

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF101421\  
 Data File : BF125850.D  
 Acq On : 14 Oct 2021 18:08  
 Operator : JU/CG  
 Sample : M4194-03  
 Misc :  
 ALS Vial : 13 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 VNJ-209

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-BF100721.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125850.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.298	201	206	219	rBV	119391	260823	6.17%	0.819%
2	5.451	567	572	575	rBV	3696521	3663951	86.70%	11.505%
3	6.463	738	744	747	rBV	3304162	3713179	87.86%	11.659%
4	6.833	803	807	810	rBV	1216981	967409	22.89%	3.038%
5	7.392	897	902	905	rBV	2594929	2382807	56.38%	7.482%
6	8.016	1004	1008	1011	rBV	1349845	1074574	25.43%	3.374%
7	8.110	1020	1024	1028	rBV	1465052	1332883	31.54%	4.185%
8	9.186	1202	1207	1210	rBV	4780552	4226014	100.00%	13.270%
9	9.316	1225	1229	1236	rVB2	44674	58044	1.37%	0.182%
10	9.810	1309	1313	1318	rBV2	43573	61701	1.46%	0.194%
11	9.863	1318	1322	1326	rVB	1936834	1545093	36.56%	4.852%
12	10.651	1452	1456	1459	rBV	3214576	2784491	65.89%	8.743%
13	11.151	1538	1541	1549	rBV	89517	120556	2.85%	0.379%
14	11.345	1570	1574	1577	rBV	1917294	1571873	37.20%	4.936%
15	11.416	1581	1586	1589	rVB4	49529	47260	1.12%	0.148%
16	11.739	1638	1641	1645	rBV	121030	95318	2.26%	0.299%
17	11.874	1660	1664	1675	rBV2	310778	321249	7.60%	1.009%
18	12.321	1737	1740	1750	rVB	178534	205370	4.86%	0.645%
19	12.445	1755	1761	1764	rVB6	43420	46508	1.10%	0.146%
20	12.557	1777	1780	1786	rBV	119443	110999	2.63%	0.349%
21	12.657	1793	1797	1804	rBV	120051	130404	3.09%	0.409%
22	12.780	1815	1818	1821	rVB	111828	100705	2.38%	0.316%
23	12.933	1839	1844	1847	rBV	3935319	3647280	86.31%	11.452%
24	13.345	1911	1914	1923	rBV	196640	299947	7.10%	0.942%
25	13.827	1992	1996	2007	rBV2	162910	241566	5.72%	0.759%
26	13.980	2016	2022	2025	rBV	1201112	1203471	28.48%	3.779%
27	14.257	2066	2069	2084	rBV	177431	311043	7.36%	0.977%
28	15.004	2193	2196	2199	rBV	43237	60605	1.43%	0.190%
29	15.151	2218	2221	2236	rBV2	42519	131959	3.12%	0.414%
30	15.433	2263	2269	2273	rBV	905832	1129961	26.74%	3.548%

