

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
 Data File : BF130201.D
 Acq On : 09 Sep 2022 18:36
 Operator : CG\JU
 Sample : N4549-04
 Misc :
 ALS Vial : 11 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-BF083122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130201.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.875	437	440	447	rBV	79280	93608	2.67%	0.522%
2	5.293	506	511	514	rBV	1781886	1568051	44.79%	8.752%
3	6.322	682	686	697	rVB	1097526	1002166	28.63%	5.594%
4	6.692	745	749	752	rBV	835834	609087	17.40%	3.400%
5	7.257	840	845	848	rBV	2113701	1975771	56.43%	11.028%
6	7.563	892	897	904	rBV5	33901	61871	1.77%	0.345%
7	7.716	918	923	927	rBV6	28528	41596	1.19%	0.232%
8	7.892	950	953	963	rVB2	75267	126719	3.62%	0.707%
9	7.975	963	967	970	rBV	961377	798810	22.82%	4.459%
10	9.051	1145	1150	1153	rBV	4222237	3501016	100.00%	19.542%
11	9.469	1218	1221	1225	rVB4	32719	43621	1.25%	0.243%
12	9.633	1245	1249	1255	rBV	171759	198707	5.68%	1.109%
13	9.722	1260	1264	1268	rVV	972110	789688	22.56%	4.408%
14	9.798	1275	1277	1284	rVB3	34351	41171	1.18%	0.230%
15	10.010	1311	1313	1317	rBV4	40893	49105	1.40%	0.274%
16	10.298	1360	1362	1365	rBV4	44221	47988	1.37%	0.268%
17	10.445	1383	1387	1392	rBV	228971	264677	7.56%	1.477%
18	10.510	1392	1398	1401	rBV	2330352	1984152	56.67%	11.075%
19	11.204	1513	1516	1519	rBV	771737	637223	18.20%	3.557%
20	11.745	1605	1608	1612	rVB	144983	135463	3.87%	0.756%
21	12.527	1738	1741	1746	rBV2	100860	93291	2.66%	0.521%
22	12.792	1781	1786	1789	rBV	2844809	2511544	71.74%	14.019%
23	13.727	1943	1945	1951	rVB5	41657	48809	1.39%	0.272%
24	13.833	1959	1963	1966	rBV	606626	530239	15.15%	2.960%
25	14.651	2099	2102	2109	rVB3	51806	55346	1.58%	0.309%
26	15.233	2196	2201	2205	rBV	597433	661800	18.90%	3.694%
27	15.674	2274	2276	2285	rVB4	30217	44062	1.26%	0.246%

