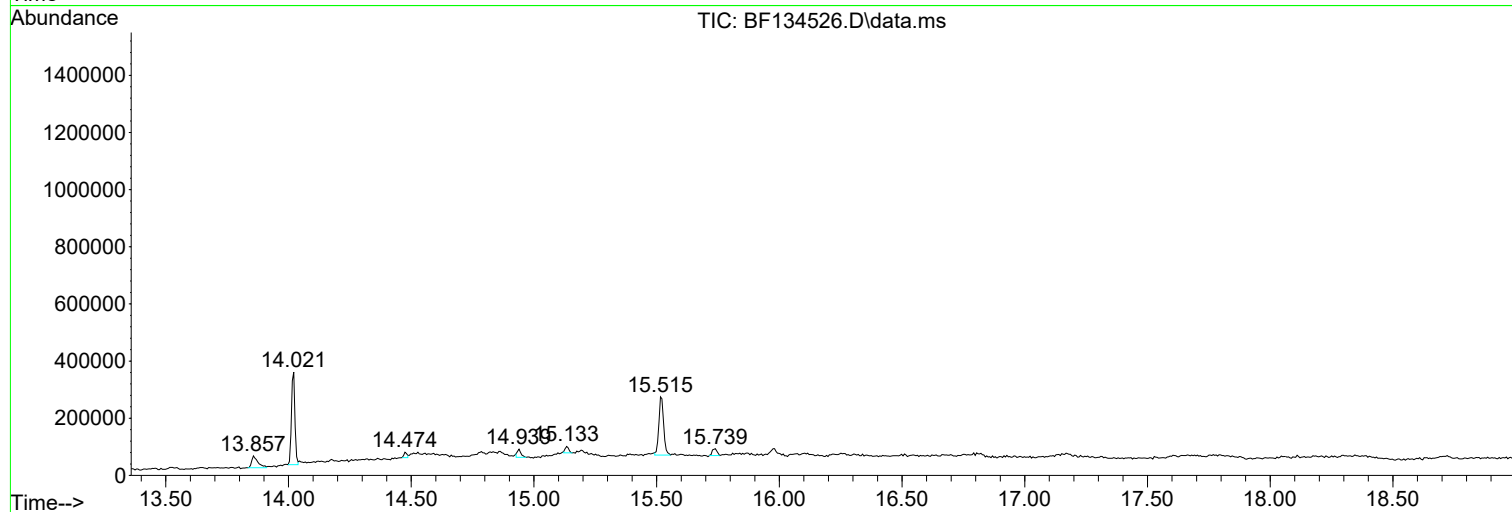
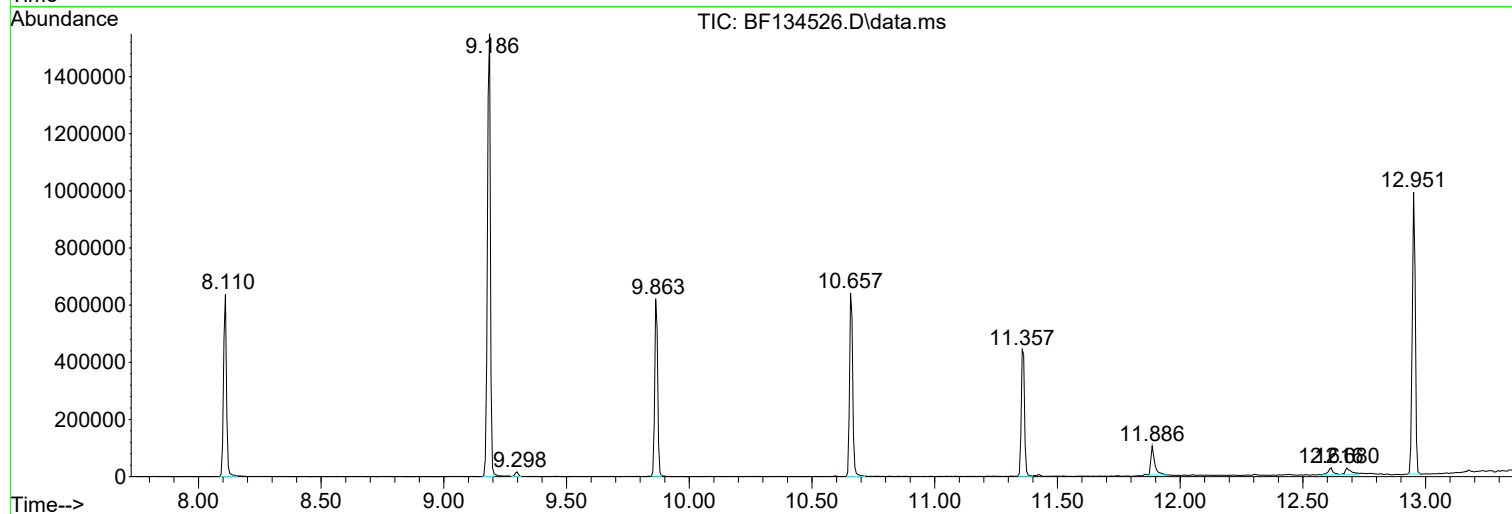
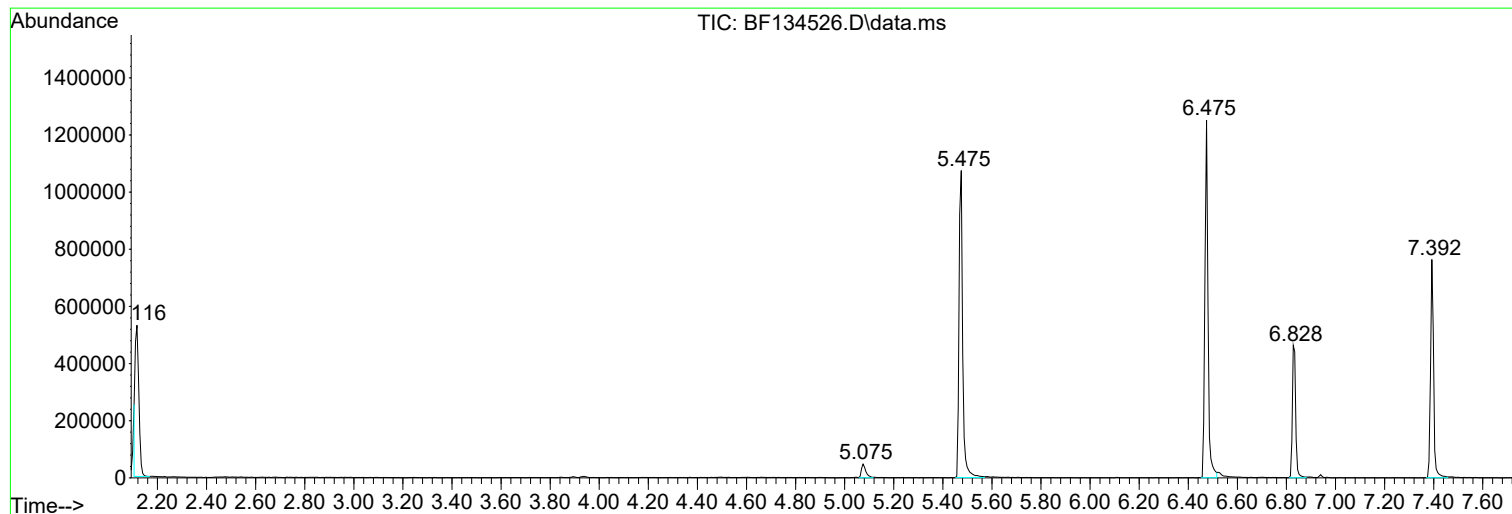
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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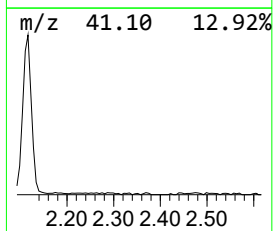
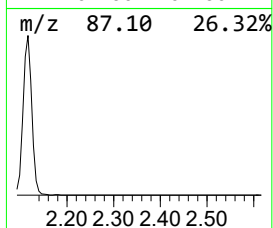
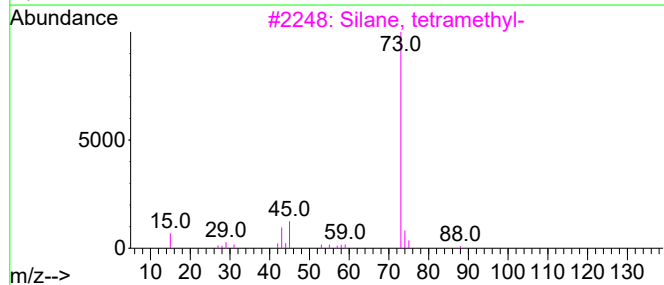
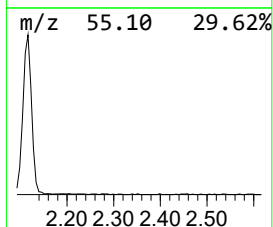
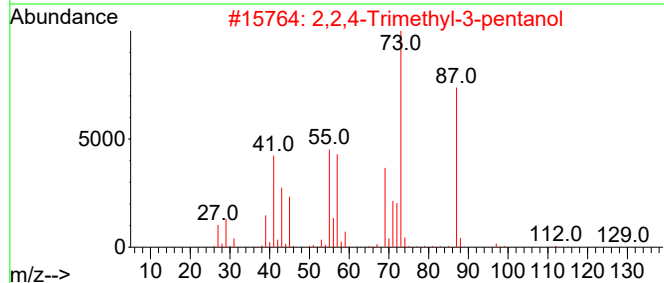
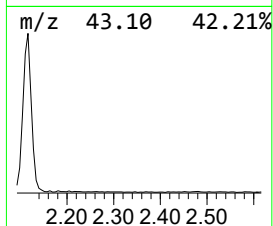
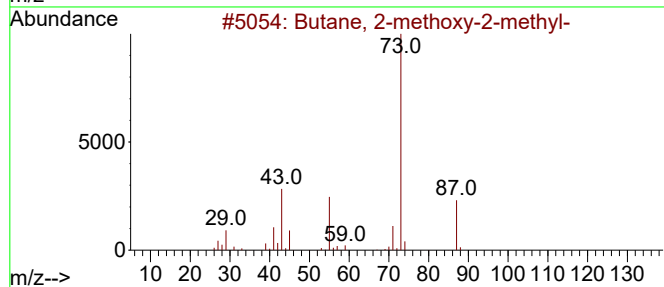
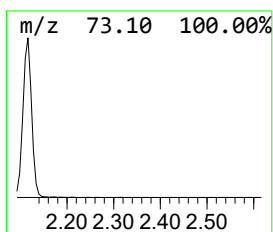
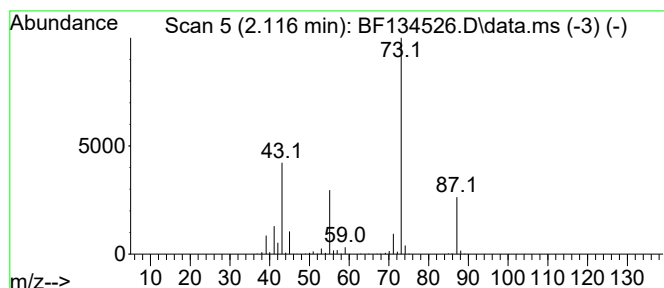
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.116	25.47 ng	553947	1,4-Dichlorobenzene-d4	6.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	16
