

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091522\
 Data File : BF130280.D
 Acq On : 15 Sep 2022 19:56
 Operator : CG\JU
 Sample : N4549-04
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-49

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-BF091422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130280.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.863	468	472	478	rBV	74342	96668	2.49%	0.484%
2	5.275	537	542	545	rBV	1826607	1674944	43.21%	8.391%
3	6.304	713	717	729	rBV	1213551	1104105	28.48%	5.531%
4	6.675	776	780	783	rBV	767443	596588	15.39%	2.989%
5	7.245	871	877	880	rVB	2300897	2195874	56.65%	11.001%
6	7.698	949	954	958	rVB5	32400	46861	1.21%	0.235%
7	7.957	992	998	1001	rBV	1027375	851623	21.97%	4.267%
8	8.204	1036	1040	1044	rBV2	41830	43471	1.12%	0.218%
9	8.322	1054	1060	1062	rBV4	34187	57921	1.49%	0.290%
10	8.687	1115	1122	1123	rBV6	23919	45473	1.17%	0.228%
11	8.734	1126	1130	1133	rBV3	50972	57992	1.50%	0.291%
12	8.904	1155	1159	1161	rBV2	63152	59716	1.54%	0.299%
13	9.039	1176	1182	1185	rBV	4474337	3876173	100.00%	19.419%
14	9.457	1250	1253	1257	rVB5	45547	53964	1.39%	0.270%
15	9.634	1278	1283	1287	rVB	191910	218533	5.64%	1.095%
16	9.704	1292	1295	1298	rVV	992746	821671	21.20%	4.116%
17	9.792	1307	1310	1317	rVB5	49152	63086	1.63%	0.316%
18	9.963	1336	1339	1343	rBV5	37377	60427	1.56%	0.303%
19	9.998	1343	1345	1350	rVV6	50335	70079	1.81%	0.351%
20	10.051	1351	1354	1358	rVB5	63918	82485	2.13%	0.413%
21	10.386	1408	1411	1416	rVB6	48023	71119	1.83%	0.356%
22	10.439	1416	1420	1424	rBV	285580	337972	8.72%	1.693%
23	10.498	1424	1430	1439	rBV	2180821	2589223	66.80%	12.972%
24	11.063	1524	1526	1529	rVB2	57118	44658	1.15%	0.224%
25	11.186	1543	1547	1550	rBV	999530	777555	20.06%	3.895%
26	11.728	1636	1639	1647	rVB	189604	212597	5.48%	1.065%
27	12.510	1769	1772	1783	rVB2	105064	124690	3.22%	0.625%
28	12.775	1812	1817	1820	rBV	3342818	2767146	71.39%	13.863%
29	13.810	1990	1993	1997	rBV	464087	436846	11.27%	2.189%
30	14.633	2130	2133	2140	rVB2	37353	46173	1.19%	0.231%
31	15.204	2225	2230	2236	rBV2	416446	474827	12.25%	2.379%

