

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
 Data File : BF125950.D
 Acq On : 26 Oct 2021 23:51
 Operator : JU/CG
 Sample : M4348-08
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 287

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-BF102521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125950.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	6	14	20	rBV	2911262	3880991	81.54%	9.853%
2	5.098	509	512	517	rVB	42569	48982	1.03%	0.124%
3	5.481	572	577	580	rBV	4535671	4759730	100.00%	12.084%
4	6.487	742	748	751	rBV	4193995	4686878	98.47%	11.899%
5	6.863	807	812	816	rBV	1297342	1172604	24.64%	2.977%
6	7.428	901	908	911	rBV	3376153	3058062	64.25%	7.764%
7	8.051	1010	1014	1017	rBV	996038	713820	15.00%	1.812%
8	8.145	1026	1030	1034	rBV	1642588	1452622	30.52%	3.688%
9	9.222	1209	1213	1217	rBV	4064691	3858266	81.06%	9.795%
10	9.357	1230	1236	1239	rBV	480208	574693	12.07%	1.459%
11	9.845	1316	1319	1325	rBV3	50275	59671	1.25%	0.151%
12	9.904	1325	1329	1332	rVB	1566725	1425773	29.95%	3.620%
13	10.686	1458	1462	1465	rBV	2877451	2395386	50.33%	6.081%
14	11.192	1545	1548	1552	rBV	107229	96112	2.02%	0.244%
15	11.386	1577	1581	1583	rBV	1393088	1199091	25.19%	3.044%
