

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011022\
 Data File : BF126576.D
 Acq On : 10 Jan 2022 19:42
 Operator : JU/CG
 Sample : N1054-18
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20220024-CAPE-6-MODIFIED-ELUTRIATE

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-BF122921.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126576.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.969	487	490	500	rVB	38535	52219	1.99%	0.353%
2	5.386	556	561	564	rBV	1478752	1424998	54.30%	9.631%
3	6.398	729	733	745	rBV	1297785	1254748	47.81%	8.481%
4	6.769	792	796	799	rBV	597584	487960	18.59%	3.298%
5	7.333	886	892	895	rBV	1671224	1680370	64.03%	11.357%
6	7.957	995	998	1007	rBV	116104	103085	3.93%	0.697%
7	8.051	1010	1014	1017	rBV	828297	682303	26.00%	4.612%
8	8.327	1058	1061	1064	rVB	41170	32525	1.24%	0.220%
9	9.133	1192	1198	1201	rBV	2762110	2624466	100.00%	17.738%
10	9.521	1261	1264	1267	rBV	164836	140156	5.34%	0.947%
11	9.810	1308	1313	1316	rBV	788022	722713	27.54%	4.885%
12	10.227	1380	1384	1386	rBV2	27366	27932	1.06%	0.189%
13	10.598	1442	1447	1451	rBV	1609340	1588240	60.52%	10.735%
14	10.704	1462	1465	1472	rVB	84952	70175	2.67%	0.474%
15	11.292	1561	1565	1569	rBV	762558	657779	25.06%	4.446%
16	11.686	1628	1632	1637	rVB3	23938	31142	1.19%	0.210%
17	11.833	1653	1657	1661	rBV	105188	110282	4.20%	0.745%
18	12.621	1786	1791	1800	rBV2	35791	51130	1.95%	0.346%
19	12.886	1831	1836	1839	rBV	2091781	1917243	73.05%	12.958%
20	13.792	1983	1990	2006	rBV	117121	186173	7.09%	1.258%
21	13.939	2011	2015	2018	rBV	434829	408908	15.58%	2.764%
22	14.033	2027	2031	2037	rBV	68380	71592	2.73%	0.484%
23	15.386	2256	2261	2265	rBV	389384	440384	16.78%	2.977%
24	15.921	2345	2352	2356	rBV5	12580	28817	1.10%	0.195%

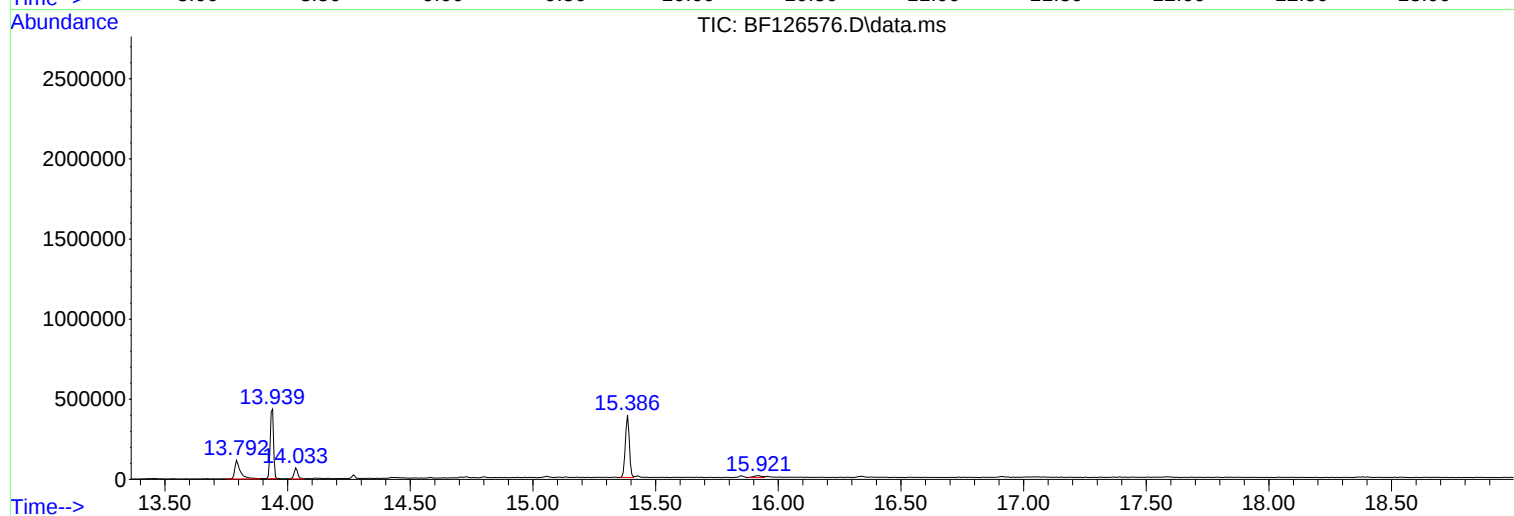
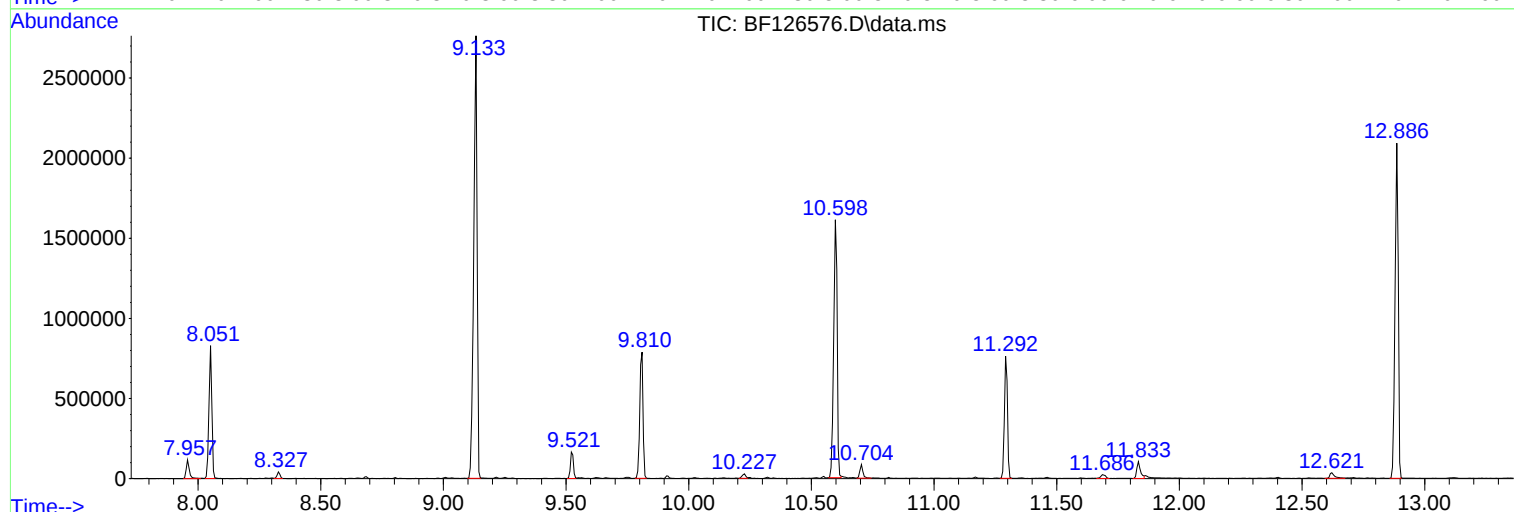
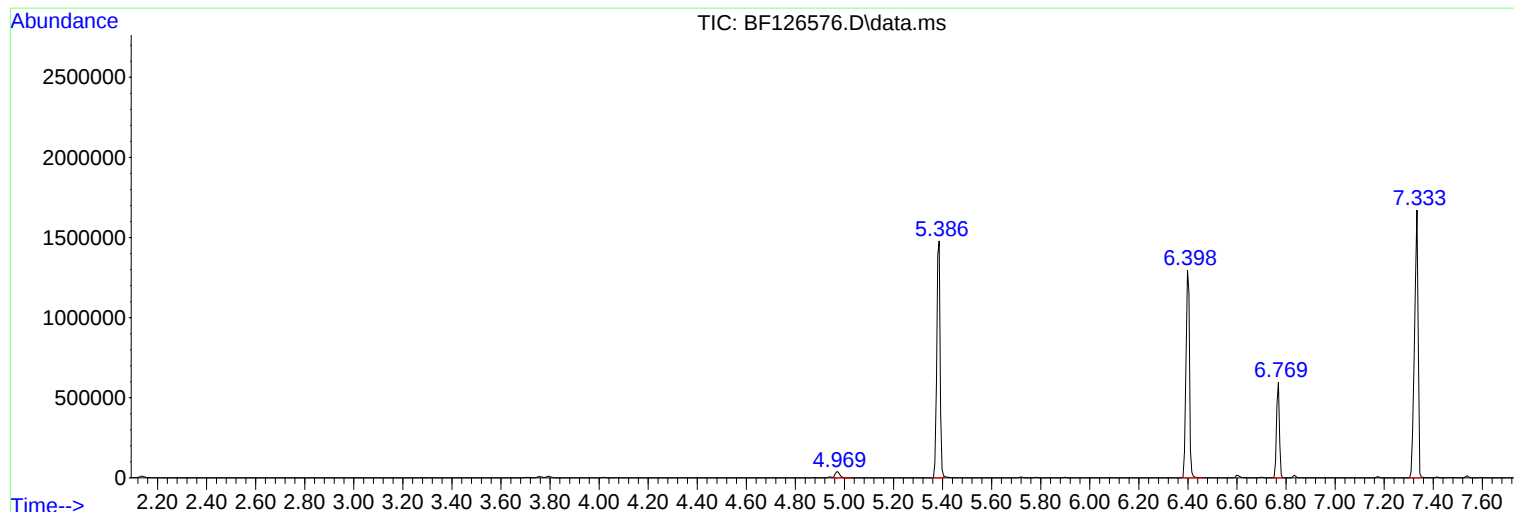
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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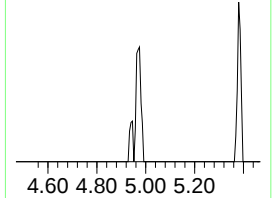
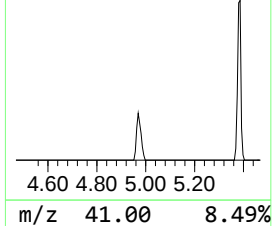