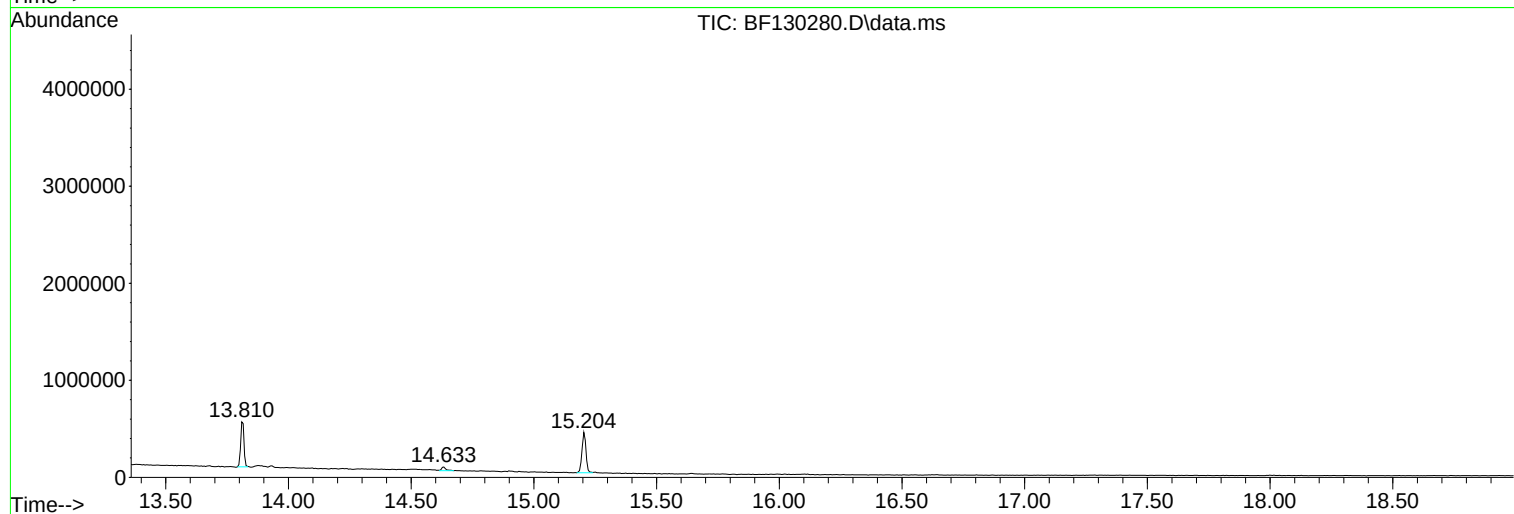
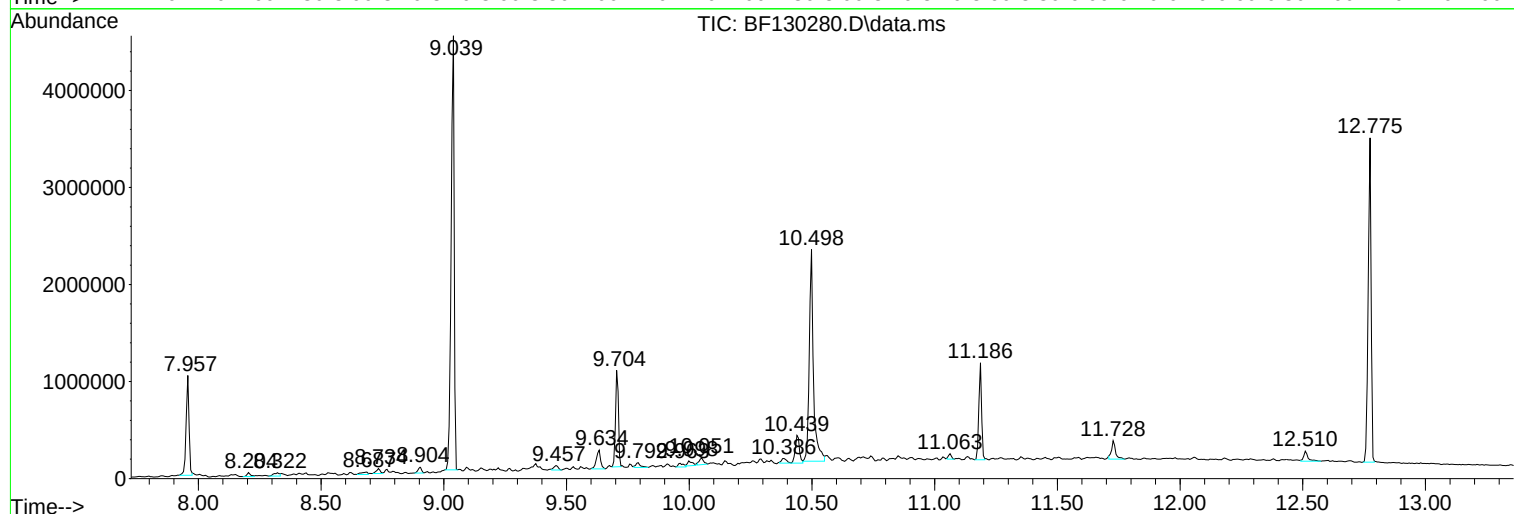
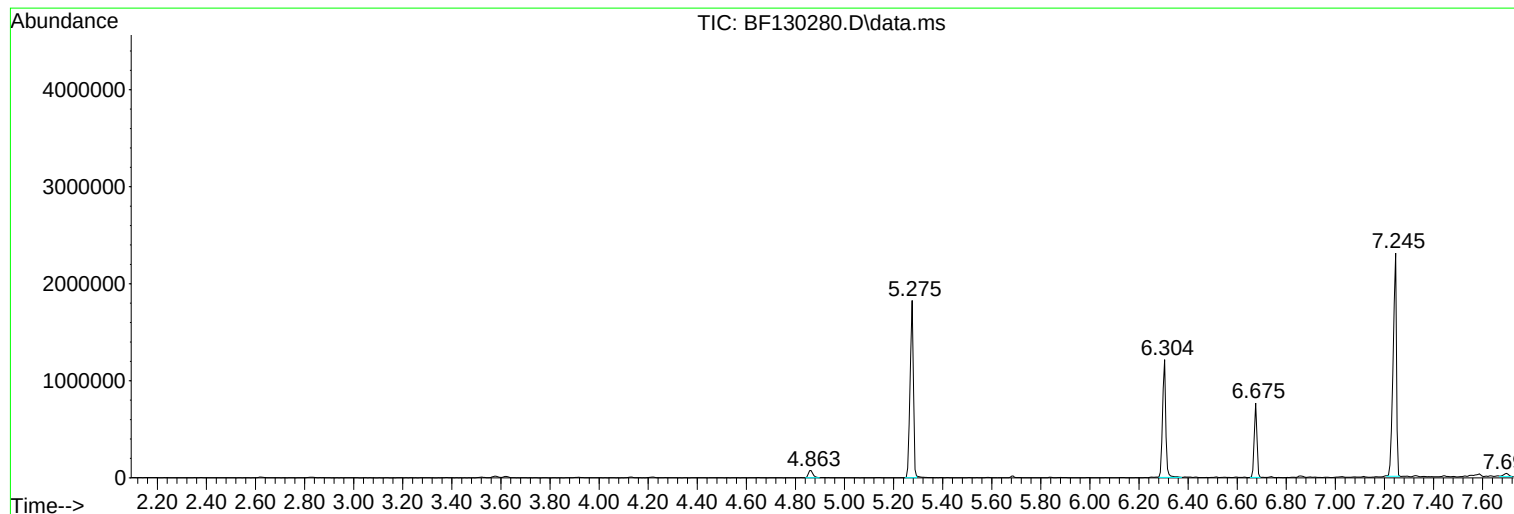
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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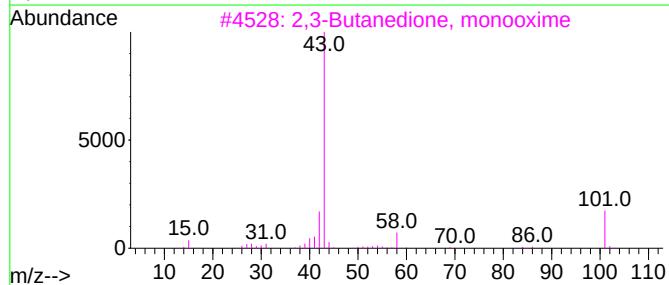
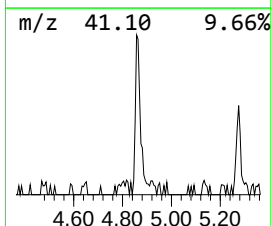
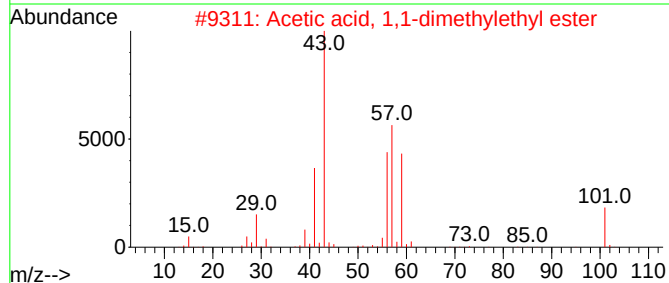