16	11.916	1667	1671	1677	rBV2	190858	186336	3.91%	0.473%
17	12.363	1744	1747	1756	rBV	379608	337534	7.09%	0.857%
18	12.592	1783	1786	1790	rBV	151194	143788	3.02%	0.365%
19	12.698	1800	1804	1810	rBV2	86292	96363	2.02%	0.245%
20	12.821	1818	1825	1828	rBV	152022	161833	3.40%	0.411%
21	12.974	1846	1851	1854	rVB	2777103	2543455	53.44%	6.457%
22	13.392	1919	1922	1931	rBV	769434	718936	15.10%	1.825%
23	13.874	1999	2004	2009	rBV2	252759	249363	5.24%	0.633%
24	14.021	2025	2029	2032	rBV	1210730	1122556	23.58%	2.850%
25	14.045	2032	2033	2037	rVB	92437	62361	1.31%	0.158%
26	14.310	2074	2078	2086	rBV	1344565	1208208	25.38%	3.067%
27	14.510	2109	2112	2115	rBV4	53505	57719	1.21%	0.147%
28	14.898	2175	2178	2182	rVB2	62170	60179	1.26%	0.153%
29	15.062	2202	2206	2208	rBV	97487	124036	2.61%	0.315%
30	15.221	2228	2233	2243	rBV	949618	1140377	23.96%	2.895%
31	15.368	2254	2258	2261	rVB	61813	81356	1.71%	0.207%
32	15.427	2265	2268	2271	rVB	62068	72383	1.52%	0.184%
33	15.492	2274	2279	2283	rBV	916908	1081452	22.72%	2.746%
34	16.033	2368	2371	2379	rVB8	68404	107499	2.26%	0.273%
35	16.456	2437	2443	2450	rBV	256356	450550	9.47%	1.144%

