

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
 Data File : BF125947.D
 Acq On : 26 Oct 2021 22:15
 Operator : JU/CG
 Sample : M4348-04
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 358

Integration Parameters: rteint.p

Integrator: RTE

Smoother: 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: BF125947.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	6	13	21	rVB	2980068	3836989	91.62%	11.134%
2	5.092	508	511	518	rVB	49688	58075	1.39%	0.169%
3	5.481	572	577	580	rBV	4409631	4146085	99.00%	12.031%
4	6.486	743	748	751	rBV	4088489	4187813	100.00%	12.152%
5	6.863	806	812	816	rBV	1241221	1147278	27.40%	3.329%
6	7.428	903	908	911	rBV	2887278	2706226	64.62%	7.853%
7	8.022	1005	1009	1011	rBV	65825	67580	1.61%	0.196%
8	8.051	1011	1014	1017	rVB	870209	610458	14.58%	1.771%
9	8.145	1026	1030	1034	rBV	1593433	1386939	33.12%	4.024%
10	8.227	1041	1044	1053	rVB2	111674	106279	2.54%	0.308%
11	9.222	1209	1213	1217	rBV	3706625	3514859	83.93%	10.199%
12	9.351	1231	1235	1238	rBV	308202	330855	7.90%	0.960%
13	9.904	1325	1329	1332	rVB	1644075	1431549	34.18%	4.154%
14	10.310	1395	1398	1406	rVB4	37446	55709	1.33%	0.162%
15	10.686	1458	1462	1465	rBV	2819891	2345540	56.01%	6.806%
16	10.827	1481	1486	1491	rVB2	40611	55403	1.32%	0.161%
17	10.933	1502	1504	1507	rVB	135370	100968	2.41%	0.293%
18	11.292	1561	1565	1568	rVB3	33597	43205	1.03%	0.125%
19	11.386	1577	1581	1583	rBV	1525324	1314154	31.38%	3.813%
20	11.410	1583	1585	1588	rVV	271580	211217	5.04%	0.613%
21	11.457	1591	1593	1597	rVB2	65467	52052	1.24%	0.151%
22	11.915	1668	1671	1676	rBV	249476	208364	4.98%	0.605%
23	11.998	1681	1685	1687	rBV2	48566	51011	1.22%	0.148%
24	12.433	1757	1759	1763	rVB2	63201	61952	1.48%	0.180%
25	12.598	1783	1787	1790	rBV	308143	290748	6.94%	0.844%
26	12.698	1801	1804	1807	rBV2	79175	80651	1.93%	0.234%
27	12.821	1820	1825	1828	rBV	255508	251524	6.01%	0.730%
28	12.974	1846	1851	1854	rVB	2494018	2342082	55.93%	6.796%
29	13.768	1982	1986	1990	rBV5	27376	45375	1.08%	0.132%
30	13.874	1999	2004	2014	rBV2	285007	318792	7.61%	0.925%
31	14.021	2024	2029	2032	rBV2	1197512	1232547	29.43%	3.576%