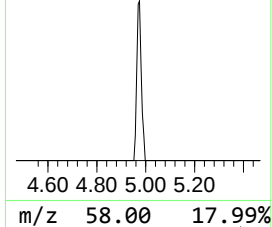
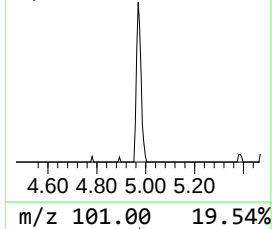
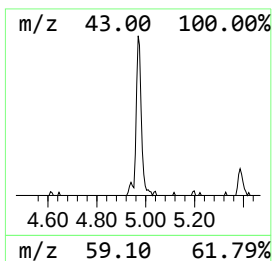
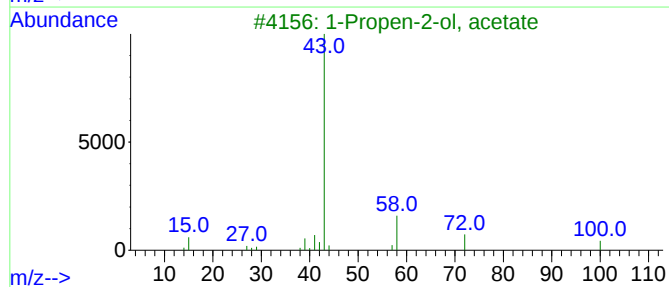
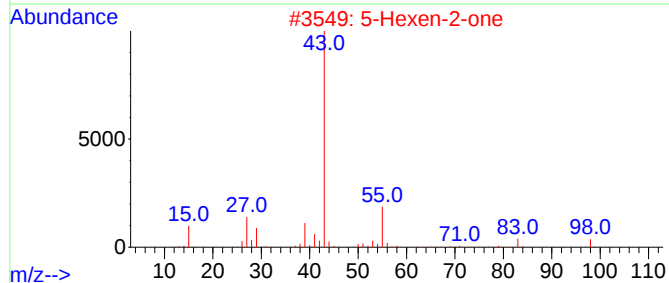
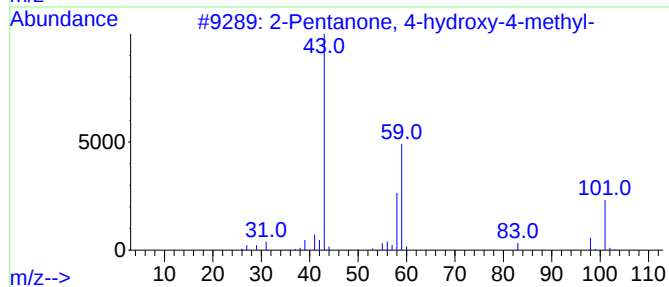
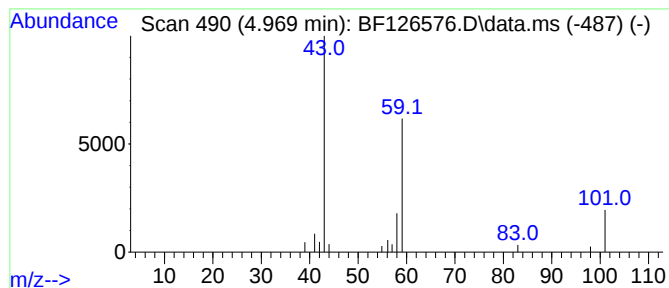
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.969	2.14 ng	52219	1,4-Dichlorobenzene-d4	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9		
4	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	9		
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9		



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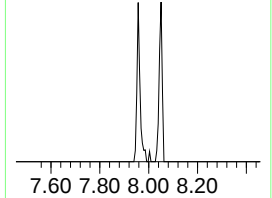
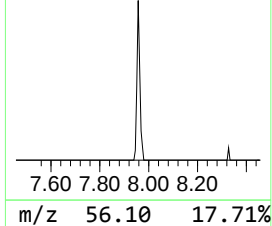
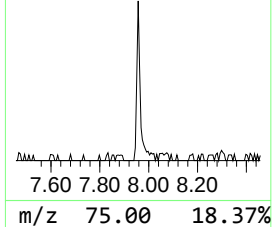
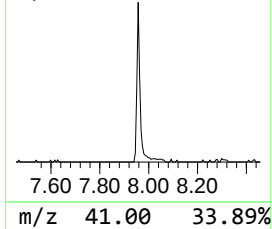
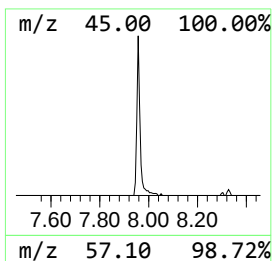
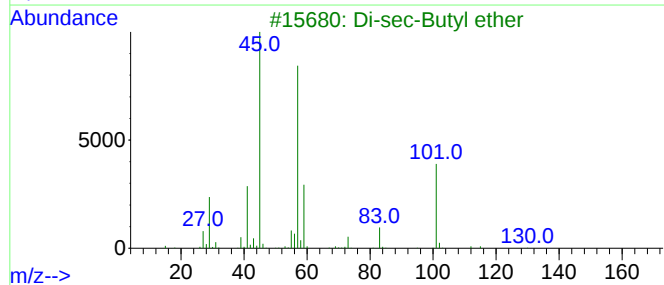
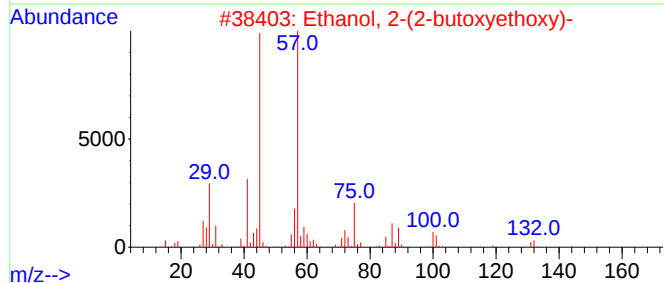
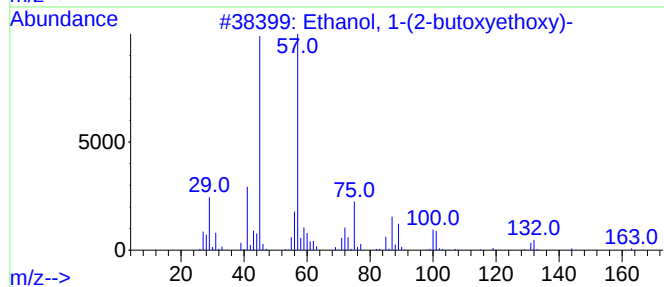
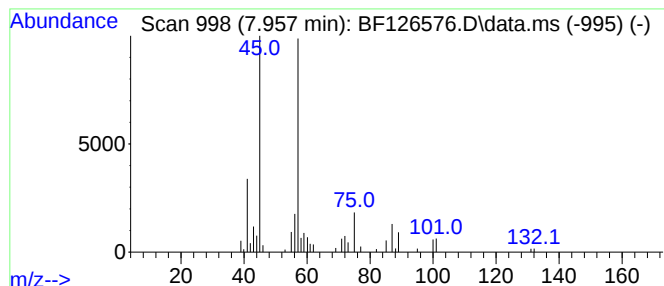