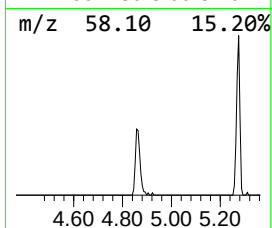
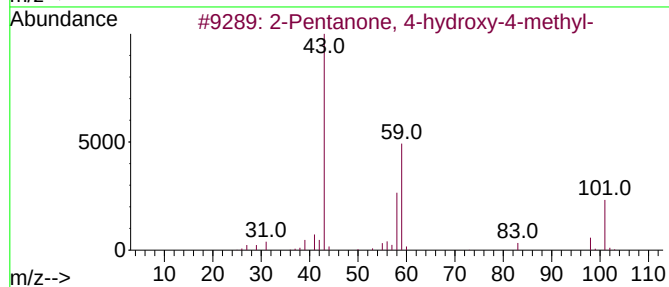
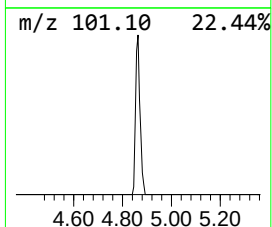
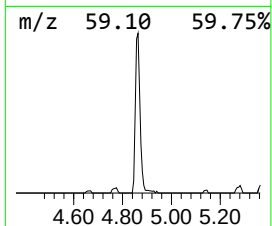
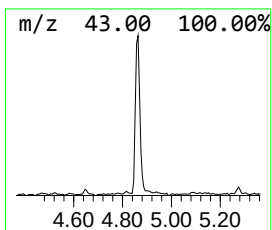
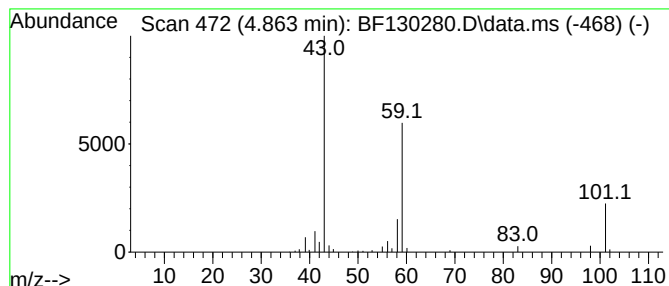
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.863	3.24 ng	96668	1,4-Dichlorobenzene-d4	6.675

