

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
 Data File : BF135292.D
 Acq On : 15 Sep 2023 21:59
 Operator : CG\JU
 Sample : 04409-13
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-5(0-6)COMP

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-BF091123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135292.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	17	rVB3	34285	47868	2.70%	0.303%
2	4.987	489	493	503	rVB	51667	66149	3.73%	0.419%
3	5.387	557	561	580	rBV	1884218	1773260	100.00%	11.229%
4	6.398	729	733	736	rBV	1921210	1706819	96.25%	10.808%
5	6.592	763	766	778	rBV	45815	63563	3.58%	0.402%
6	6.757	790	794	803	rBV	787284	629965	35.53%	3.989%
7	7.322	885	890	893	rBV	1171056	1097560	61.90%	6.950%
8	8.033	1007	1011	1015	rBV	898182	753324	42.48%	4.770%
9	9.116	1190	1195	1198	rBV	2071355	1766896	99.64%	11.188%
10	9.239	1210	1216	1219	rBV	1608072	1510853	85.20%	9.567%
11	9.792	1306	1310	1313	rBV	889736	720864	40.65%	4.565%
12	10.586	1441	1445	1458	rBV	957081	915688	51.64%	5.798%
13	10.763	1471	1475	1490	rBV2	27969	58715	3.31%	0.372%
14	10.874	1490	1494	1501	rBV	29188	40473	2.28%	0.256%