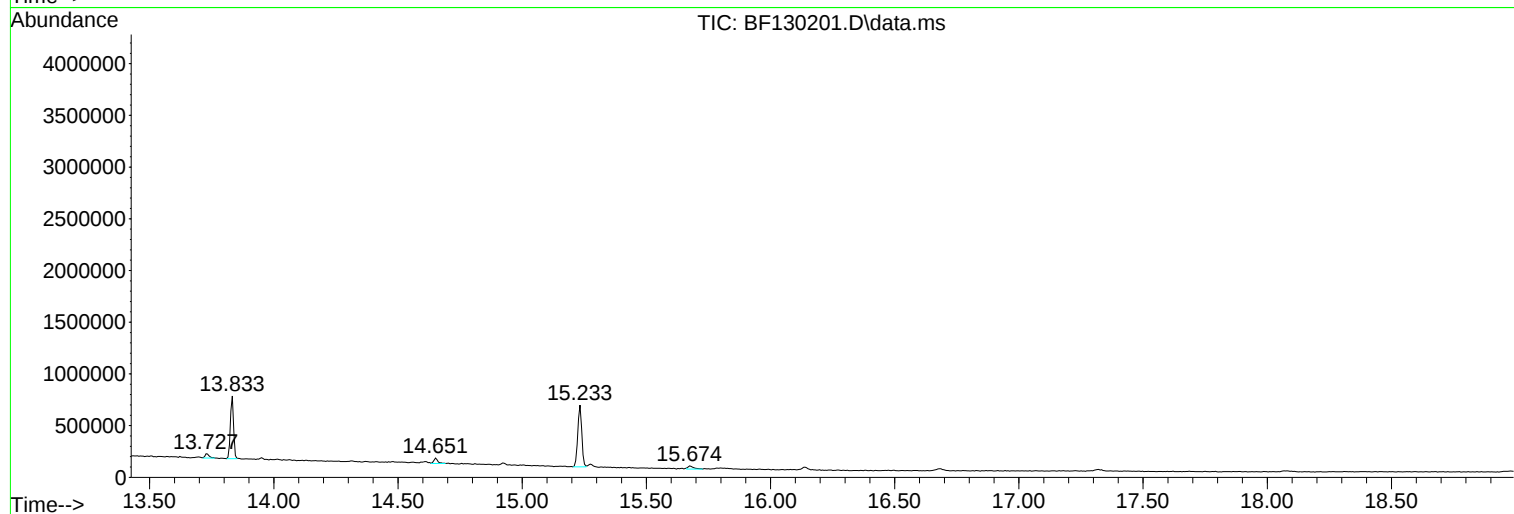
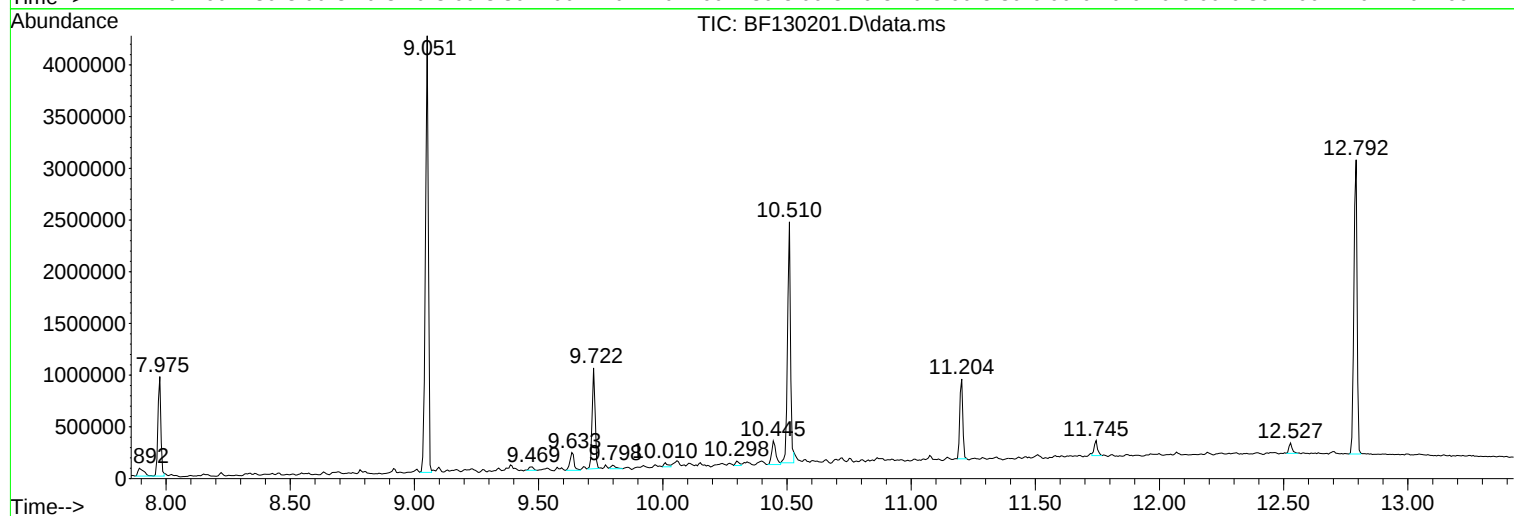
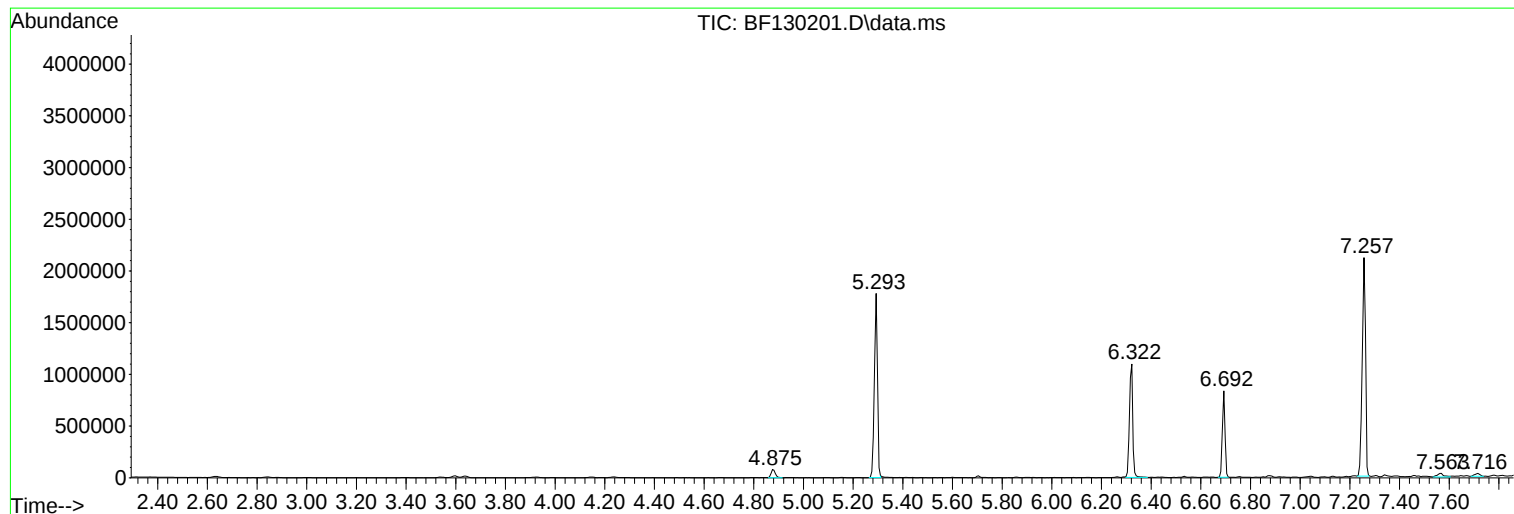
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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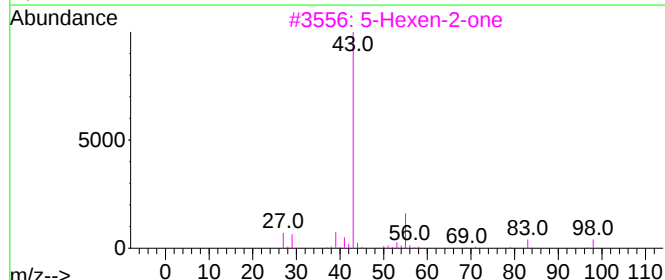
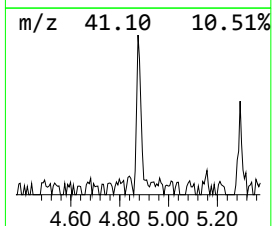
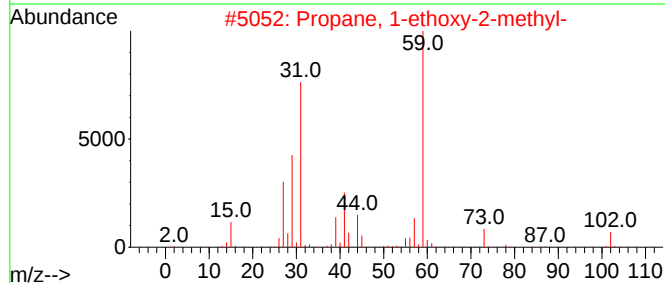
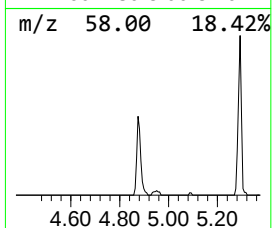
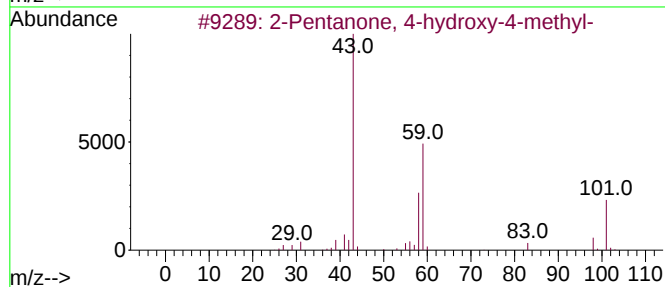
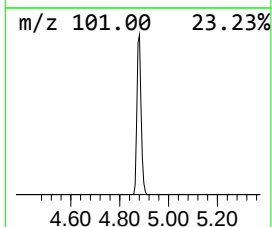
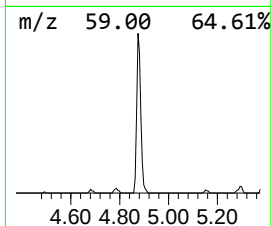
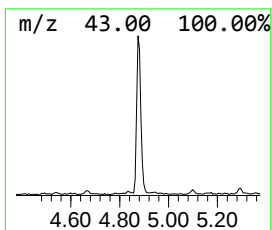
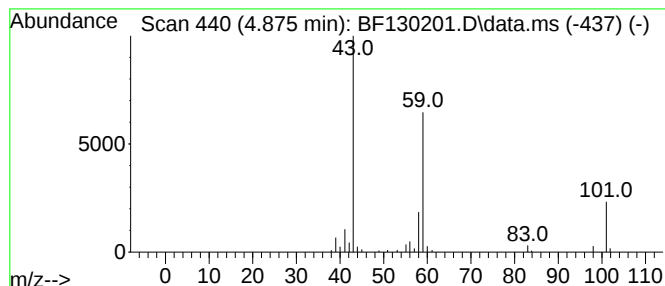
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.875	3.07 ng	93608	1,4-Dichlorobenzene-d4	6.692

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	17
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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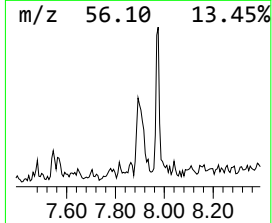