32	14.045	2032	2033	2040	rVB	115825	102357	2.44%	0.297%
33	14.898	2174	2178	2182	rVB	243907	240030	5.73%	0.696%
34	15.062	2202	2206	2209	rBV	94175	139167	3.32%	0.404%
35	15.162	2221	2223	2230	rVB4	29808	45079	1.08%	0.131%
36	15.368	2254	2258	2264	rBV	60549	81137	1.94%	0.235%

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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

37	15.421	2264	2267	2273	rVB	71686	91424	2.18%	0.265%
38	15.492	2274	2279	2284	rBV	852033	1041320	24.87%	3.022%
39	16.039	2369	2372	2378	rVB8	36039	56568	1.35%	0.164%
40	16.950	2522	2527	2535	rVB5	32004	73114	1.75%	0.212%

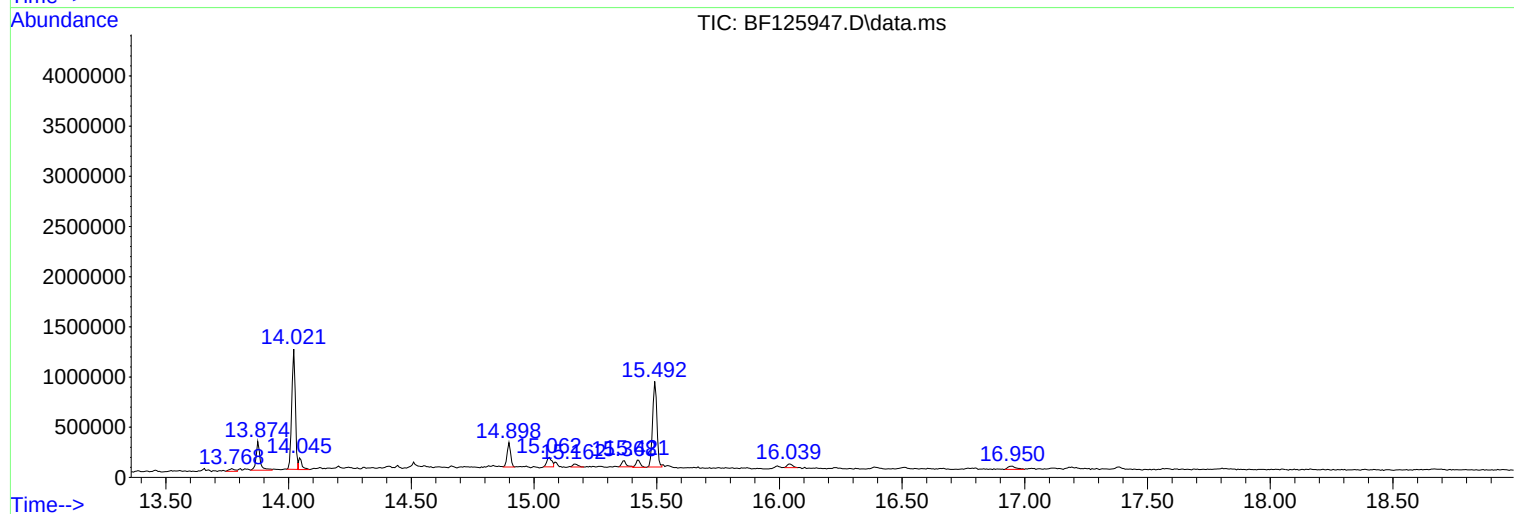
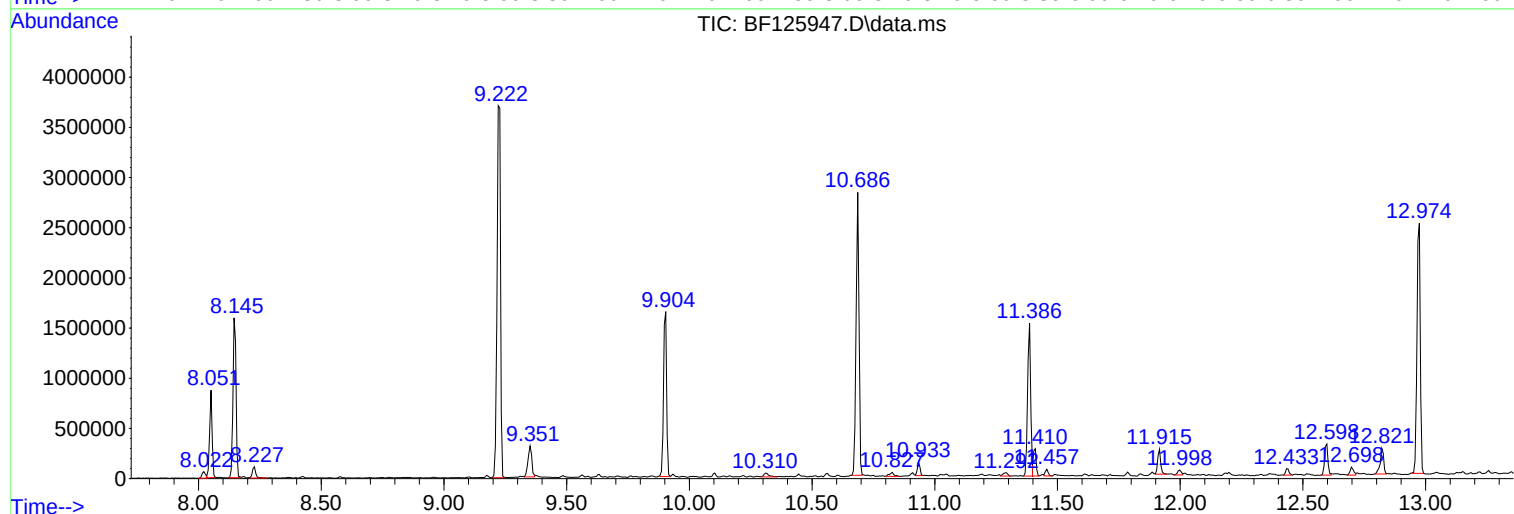
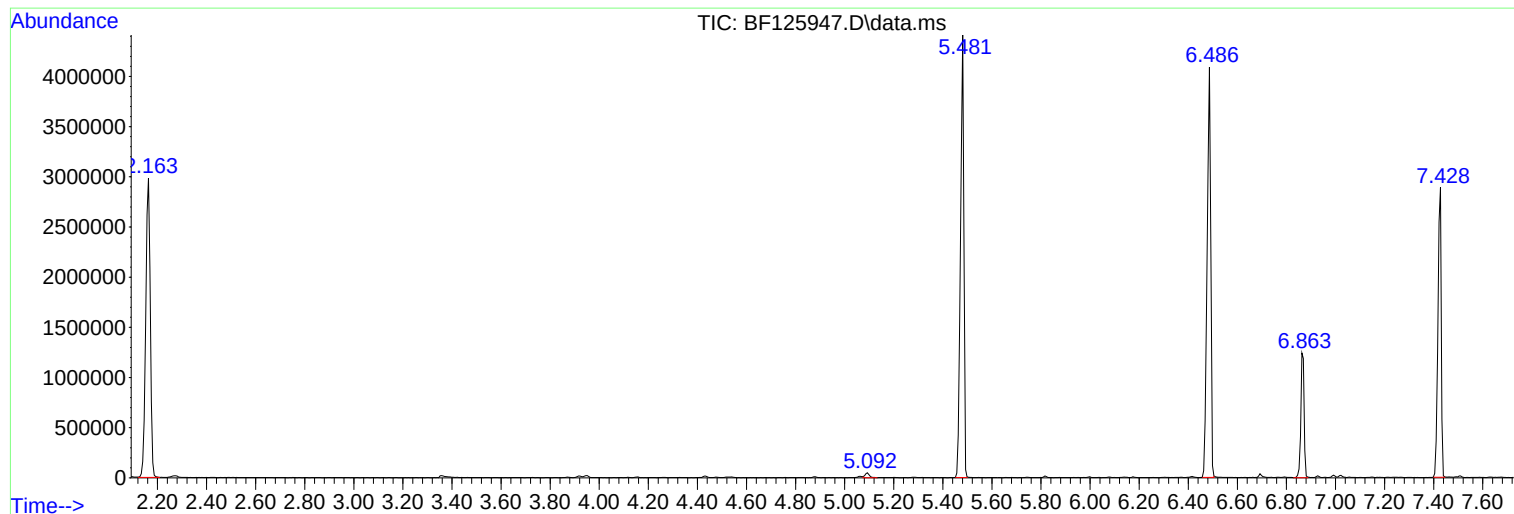
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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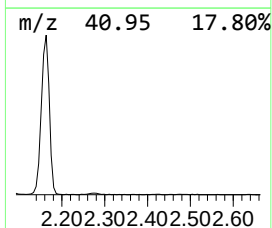
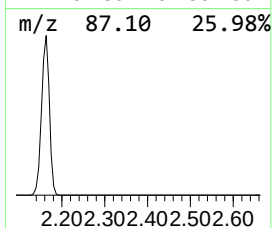
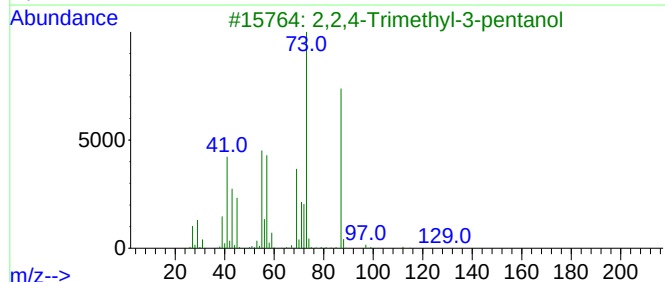
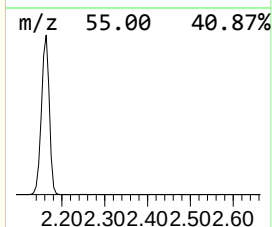