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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-BF102521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

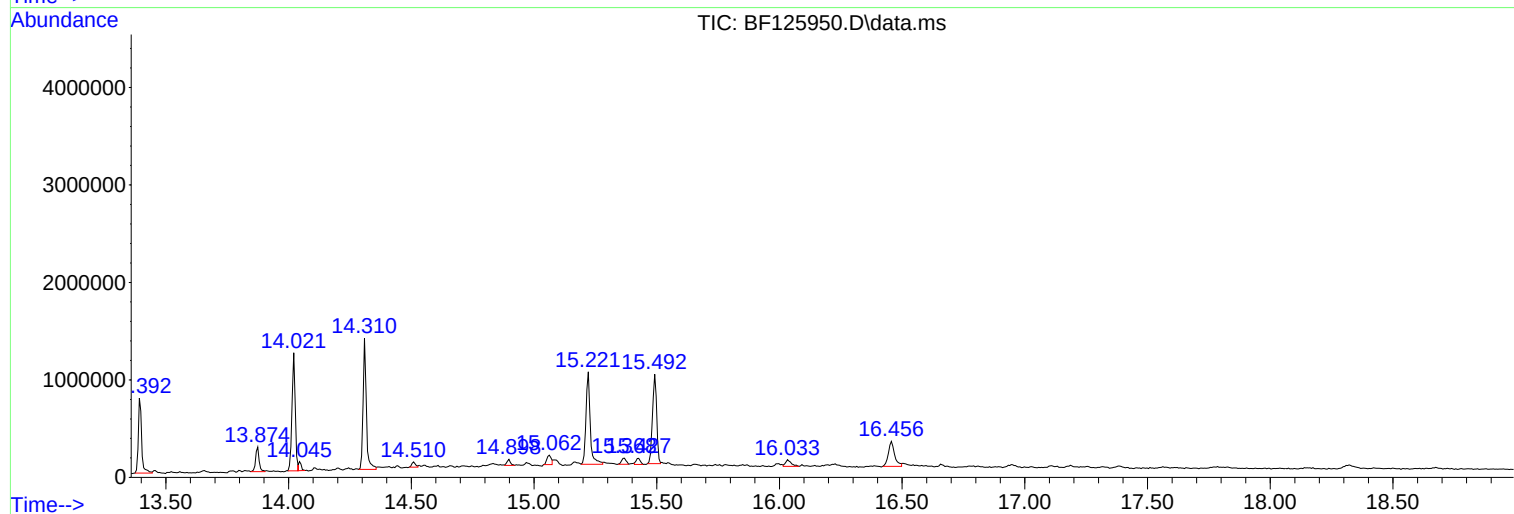
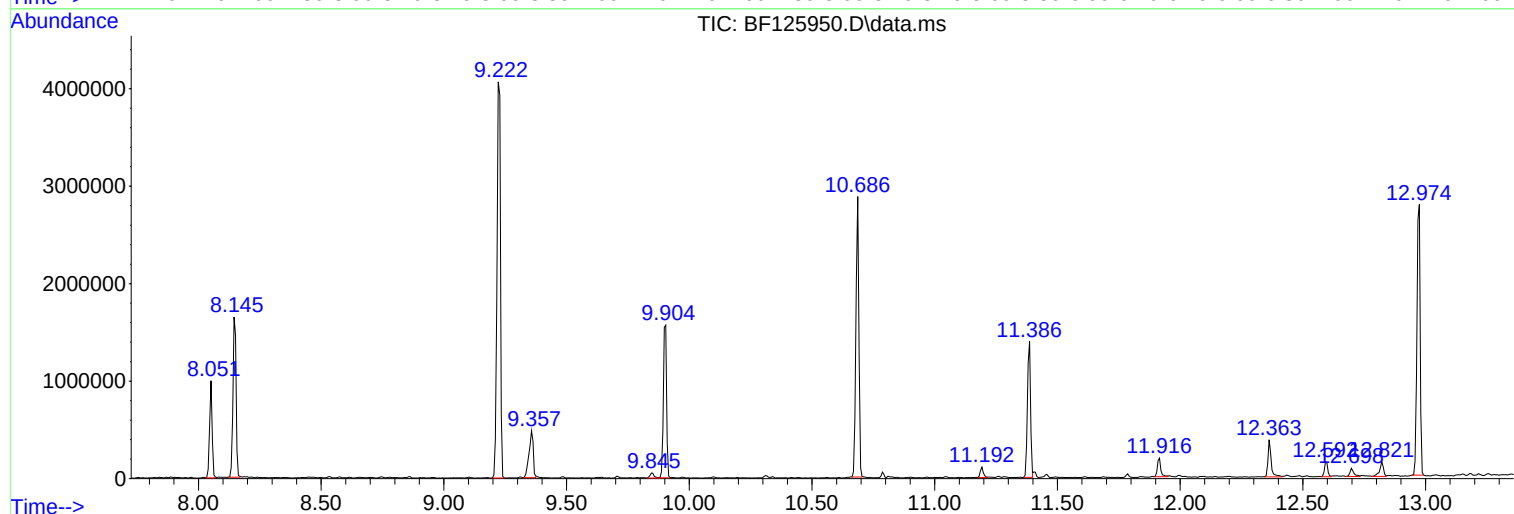
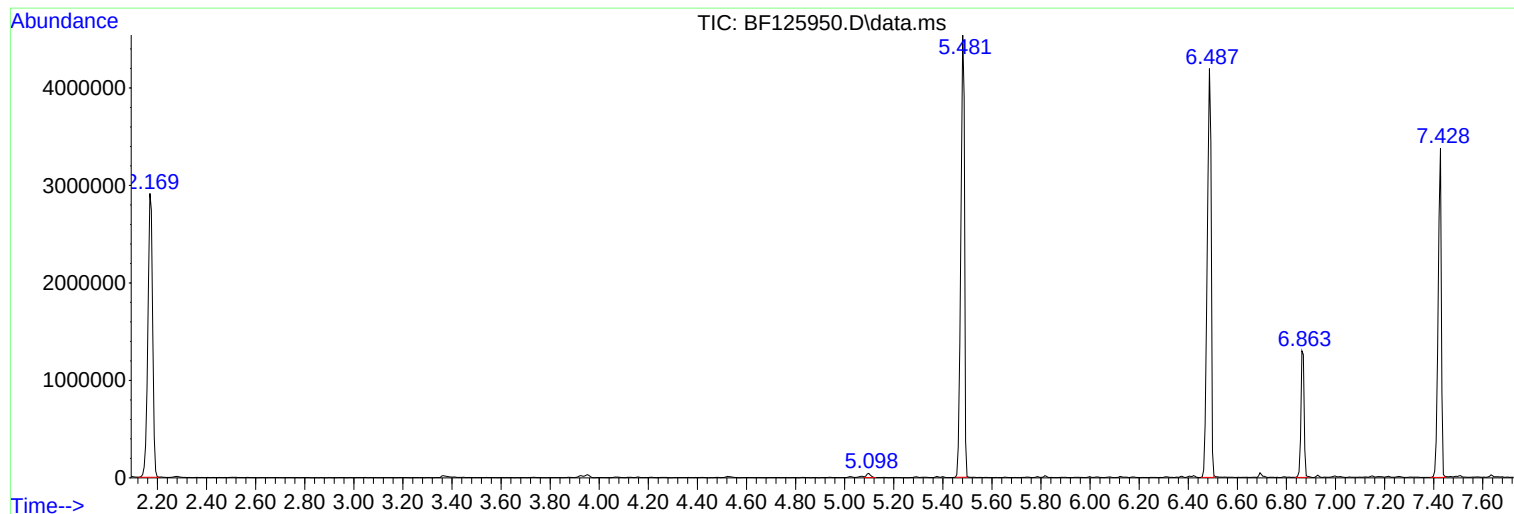
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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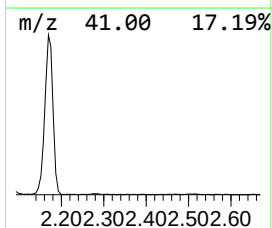
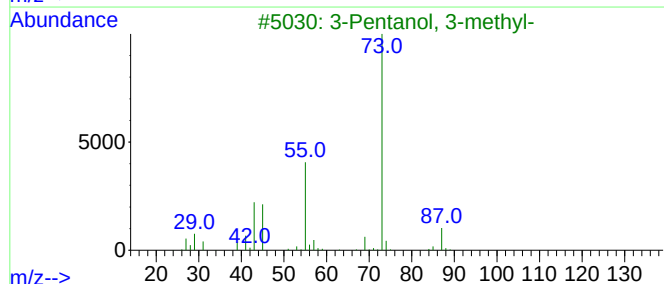
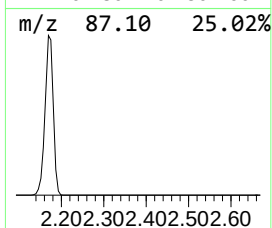
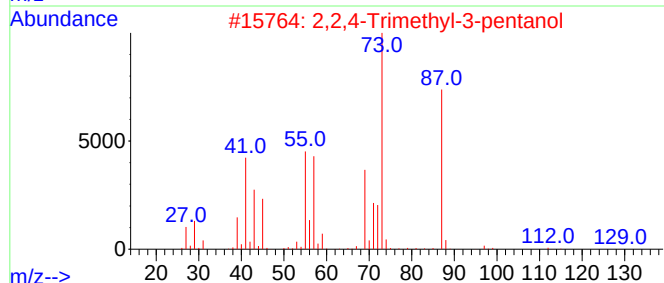
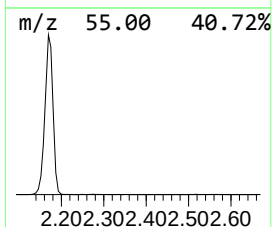
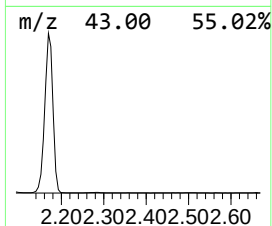
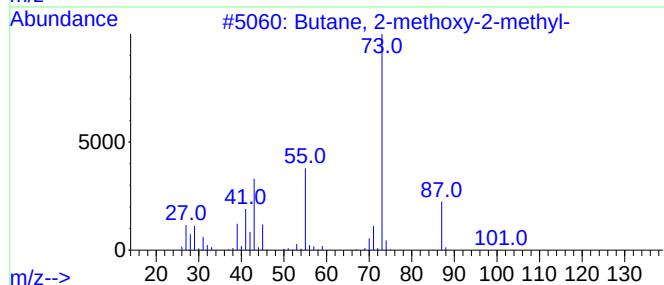
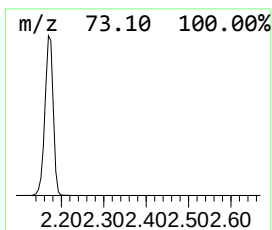
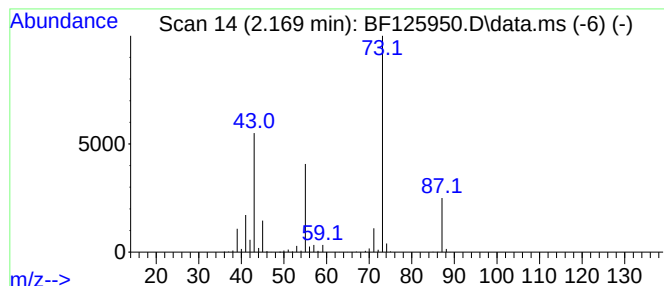
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	66.19 ng	3880990	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	25
4			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
287

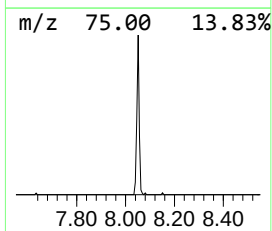
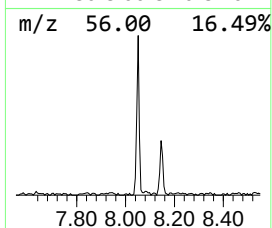
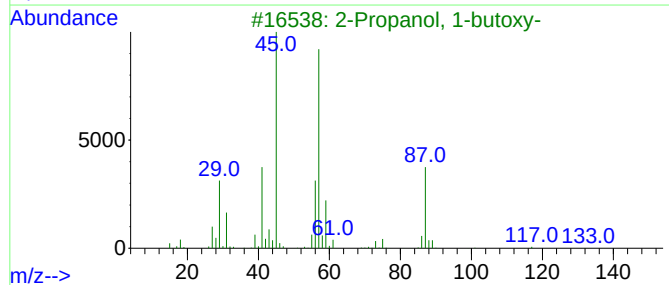
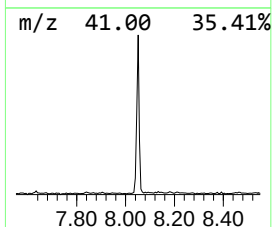
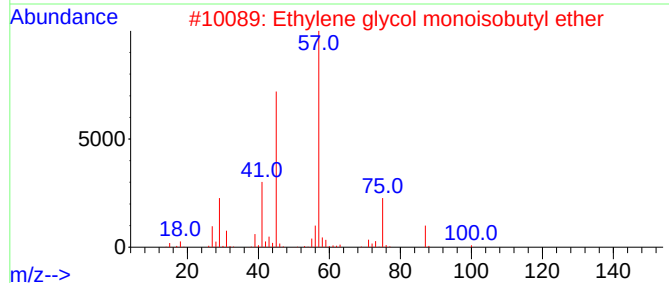
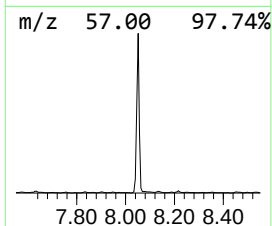
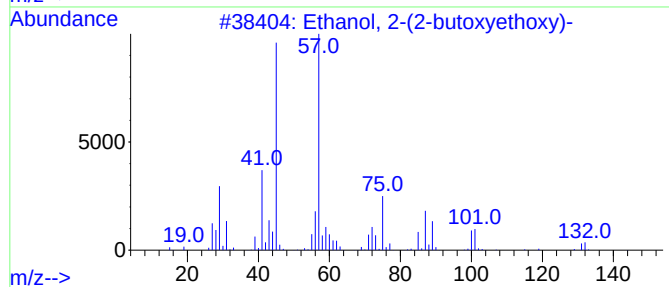