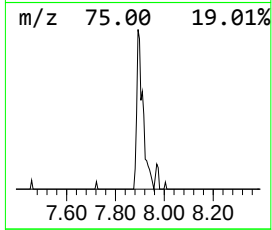
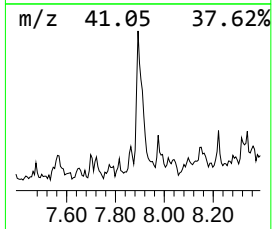
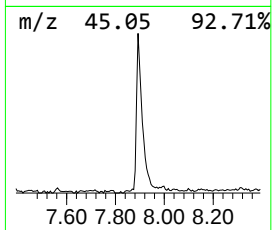
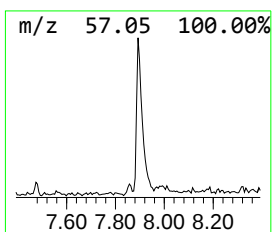
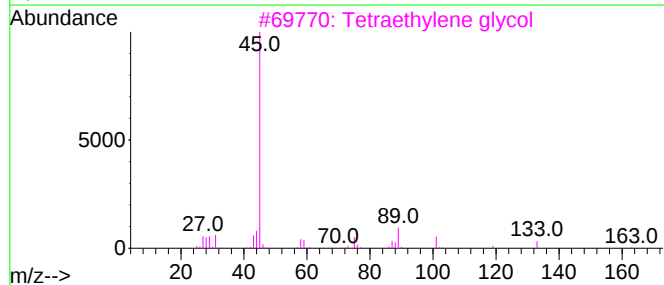
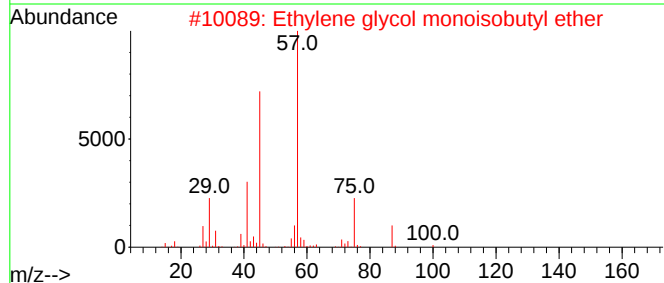
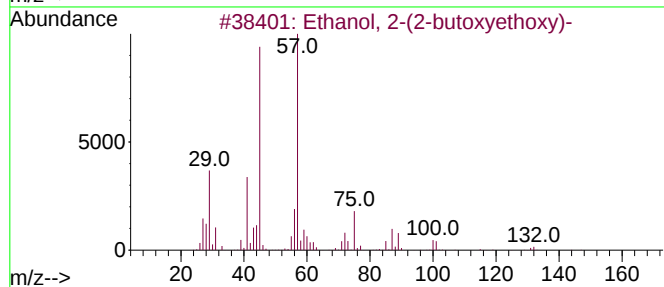
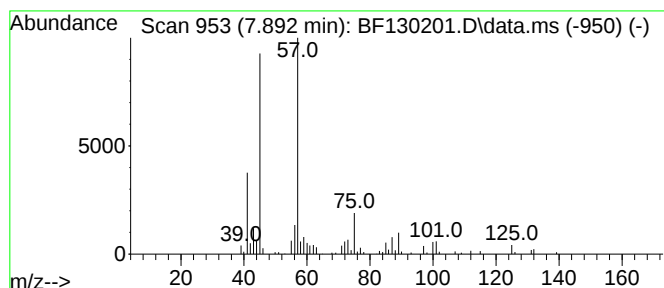
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.892	3.17 ng	126719	Naphthalene-d8	7.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	86
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
3			Tetraethylene glycol	194	C8H18O5	000112-60-7	53
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50
5			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50



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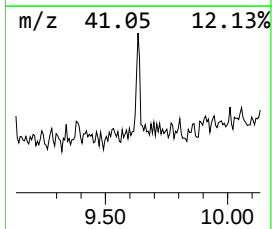
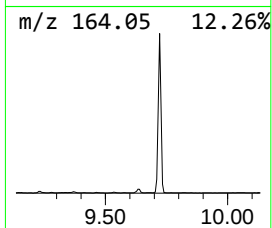
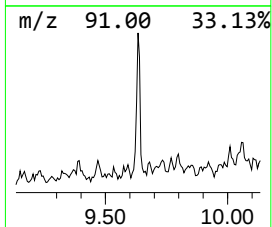
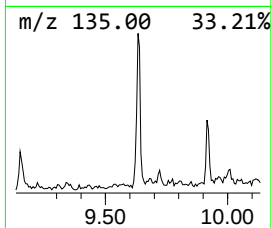
