

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021522\
 Data File : BF126889.D
 Acq On : 15 Feb 2022 14:07
 Operator : CG\JU
 Sample : N1511-02
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20220041-AMENDED-NACOTE-1-COMP

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-BF020922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126889.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.181	487	492	499	rVB	175560	224712	4.73%	0.772%
2	5.563	551	557	560	rBV	3240538	3280651	69.04%	11.274%
3	6.481	709	713	720	rBV	109673	129116	2.72%	0.444%
4	6.563	720	727	730	rBV	3213844	3862553	81.28%	13.274%
5	6.940	787	791	794	rBV	822214	673545	14.17%	2.315%
6	7.504	881	887	890	rBV	2634355	2611943	54.97%	8.976%
7	8.110	987	990	1001	rBV	106287	110944	2.33%	0.381%
8	8.222	1004	1009	1012	rBV	1068635	933720	19.65%	3.209%
9	8.351	1028	1031	1042	rBV	100508	150434	3.17%	0.517%
10	9.298	1186	1192	1195	rBV	4699522	4319010	90.89%	14.843%
11	9.775	1269	1273	1279	rBV3	36977	57726	1.21%	0.198%
12	9.975	1303	1307	1311	rVB	1186289	1052152	22.14%	3.616%
13	10.769	1437	1442	1445	rBV	3079116	2732658	57.51%	9.391%
14	11.116	1496	1501	1506	rBV5	33999	54094	1.14%	0.186%