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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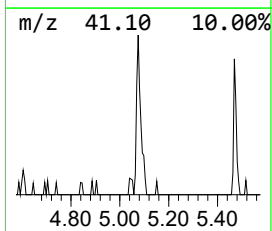
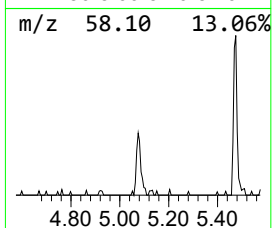
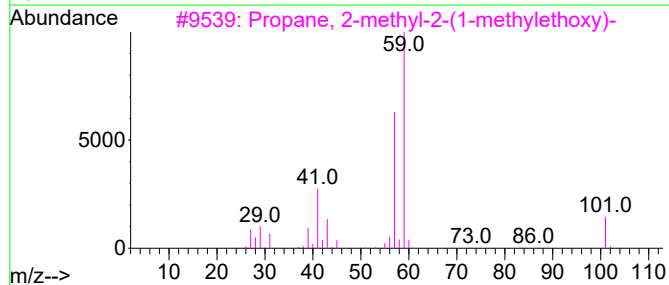
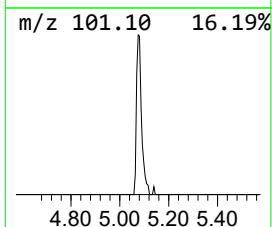
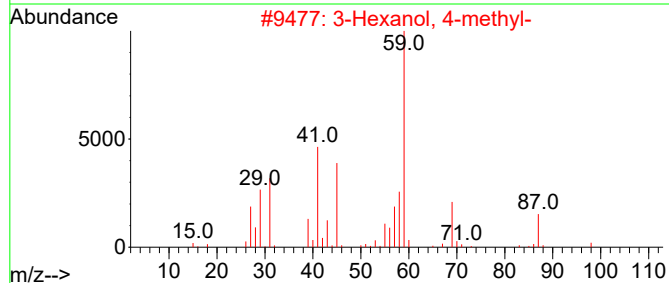
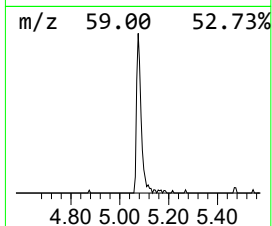
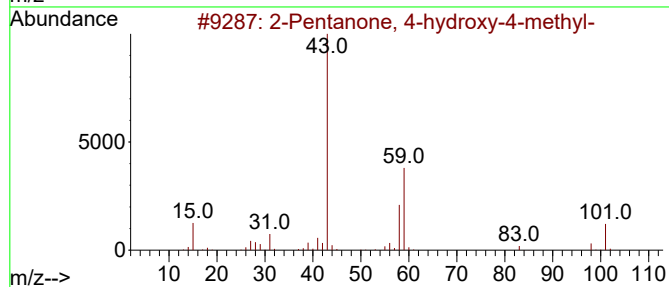
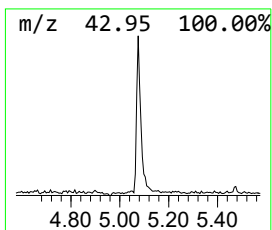
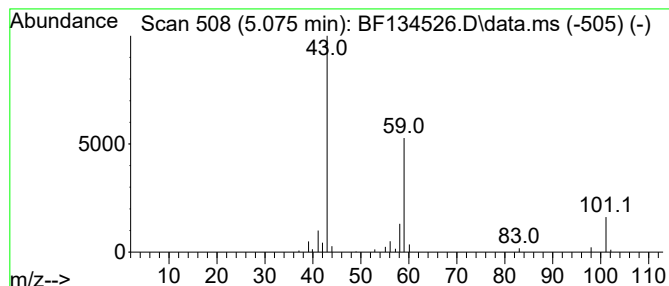
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	2.73 ng	59278	1,4-Dichlorobenzene-d4	6.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4			2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	28