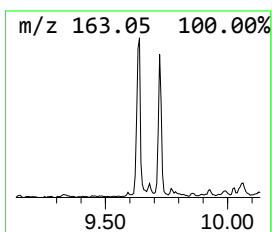
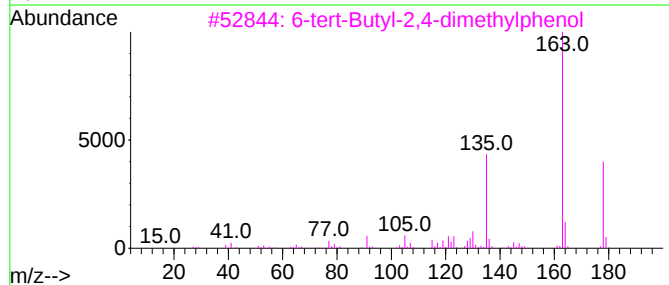
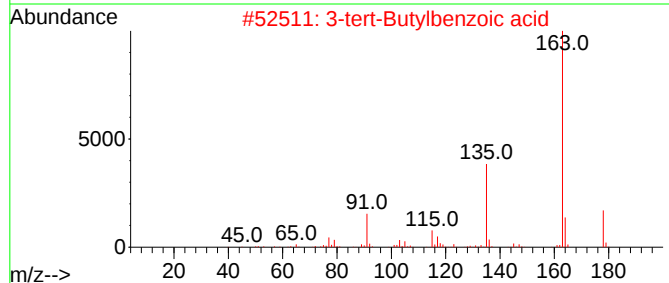
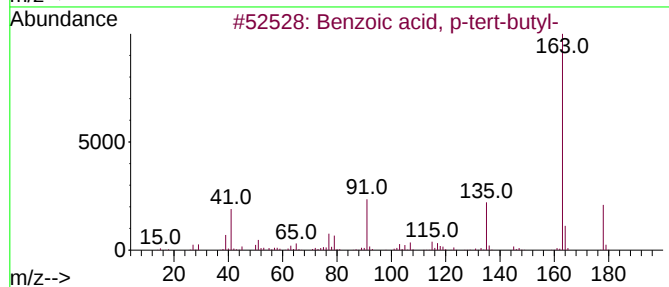
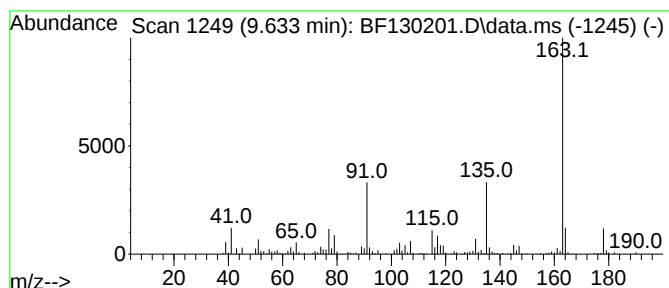
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzoic acid, p-tert-butyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.633	5.03 ng	198707	Acenaphthene-d10	9.722

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	94
2			3-tert-Butylbenzoic acid	178	C11H14O2	007498-54-6	80
3			6-tert-Butyl-2,4-dimethylphenol	178	C12H18O	001879-09-0	80
4			Benzoic acid, 4-acetyl-, methyl ...	178	C10H10O3	003609-53-8	64
5			2,4-Diamino-3,5-diethyltoluene	178	C11H18N2	002095-02-5	64



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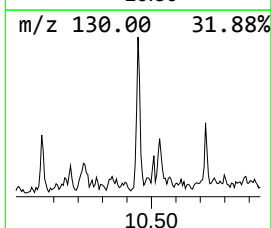
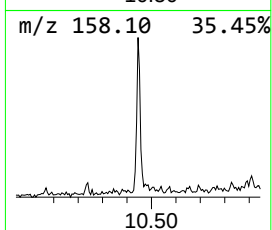
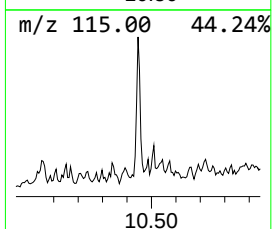
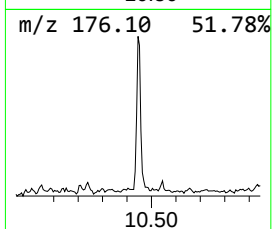
