

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
 Data File : BF130198.D
 Acq On : 09 Sep 2022 16:58
 Operator : CG\JU
 Sample : N4549-12
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-56

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: BF130198.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.863	92	98	105	rBV	72124	122028	1.98%	0.372%
2	4.157	311	318	326	rBV2	49104	80014	1.30%	0.244%
3	4.881	437	441	447	rBV	220366	237555	3.85%	0.724%
4	5.293	507	511	515	rBV	2199871	2000413	32.44%	6.101%
5	6.322	682	686	691	rVB	1271150	1188514	19.27%	3.625%
6	6.692	745	749	752	rBV	1180520	908990	14.74%	2.772%
7	7.263	838	846	848	rVB	3039649	3373309	54.70%	10.288%
8	7.463	874	880	884	rVB3	72926	89684	1.45%	0.274%
9	7.892	950	953	963	rBV2	121614	264150	4.28%	0.806%
10	7.975	963	967	970	rBV	1856943	1517762	24.61%	4.629%
11	8.534	1059	1062	1065	rBV	74419	66685	1.08%	0.203%
12	8.669	1083	1085	1093	rBV	44298	67422	1.09%	0.206%
13	8.898	1119	1124	1129	rVB4	45981	67167	1.09%	0.205%
14	9.051	1145	1150	1153	rBV	6057730	6167329	100.00%	18.809%
15	9.498	1223	1226	1228	rBV	97537	69516	1.13%	0.212%
16	9.581	1237	1240	1244	rBV2	129853	117509	1.91%	0.358%
17	9.722	1258	1264	1267	rBV	1962532	1709971	27.73%	5.215%
18	9.757	1267	1270	1273	rVB	89334	92326	1.50%	0.282%
19	9.928	1296	1299	1302	rBV2	68818	73345	1.19%	0.224%
20	10.039	1315	1318	1323	rVB3	56312	76576	1.24%	0.234%
21	10.333	1363	1368	1374	rBV2	226820	242633	3.93%	0.740%
22	10.510	1391	1398	1402	rBV	4098323	4078244	66.13%	12.438%
23	10.804	1444	1448	1452	rVB2	46727	82791	1.34%	0.252%
24	10.845	1452	1455	1457	rBV	71033	67968	1.10%	0.207%
25	11.204	1513	1516	1519	rVB	1944089	1533988	24.87%	4.678%
26	11.316	1531	1535	1538	rBV3	64657	69181	1.12%	0.211%
27	11.739	1604	1607	1611	rBV	311756	262015	4.25%	0.799%
28	12.527	1737	1741	1750	rVB	335433	347747	5.64%	1.061%
29	12.792	1781	1786	1789	rBV	5671314	5713907	92.65%	17.426%
30	13.757	1946	1950	1959	rBV2	92209	179726	2.91%	0.548%
31	13.833	1959	1963	1966	rBV	1167000	984426	15.96%	3.002%
32	14.651	2099	2102	2105	rBV	130403	119302	1.93%	0.364%
33	15.233	2196	2201	2205	rBV	740967	817003	13.25%	2.492%