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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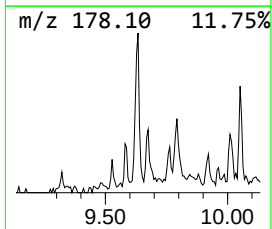
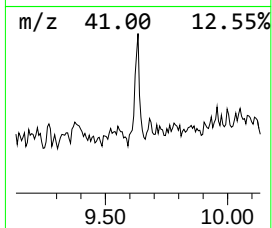
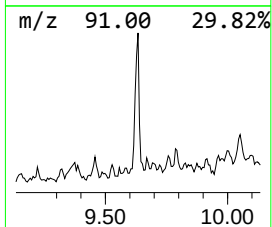
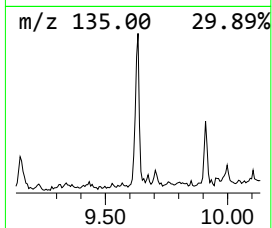
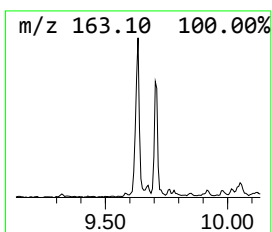
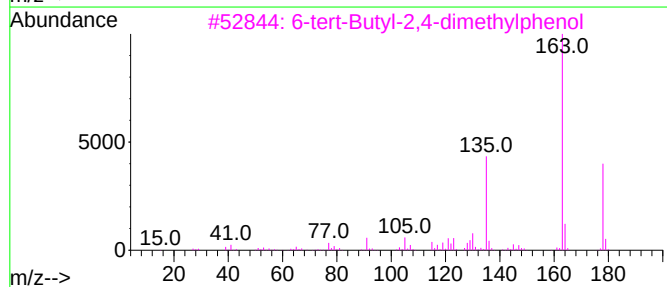
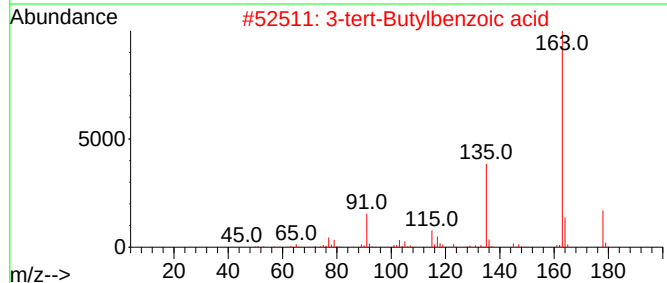
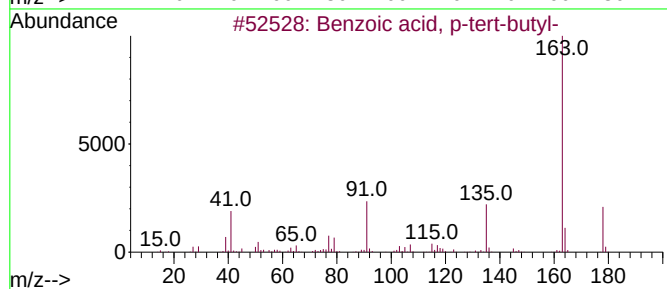
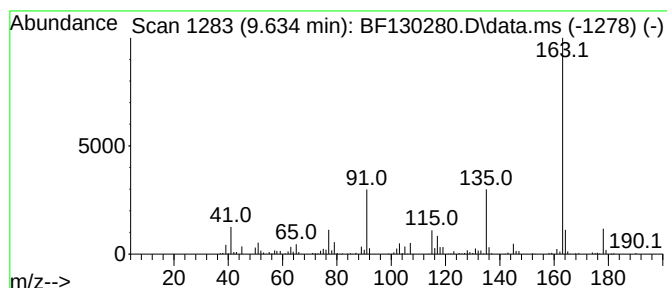
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzoic acid, p-tert-butyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.634	5.32 ng	218533	Acenaphthene-d10	9.704