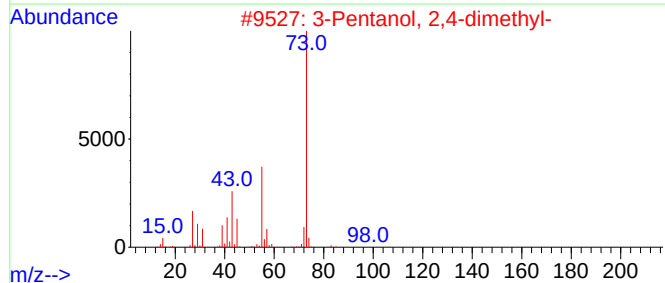
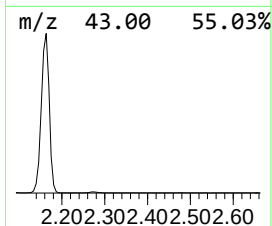
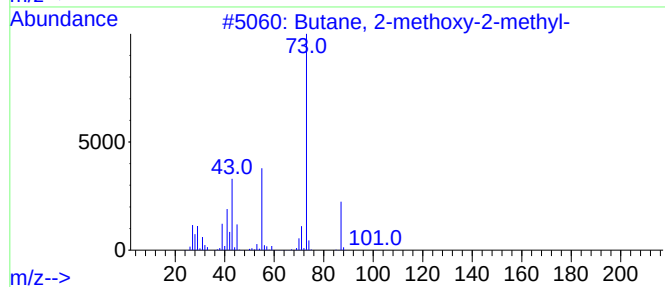
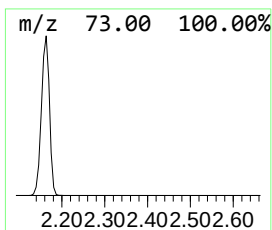
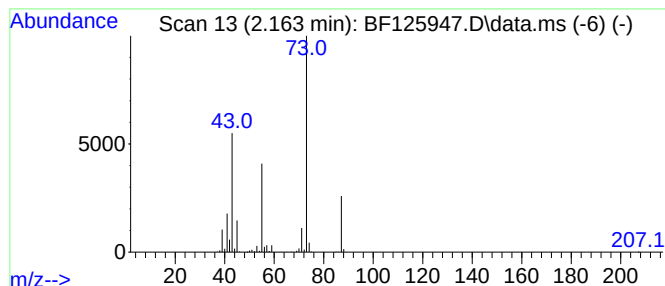
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.163	66.89 ng	3836990	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			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	32
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	25



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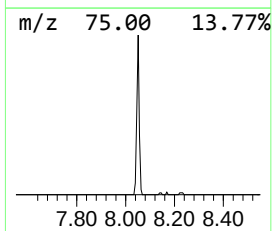
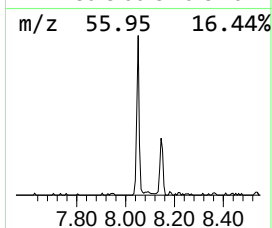
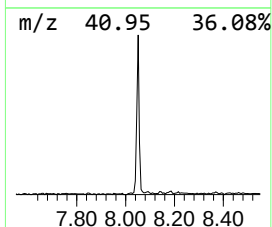
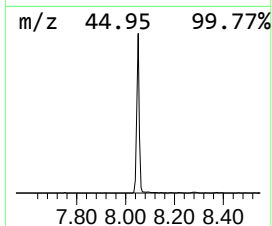
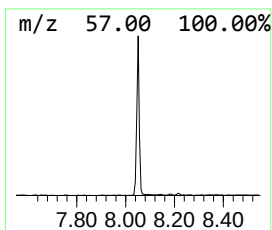
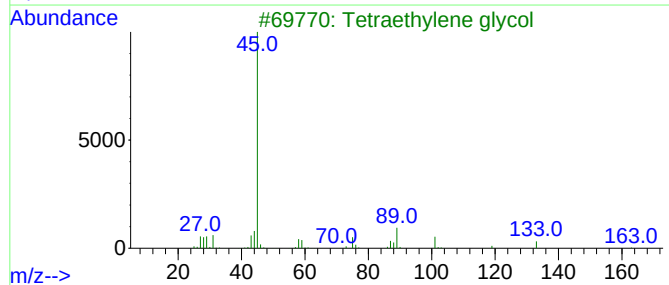
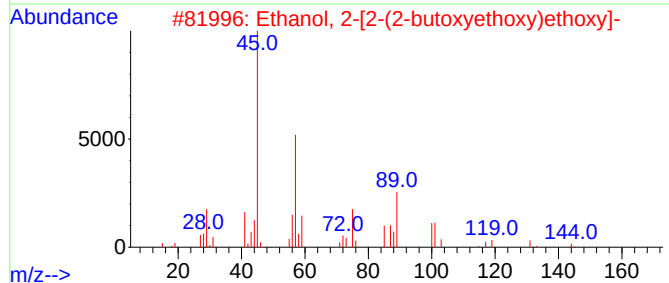
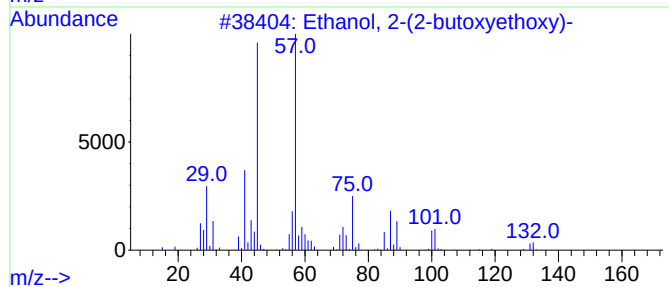
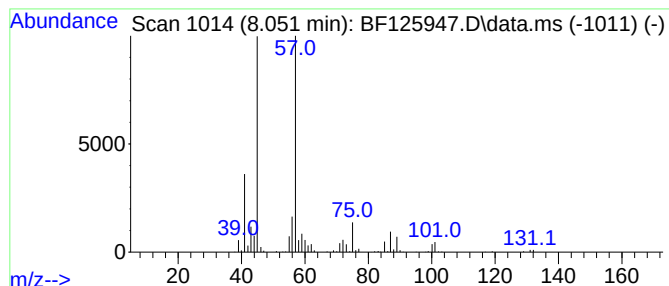
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	8.80 ng	610458	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			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	50