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Peak Number 2 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.957	3.02 ng	103085	Naphthalene-d8	8.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
2			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
3			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50
5			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	50



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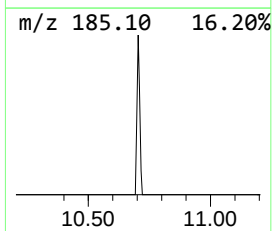
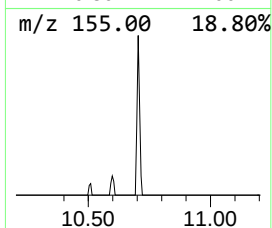
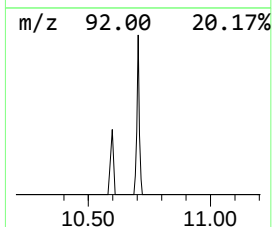
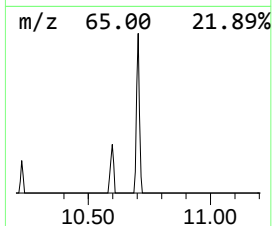
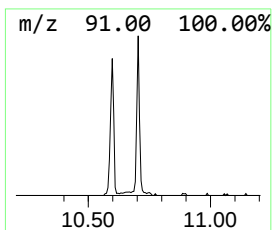
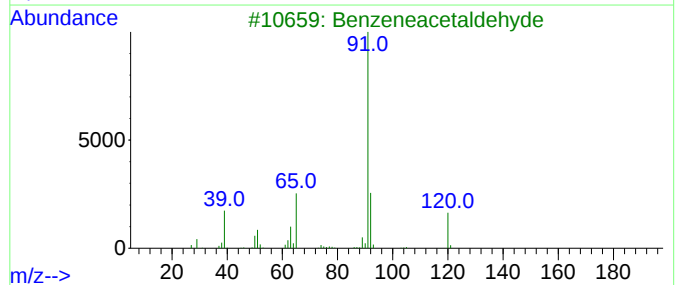
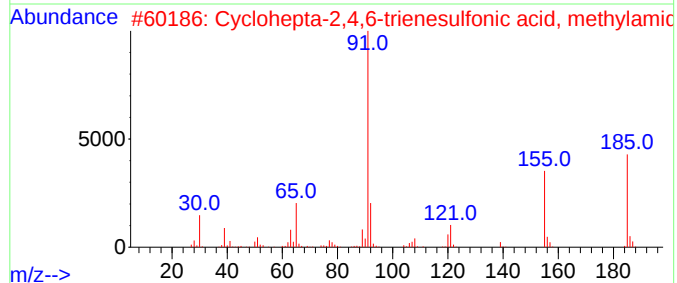
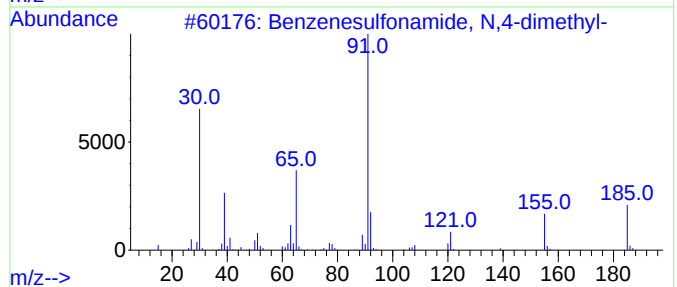
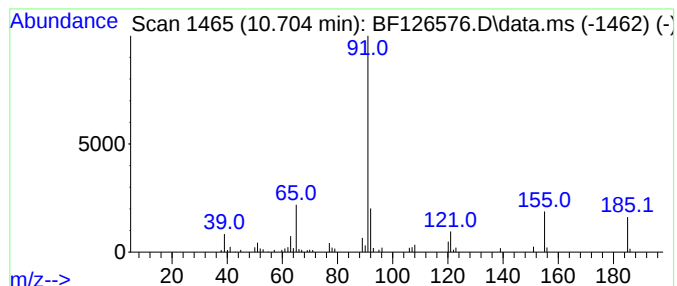
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzenesulfonamide, N,4-dim... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.704	2.13 ng	70175	Phenanthrene-d10	11.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	95