15	10.933	1501	1504	1507	rBV2	22495	28794	1.62%	0.182%
16	11.286	1560	1564	1566	rBV	706565	646719	36.47%	4.095%
17	11.304	1566	1567	1571	rVV	97608	79448	4.48%	0.503%
18	11.357	1571	1576	1580	rVB	26142	26687	1.50%	0.169%
19	11.821	1651	1655	1665	rBV2	171349	203491	11.48%	1.289%
20	12.374	1746	1749	1750	rBV2	23022	19816	1.12%	0.125%
21	12.398	1750	1753	1756	rVB	76752	67496	3.81%	0.427%
22	12.504	1765	1771	1775	rBV	177497	163160	9.20%	1.033%
23	12.545	1775	1778	1780	rVV	79143	68680	3.87%	0.435%
24	12.610	1786	1789	1794	rBV5	19358	26664	1.50%	0.169%
25	12.733	1804	1810	1813	rBV	160443	156177	8.81%	0.989%
26	12.880	1831	1835	1843	rVB	1654097	1365304	76.99%	8.645%
27	13.580	1951	1954	1957	rVB2	24381	23573	1.33%	0.149%
28	13.739	1979	1981	1983	rBV	21548	21108	1.19%	0.134%
29	13.815	1986	1994	2004	rVV4	103259	260078	14.67%	1.647%
30	13.939	2010	2015	2018	rBV	707479	707658	39.91%	4.481%
31	13.968	2018	2020	2023	rVB	73876	63408	3.58%	0.402%
32	14.039	2029	2032	2036	rVB3	29032	35805	2.02%	0.227%
33	14.980	2189	2192	2195	rBV	66851	92436	5.21%	0.585%
34	15.280	2240	2243	2249	rBV	34469	47969	2.71%	0.304%
35	15.339	2251	2253	2259	rVB	52139	65253	3.68%	0.413%