15	11.469	1557	1561	1564	rBV	1410658	1152539	24.25%	3.961%
16	11.980	1645	1648	1657	rBV2	241104	233436	4.91%	0.802%
17	12.233	1686	1691	1696	rVB	146397	115249	2.43%	0.396%
18	13.063	1826	1832	1834	rBV	4549704	4751889	100.00%	16.330%
19	13.939	1978	1981	1993	rBV	459545	673778	14.18%	2.316%
20	14.110	2006	2010	2014	rBV	986137	852662	17.94%	2.930%
21	14.880	2136	2141	2145	rVB2	36561	51295	1.08%	0.176%
22	14.963	2152	2155	2163	rVB	107852	122391	2.58%	0.421%
23	15.233	2198	2201	2206	rVB2	51200	59780	1.26%	0.205%
24	15.616	2261	2266	2277	rVB2	519575	733863	15.44%	2.522%
25	16.092	2343	2347	2353	rVB2	37711	55074	1.16%	0.189%
26	16.163	2353	2359	2365	rBV3	40575	103167	2.17%	0.355%

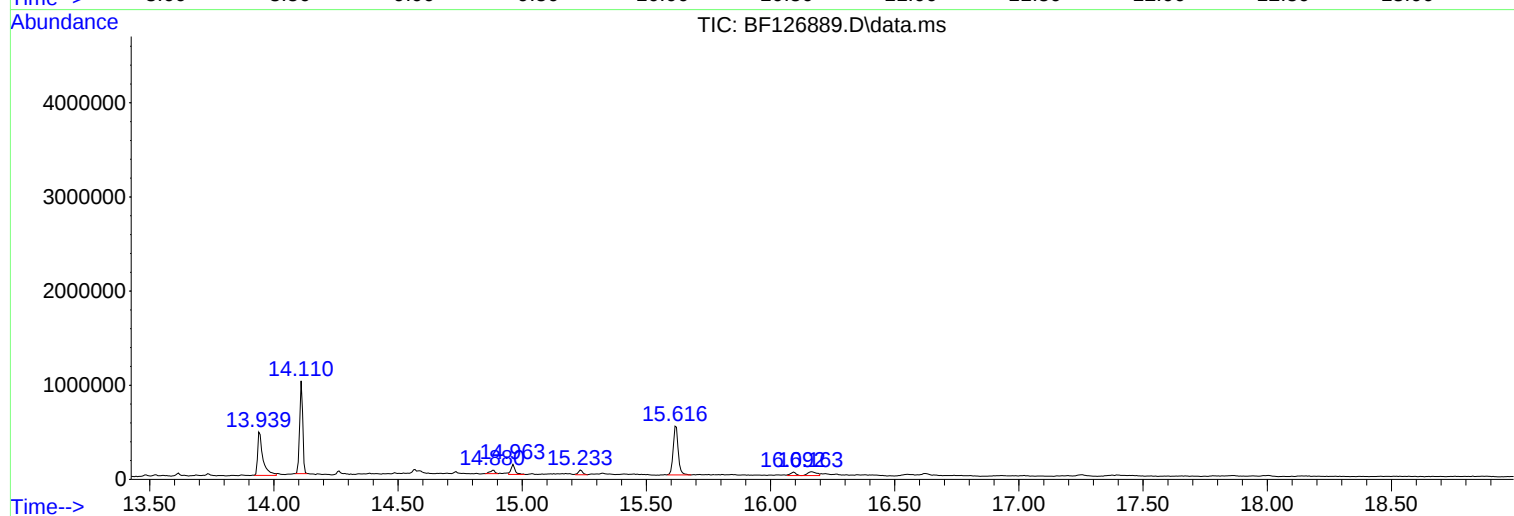
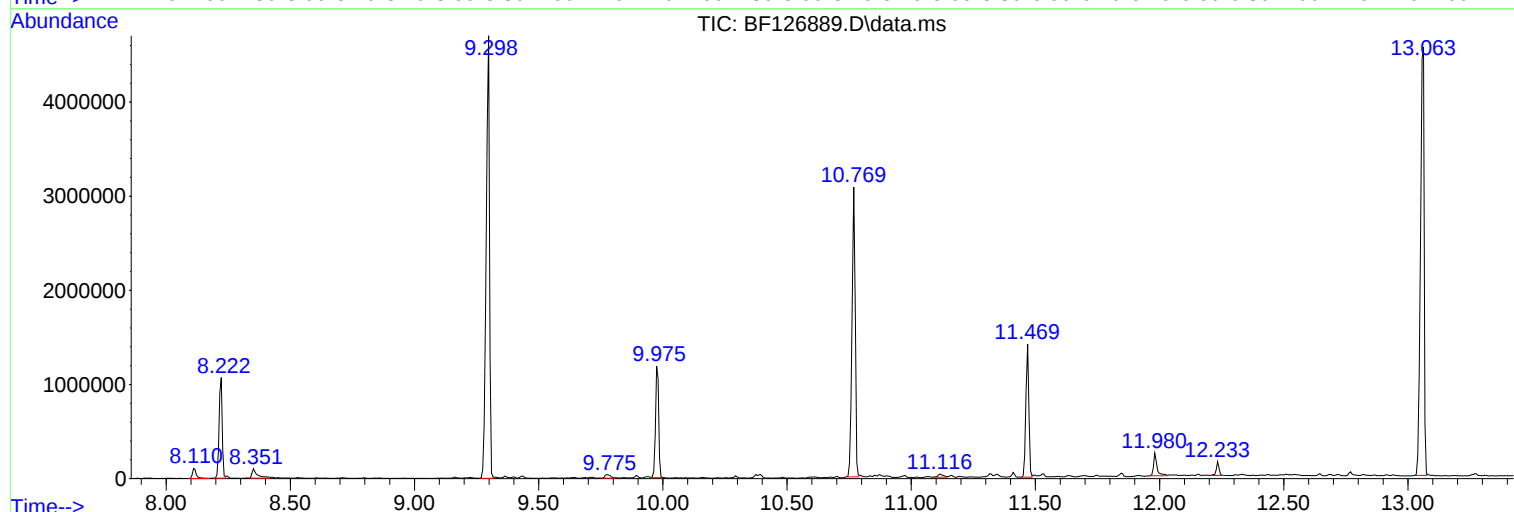
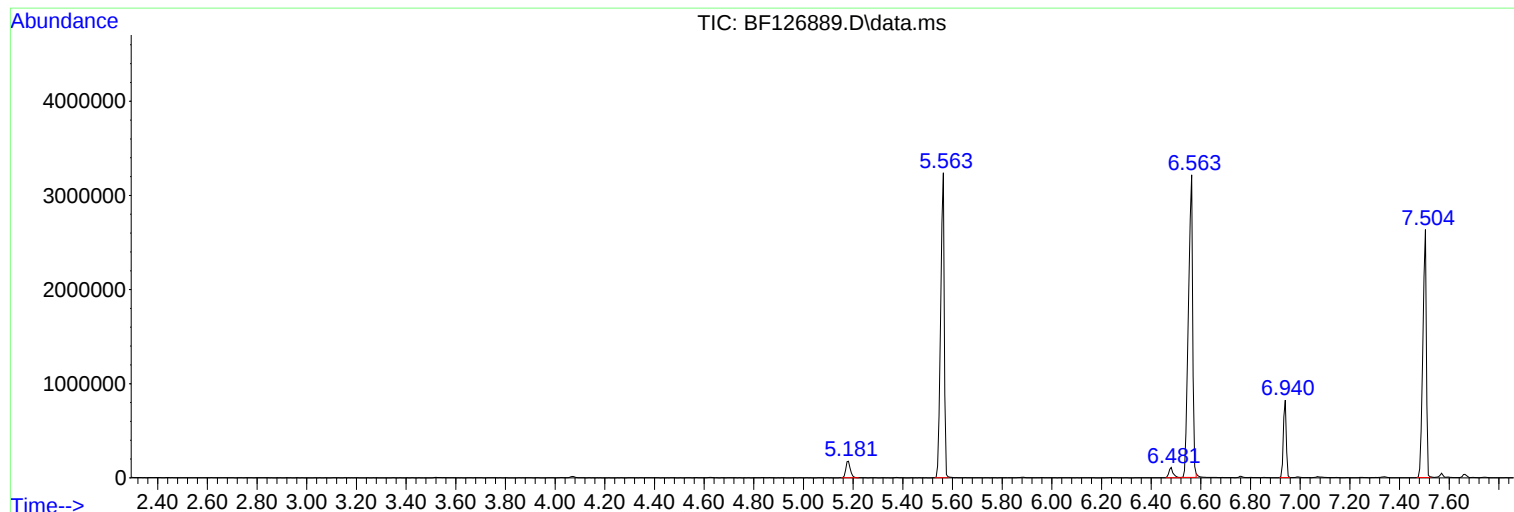
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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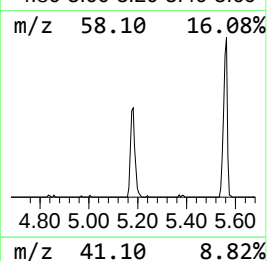
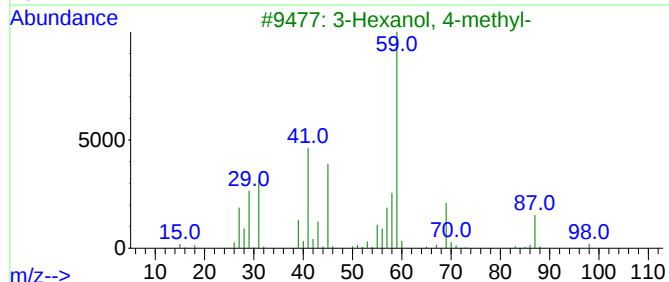
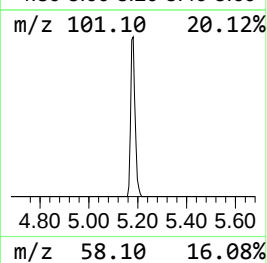
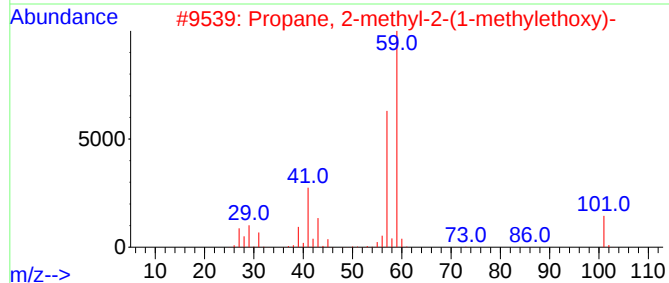
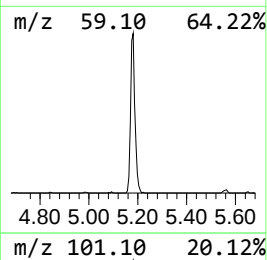
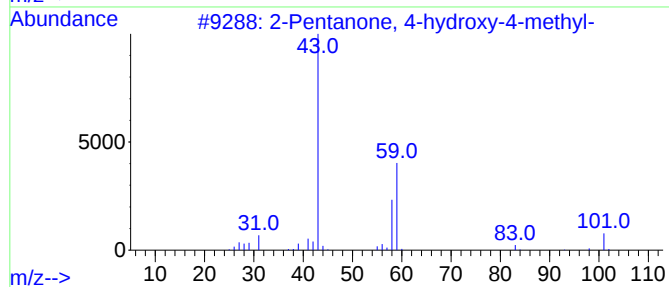