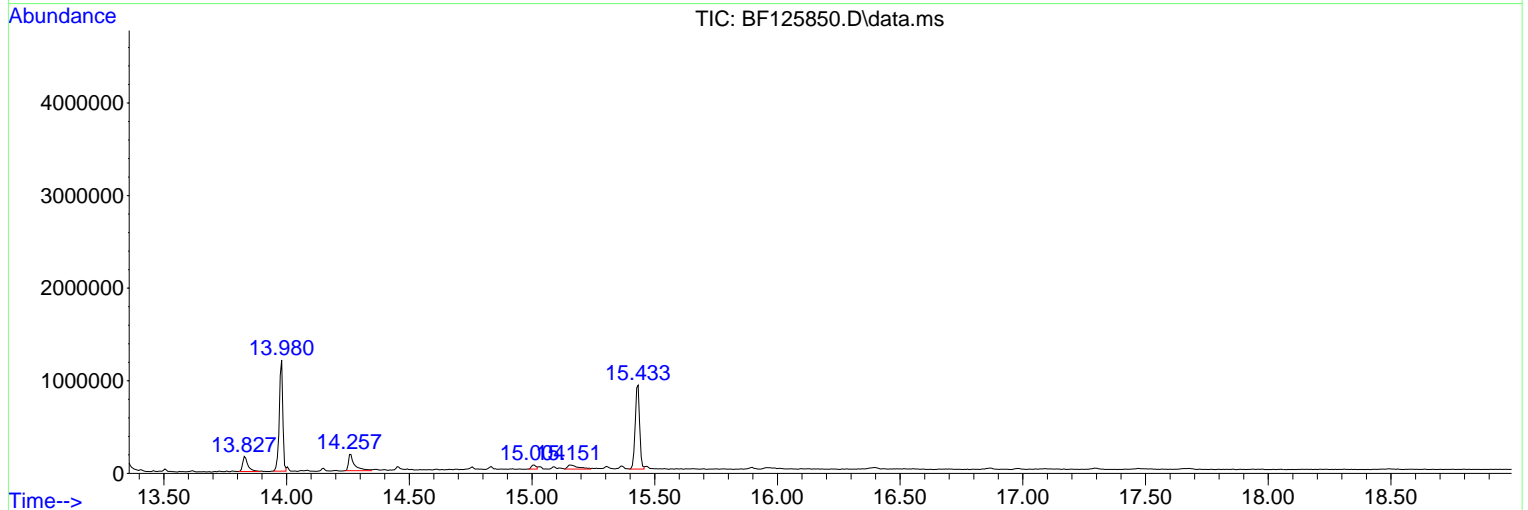
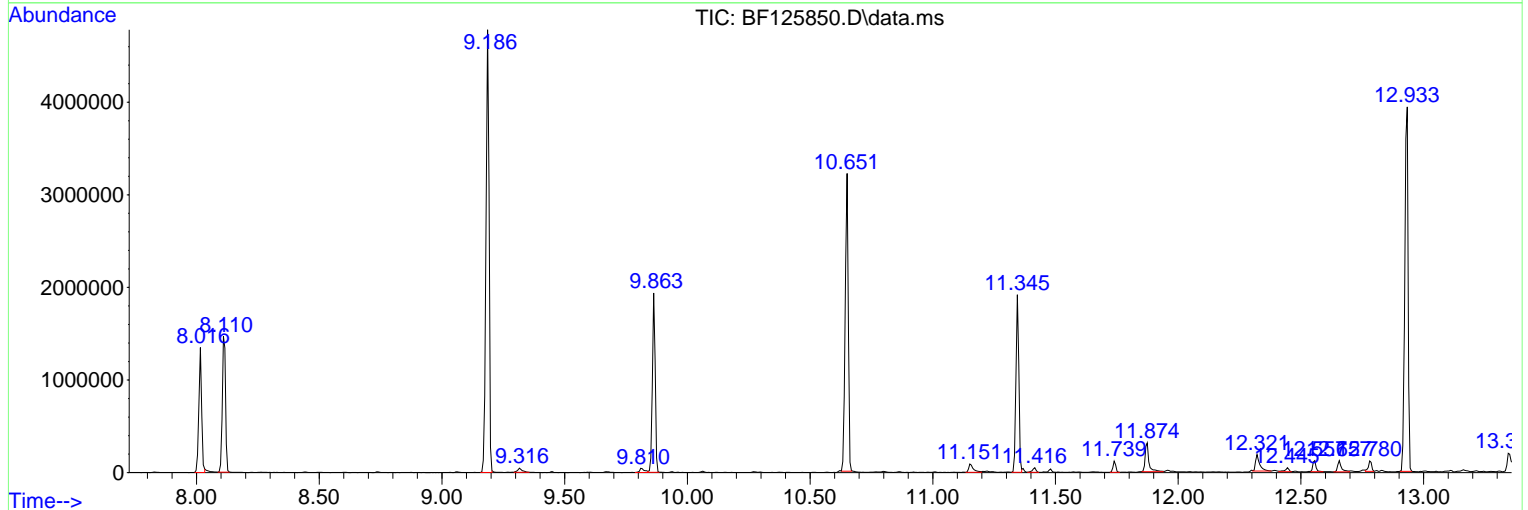
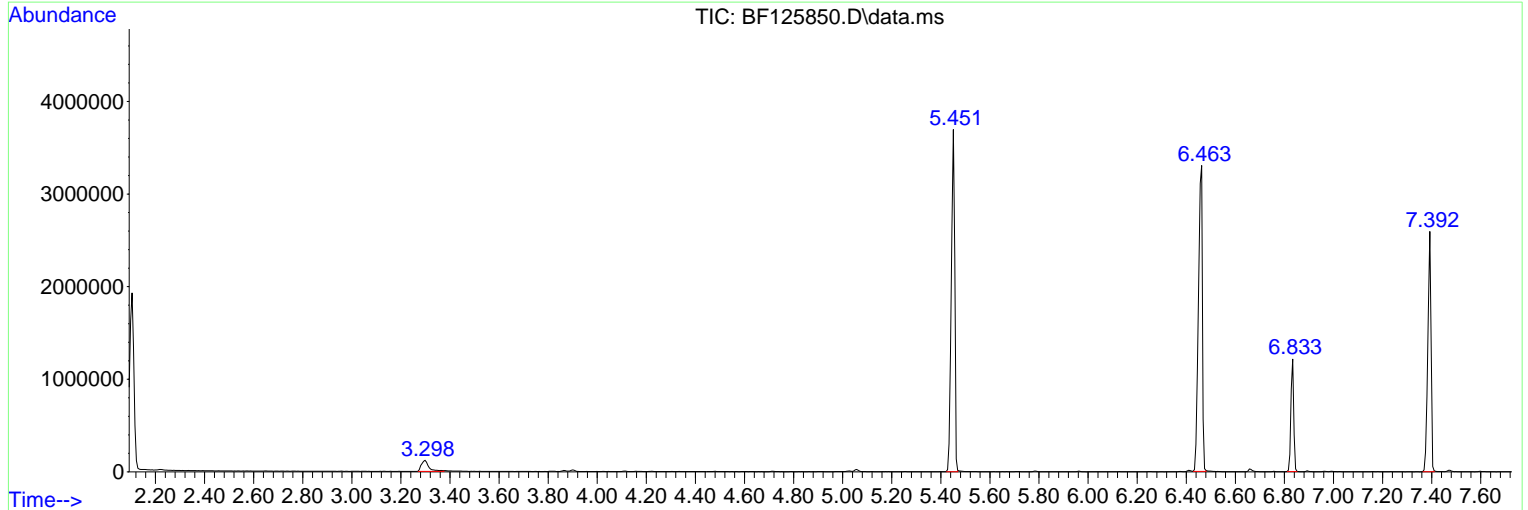
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF100721.M  
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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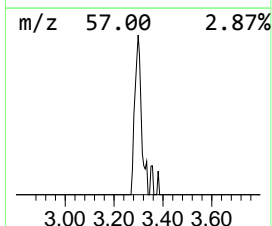
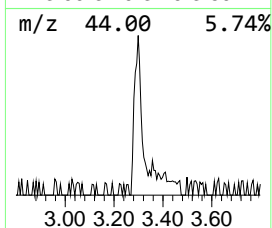
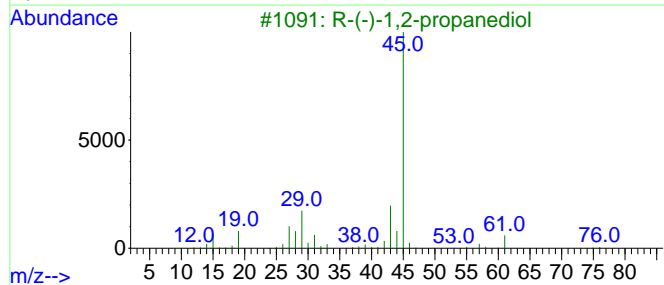
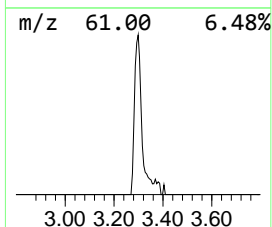