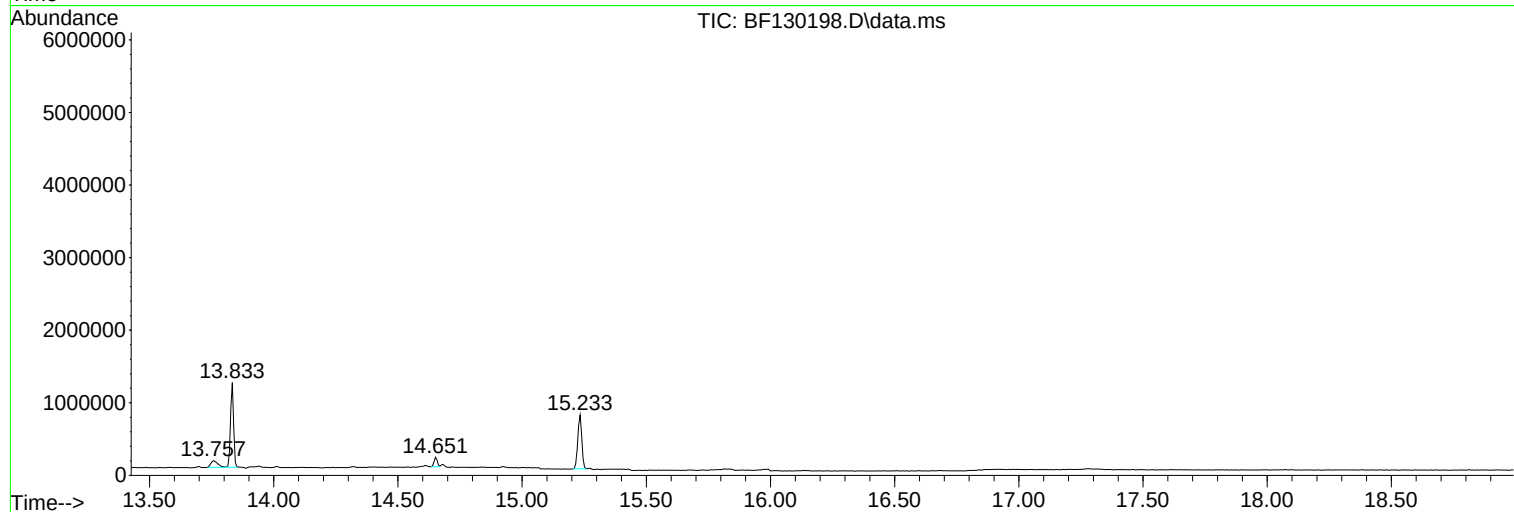
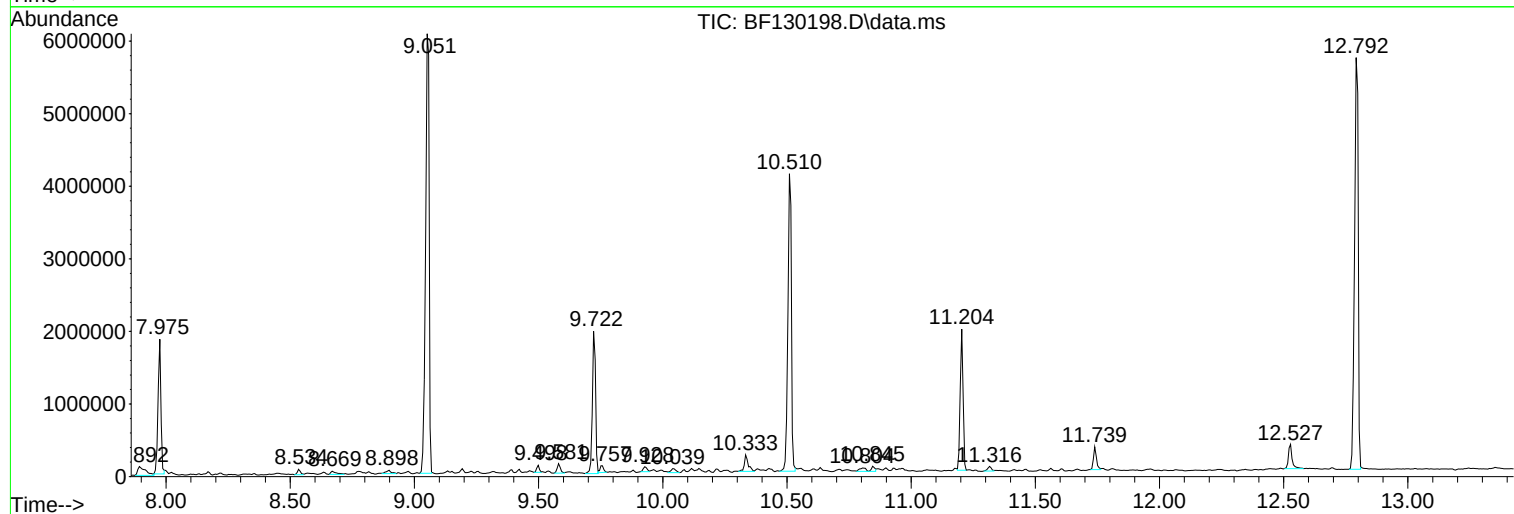
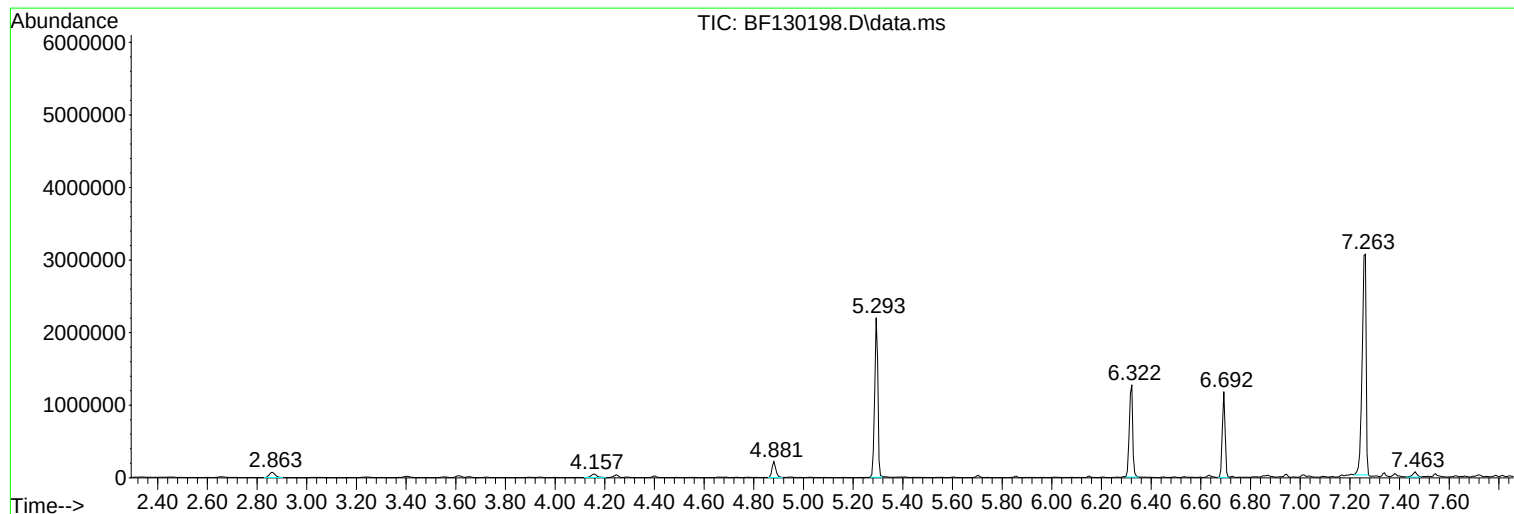
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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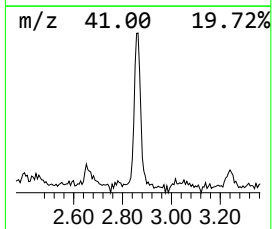
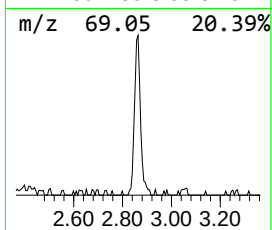
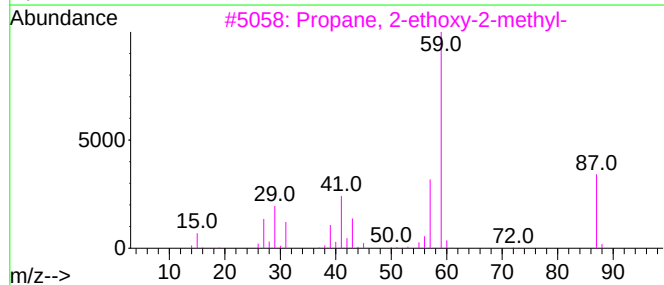
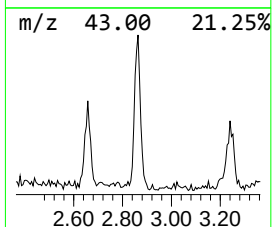