36	15.404	2260	2264	2269	rBV	389320	470565	26.54%	2.980%

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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-BF091123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

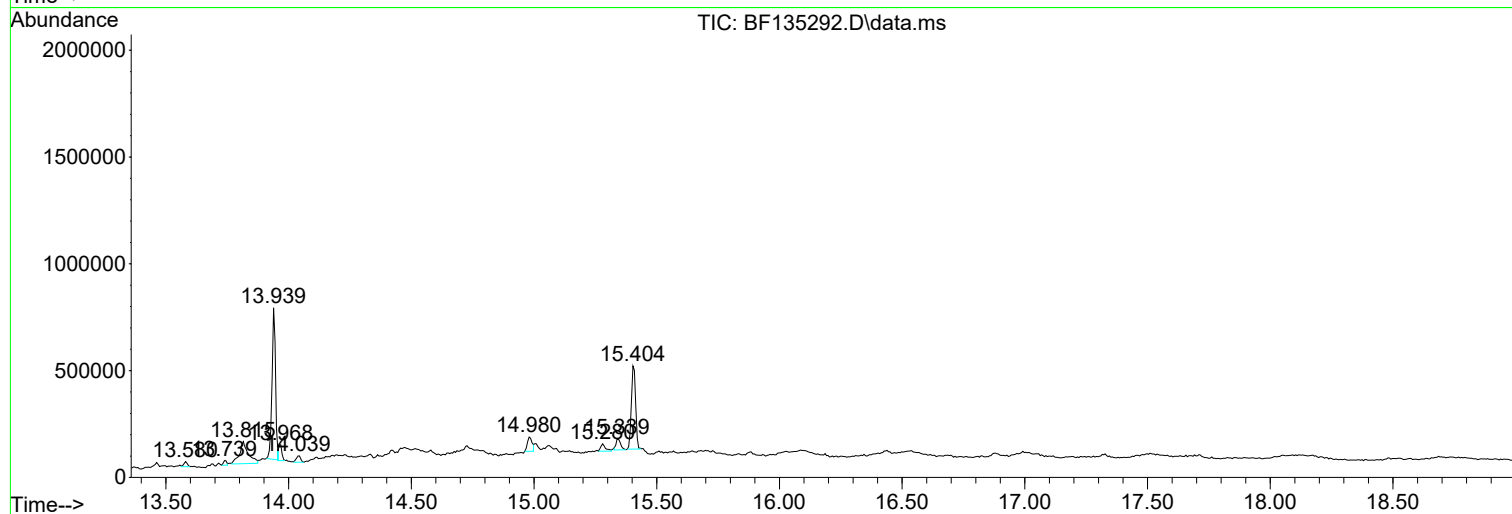
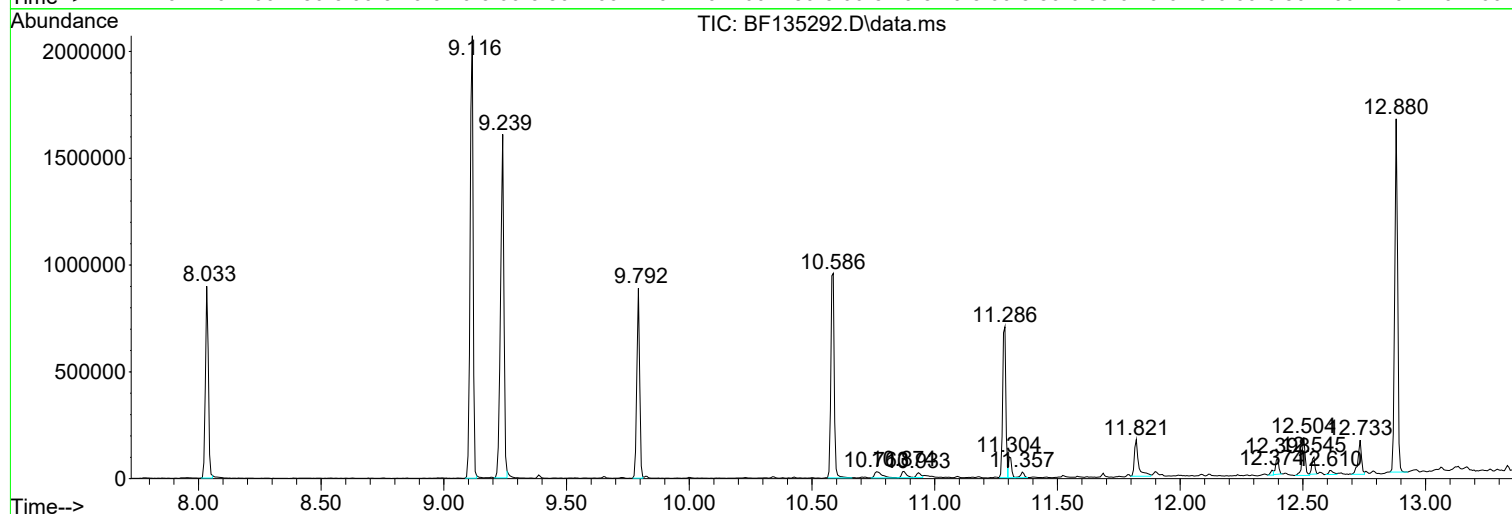
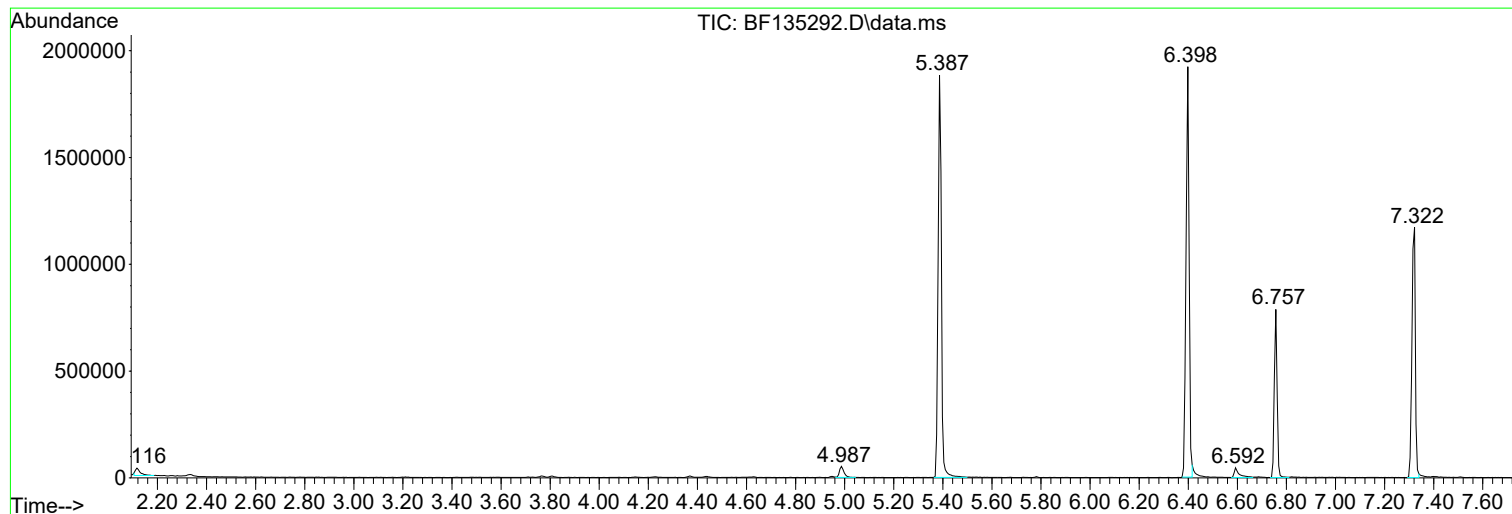
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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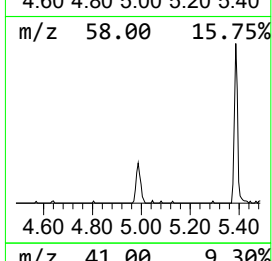
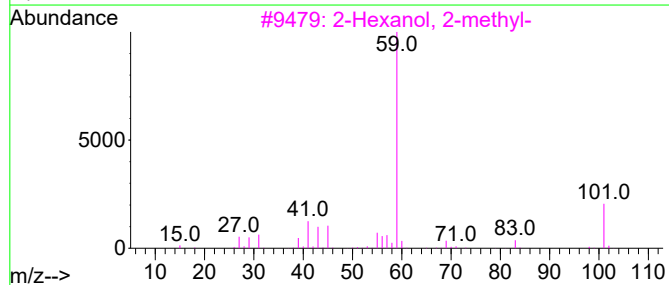
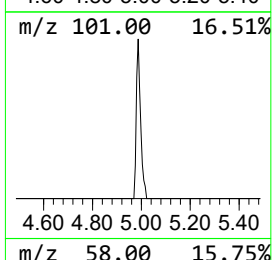
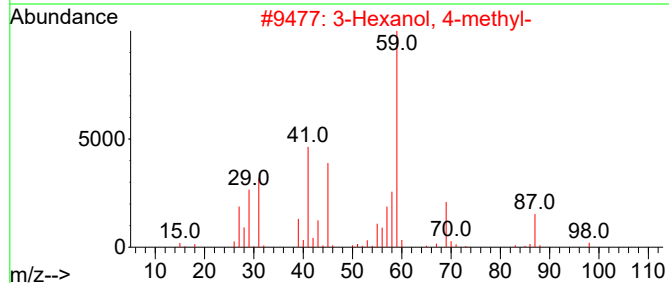
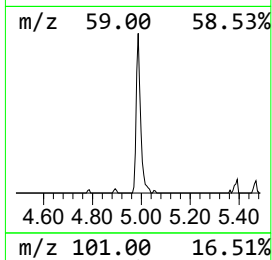
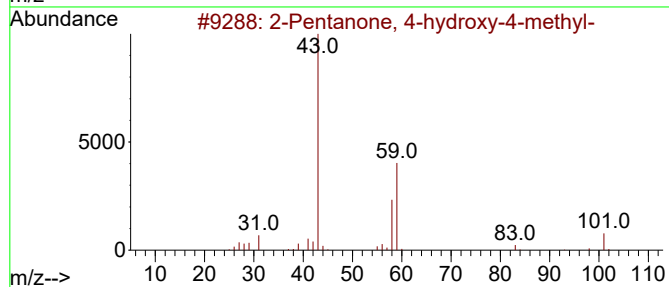
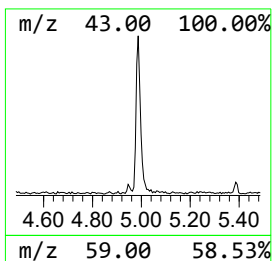
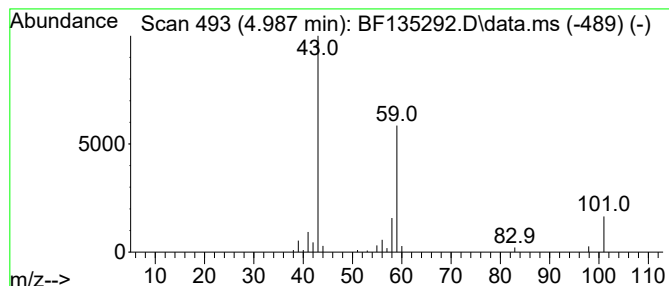
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.987	2.10 ng	66149	1,4-Dichlorobenzene-d4	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		



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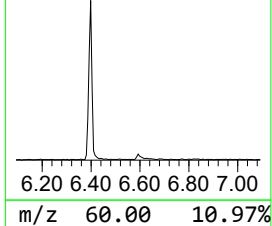
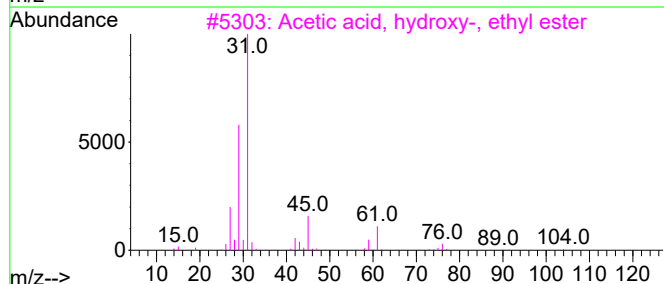
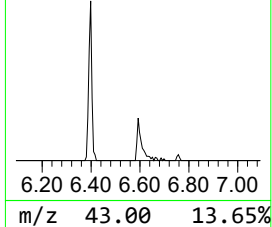