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	91
2			3-tert-Butylbenzoic acid	178	C11H14O2	007498-54-6	90
3			6-tert-Butyl-2,4-dimethylphenol	178	C12H18O	001879-09-0	72
4			2-Propenal, 3-(2,6,6-trimethyl-1...	178	C12H18O	004951-40-0	59
5			Benzonitrile, 2,4-dimethoxy-	163	C9H9NO2	004107-65-7	53



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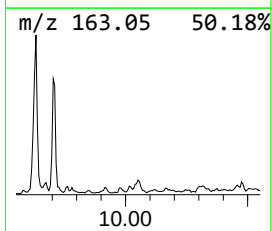
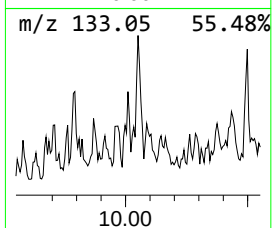
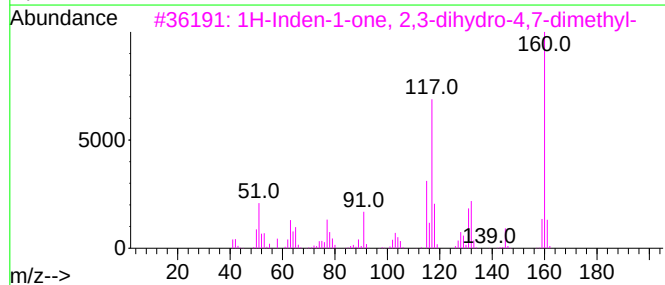
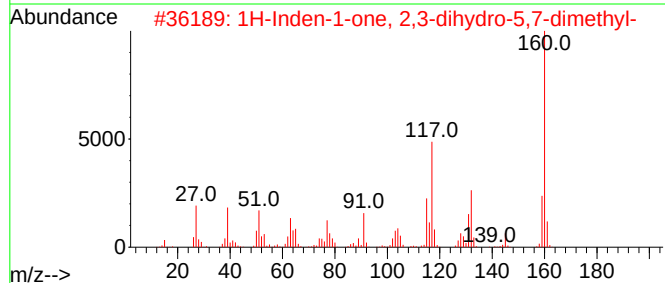
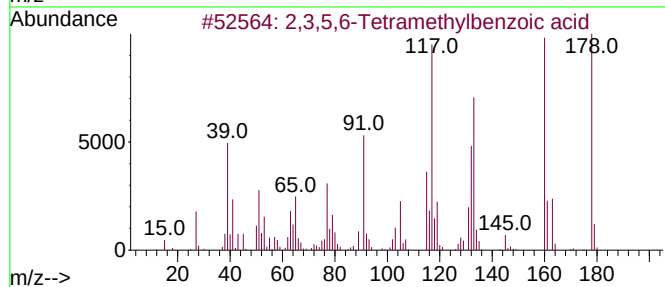
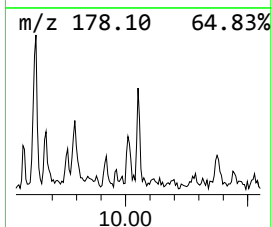
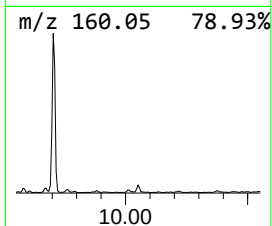
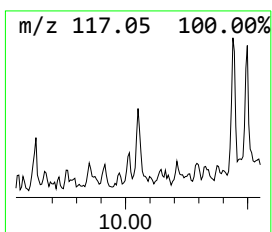
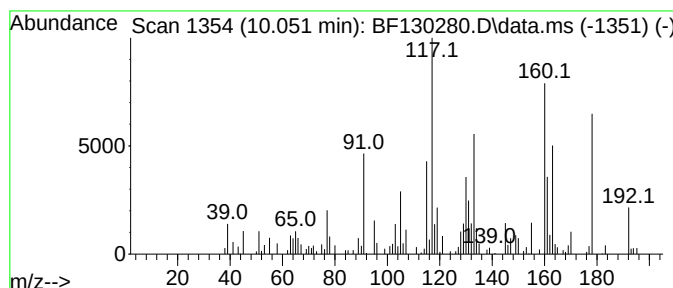
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TIC Integration Parameters: LSCINT.P