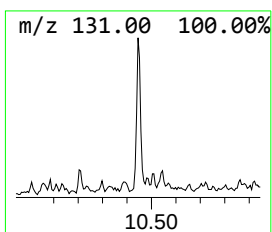
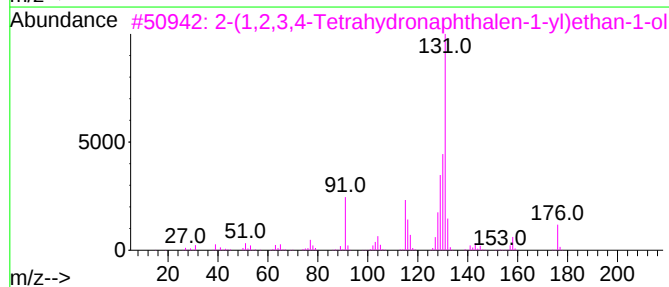
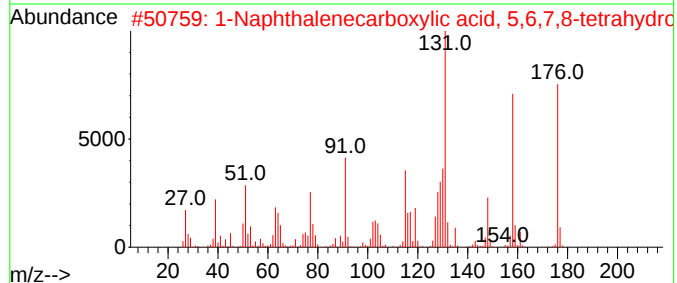
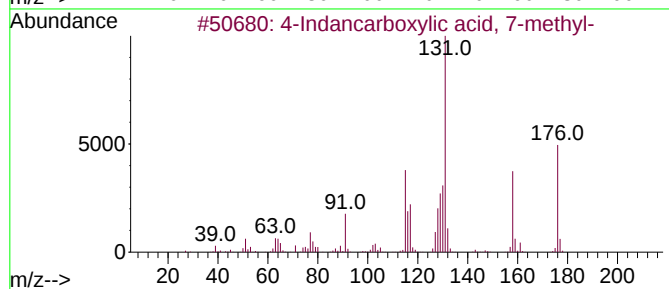
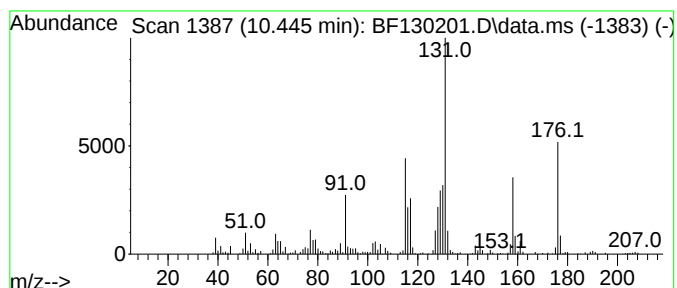
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Peak Number 4 4-Indancarboxylic acid, 7-m... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.445	6.70 ng	264677	Acenaphthene-d10	9.722	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Indancarboxylic acid, 7-methyl-	176	C11H12O2	071042-74-5	98
2	1-Naphthalenecarboxylic acid, 5,...	176	C11H12O2	004242-18-6	95
3	2-(1,2,3,4-Tetrahydronaphthalen-...	176	C12H16O	068480-12-6	87
4	1-(p-Tolyl)cyclopropanecarboxyli...	176	C11H12O2	083846-66-6	50
5	1,2,3,4-Tetrahydro-1-naphthalene...	164	C10H12S	103324-34-1	47



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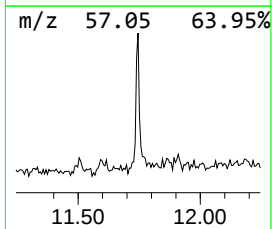
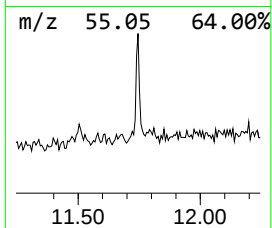