5			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28



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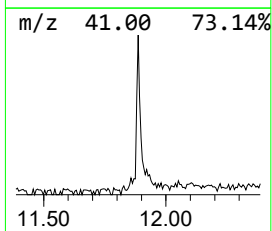
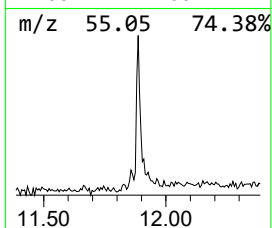
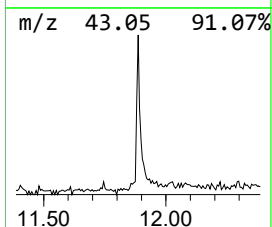
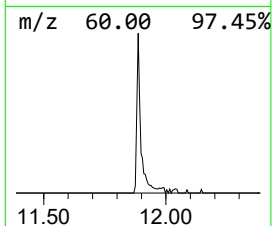
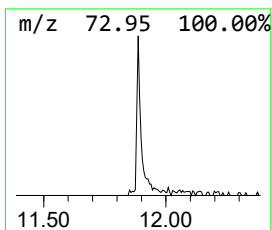
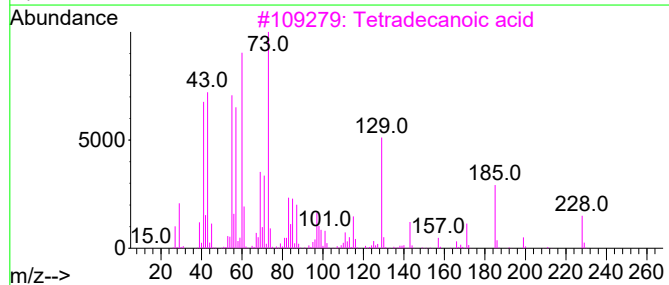
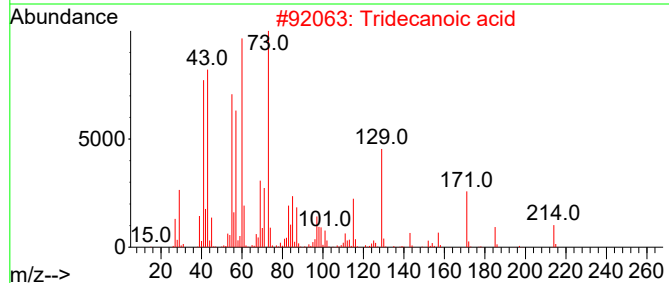
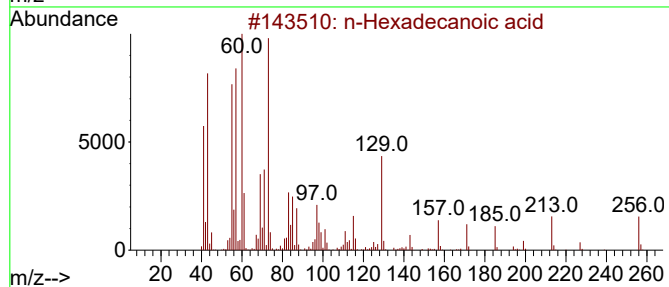
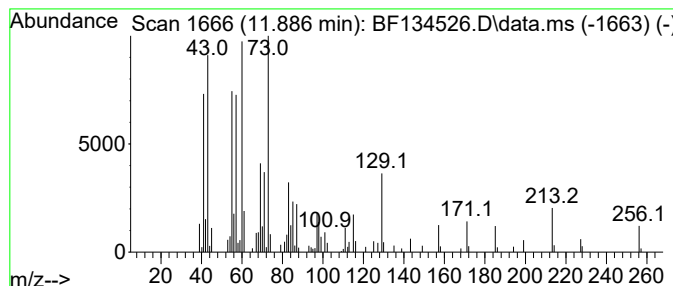
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	5.25 ng	107859	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5			Undecanoic acid	186	C11H22O2	000112-37-8	62