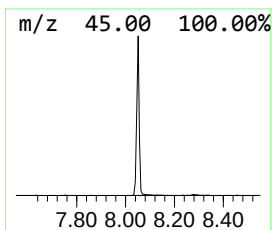
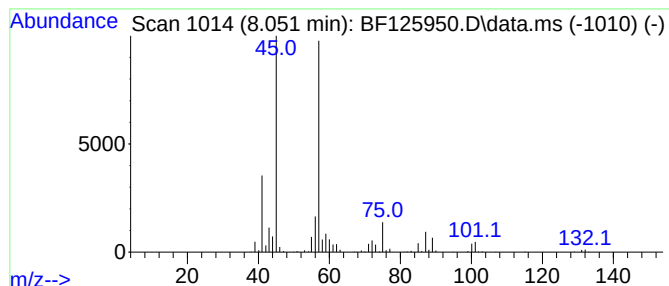
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	9.83 ng	713820	Naphthalene-d8	8.145

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	64
3			2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	59
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
5			Tetraethylene glycol	194	C8H18O5	000112-60-7	50



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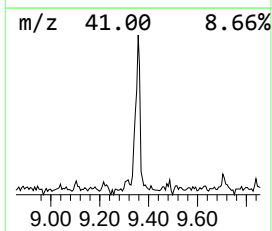
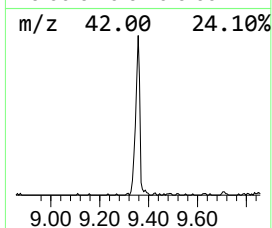
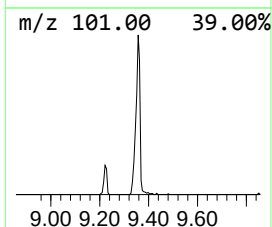
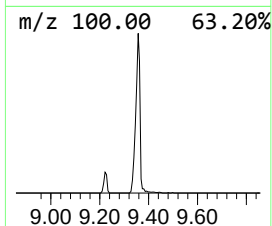
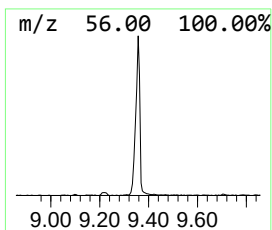
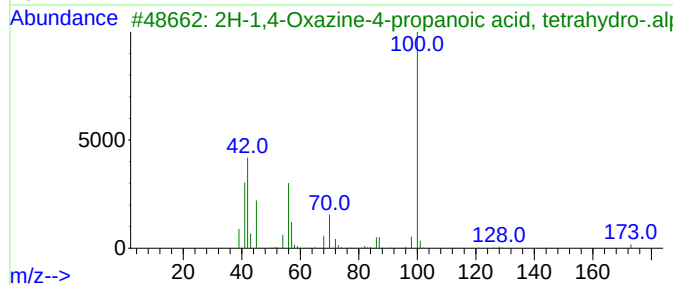
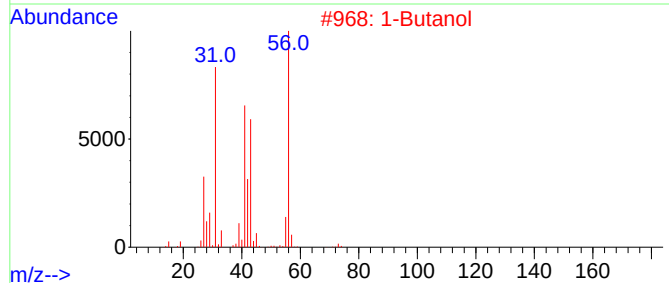
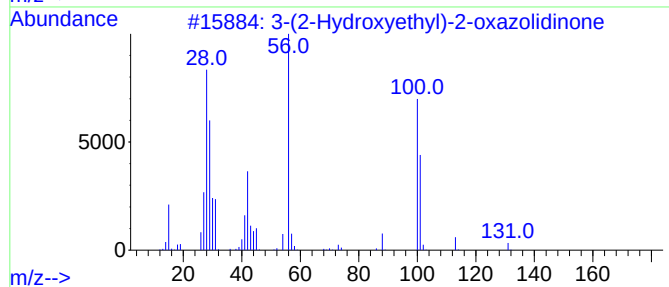
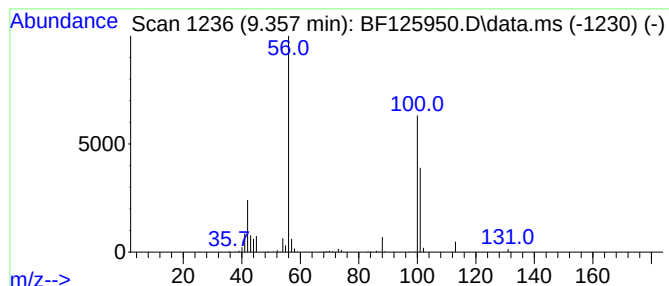
Instrument :
BNA_F
ClientSampleId :
287

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 3-(2-Hydroxyethyl)-2-oxazol... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD			R.T.
9.357	8.06 ng	574693	Acenaphthene-d10			9.904
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	3-(2-Hydroxyethyl)-2-oxazolidinone		131	C5H9NO3	003356-88-5	64