3			Tetraethylene glycol	194	C8H18O5	000112-60-7	50
4			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
5			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50



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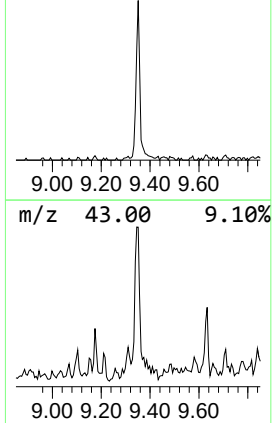
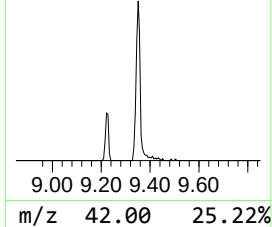
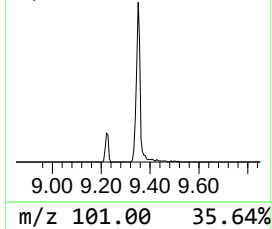
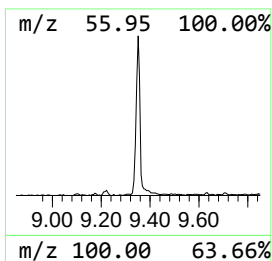
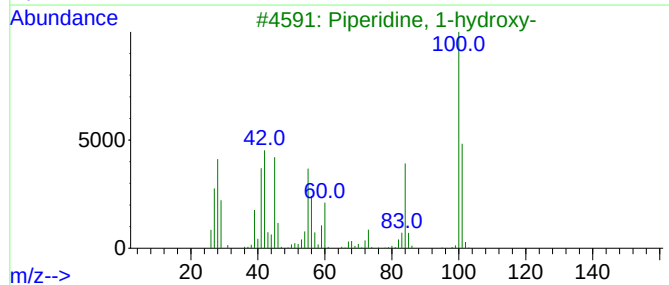
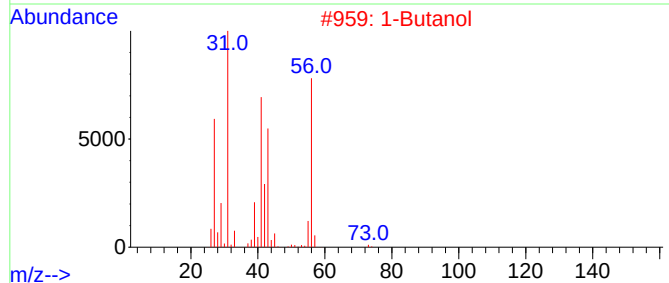
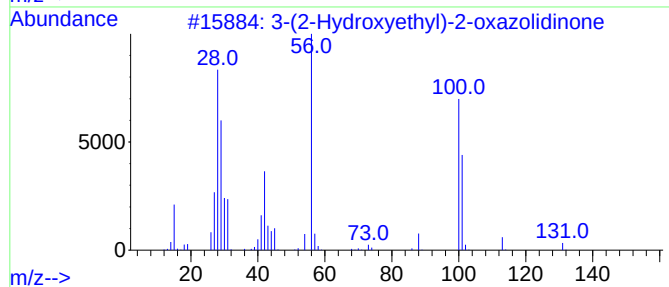
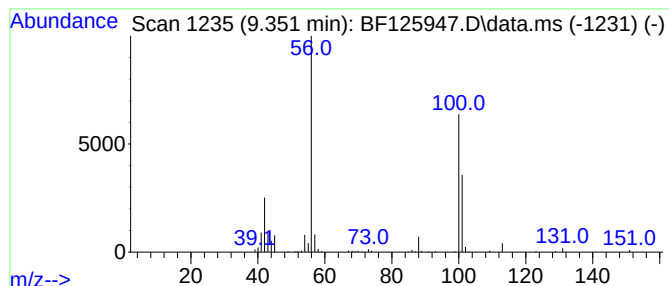
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 3-(2-Hydroxyethyl)-2-oxazol... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.351	4.62 ng	330855	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	43
3			Piperidine, 1-hydroxy-	101	C5H11NO	004801-58-5	32
4			4-Morpholineethanol	131	C6H13NO2	000622-40-2	25
5			Methanamine, N-(1-methylbutylidene...	99	C6H13N	022431-09-0	25



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ALS Vial : 14 Sample Multiplier: 1