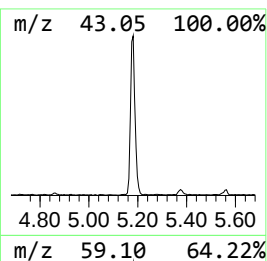
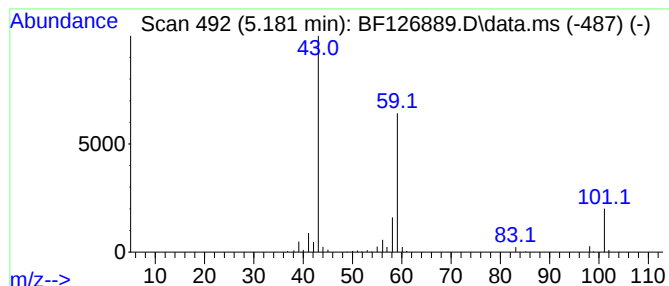
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.181	6.67 ng	224712	1,4-Dichlorobenzene-d4	6.940

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		



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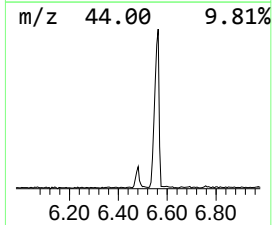
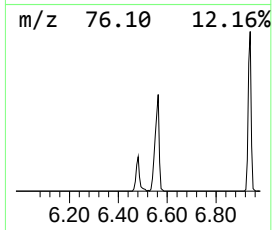
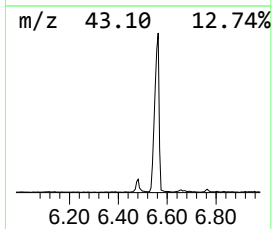
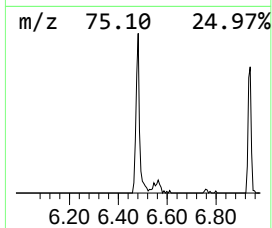
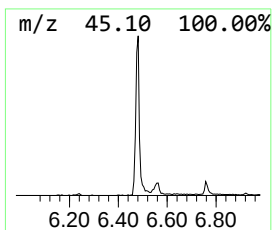
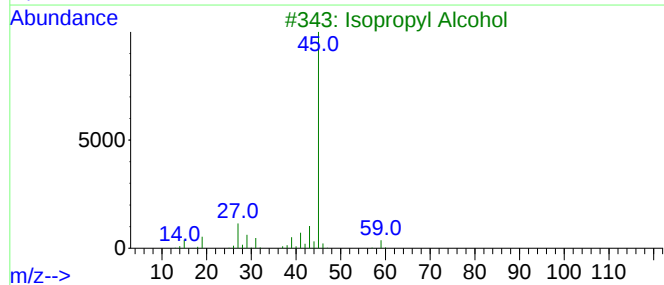
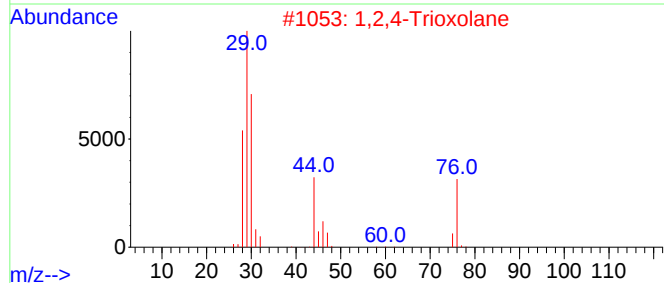
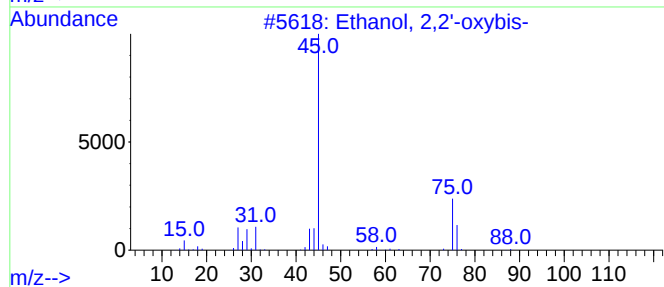
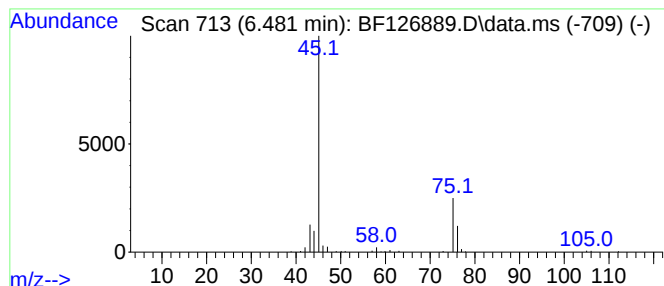
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2,2'-oxybis- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.481	3.83 ng	129116	1,4-Dichlorobenzene-d4	6.940

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2,2'-oxybis-	106	C4H10O3	000111-46-6	78
2			1,2,4-Trioxolane	76	C2H4O3	000289-14-5	9
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4			2-Hydrazinoethanol	76	C2H8N2O	000109-84-2	9
5			Ethanol, 2-methoxy-	76	C3H8O2	000109-86-4	9