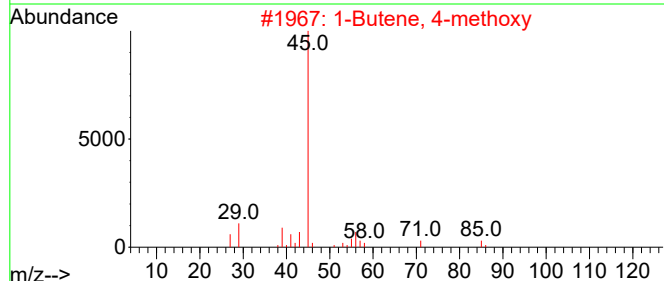
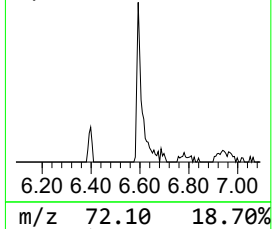
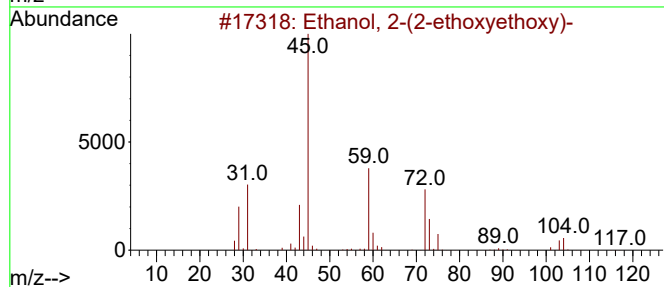
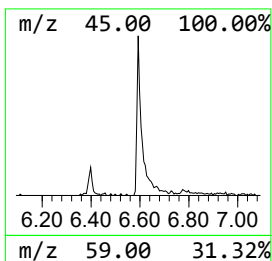
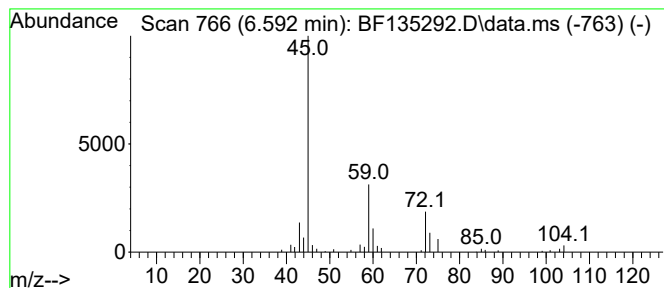
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.592	2.02 ng	63563	1,4-Dichlorobenzene-d4	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	78
2			1-Butene, 4-methoxy	86	C5H10O	004696-30-4	47
3			Acetic acid, hydroxy-, ethyl ester	104	C4H8O3	000623-50-7	45
4			2-Butanol	74	C4H10O	000078-92-2	45
5			.beta.-Methoxyethoxymethyl chloride	124	C4H9ClO2	003970-21-6	39



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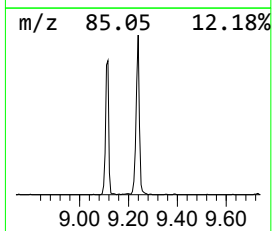
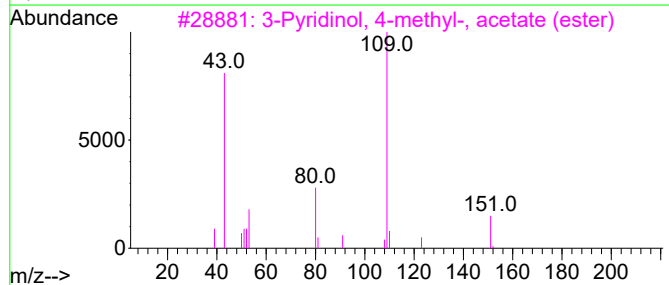
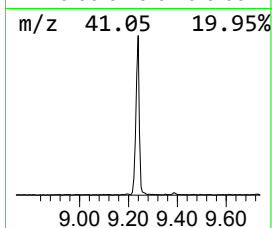
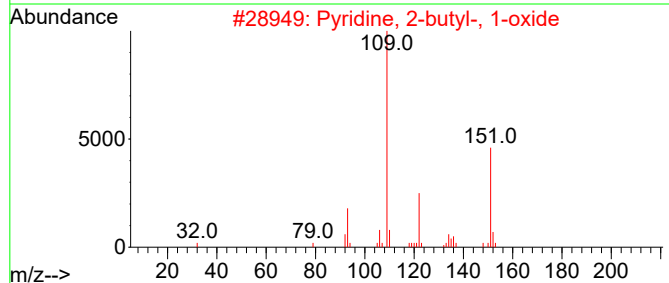
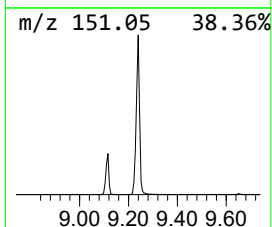
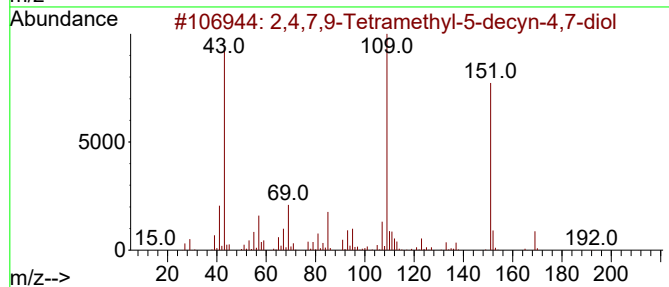
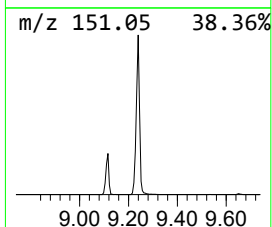
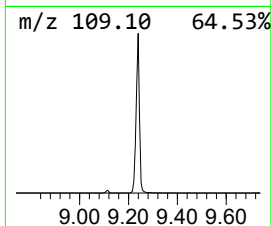
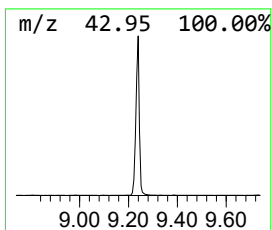
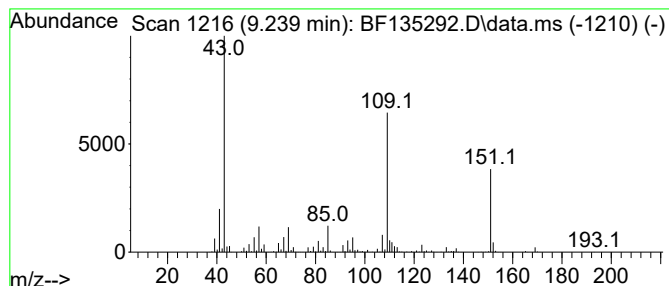
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD			R.T.
9.239	41.92 ng	1510850	Acenaphthene-d10			9.792