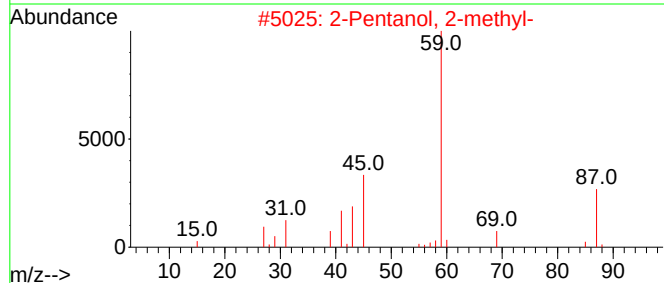
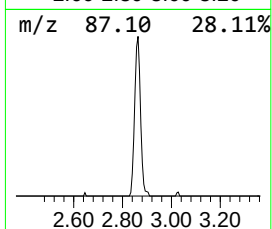
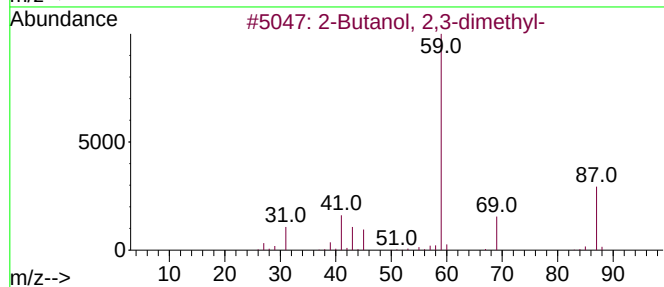
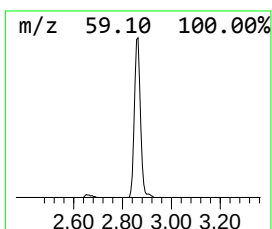
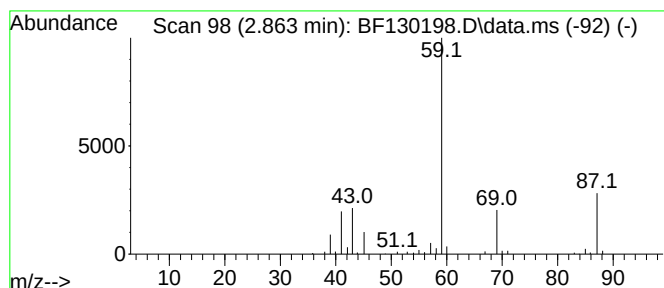
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Butanol, 2,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.863	2.68 ng	122028	1,4-Dichlorobenzene-d4	6.692