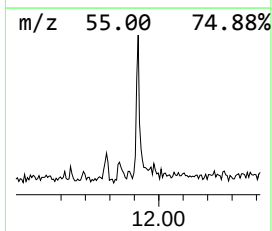
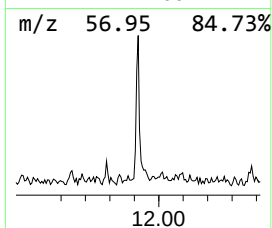
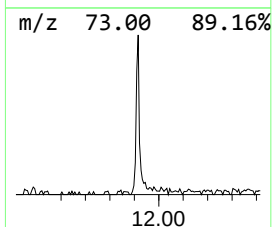
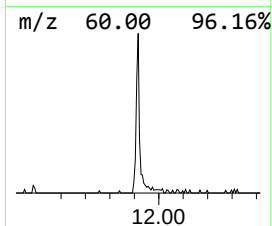
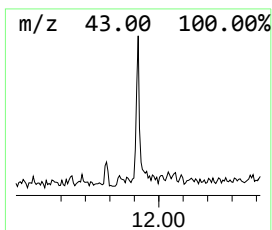
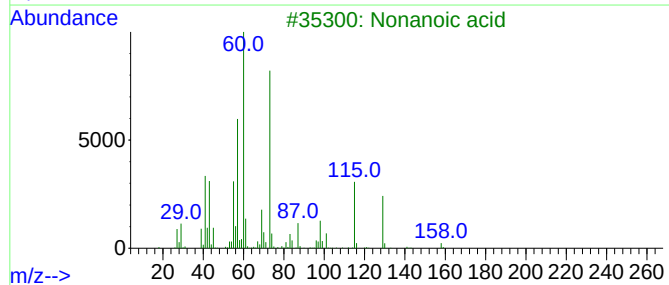
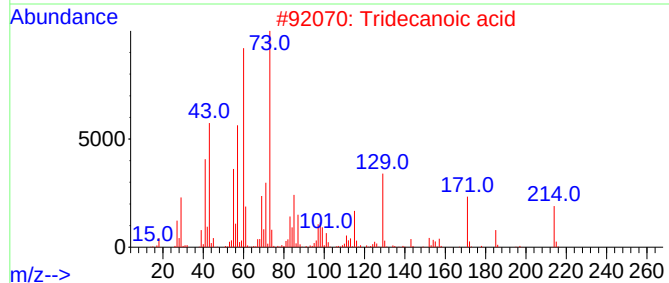
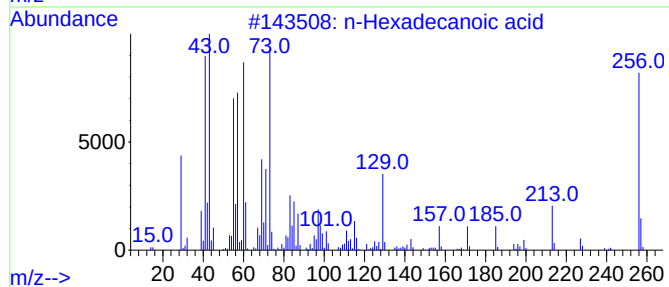
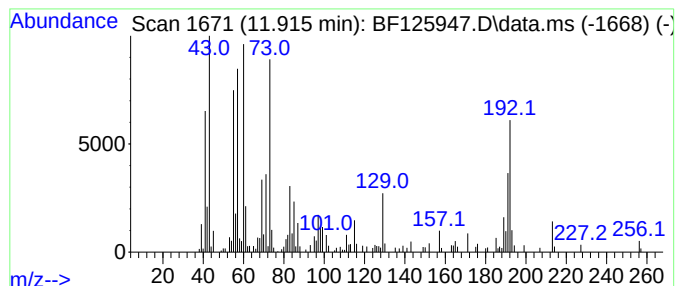
Instrument :
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ClientSampled :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.916	3.17 ng	208364	Phenanthrene-d10		11.386	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	98
2	Tridecanoic acid		214	C13H26O2	000638-53-9	91
3	Nonanoic acid		158	C9H18O2	000112-05-0	50
4	Phenanthrene, 1-methyl-		192	C15H12	000832-69-9	35
5	Phenanthrene, 2-methyl-		192	C15H12	002531-84-2	35



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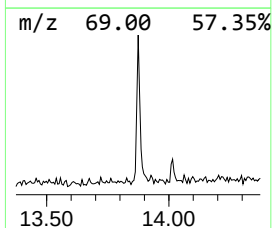
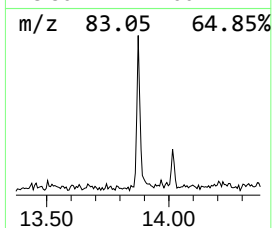
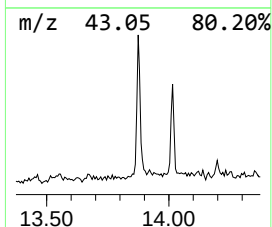
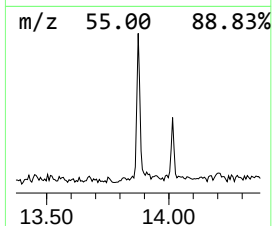
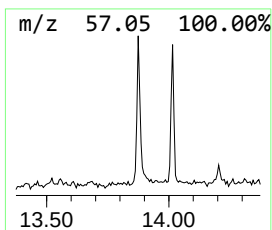