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...		226	C14H26O2	000126-86-3	87
2	Pyridine, 2-butyl-, 1-oxide		151	C9H13NO	031396-32-4	59
3	3-Pyridinol, 4-methyl-, acetate ...		151	C8H9NO2	001006-96-8	53
4	Metacetamol		151	C8H9NO2	000621-42-1	53
5	2-Thiophenecarbonitrile		109	C5H3NS	001003-31-2	35



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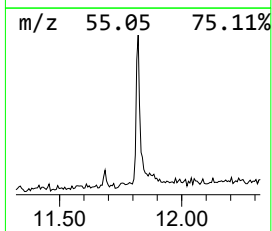
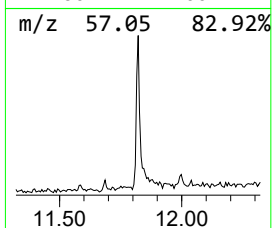
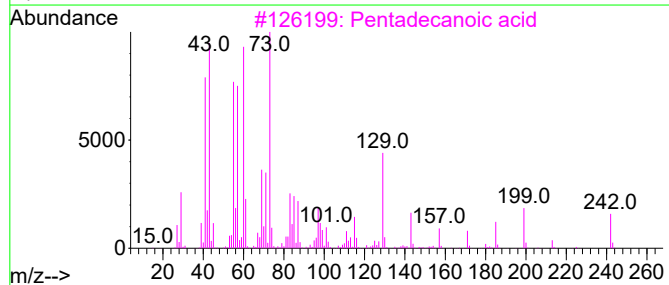
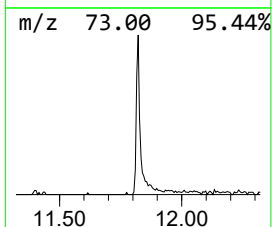
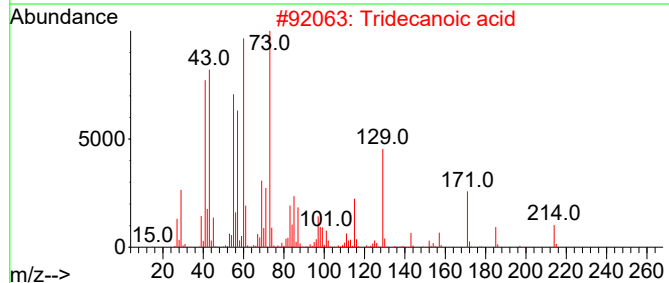
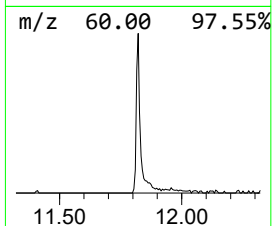
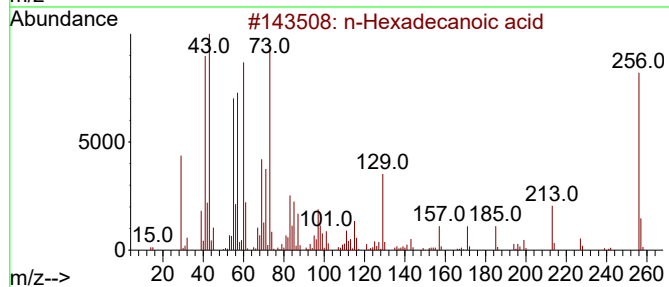
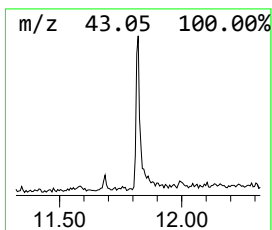
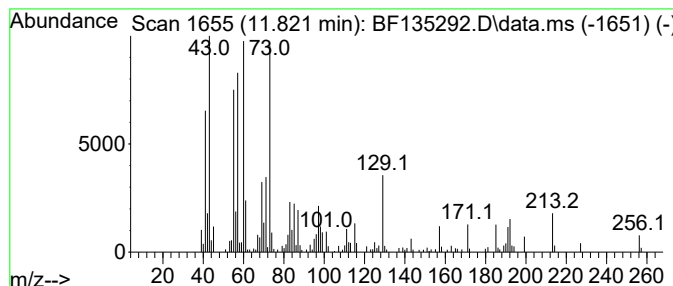
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.822	6.29 ng	203491	Phenanthrene-d10	11.286

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	92
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			n-Decanoic acid	172	C10H20O2	000334-48-5	83
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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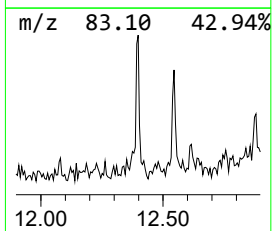