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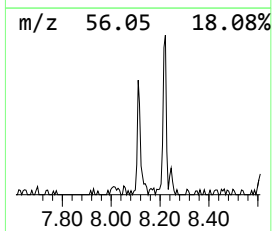
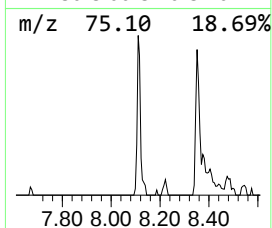
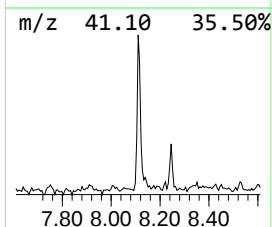
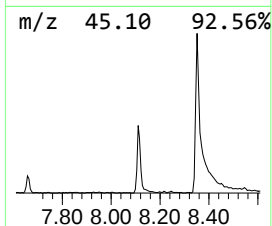
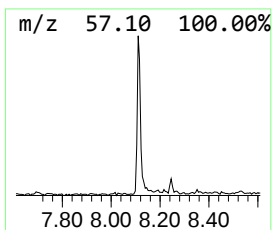
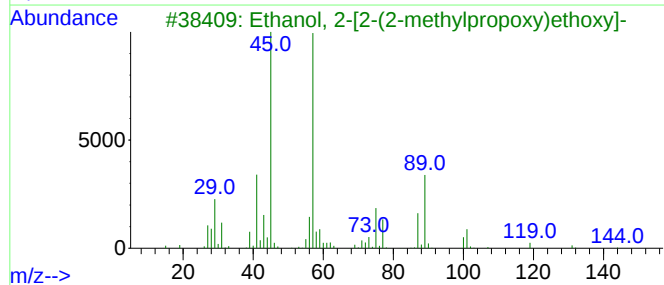
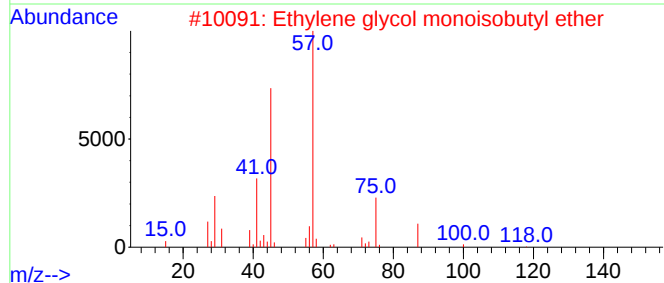
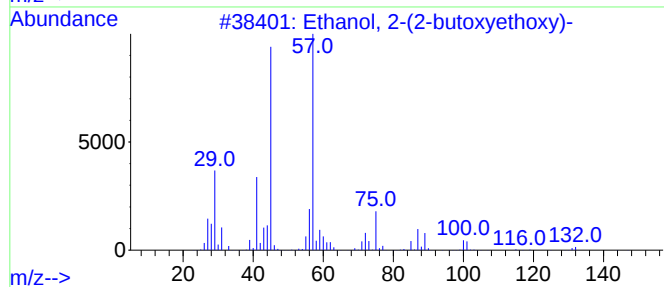
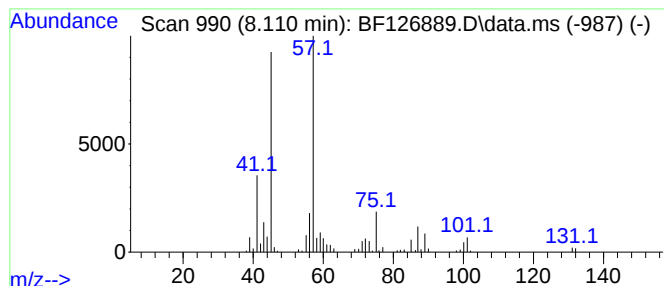
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	2.38 ng	110944	Naphthalene-d8	8.222

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	64
3			Ethanol, 2-[2-(2-methylpropoxy)ethoxy]-	162	C8H18O3	018912-80-6	56
4			2-Pentanol, 4,4-dimethyl-	116	C7H16O	006144-93-0	50
5			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50



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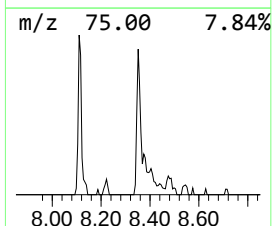
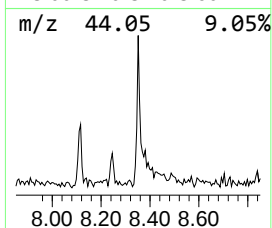
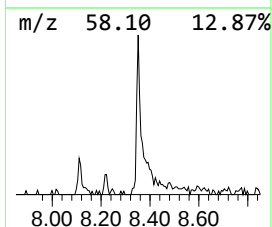
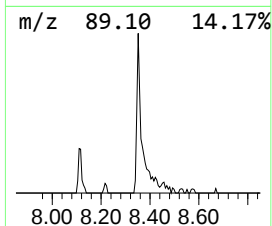
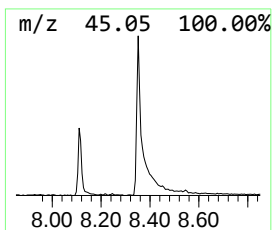
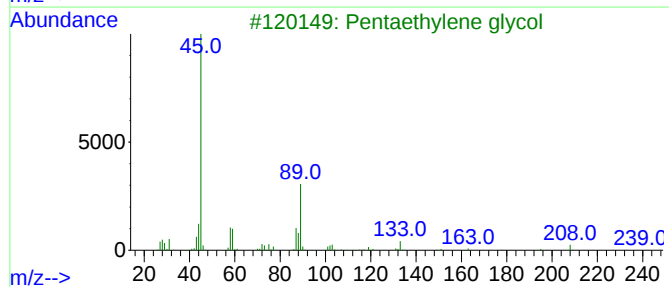
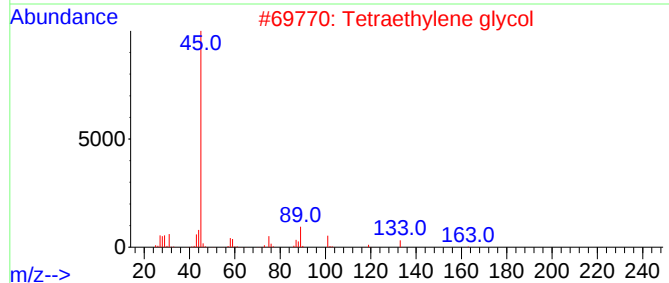
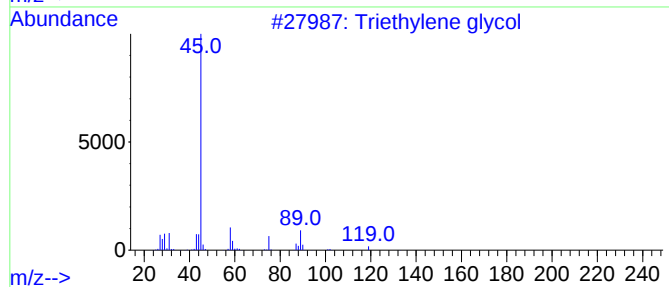
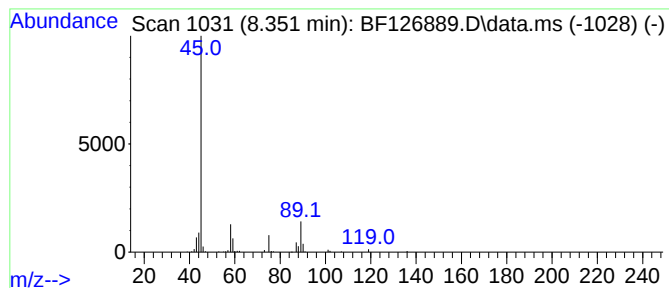