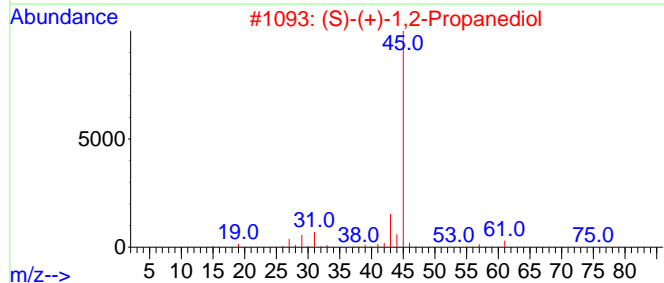
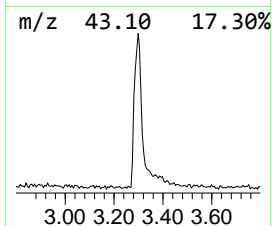
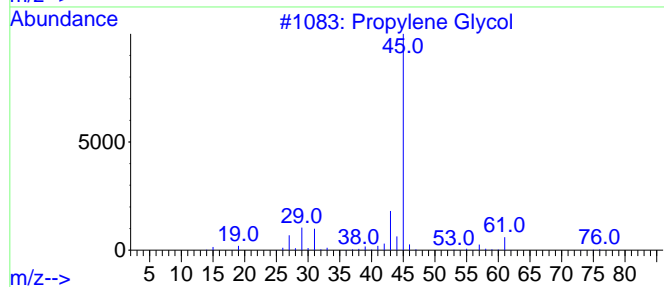
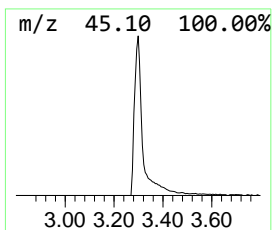
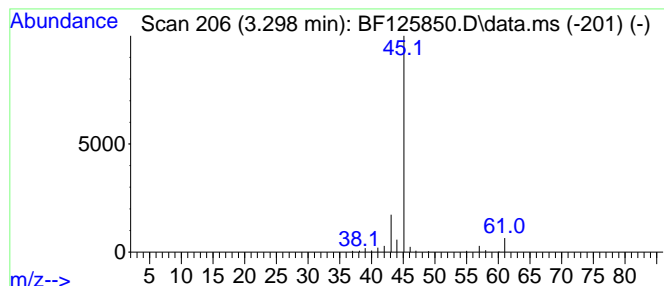
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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 Peak Number 1 unknown3.298 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.298	5.39 ng	260823	1,4-Dichlorobenzene-d4	6.833