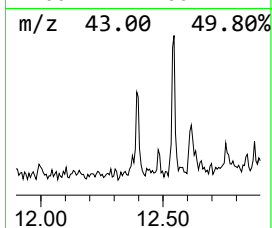
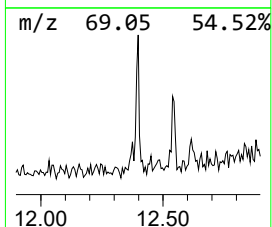
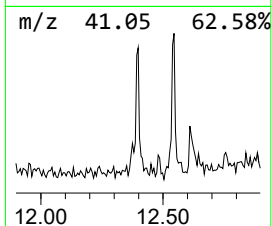
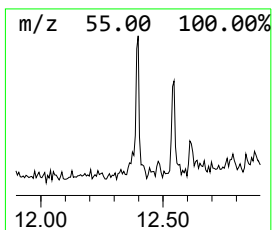
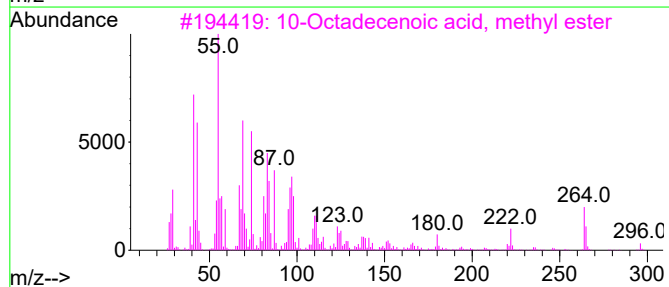
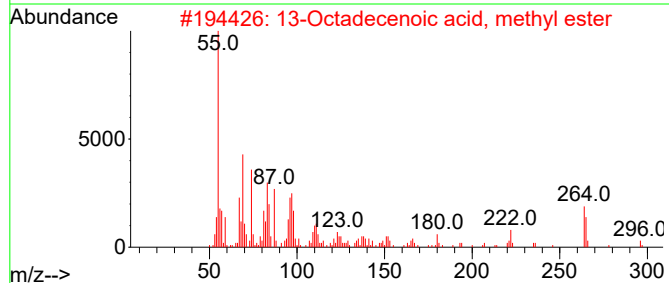
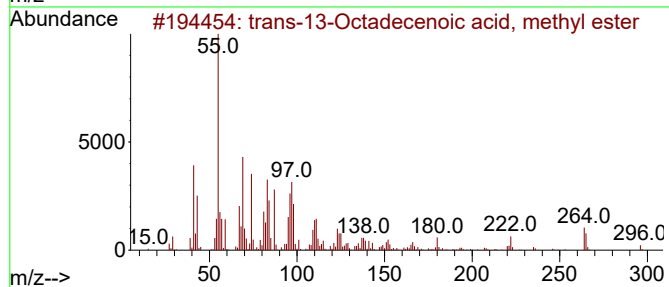
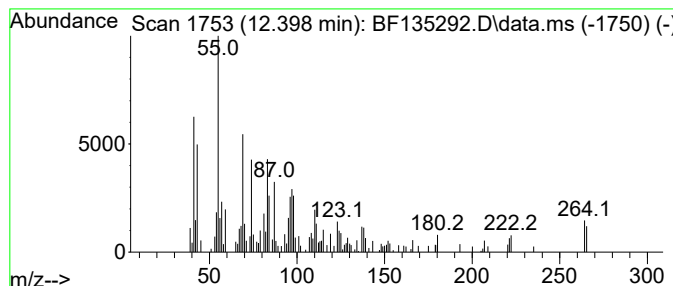
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TIC Integration Parameters: LSCINT.P

Peak Number 5 trans-13-Octadecenoic acid,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.398	2.09 ng	67496	Phenanthrene-d10	11.286	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	91
2	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	91
3	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	81
4	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	81
5	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
Data File : BF135292.D
Acq On : 15 Sep 2023 21:59
Operator : CG\JU
Sample : 04409-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

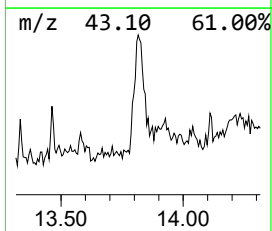
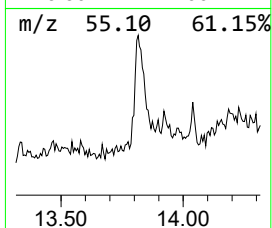
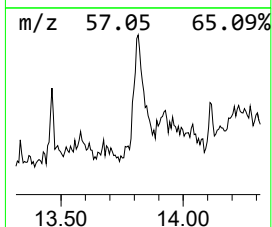
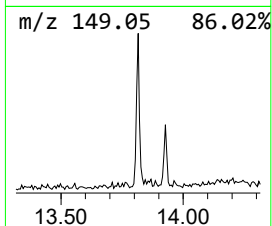