2	1-Butanol		74	C4H10O	000071-36-3	38
3	2H-1,4-Oxazine-4-propanoic acid,...		173	C8H15NO3	322725-55-3	12
4	Propanamide, N-ethyl-		101	C5H11NO	005129-72-6	9
5	Aminothiazole		100	C3H4N2S	000096-50-4	9



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Instrument :
BNA_F
ClientSampled :
287

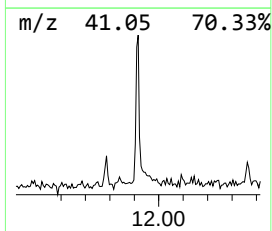
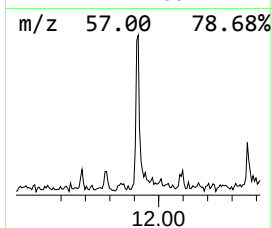
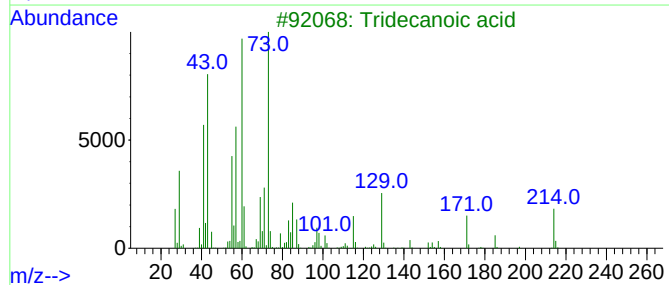
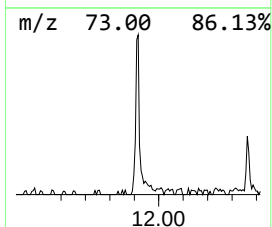
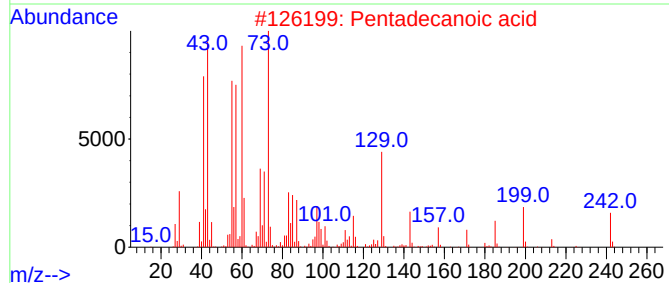
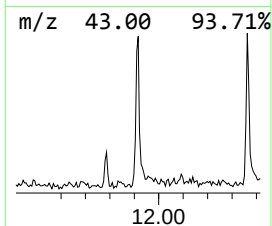
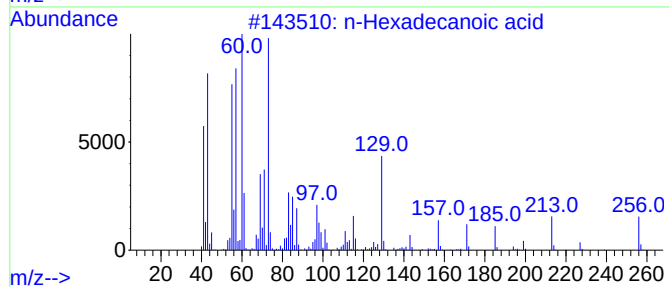
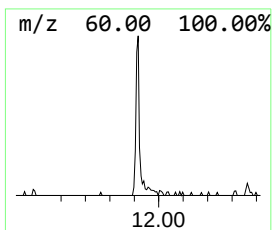
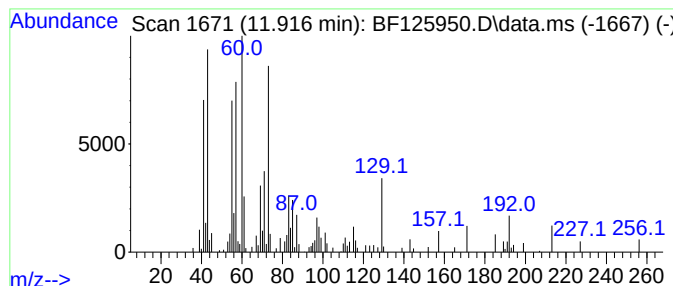
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	3.11 ng	186336	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3			Tridecanoic acid	214	C13H26O2	000638-53-9	72
4			Undecanoic acid	186	C11H22O2	000112-37-8	64
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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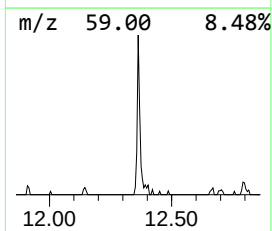
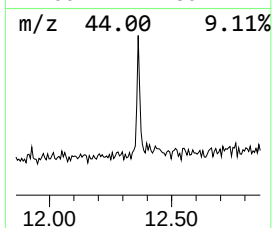
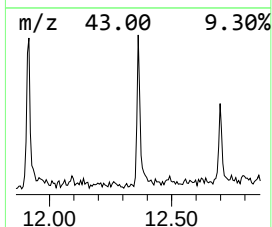
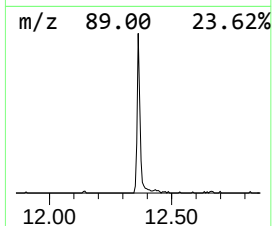
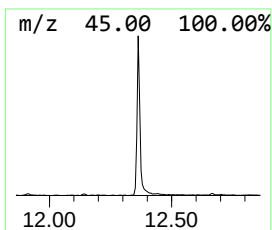