2			Cyclohepta-2,4,6-trienesulfonic ...	185	C8H11NO2S	1000187-28-7	58
3			Benzeneacetaldehyde	120	C8H8O	000122-78-1	53
4			Tetracyclo[3.2.0.0(2,7).0(4,6)]h...	92	C7H8	000278-06-8	46
5			phosphonic acid, P-ethyl-, bis(p...	290	C16H19O3P	1000402-03-1	43



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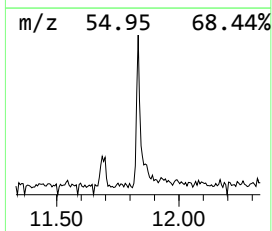
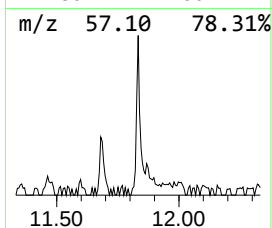
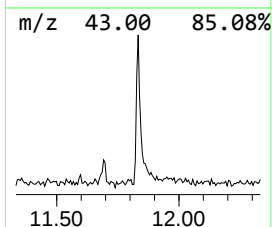
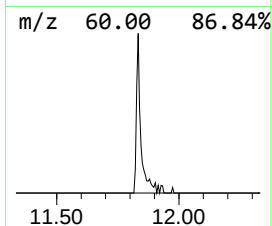
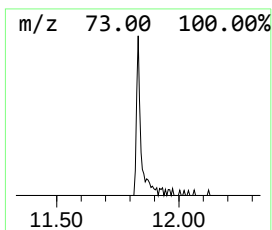
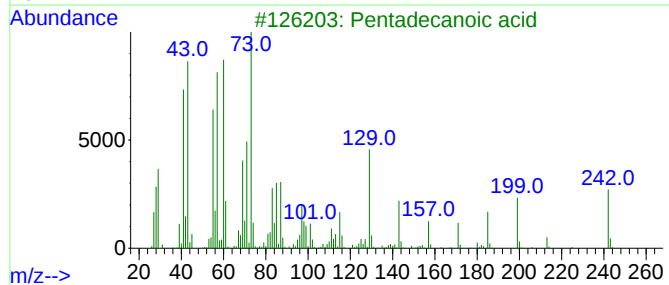
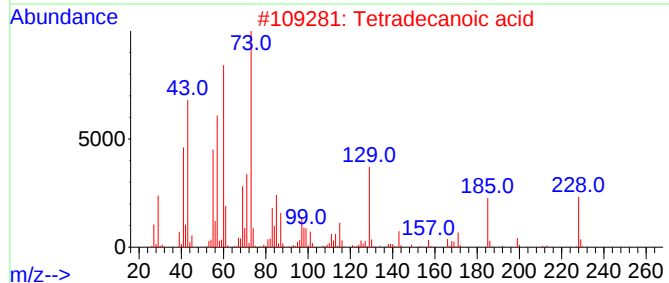
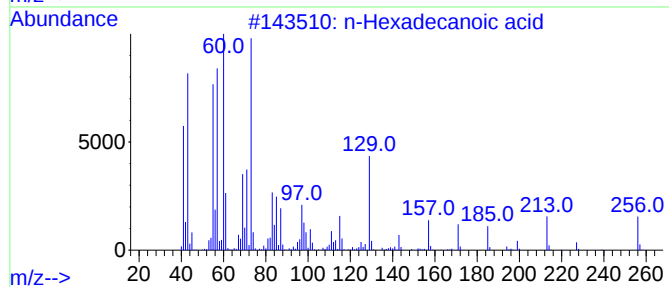
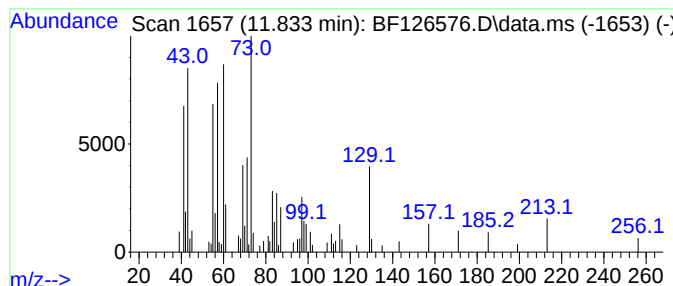
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.833	3.35 ng	110282	Phenanthrene-d10	11.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Tridecanoic acid	214	C13H26O2	000638-53-9	80
5			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	11



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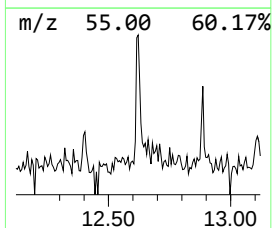