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propylene Glycol	76	C3H8O2	000057-55-6	43
2		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	43
3		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
4		Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5		Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9



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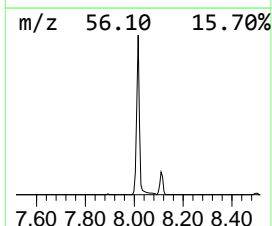
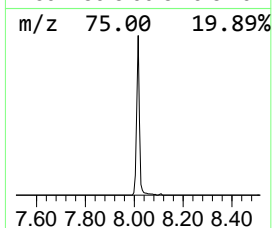
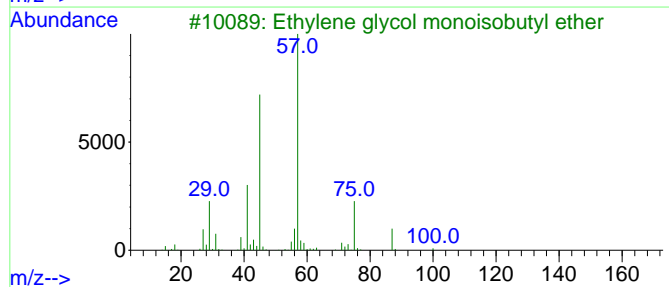
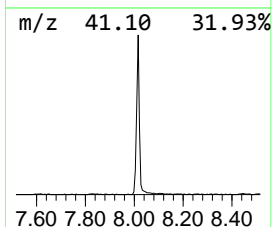
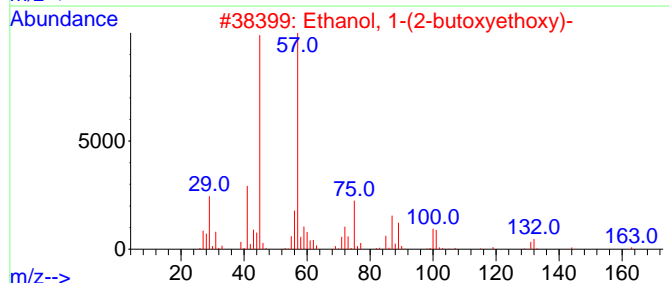
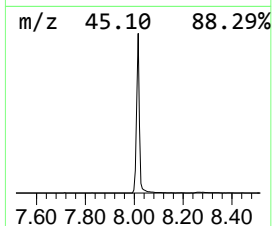
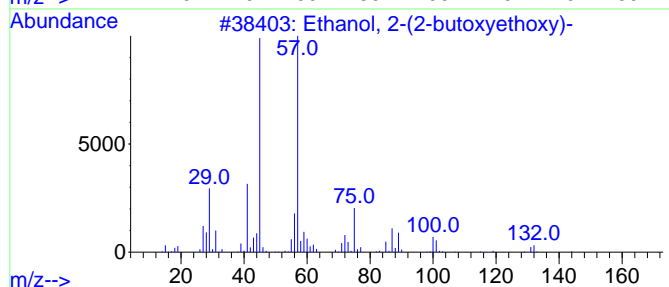
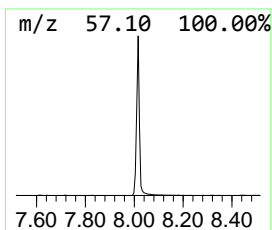
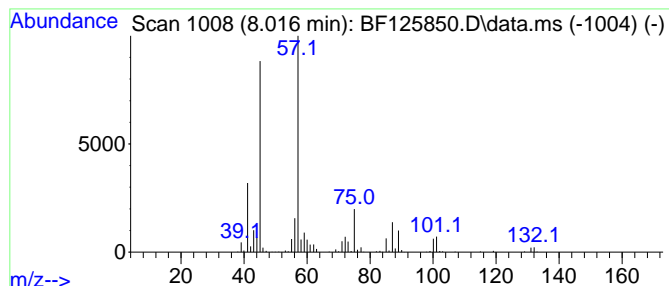
TIC Library : C:\Database\NIST20.L  
 TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.016	16.12 ng	1074570	Naphthalene-d8	8.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4			Ethanol, 2-[2-(2-methylpropoxy)e...]	162	C8H18O3	018912-80-6	56
5			Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	53