Peak Number 3 2,3,5,6-Tetramethylbenzoic ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.051	2.01 ng	82485	Acenaphthene-d10	9.704	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3,5,6-Tetramethylbenzoic acid	178	C11H14O2	002604-45-7	62
2	1H-Inden-1-one, 2,3-dihydro-5,7-...	160	C11H12O	006682-69-5	43
3	1H-Inden-1-one, 2,3-dihydro-4,7-...	160	C11H12O	005037-60-5	43
4	7-Methoxy-1-indanone oxime, (E)-	177	C10H11NO2	179899-16-2	30
5	6-Methylquinazolin-4(3H)-one	160	C9H8N2O	019181-53-4	18



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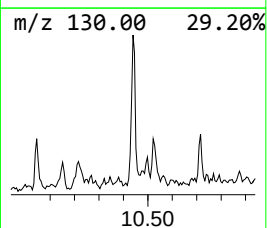
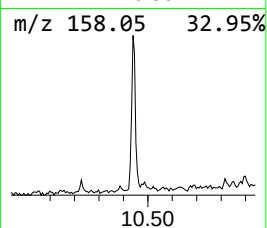
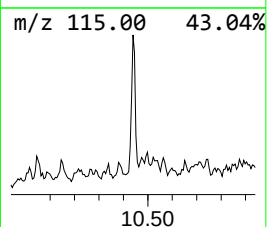
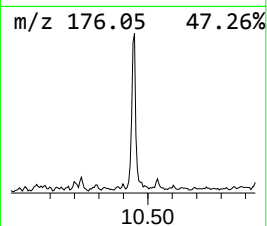
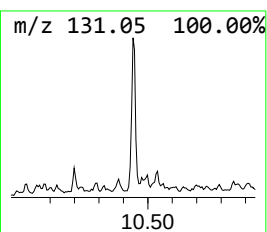
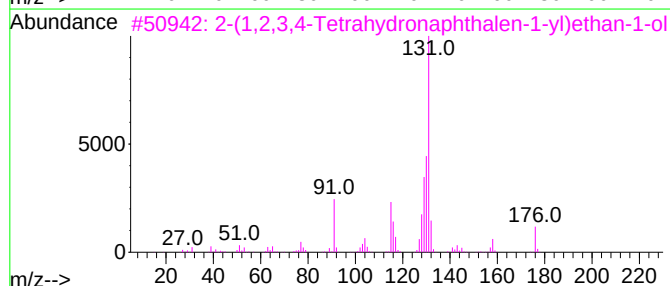
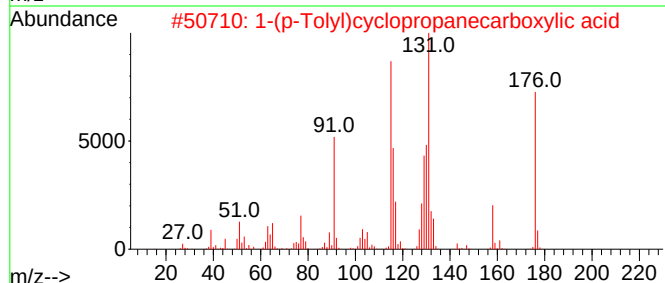
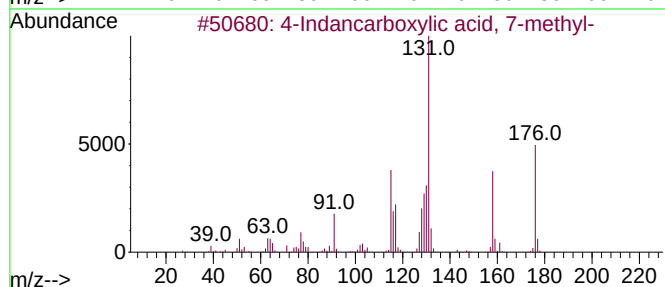
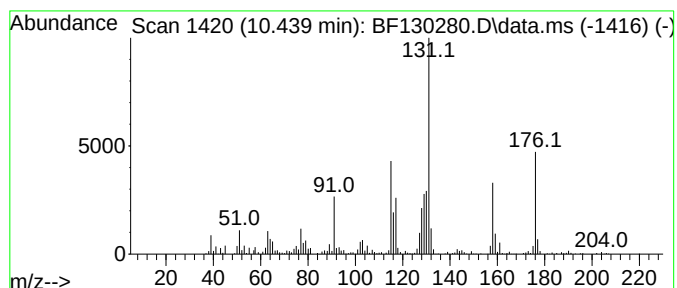
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Peak Number 4 4-Indancarboxylic acid, 7-m... Concentration Rank 1