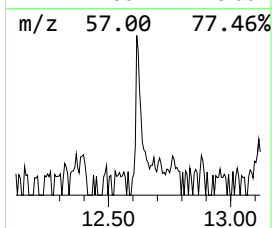
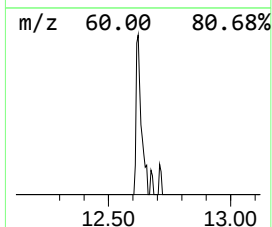
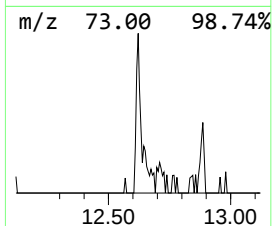
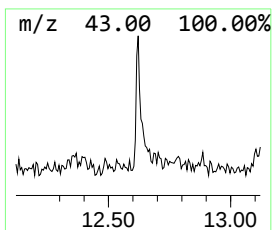
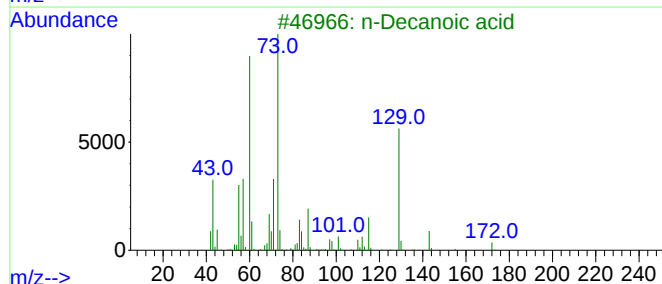
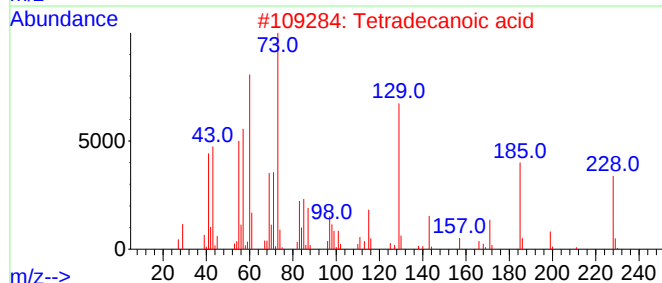
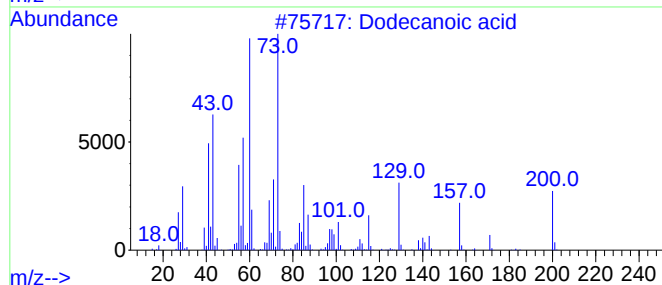
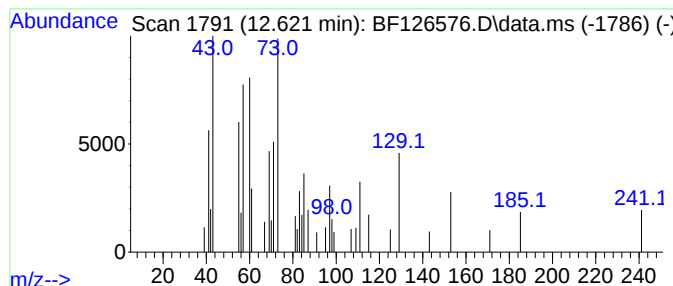
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Peak Number 5 Dodecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.621	2.50 ng	51130	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	53
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	53
3			n-Decanoic acid	172	C10H20O2	000334-48-5	47
4			1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	18
5			1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	18



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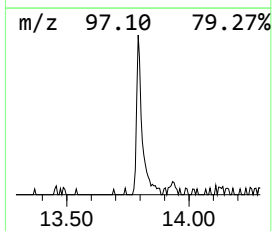
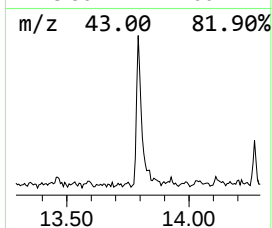
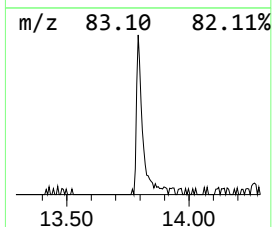
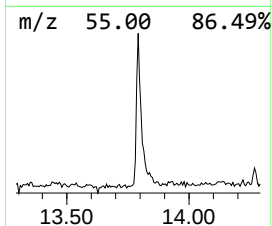