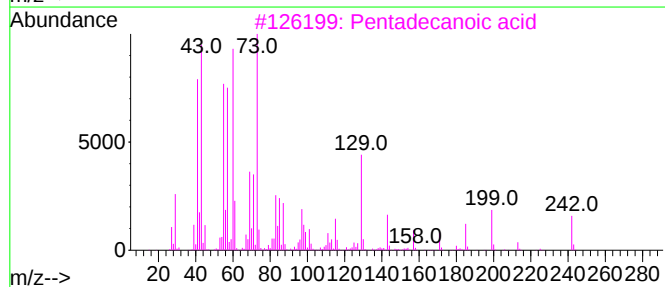
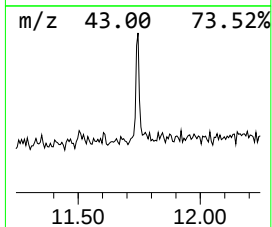
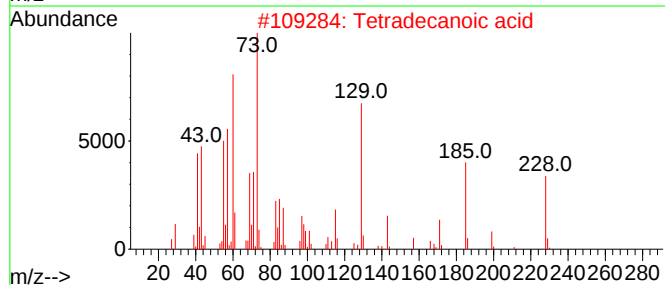
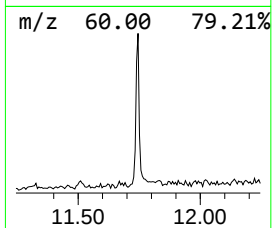
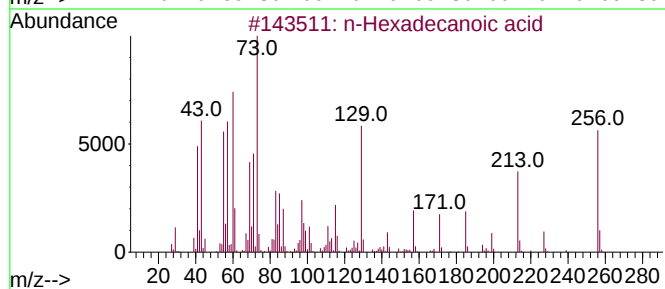
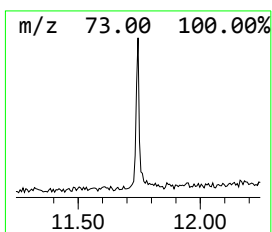
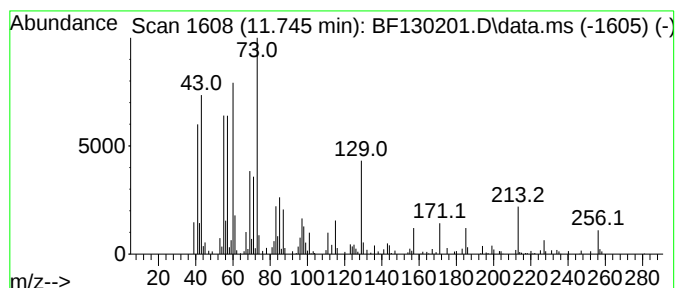
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.745	4.25 ng	135463	Phenanthrene-d10	11.204

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Dodecanoic acid	200	C12H24O2	000143-07-7	72
5			Undecanoic acid	186	C11H22O2	000112-37-8	68



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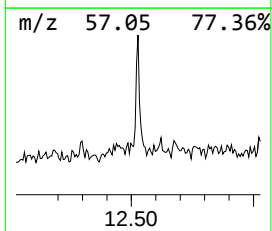
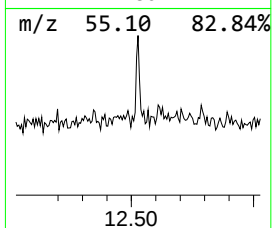
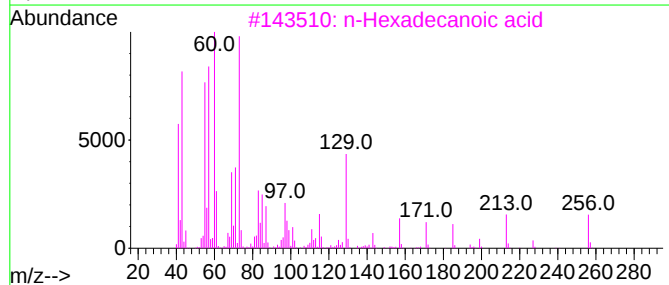
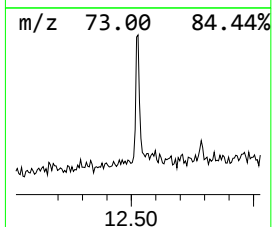
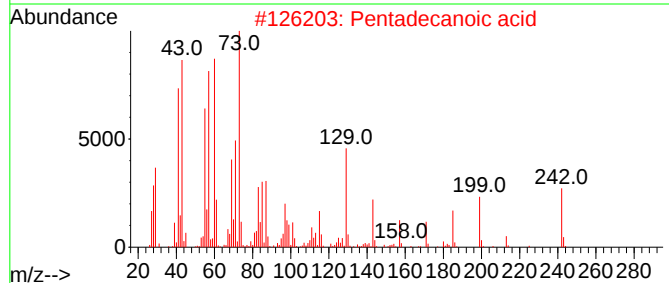
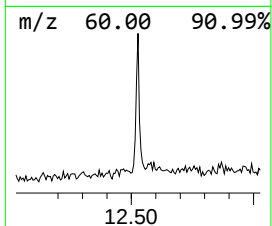
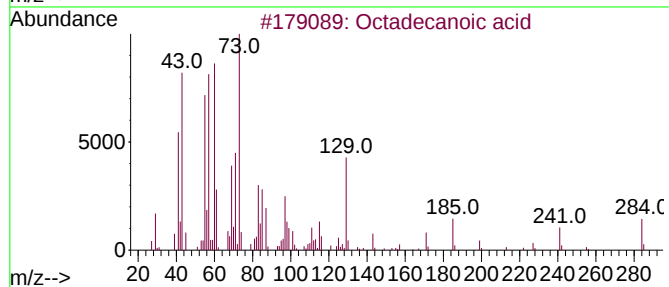
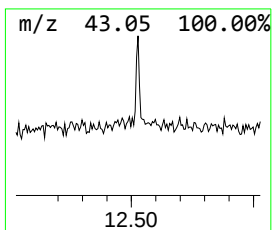