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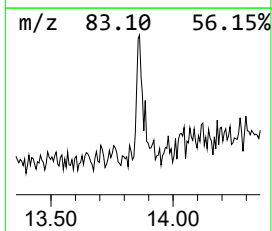
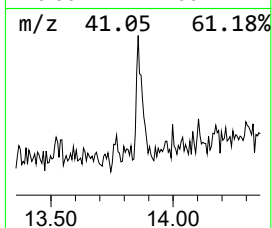
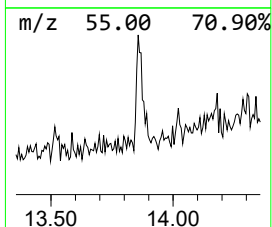
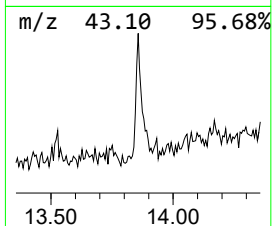
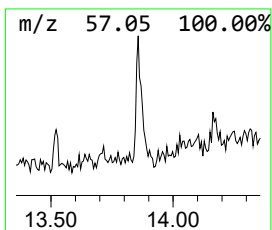
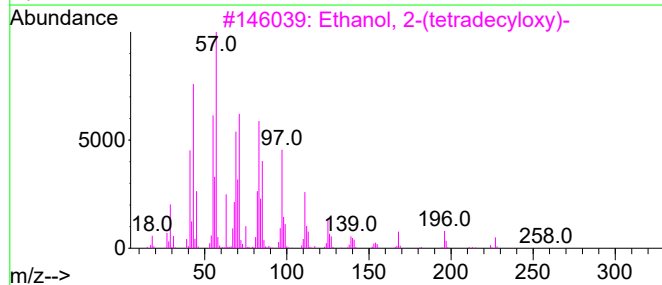
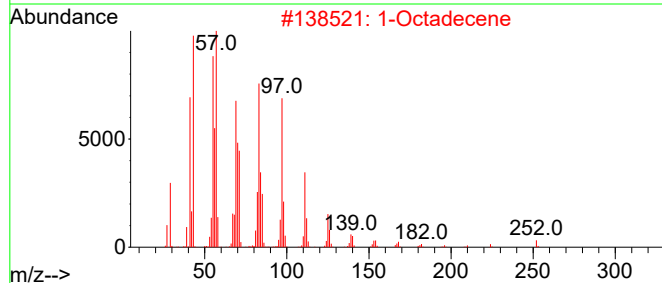
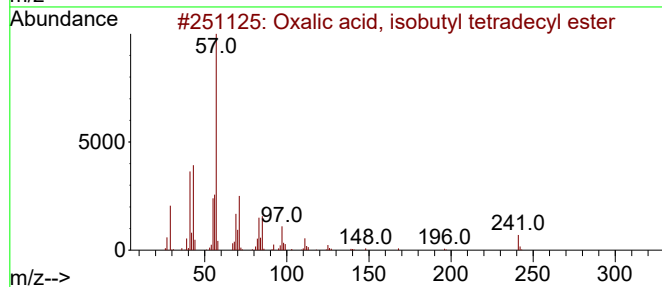
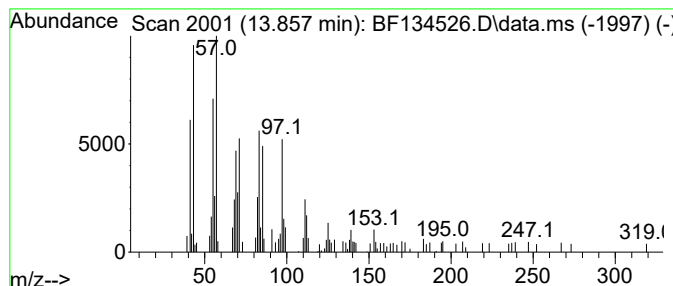
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Peak Number 4 Oxalic acid, isobutyl tetra... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.857	4.61 ng	73416	Chrysene-d12	14.021	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	83