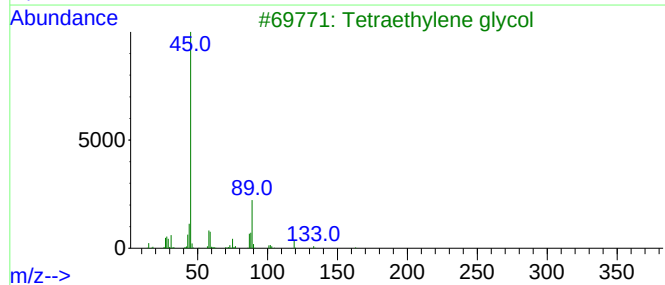
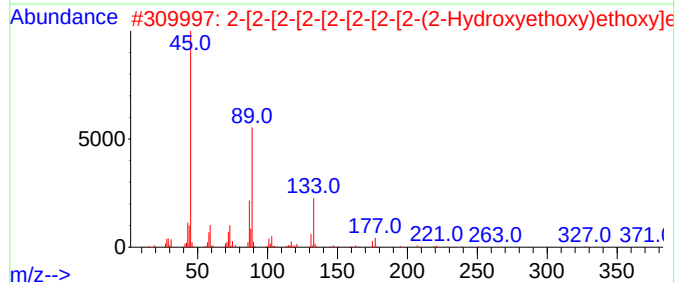
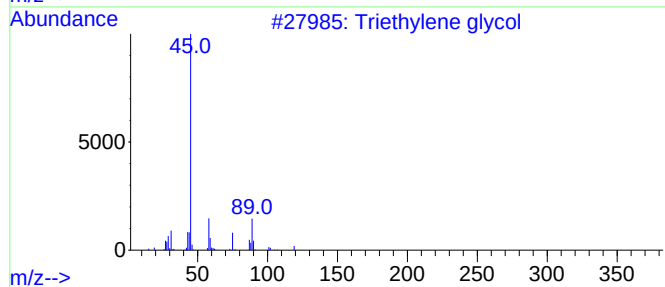
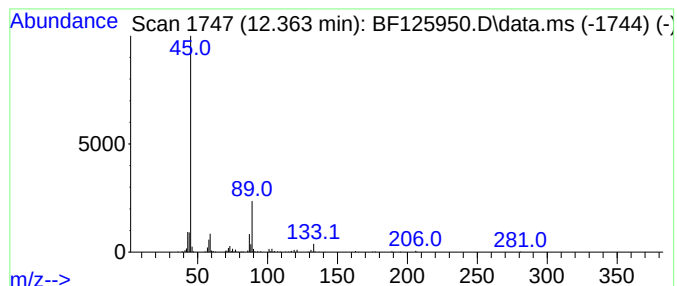
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Triethylene glycol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.363	5.63 ng	337534	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triethylene glycol	150	C6H14O4	000112-27-6	78
2			2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	003386-18-3	74
3			Tetraethylene glycol	194	C8H18O5	000112-60-7	64
4			Ethanol, 2-[2-(2-methoxyethoxy)e...	164	C7H16O4	000112-35-6	64
5			3,6,9,12-Tetraoxahexadecan-1-ol	250	C12H26O5	001559-34-8	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125950.D
Acq On : 26 Oct 2021 23:51
Operator : JU/CG
Sample : M4348-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
287

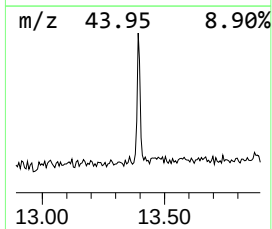
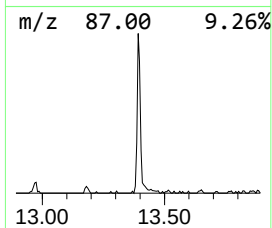
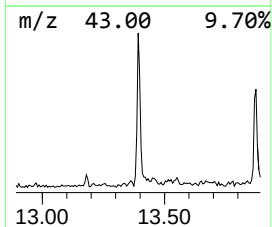
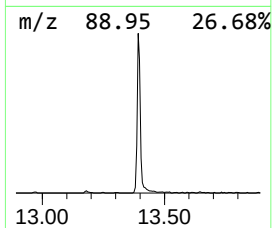
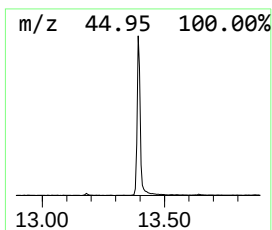
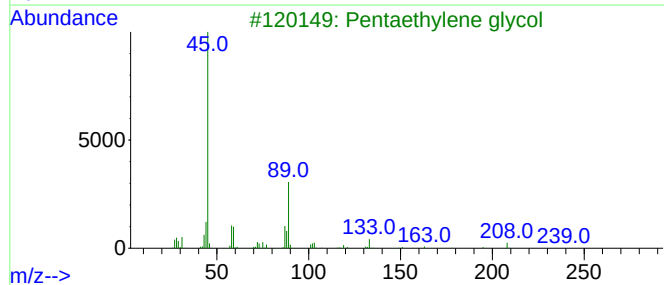
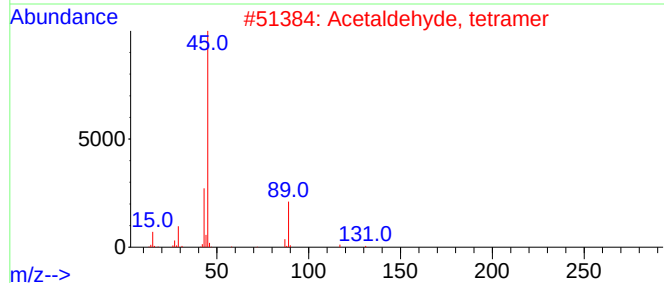
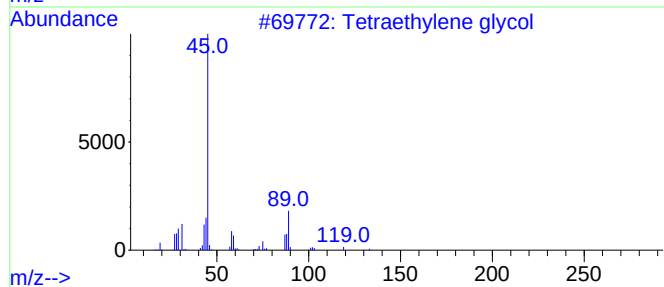