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Triethylene glycol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.351	3.22 ng	150434	Naphthalene-d8	8.222

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triethylene glycol	150	C6H14O4	000112-27-6	83
2			Tetraethylene glycol	194	C8H18O5	000112-60-7	78
3			Pentaethylene glycol	238	C10H22O6	004792-15-8	78
4			Ethanol, 2-[2-(2-methoxyethoxy)e...	164	C7H16O4	000112-35-6	56
5			Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	50



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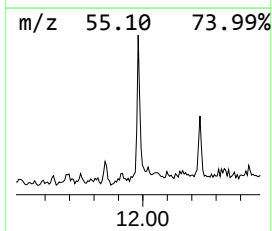
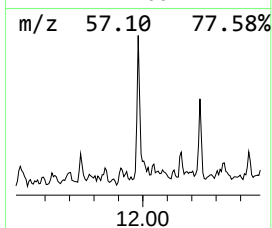
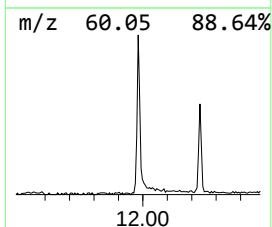
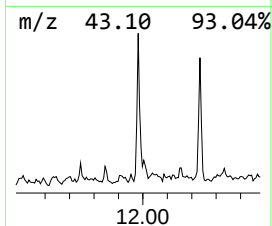
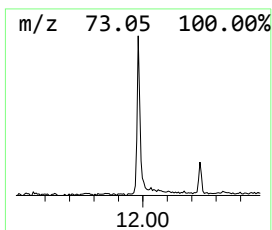
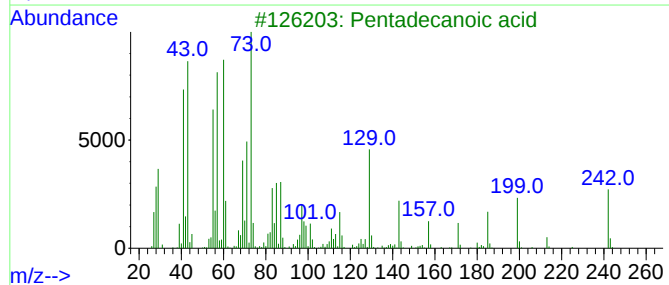
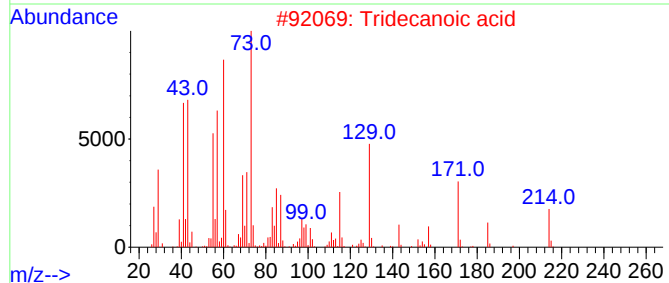
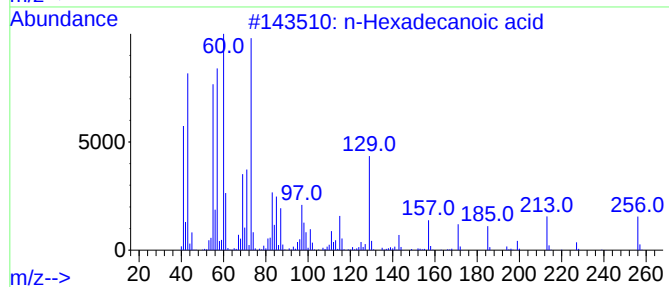
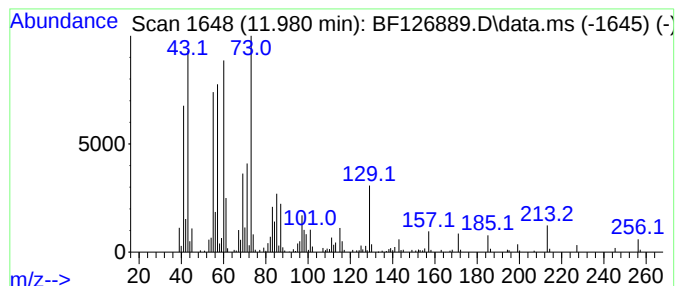
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.980	4.05 ng	233436	Phenanthrene-d10	11.469	
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	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	64