2	1-Octadecene	252	C18H36	000112-88-9	83
3	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	76
4	Octacosyl propyl ether	452	C31H64O	1000406-28-5	76
5	Butyl eicosyl ether	354	C24H50O	1000406-40-7	74



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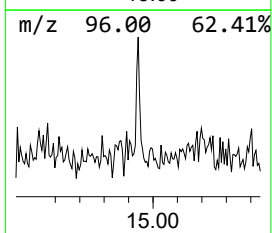
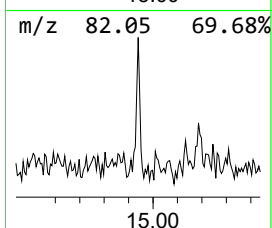
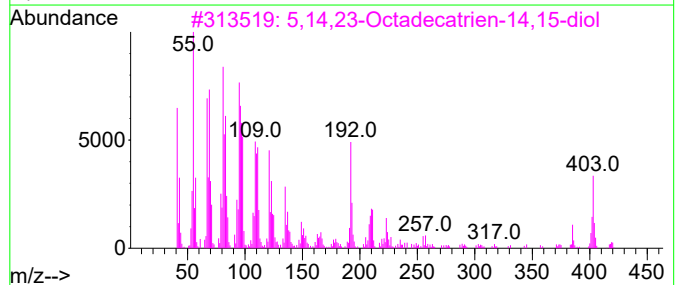
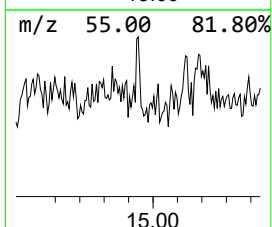
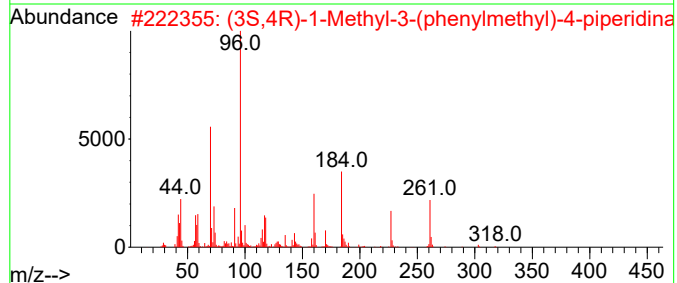
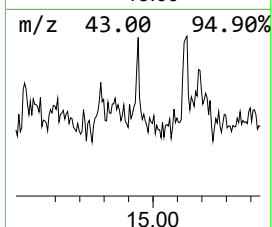
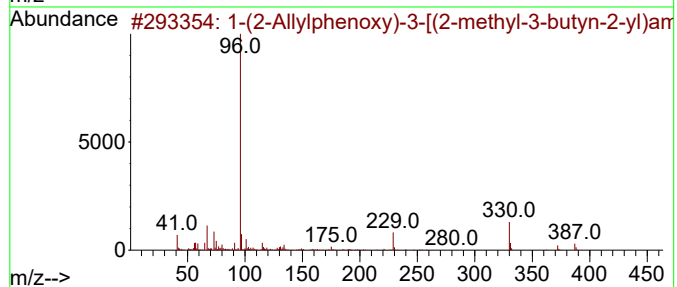
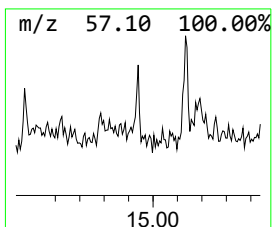
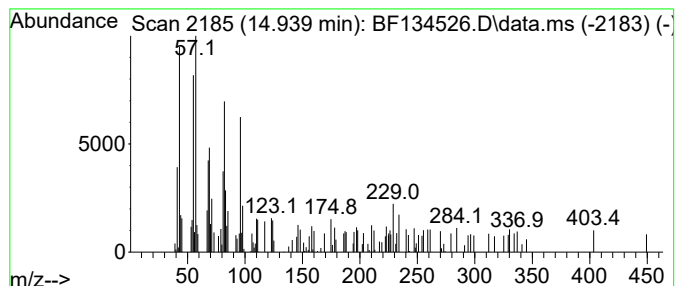