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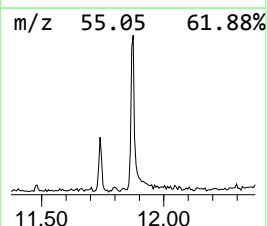
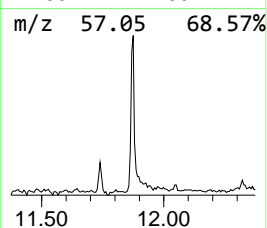
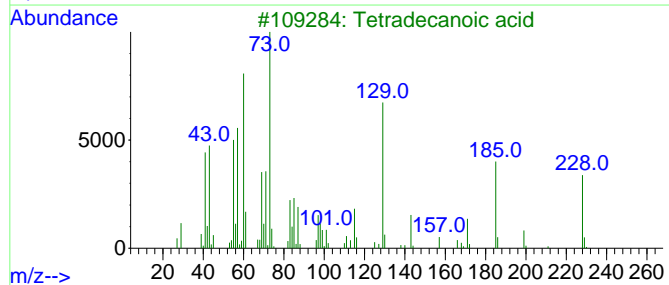
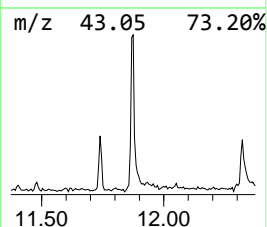
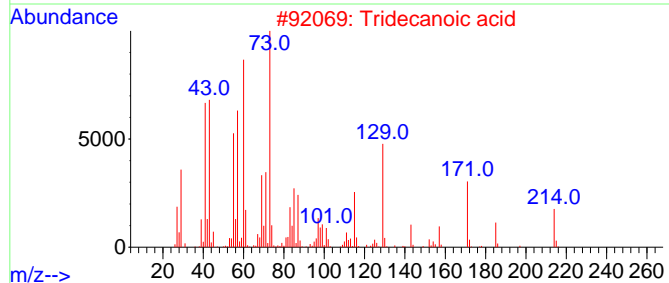
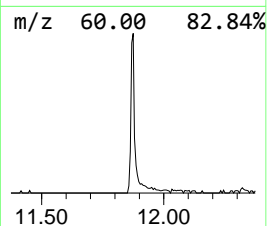
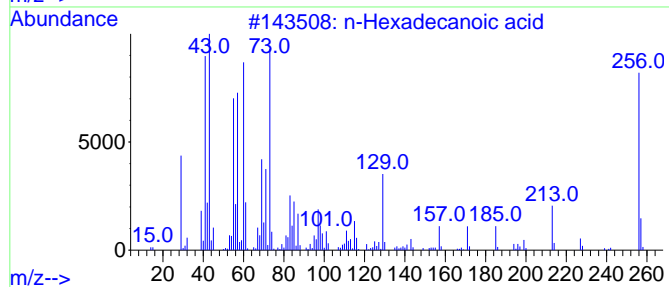
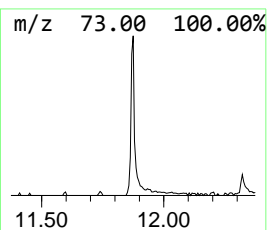
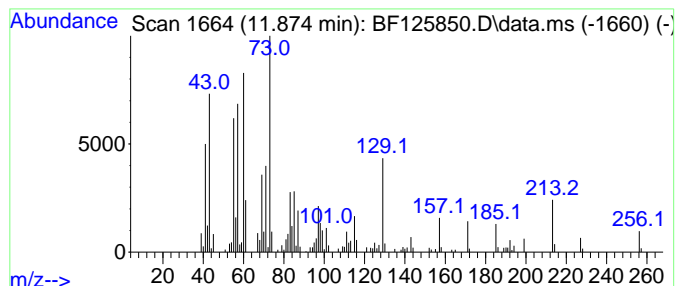
TIC Library : C:\Database\NIST20.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.874	4.09 ng	321249	Phenanthrene-d10	11.345

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	94
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5		n-Decanoic acid	172	C10H20O2	000334-48-5	76



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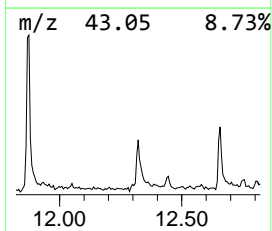
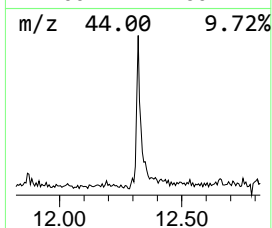
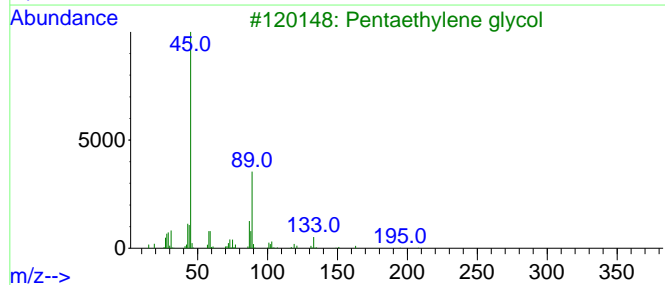
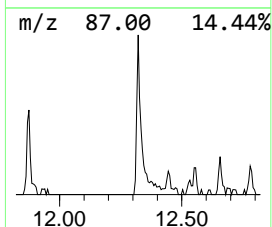
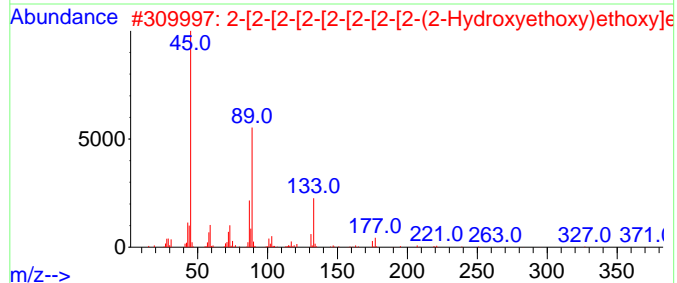
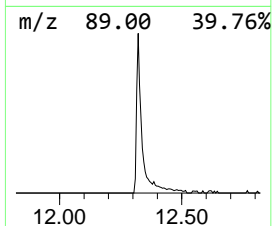
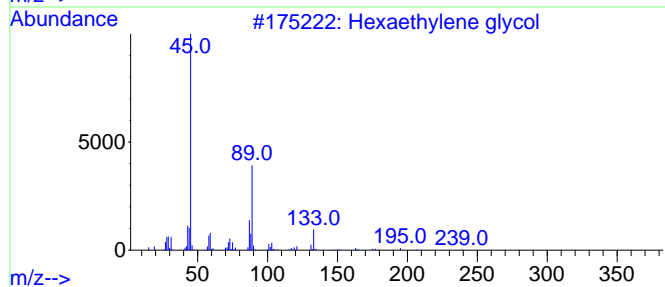
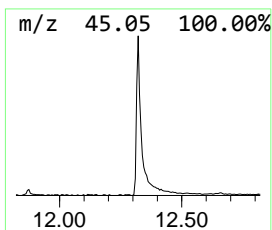
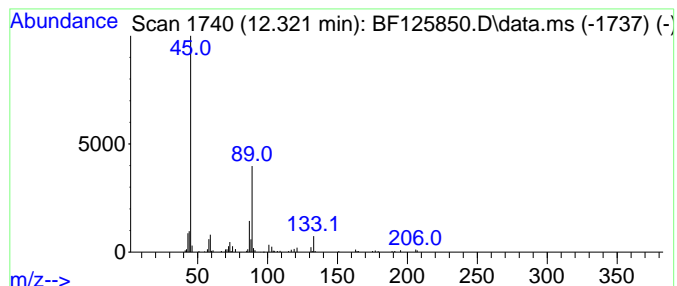
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 Peak Number 4 Hexaethylene glycol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.321	2.61 ng	205370	Phenanthrene-d10	11.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexaethylene glycol	282	C12H26O7	002615-15-8	91
2			2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	003386-18-3	83
3			Pentaethylene glycol	238	C10H22O6	004792-15-8	80
4			Ethanol, 2-[2-(2-methylprooxy)e...	162	C8H18O3	018912-80-6	64
5			2,5,8,11,14-Pentaoxahexadecan-16-ol	252	C11H24O6	023778-52-1	64