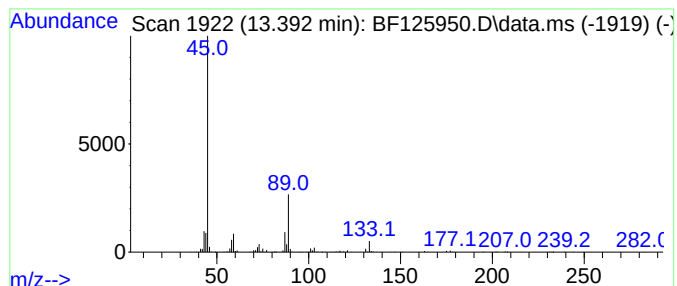
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetraethylene glycol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.392	12.81 ng	718936	Chrysene-d12	14.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetraethylene glycol	194	C8H18O5	000112-60-7	78
2			Acetaldehyde, tetramer	176	C8H16O4	000108-62-3	64
3			Pentaethylene glycol	238	C10H22O6	004792-15-8	64
4			Triethylene glycol	150	C6H14O4	000112-27-6	56
5			3,6,9,12-Tetraoxahexadecan-1-ol	250	C12H26O5	001559-34-8	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125950.D
Acq On : 26 Oct 2021 23:51
Operator : JU/CG
Sample : M4348-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
287

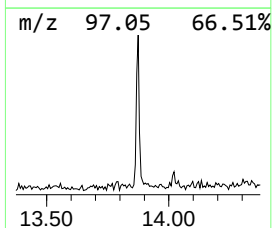
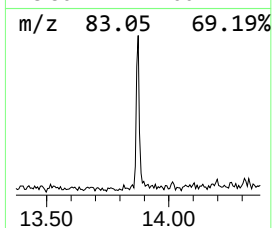
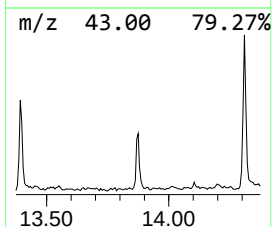
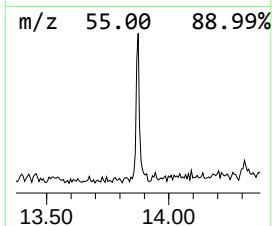
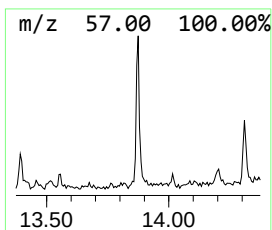
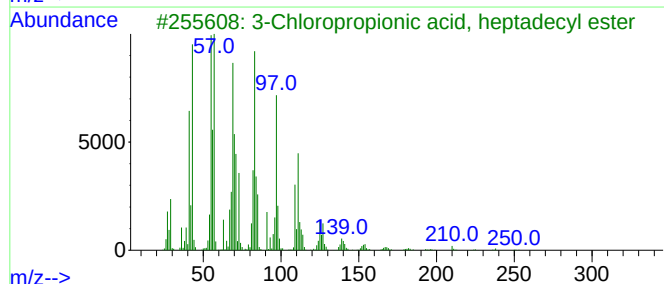
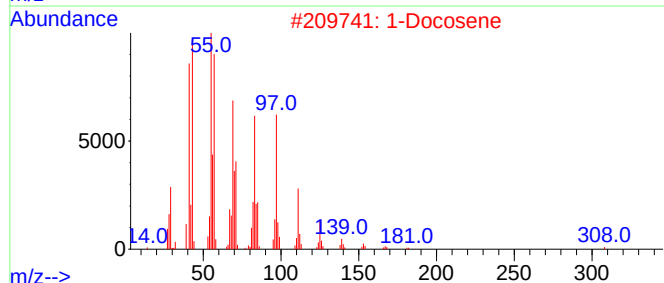
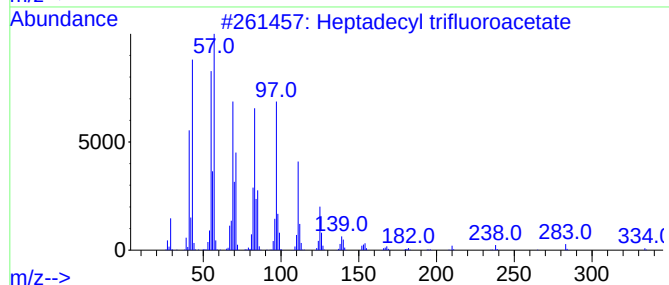
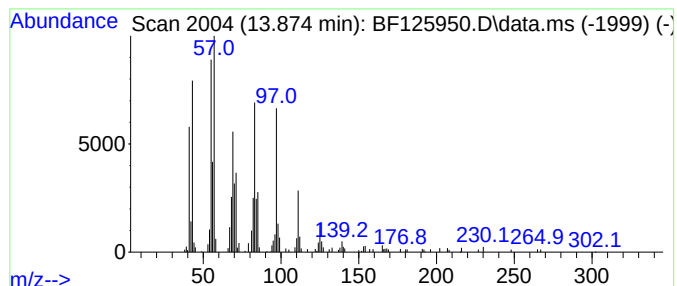
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecyl trifluoroacetate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	4.44 ng	249363	Chrysene-d12	14.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91