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	83	
2	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	56	
3	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	50	
4	Butane, 2-methoxy-	88	C5H12O	006795-87-5	45	
5	3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	40	



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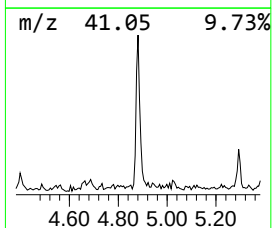
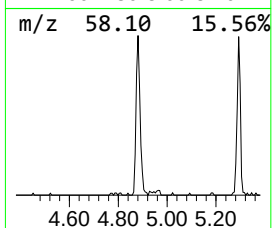
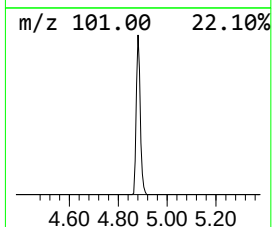
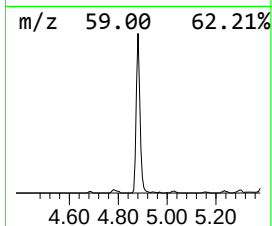
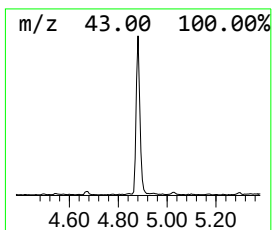
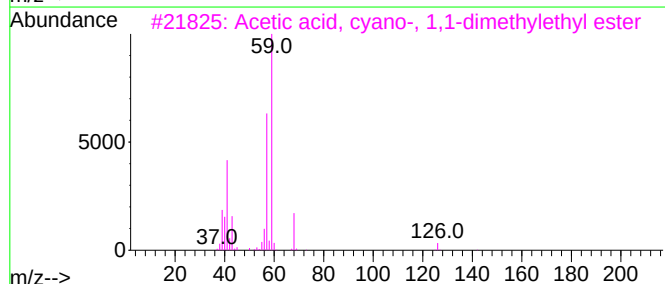
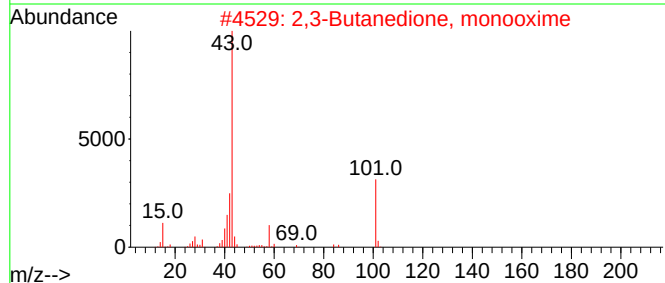
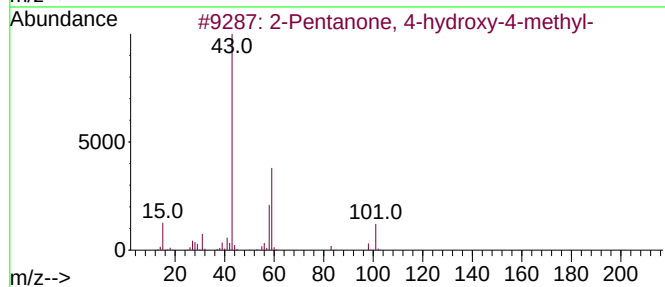
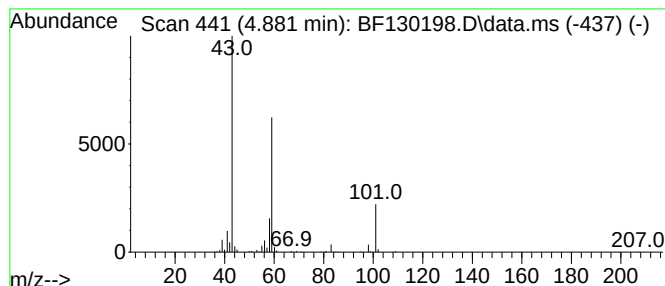
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.881	5.23 ng	237555	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	56
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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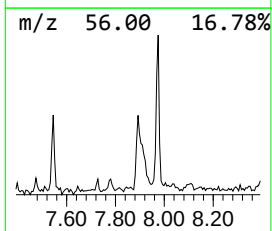
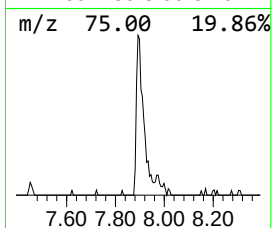
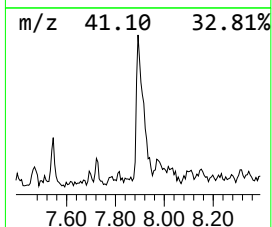
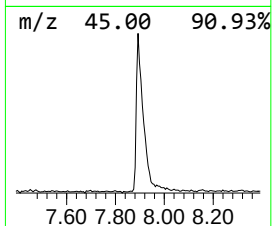
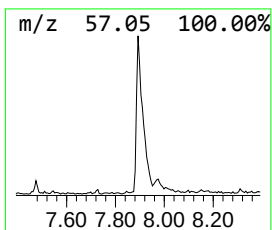
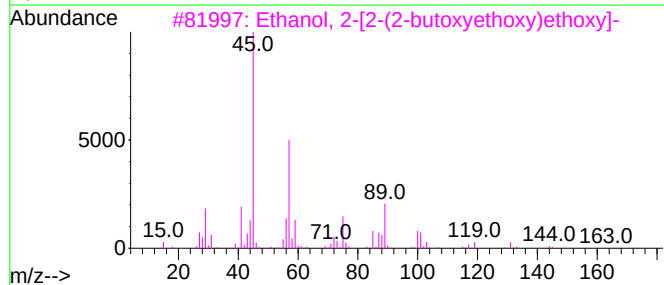
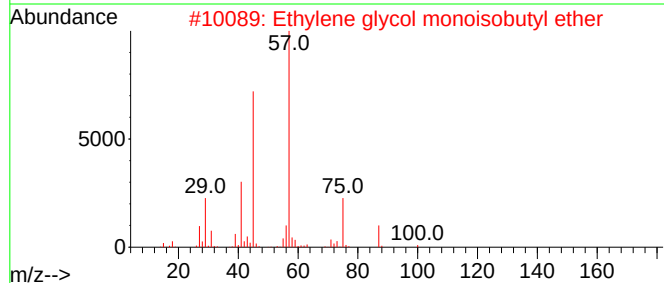
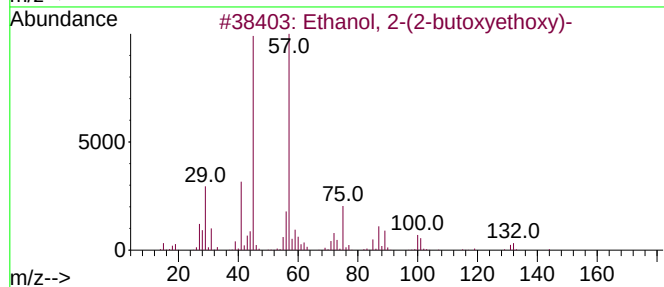
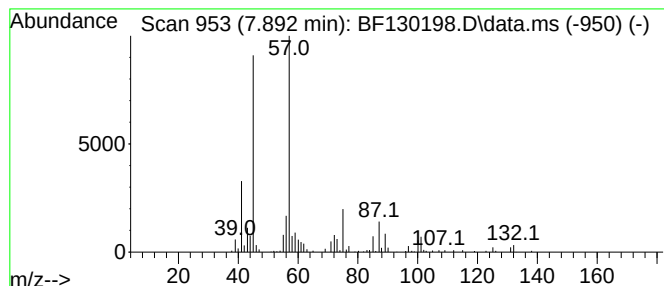
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.892	3.48 ng	264150	Naphthalene-d8	7.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	72
3			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	64
4			Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	59
5			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56