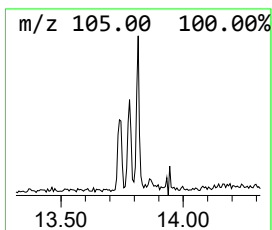
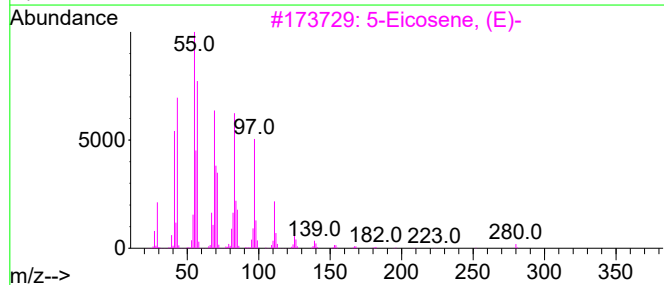
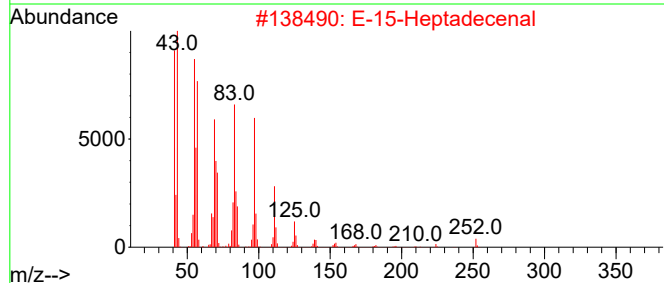
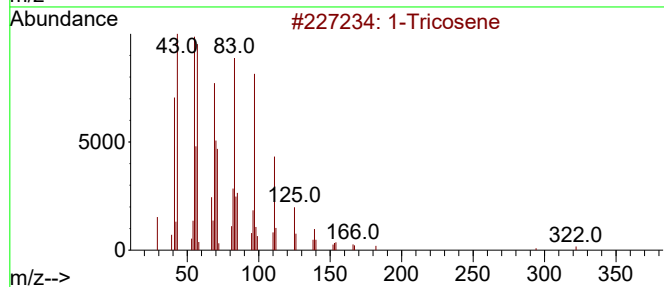
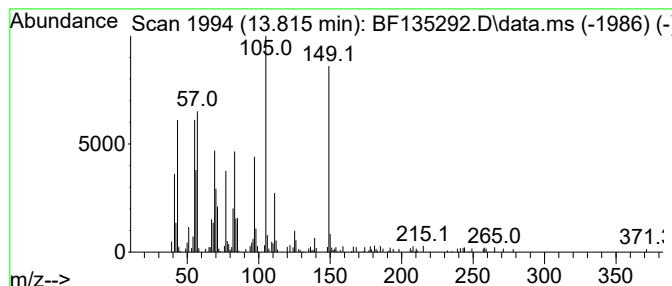
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ClientSampleId :
WC-5(0-6)COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Tricosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.816	7.35 ng	260078	Chrysene-d12	13.939	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene	322	C23H46	018835-32-0	53
2	E-15-Heptadecenal	252	C17H32O	1000130-97-9	50
3	5-Eicosene, (E)-	280	C20H40	074685-30-6	50
4	E-14-Hexadecenal	238	C16H30O	330207-53-9	50
5	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
Data File : BF135292.D
Acq On : 15 Sep 2023 21:59
Operator : CG\JU
Sample : 04409-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-5(0-6)COMP

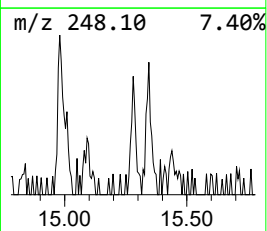
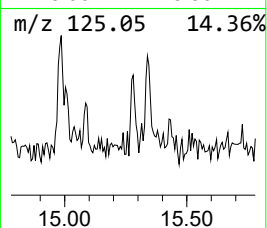
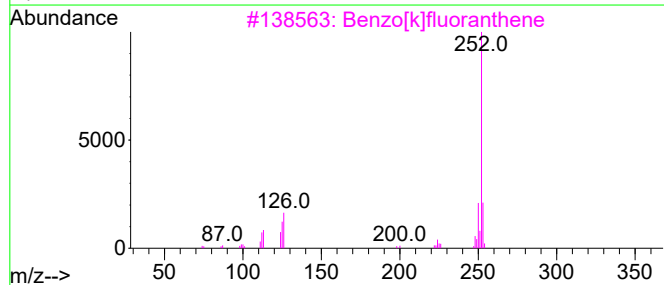
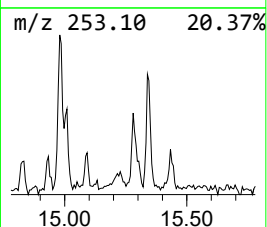
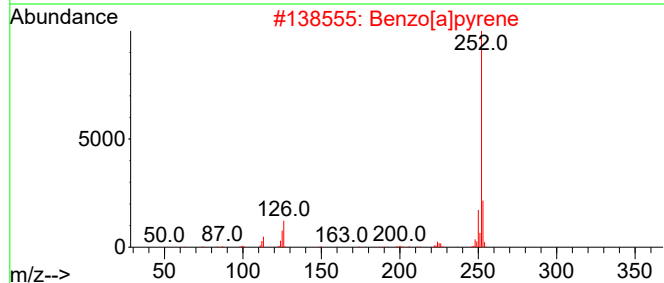
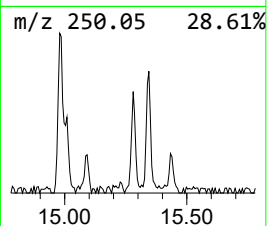