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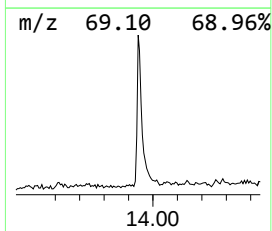
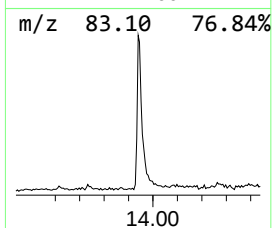
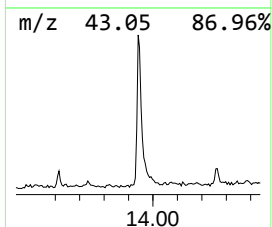
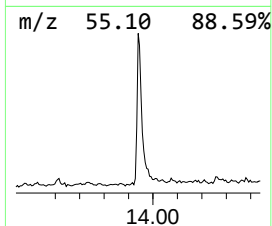
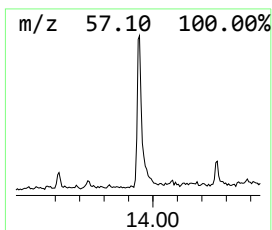
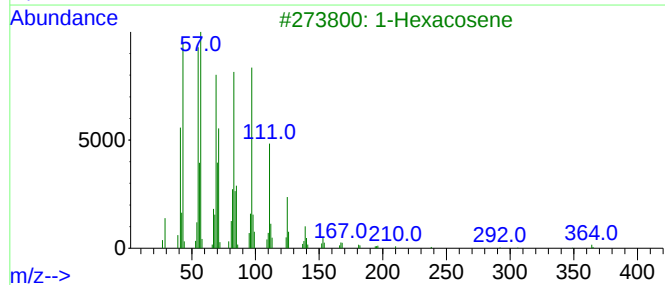
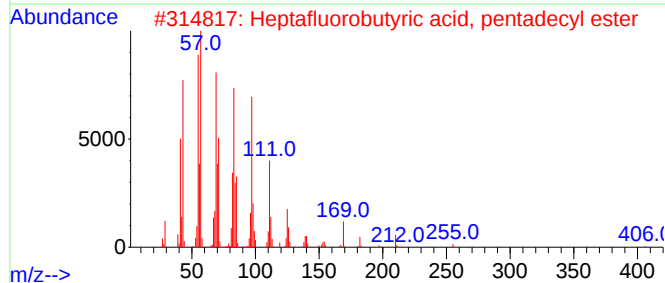
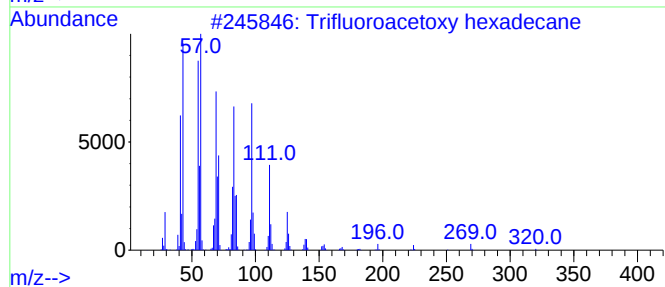
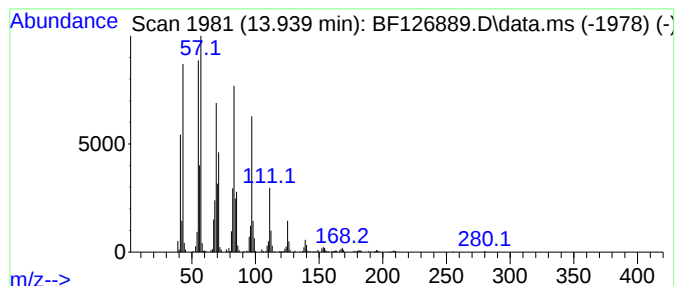
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.939	15.80 ng	673778	Chrysene-d12	14.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3			1-Hexacosene	364	C26H52	018835-33-1	94
4			1-Docosene	308	C22H44	001599-67-3	94
5			1-Heneicosanol	312	C21H44O	015594-90-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021522\
Data File : BF126889.D
Acq On : 15 Feb 2022 14:07
Operator : CG\JU
Sample : N1511-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220041-AMENDED-NACOTE-1-COMP

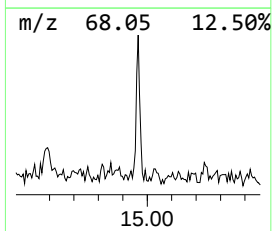
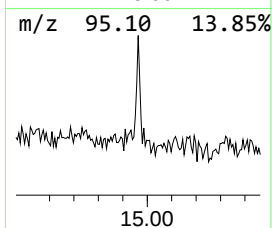
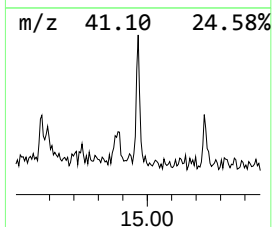
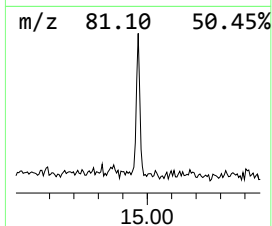
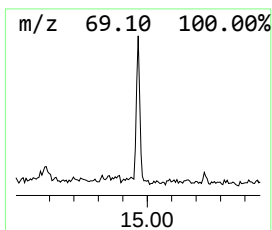
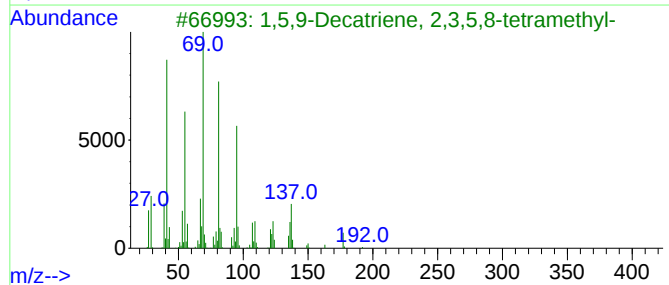