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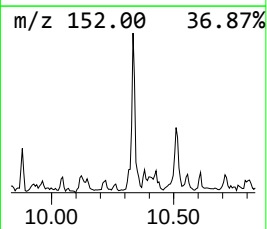
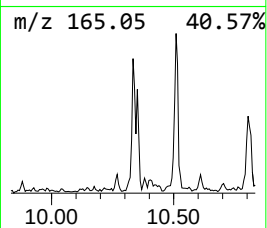
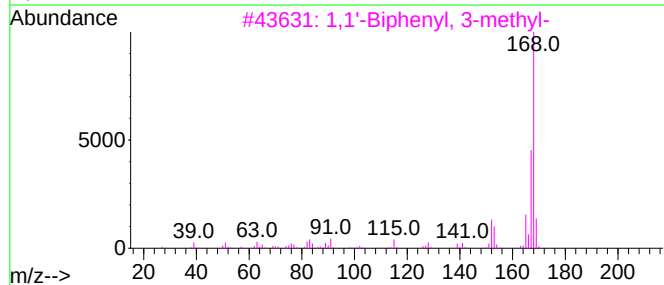
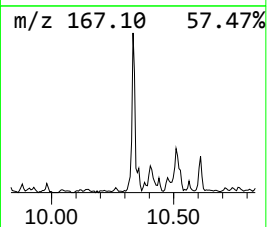
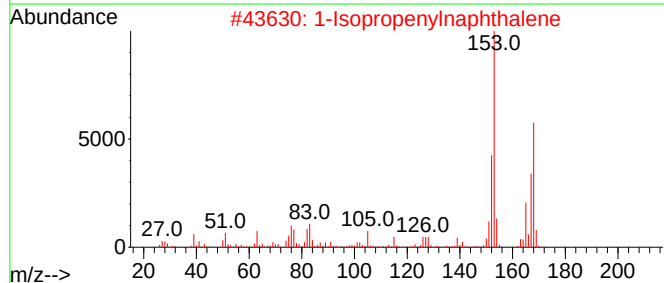
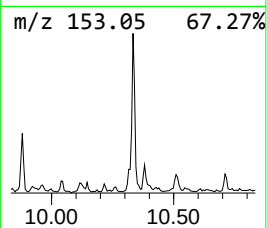
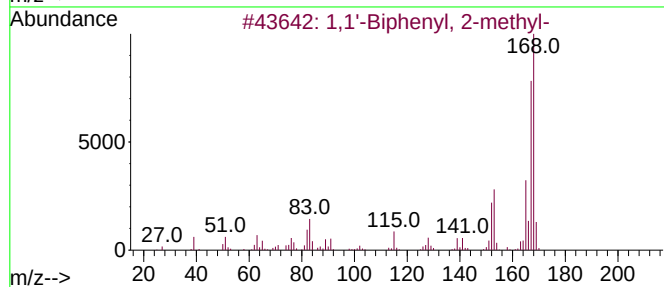
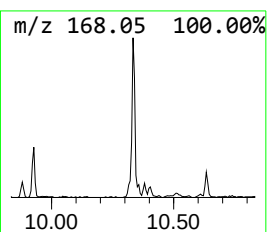
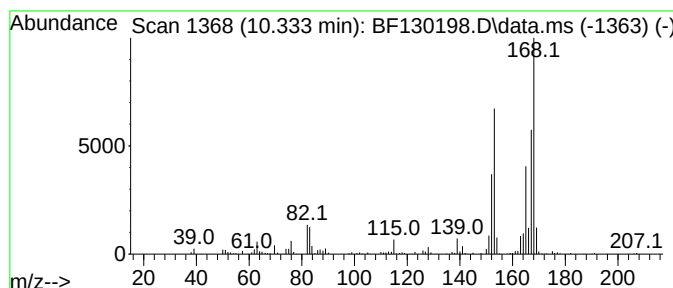
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Peak Number 4 1,1'-Biphenyl, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.333	2.84 ng	242633	Acenaphthene-d10	9.722

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Biphenyl, 2-methyl-		168	C13H12		000643-58-3	74
2	1-Isopropenylnaphthalene		168	C13H12		001855-47-6	74
3	1,1'-Biphenyl, 3-methyl-		168	C13H12		000643-93-6	62
4	1,1-Diphenyl-2-propanol		212	C15H16O		029338-49-6	53
5	Naphthalene, 1-(2-propenyl)-		168	C13H12		002489-86-3	52