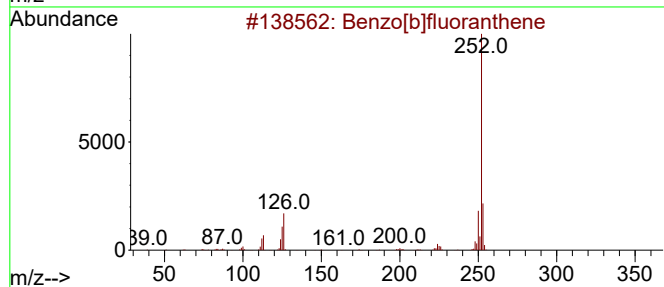
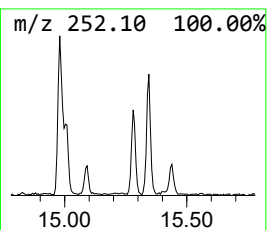
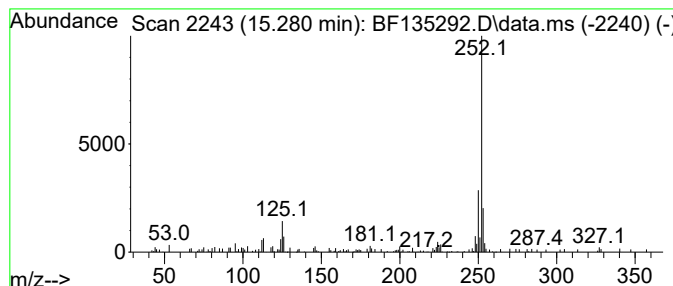
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.280	2.04 ng	47969	Perylene-d12	15.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
2			Benzo[a]pyrene	252	C20H12	000050-32-8	91
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
4			Benzo[e]pyrene	252	C20H12	000192-97-2	90
5			Perylene	252	C20H12	000198-55-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
Data File : BF135292.D
Acq On : 15 Sep 2023 21:59
Operator : CG\JU
Sample : 04409-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-5(0-6)COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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
2-Pentanone, 4-...	4.987	2.1	ng	66149	1	6.757	629965	20.0
Ethanol, 2-(2-e...	6.592	2.0	ng	63563	1	6.757	629965	20.0
2,4,7,9-Tetrame...	9.239	41.9	ng	1510850	3	9.792	720864	20.0
n-Hexadecanoic ...	11.822	6.3	ng	203491	4	11.286	646719	20.0
trans-13-Octade...	12.398	2.1	ng	67496	4	11.286	646719	20.0
1-Tricosene	13.816	7.3	ng	260078	5	13.939	707658	20.0
Benzo[e]pyrene	15.280	2.0	ng	47969	6	15.410	470565	20.0