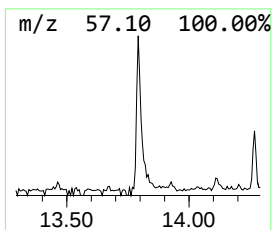
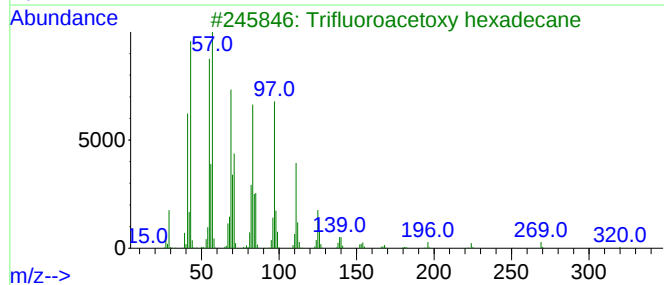
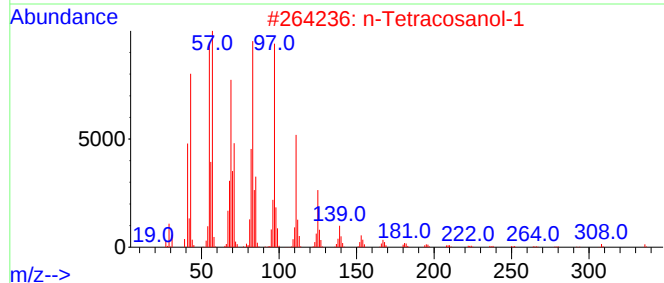
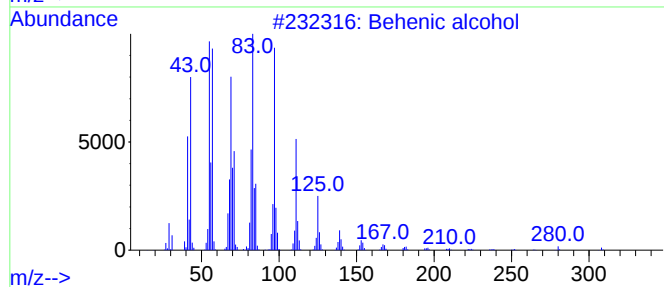
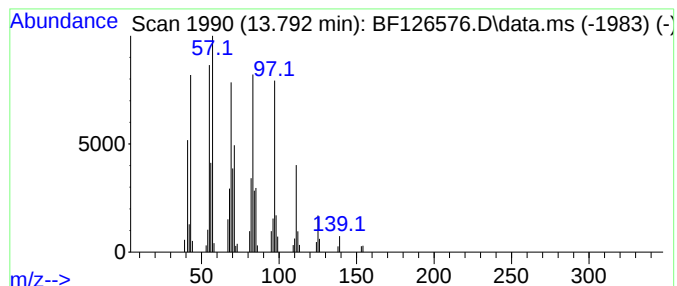
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Behenic alcohol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.792	9.11 ng	186173	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	94
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
4			1-Nonadecene	266	C19H38	018435-45-5	91
5			3-Eicosene, (E)-	280	C20H40	074685-33-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011022\
Data File : BF126576.D
Acq On : 10 Jan 2022 19:42
Operator : JU/CG
Sample : N1054-18
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220024-CAPE-6-MODIFIED-ELUTRIATE

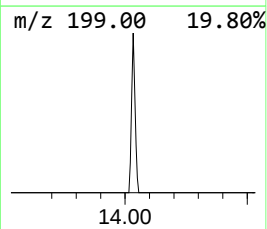
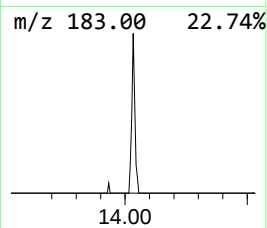
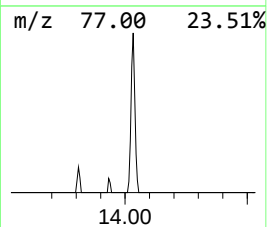
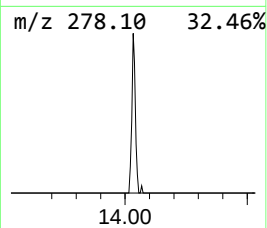
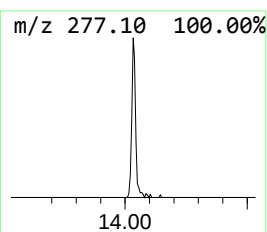
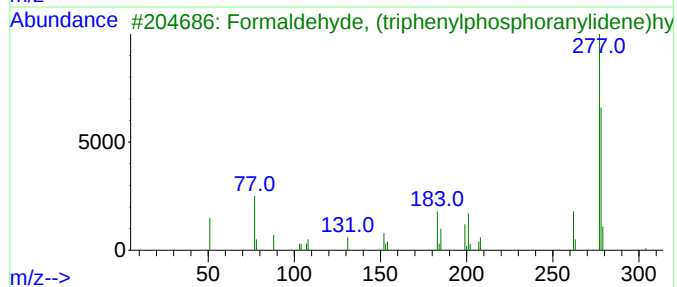