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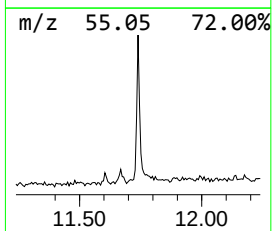
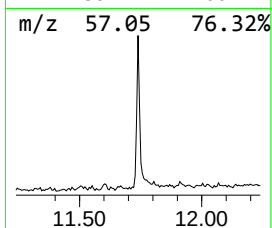
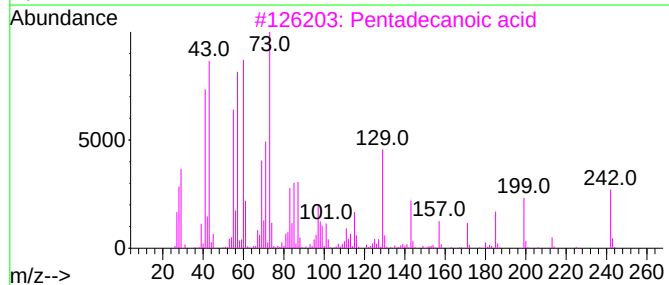
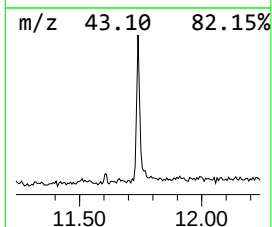
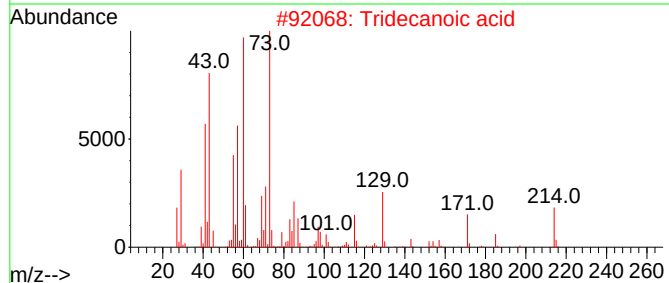
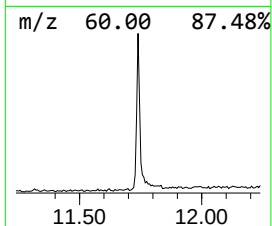
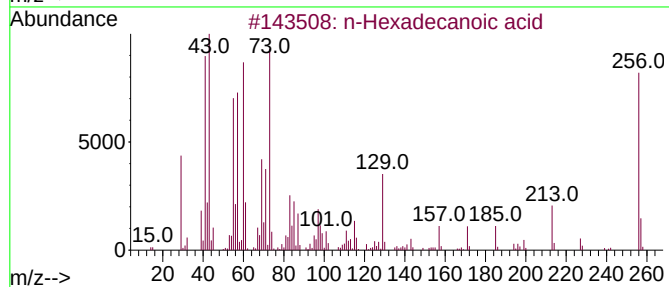
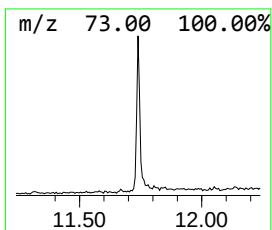
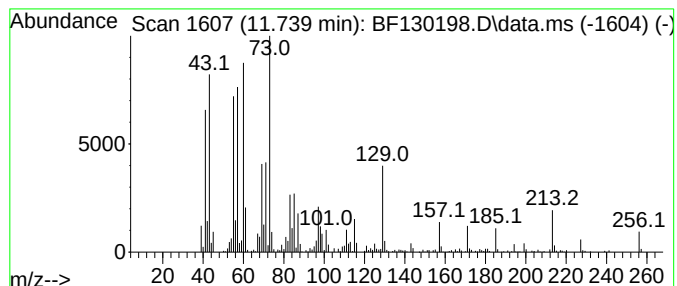
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.739	3.42 ng	262015	Phenanthrene-d10	11.204	
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	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	74



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MW-56

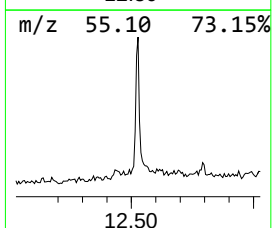
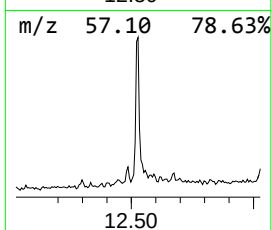
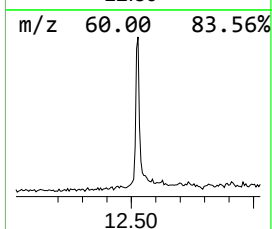
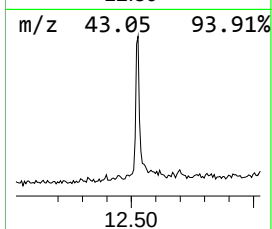
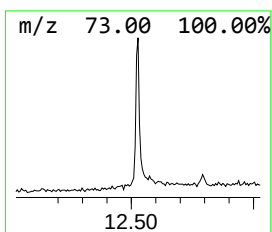
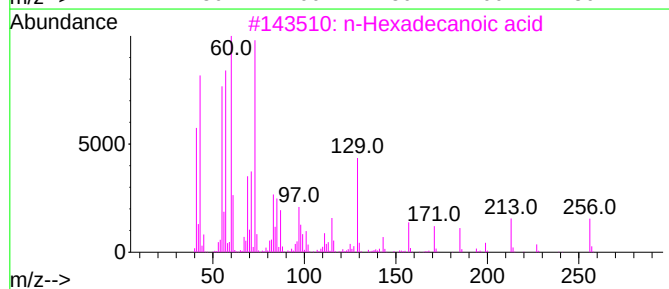
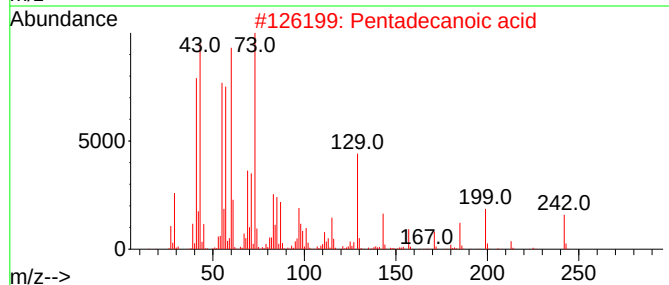
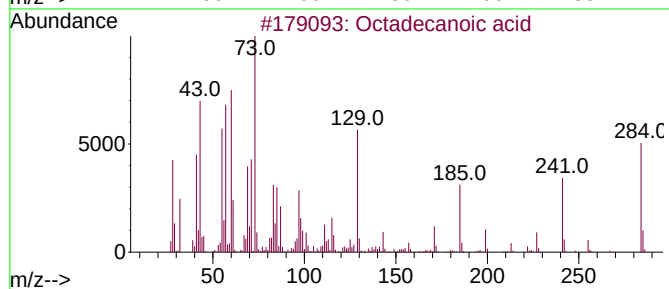
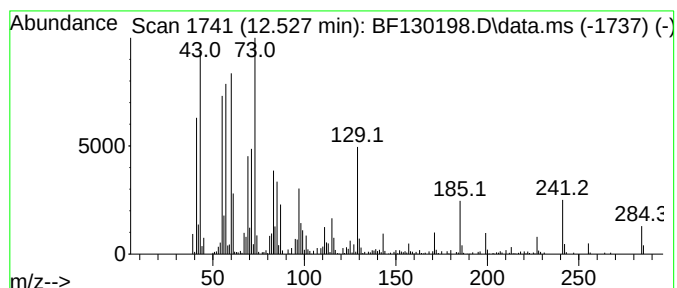
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.527	7.06 ng	347747	Chrysene-d12	13.833