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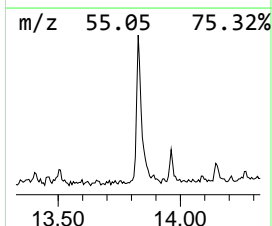
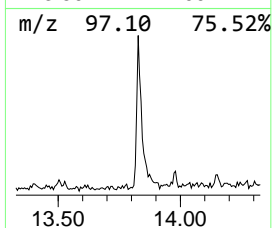
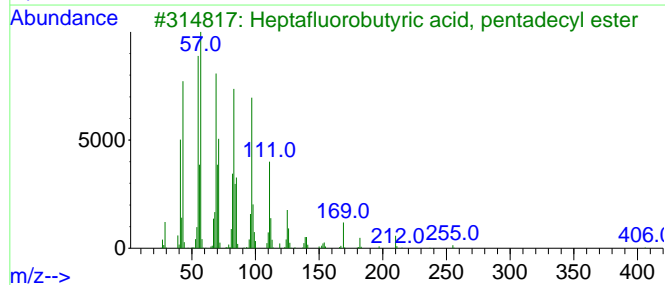
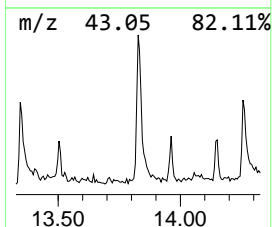
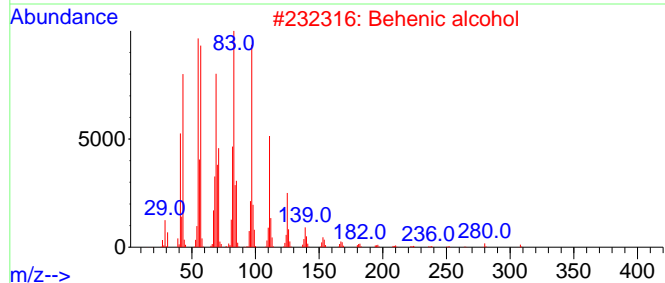
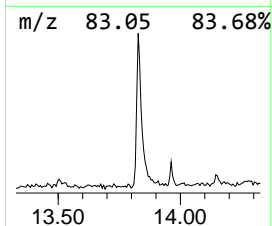
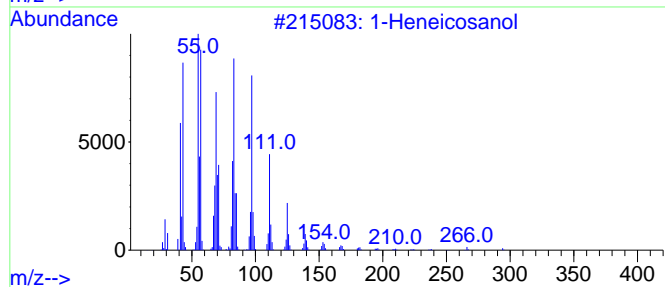
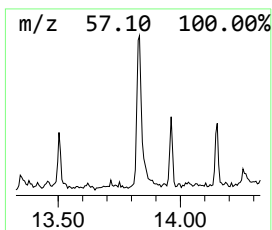
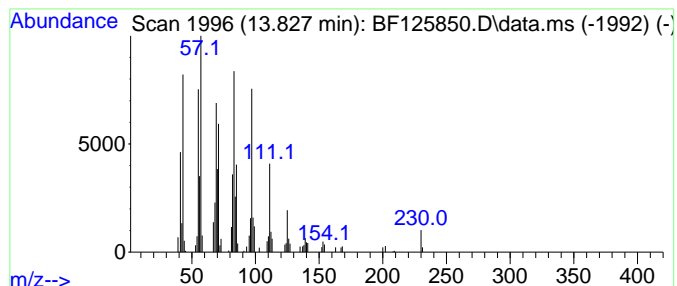
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TIC Library : C:\Database\NIST20.L  
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 Peak Number 6 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	4.01 ng	241566	Chrysene-d12	13.980