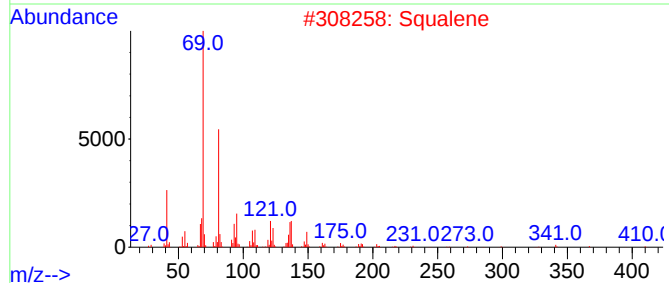
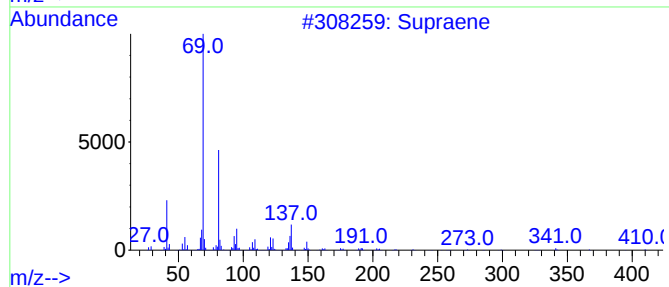
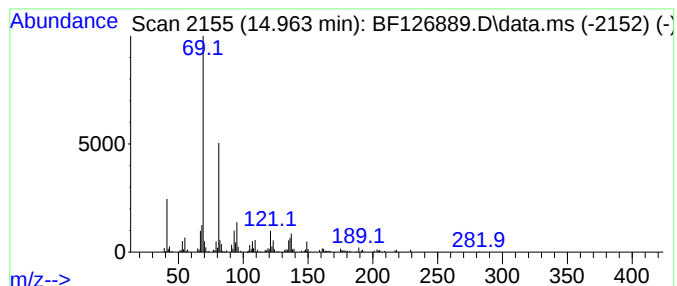
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.963	3.34 ng	122391	Perylene-d12	15.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			Squalene	410	C30H50	000111-02-4	90
3			1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	72
4			3,7,11-Tridecatricienoic acid, 4,8...	264	C17H28O2	036237-69-1	64
5			2-Octene, 2-methyl-6-methylene-	138	C10H18	010054-09-8	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021522\
Data File : BF126889.D
Acq On : 15 Feb 2022 14:07
Operator : CG\JU
Sample : N1511-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220041-AMENDED-NACOTE-1-COMP

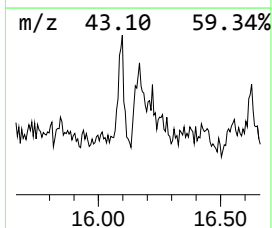
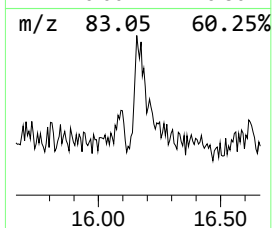
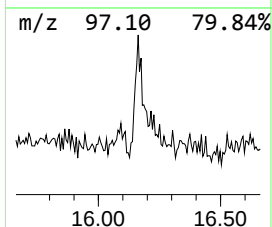
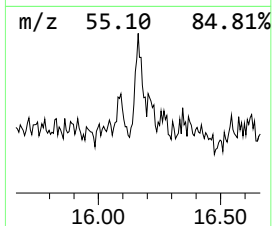
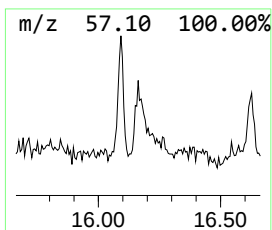
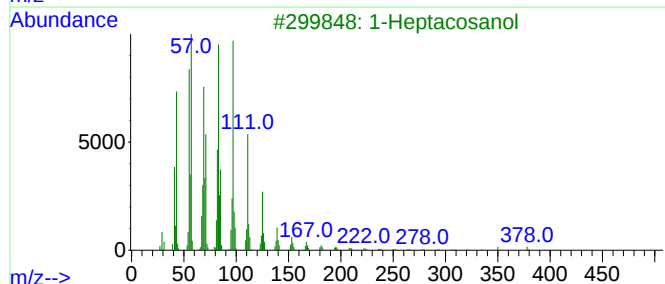
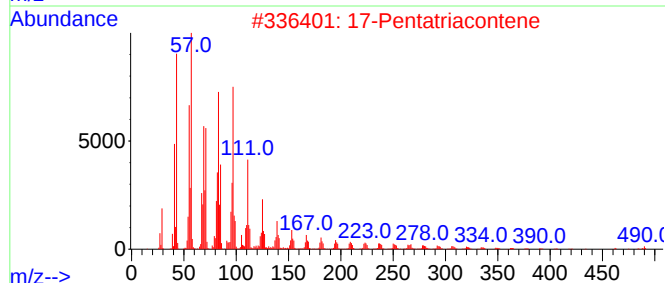
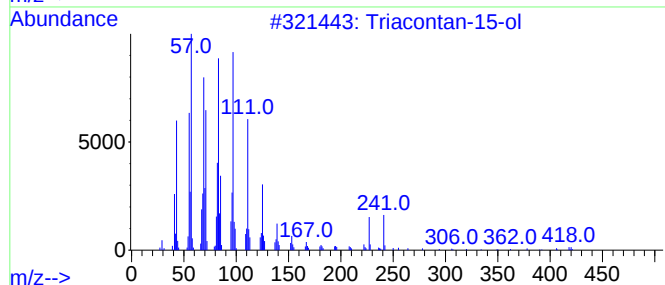
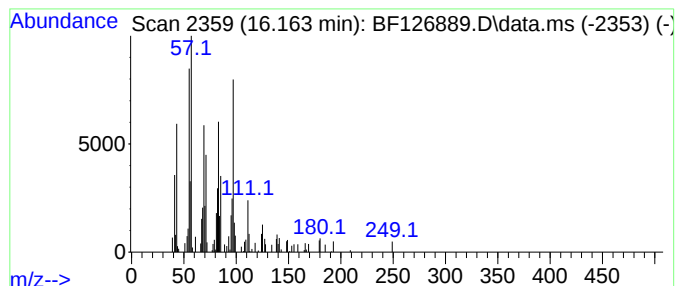