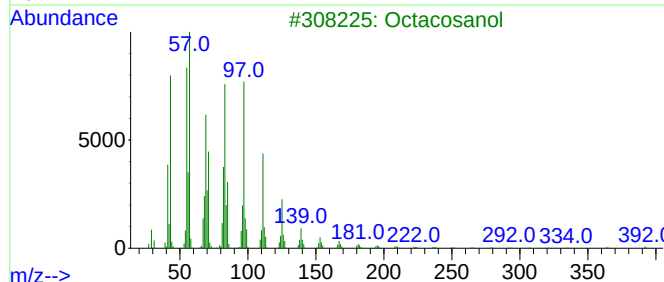
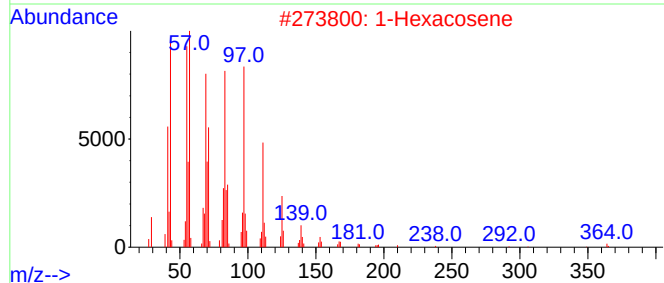
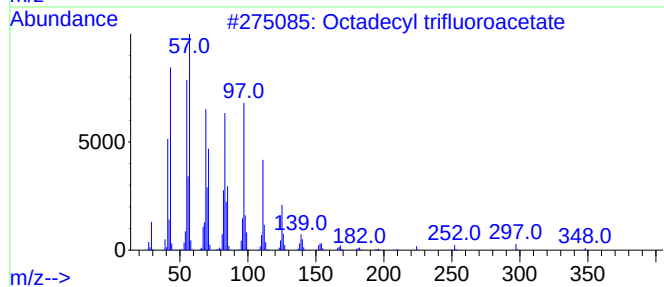
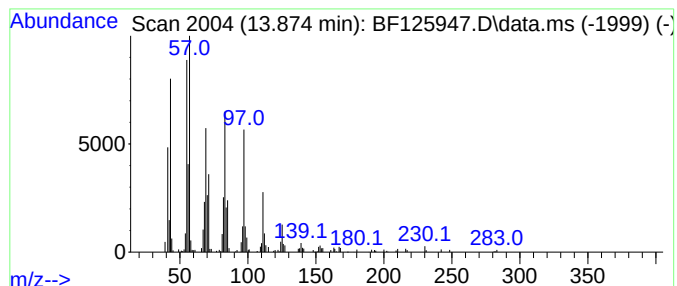
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecyl trifluoroacetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	5.17 ng	318792	Chrysene-d12	14.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
2			1-Hexacosene	364	C26H52	018835-33-1	91
3			Octacosanol	410	C28H58O	000557-61-9	91
4			1-Octadecanol	270	C18H38O	000112-92-5	91
5			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125947.D
Acq On : 26 Oct 2021 22:15
Operator : JU/CG
Sample : M4348-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
358

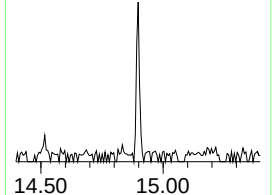
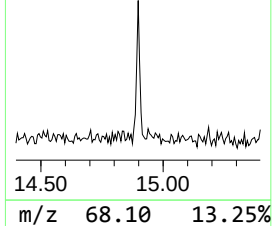
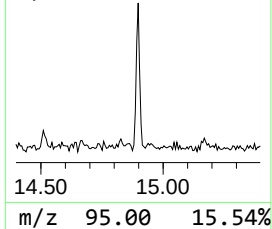
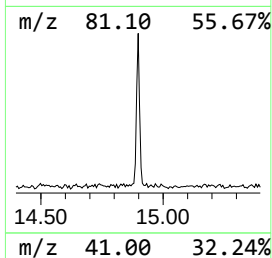
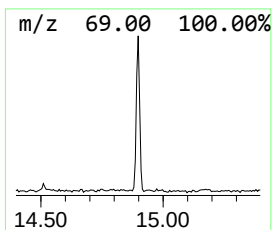
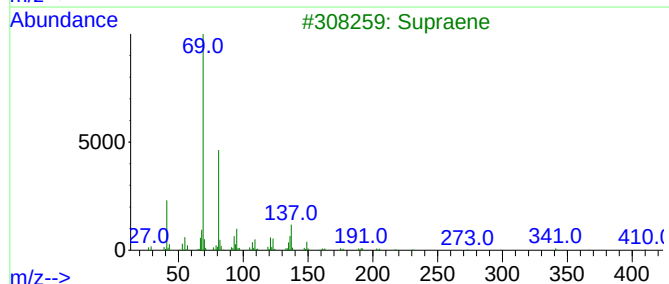
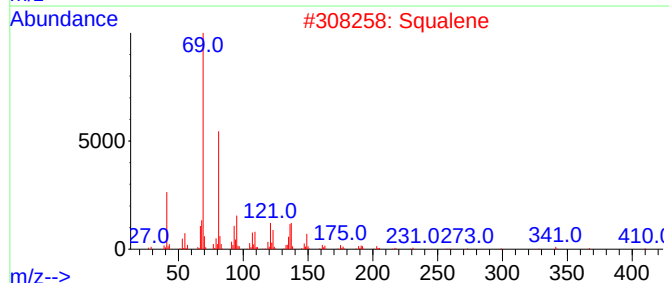
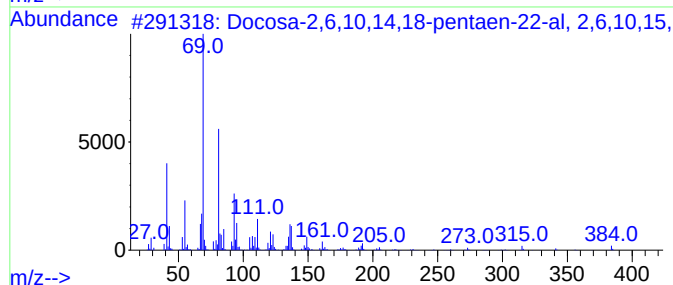