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	93
2		Behenic alcohol	326	C22H46O	000661-19-8	93
3		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
4		1-Hexacosene	364	C26H52	018835-33-1	90
5		1-Docosene	308	C22H44	001599-67-3	90





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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

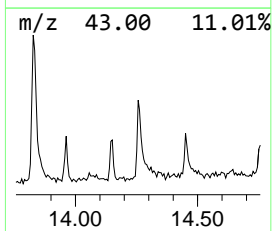
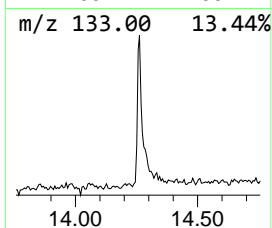
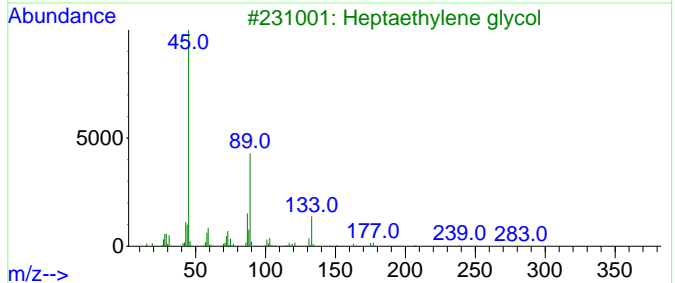
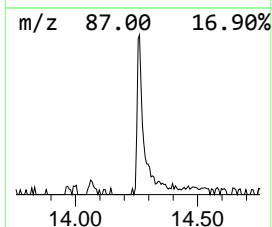
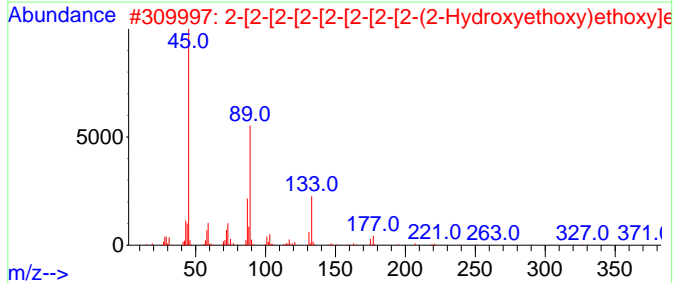
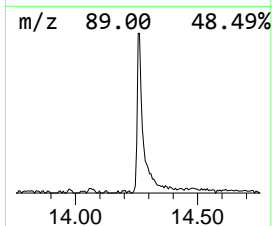
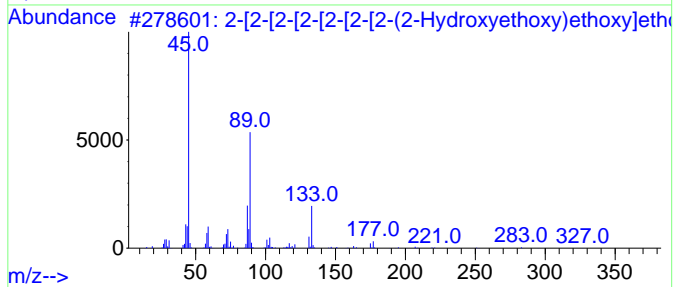
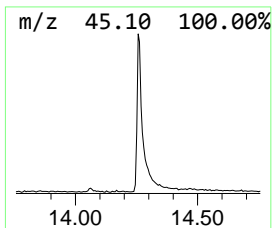
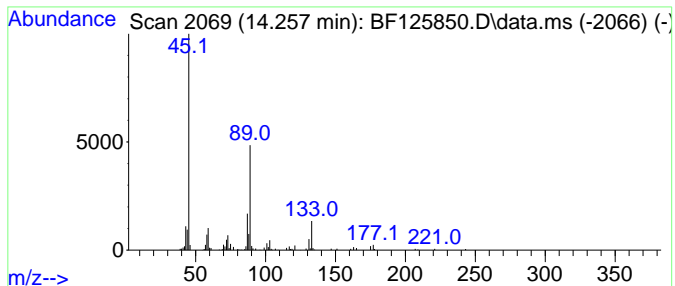
TIC Library : C:\Database\NIST20.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 7 2-[2-[2-[2-[2-[2-(2-Hydr... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.257	5.17 ng	311043	Chrysene-d12	13.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H3409	005117-19-1	91		
2	2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38010	003386-18-3	91		
3	Heptaethylene glycol	326	C14H3008	005617-32-3	91		
4	Hexaethylene glycol	282	C12H2607	002615-15-8	91		
5	Pentaethylene glycol	238	C10H2206	004792-15-8	59		



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF101421\  
 Data File : BF125850.D  
 Acq On : 14 Oct 2021 18:08  
 Operator : JU/CG  
 Sample : M4194-03  
 Misc :  
 ALS Vial : 13 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampled :  
 VNJ-209

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF100721.M  
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