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	62
5			Oxalic acid, propyl tetradecyl e...	328	C19H36O4	1000309-26-7	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130198.D
Acq On : 09 Sep 2022 16:58
Operator : CG\JU
Sample : N4549-12
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-56

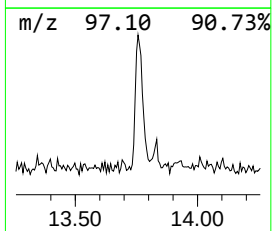
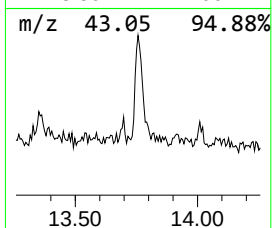
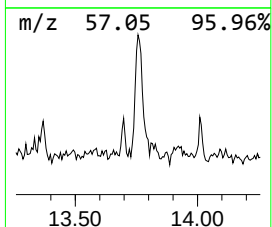
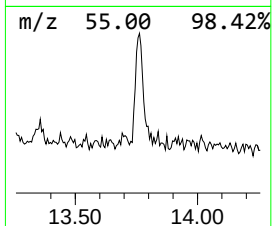
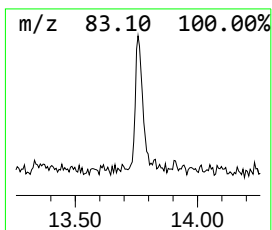
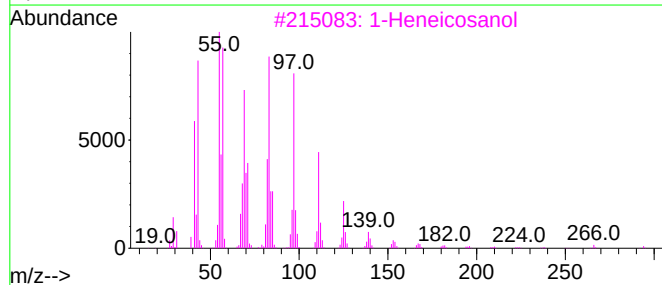
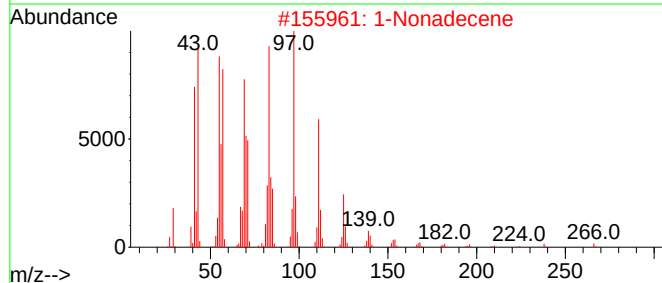
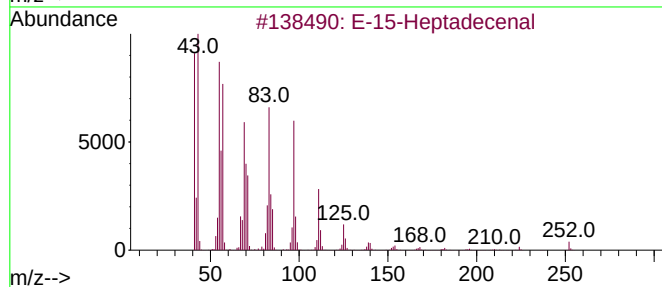
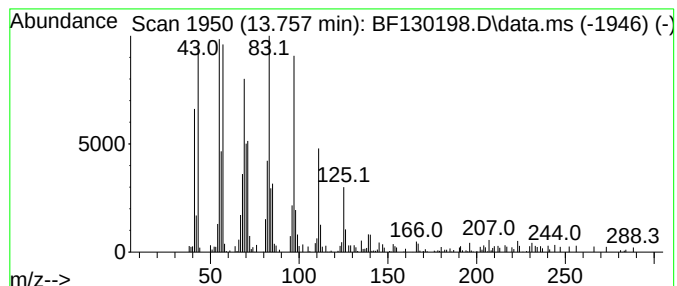
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 E-15-Heptadecenal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.757	3.65 ng	179726	Chrysene-d12	13.833