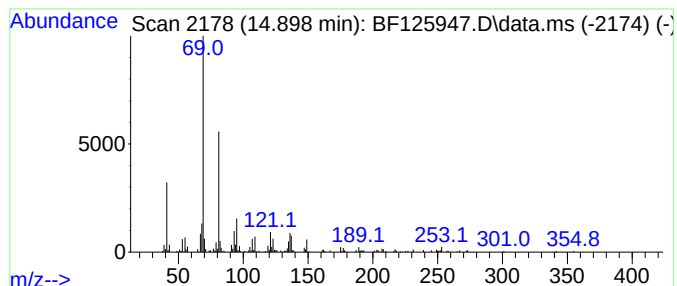
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Docosa-2,6,10,14,18-pentaen... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.898	4.61 ng	240030	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	91		
2	Squalene	410	C30H50	000111-02-4	91		
3	Supraene	410	C30H50	007683-64-9	86		
4	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83		
5	Propanoic acid, 2,2-dimethyl-, [...	306	C20H34O2	1000164-38-8	72		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125947.D
Acq On : 26 Oct 2021 22:15
Operator : JU/CG
Sample : M4348-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
358

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...	2.163	66.9	ng	3836990	1	6.869	1147280	20.0
Ethanol, 2-(2-b...	8.051	8.8	ng	610458	2	8.145	1386940	20.0
3-(2-Hydroxyeth...	9.351	4.6	ng	330855	3	9.904	1431550	20.0
n-Hexadecanoic ...	11.916	3.2	ng	208364	4	11.386	1314150	20.0
Octadecyl trifl...	13.874	5.2	ng	318792	5	14.021	1232550	20.0
Docosa-2,6,10,1...	14.898	4.6	ng	240030	6	15.492	1041320	20.0