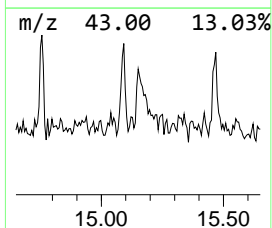
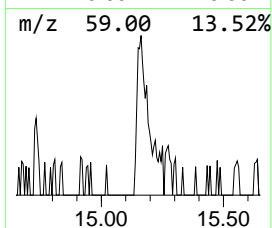
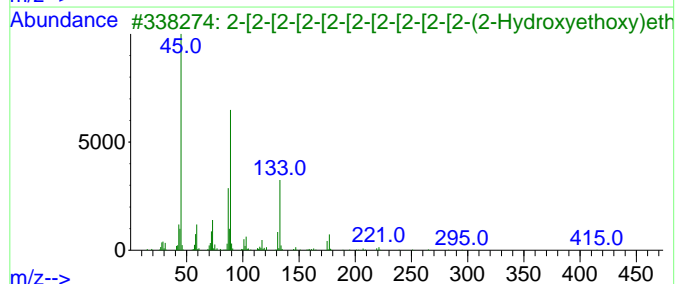
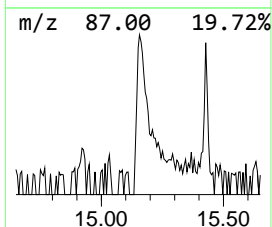
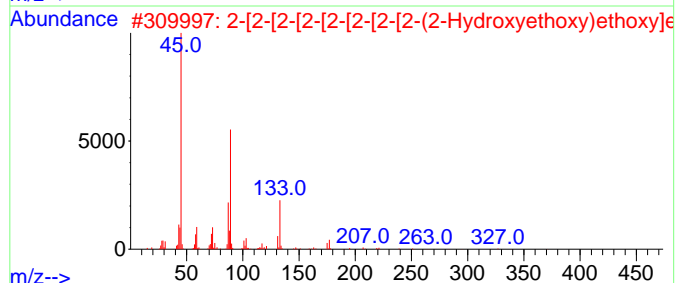
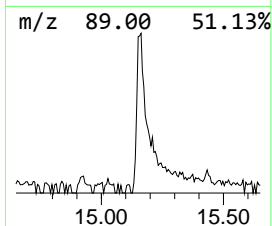
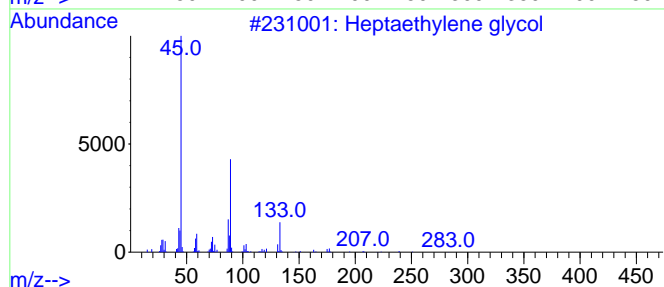
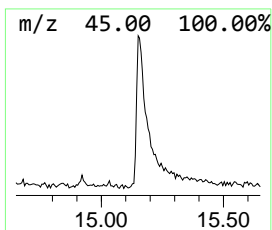
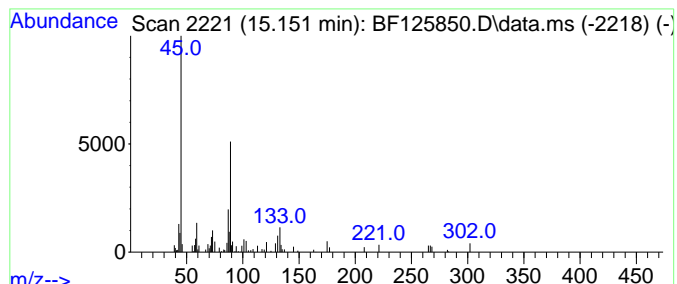
TIC Library : C:\Database\NIST20.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 8 Pentaethylene glycol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.151	2.34 ng	131959	Perylene-d12	15.433

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptaethylene glycol	326	C14H30O8	005617-32-3	86
2		2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	003386-18-3	86
3		2-[2-[2-[2-[2-[2-[2-[2-(2-...	502	C22H46O12	006809-70-7	86
4		Hexaethylene glycol	282	C12H26O7	002615-15-8	83
5		Pentaethylene glycol	238	C10H22O6	004792-15-8	78



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF101421\  
 Data File : BF125850.D  
 Acq On : 14 Oct 2021 18:08  
 Operator : JU/CG  
 Sample : M4194-03  
 Misc :  
 ALS Vial : 13 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 VNJ-209

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF100721.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
unknown3.298	3.298	5.4	ng	260823	1	6.833	967409	20.0
Ethanol, 2-(2-b...	8.016	16.1	ng	1074570	2	8.110	1332880	20.0
n-Hexadecanoic ...	11.874	4.1	ng	321249	4	11.345	1571870	20.0
Hexaethylene gl...	12.321	2.6	ng	205370	4	11.345	1571870	20.0
Heptaethylene g...	13.345	5.0	ng	299947	5	13.980	1203470	20.0
1-Heneicosanol	13.827	4.0	ng	241566	5	13.980	1203470	20.0
2-[2-[2-[2-[2-[...	14.257	5.2	ng	311043	5	13.980	1203470	20.0
Pentaethylene g...	15.151	2.3	ng	131959	6	15.433	1129960	20.0