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal			252	C17H32O	1000130-97-9	99
2	1-Nonadecene			266	C19H38	018435-45-5	95
3	1-Heneicosanol			312	C21H44O	015594-90-8	95
4	1-Octadecanol			270	C18H38O	000112-92-5	94
5	Heptafluorobutyric acid, pentade...			424	C19H31F7O2	959261-23-5	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130198.D
Acq On : 09 Sep 2022 16:58
Operator : CG\JU
Sample : N4549-12
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-56

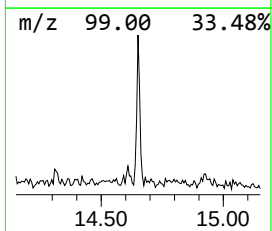
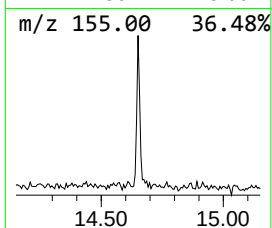
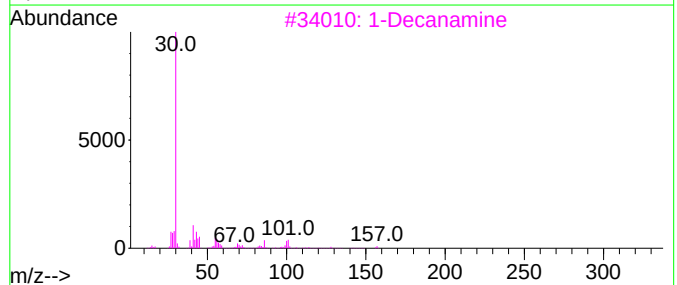
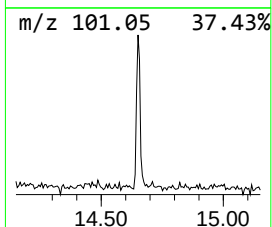
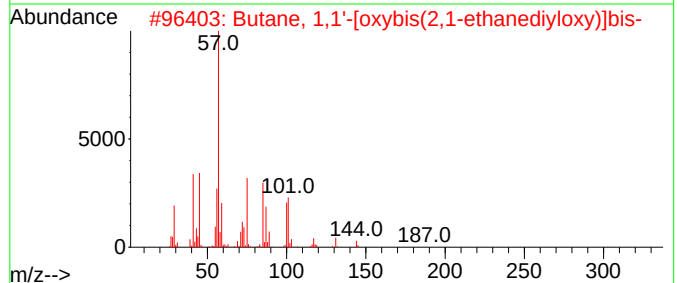
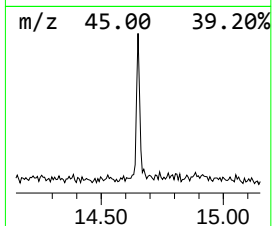
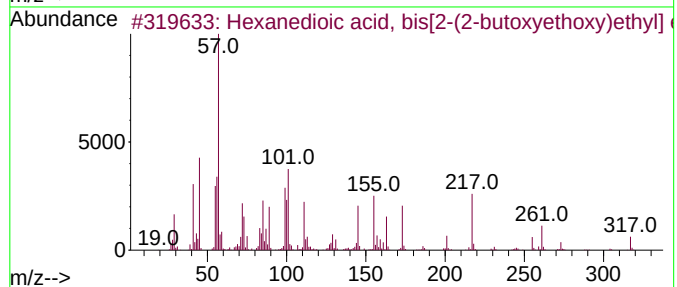
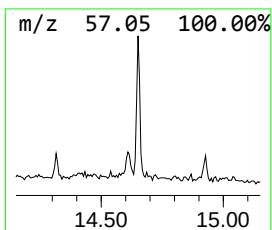
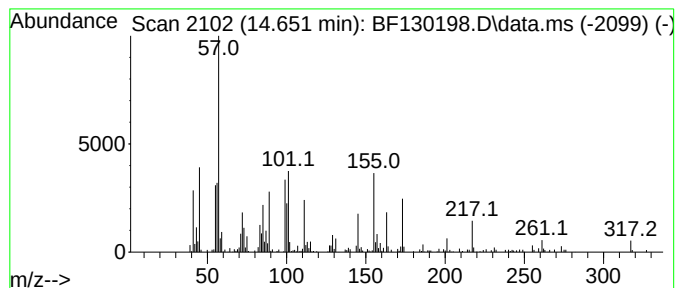
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexanedioic acid, bis[2-(2-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.651	2.92 ng	119302	Perylene-d12	15.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanedioic acid, bis[2-(2-butox...	434	C22H42O8	000141-17-3	72
2			Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	32
3			1-Decanamine	157	C10H23N	002016-57-1	27
4			di(Butoxyethyl)adipate	346	C18H34O6	000141-18-4	27
5			2-(2-Butoxyethoxy)ethyl heptanoate	274	C15H30O4	1000367-04-4	16



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130198.D
Acq On : 09 Sep 2022 16:58
Operator : CG\JU
Sample : N4549-12
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-56

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Butanol, 2,3-...	2.863	2.7	ng	122028	1	6.692	908990	20.0
2-Pentanone, 4-...	4.881	5.2	ng	237555	1	6.692	908990	20.0
Ethanol, 2-(2-b...	7.892	3.5	ng	264150	2	7.975	1517760	20.0
1,1'-Biphenyl, ...	10.333	2.8	ng	242633	3	9.722	1709970	20.0
n-Hexadecanoic ...	11.739	3.4	ng	262015	4	11.204	1533990	20.0
Octadecanoic acid	12.527	7.1	ng	347747	5	13.833	984426	20.0
E-15-Heptadecenal	13.757	3.6	ng	179726	5	13.833	984426	20.0
Hexanedioic aci...	14.651	2.9	ng	119302	6	15.233	817003	20.0