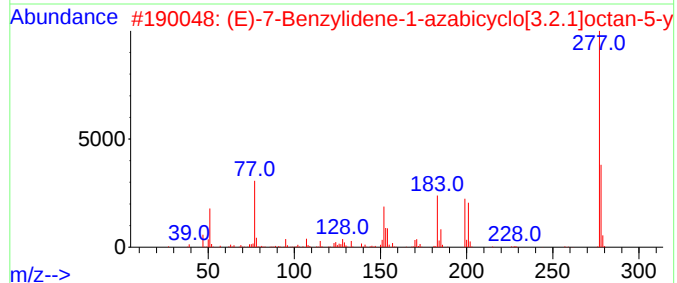
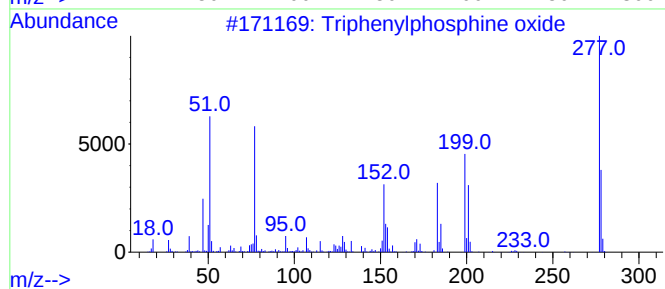
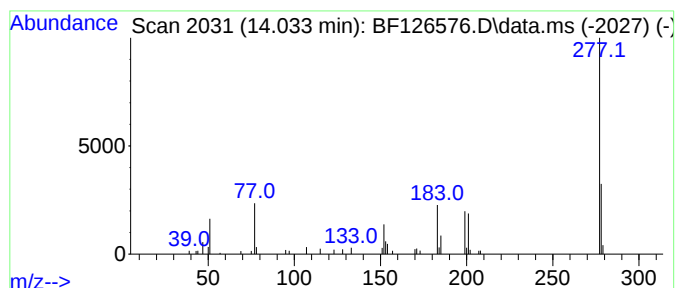
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.033	3.50 ng	71592	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	52
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	43
5			Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011022\
Data File : BF126576.D
Acq On : 10 Jan 2022 19:42
Operator : JU/CG
Sample : N1054-18
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220024-CAPE-6-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.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-...	4.969	2.1	ng	52219	1	6.769	487960	20.0
Ethanol, 1-(2-b...	7.957	3.0	ng	103085	2	8.051	682303	20.0
Benzenesulfonam...	10.704	2.1	ng	70175	4	11.292	657779	20.0
n-Hexadecanoic ...	11.833	3.4	ng	110282	4	11.292	657779	20.0
Dodecanoic acid	12.621	2.5	ng	51130	5	13.939	408908	20.0
Behenic alcohol	13.792	9.1	ng	186173	5	13.939	408908	20.0
Triphenylphosph...	14.033	3.5	ng	71592	5	13.939	408908	20.0