2			1-Docosene	308	C22H44	001599-67-3	91
3			3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
4			Cyclohexadecane	224	C16H32	000295-65-8	91
5			1-Octadecanol	270	C18H38O	000112-92-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125950.D
Acq On : 26 Oct 2021 23:51
Operator : JU/CG
Sample : M4348-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
287

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.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
Butane, 2-metho...	2.169	66.2	ng	3880990	1	6.869	1172600	20.0
Ethanol, 2-(2-b...	8.051	9.8	ng	713820	2	8.145	1452620	20.0
3-(2-Hydroxyeth...	9.357	8.1	ng	574693	3	9.904	1425770	20.0
n-Hexadecanoic ...	11.916	3.1	ng	186336	4	11.386	1199090	20.0
Triethylene glycol	12.363	5.6	ng	337534	4	11.386	1199090	20.0
Tetraethylene g...	13.392	12.8	ng	718936	5	14.021	1122560	20.0
Heptadecyl trif...	13.874	4.4	ng	249363	5	14.021	1122560	20.0
2-[2-[2-[2-[2-...	14.310	21.5	ng	1208210	5	14.021	1122560	20.0
Heptaethylene g...	15.221	21.1	ng	1140380	6	15.492	1081450	20.0
2-[2-[2-[2-[2-...	16.456	8.3	ng	450550	6	15.492	1081450	20.0