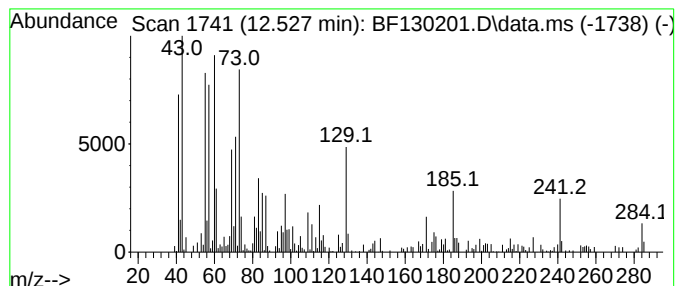
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.527	3.52 ng	93291	Chrysene-d12	13.833

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
4			Heptadecanoic acid	270	C17H34O2	000506-12-7	74
5			Heptadecane	240	C17H36	000629-78-7	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130201.D
Acq On : 09 Sep 2022 18:36
Operator : CG\JU
Sample : N4549-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-49

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.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
2-Pentanone, 4-...	4.875	3.1	ng	93608	1	6.692	609087	20.0
Ethanol, 2-(2-b...	7.892	3.2	ng	126719	2	7.975	798810	20.0
Benzoic acid, p...	9.633	5.0	ng	198707	3	9.722	789688	20.0
4-Indancarboxyl...	10.445	6.7	ng	264677	3	9.722	789688	20.0
n-Hexadecanoic ...	11.745	4.3	ng	135463	4	11.204	637223	20.0
Octadecanoic acid	12.527	3.5	ng	93291	5	13.833	530239	20.0