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown14.939 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.939	2.00 ng	27835	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-(2-Allylphenoxy)-3-[(2-methyl-...	387	C23H37NO2Si	1000116-37-4	12
2			(3S,4R)-1-Methyl-3-(phenylmethyl...	318	C19H34N2Si	1000470-01-9	12
3			5,14,23-Octadecatrien-14,15-diol	420	C28H52O2	1000131-32-4	10
4			1-Pentanol, 4-methyl-2-methylene-	114	C7H14O	121505-31-5	9
5			Astemizole	458	C28H31FN4O	068844-77-9	9



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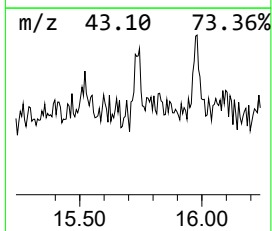
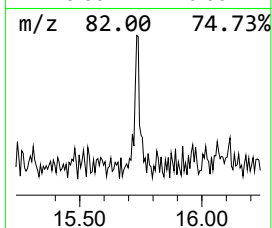
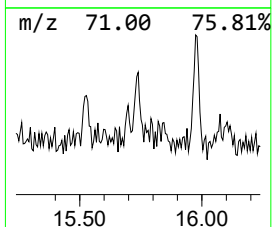
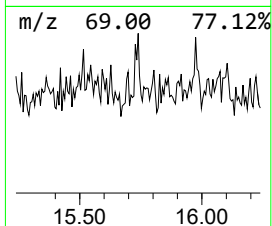