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10.439	8.23 ng	337972	Acenaphthene-d10	9.704	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Indancarboxylic acid, 7-methyl-	176	C11H12O2	071042-74-5	98
2	1-(p-Tolyl)cyclopropanecarboxyli...	176	C11H12O2	083846-66-6	70
3	2-(1,2,3,4-Tetrahydronaphthalen-...	176	C12H16O	068480-12-6	60
4	1-Naphthalenecarboxylic acid, 5,...	176	C11H12O2	004242-18-6	59
5	2,3-Dihydro-1H-inden-5-ylacetic ...	176	C11H12O2	005453-98-5	58



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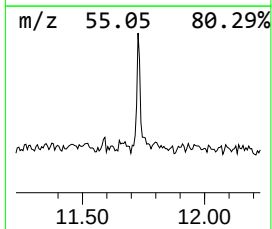
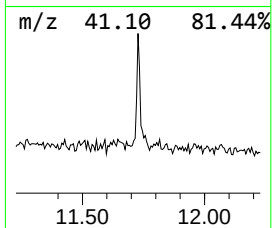
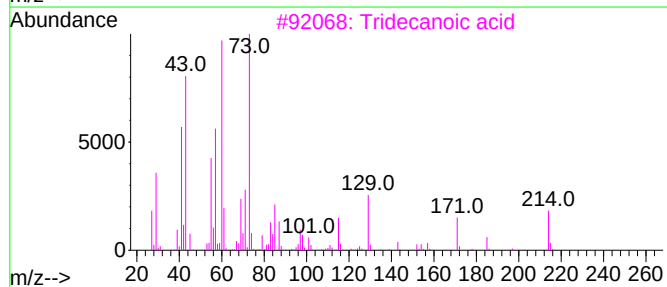
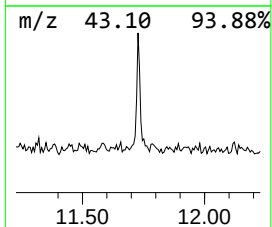
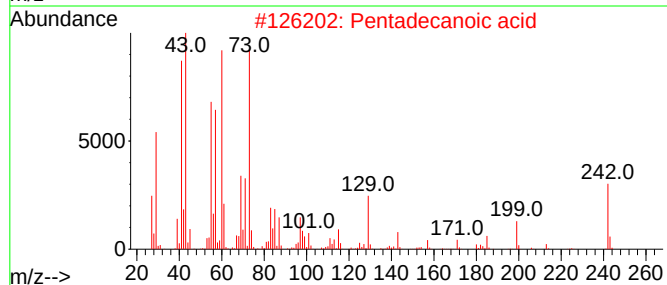
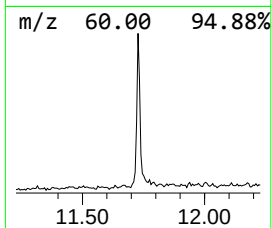
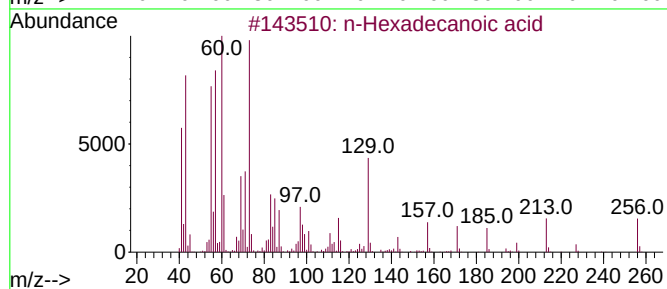
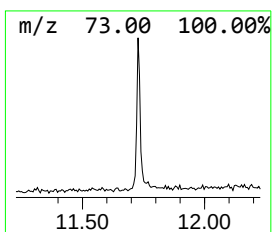
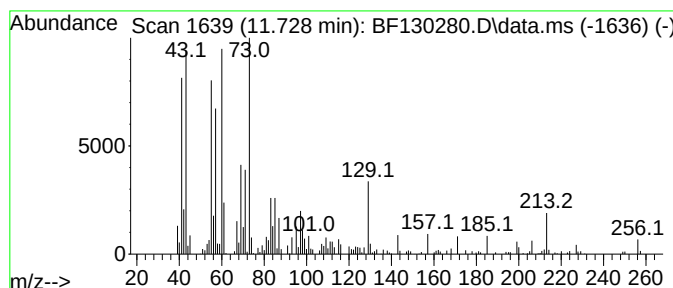
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.727	5.47 ng	212597	Phenanthrene-d10	11.186

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	87
4			Dodecanoic acid	200	C12H24O2	000143-07-7	80
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	80



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ALS Vial : 19 Sample Multiplier: 1