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Triacontan-15-ol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.163	2.81 ng	103167	Perylene-d12	15.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triacontan-15-ol	438	C30H62O	031849-26-0	83
2			17-Pentatriacontene	491	C35H70	006971-40-0	74
3			1-Heptacosanol	396	C27H56O	002004-39-9	68
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	64
5			1-Heneicosanol	312	C21H44O	015594-90-8	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021522\
Data File : BF126889.D
Acq On : 15 Feb 2022 14:07
Operator : CG\JU
Sample : N1511-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220041-AMENDED-NACOTE-1-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020922.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-...	5.181	6.7	ng	224712	1	6.940	673545	20.0
Ethanol, 2,2'-o...	6.481	3.8	ng	129116	1	6.940	673545	20.0
Ethanol, 2-(2-b...	8.110	2.4	ng	110944	2	8.222	933720	20.0
Triethylene glycol	8.351	3.2	ng	150434	2	8.222	933720	20.0
n-Hexadecanoic ...	11.980	4.0	ng	233436	4	11.469	1152540	20.0
Trifluoroacetox...	13.939	15.8	ng	673778	5	14.110	852662	20.0
Supraene	14.963	3.3	ng	122391	6	15.616	733863	20.0
Triacontan-15-ol	16.163	2.8	ng	103167	6	15.616	733863	20.0