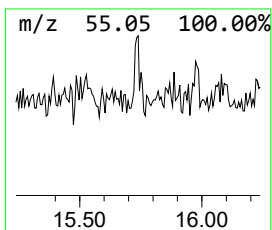
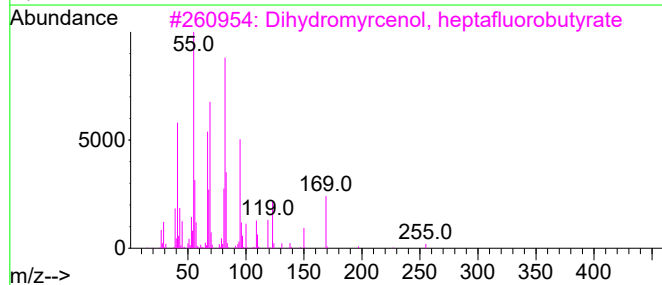
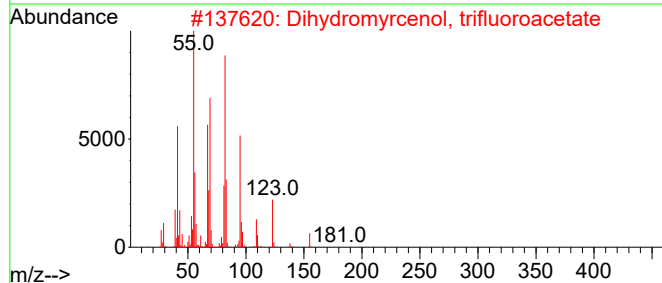
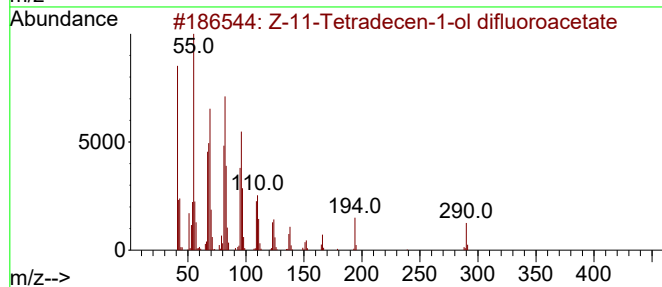
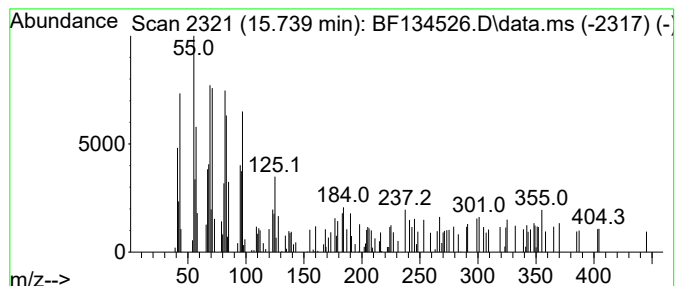
Instrument :
BNA_F
ClientSampleId :
DUP-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown15.739 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.739	2.37 ng	32969	Perylene-d12	15.515	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Z-11-Tetradecen-1-ol difluoroace...	290	C16H28F2O2	1000130-82-7	38
2	Dihydromyrcenol, trifluoroacetate	252	C12H19F3O2	1000463-72-2	35
3	Dihydromyrcenol, heptafluorobuty...	352	C14H19F7O2	1000463-72-0	35
4	Pentadecanal-	226	C15H30O	002765-11-9	35
5	Ecgonine methyl ester, trimethyl...	271	C13H25NO3Si	1000417-19-3	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072823\
Data File : BF134526.D
Acq On : 28 Jul 2023 21:06
Operator : CG\JU
Sample : 03742-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.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
Butane, 2-metho...	2.116	25.5	ng	553947	1	6.834	434913	20.0
2-Pentanone, 4-...	5.075	2.7	ng	59278	1	6.834	434913	20.0
n-Hexadecanoic ...	11.886	5.3	ng	107859	4	11.357	411244	20.0
Oxalic acid, is...	13.857	4.6	ng	73416	5	14.021	318704	20.0
unknown14.939	14.939	2.0	ng	27835	6	15.515	277697	20.0
unknown15.739	15.739	2.4	ng	32969	6	15.515	277697	20.0