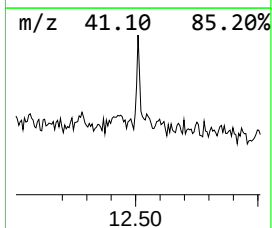
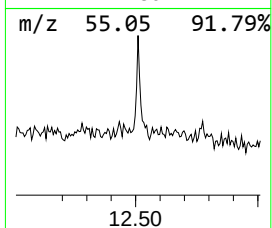
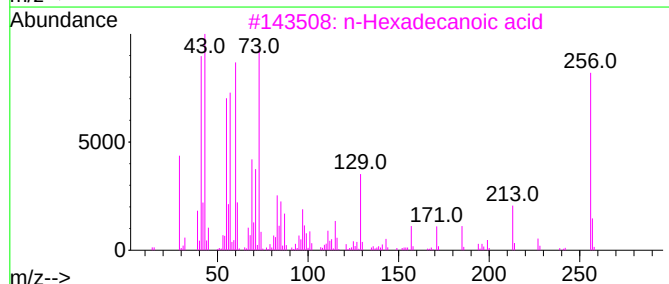
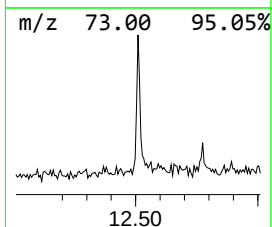
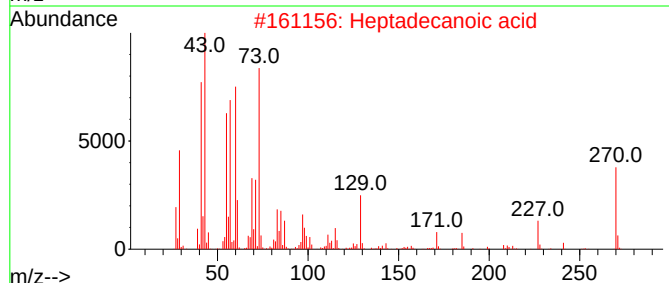
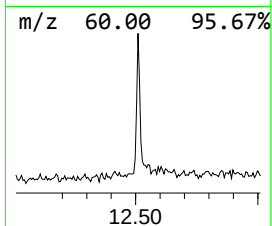
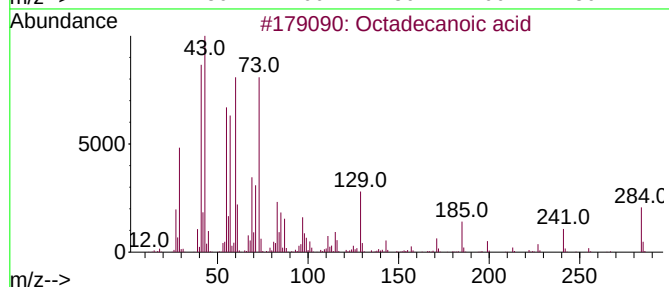
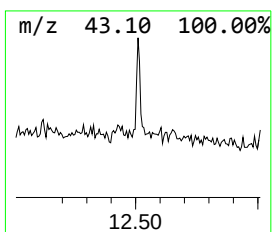
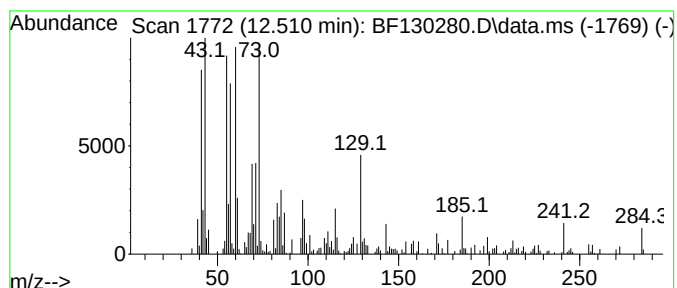
Instrument :
BNA_F
ClientSampleId :
MW-49

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.510	5.71 ng	124690	Chrysene-d12	13.816	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	Heptadecanoic acid	270	C17H34O2	000506-12-7	94
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Dodecanoic acid	200	C12H24O2	000143-07-7	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091522\
Data File : BF130280.D
Acq On : 15 Sep 2022 19:56
Operator : CG\JU
Sample : N4549-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-49

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.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-...	4.863	3.2	ng	96668	1	6.675	596588	20.0
Benzoic acid, p...	9.634	5.3	ng	218533	3	9.704	821671	20.0
2,3,5,6-Tetrame...	10.051	2.0	ng	82485	3	9.704	821671	20.0
4-Indancarboxyl...	10.439	8.2	ng	337972	3	9.704	821671	20.0
n-Hexadecanoic ...	11.727	5.5	ng	212597	4	11.186	777555	20.0
Octadecanoic acid	12.510	5.7	ng	124690	5	13.816	436846	20.0