

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082021\
 Data File : BF125133.D
 Acq On : 20 Aug 2021 14:13
 Operator : JU/CG
 Sample : M3430-08
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PE-2D

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-BF081821.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125133.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.222	17	23	29	rVB	1244555	1623823	42.35%	5.544%
2	5.146	511	520	528	rVB	86749	115406	3.01%	0.394%
3	5.534	581	586	590	rBV	3398985	3499489	91.26%	11.947%
4	6.540	751	757	760	rBV	3319917	3463831	90.33%	11.826%
5	6.922	818	822	825	rBV	1167095	964209	25.14%	3.292%
6	7.481	912	917	920	rBV	2542920	2261550	58.98%	7.721%
7	8.098	1019	1022	1034	rBV	833693	727533	18.97%	2.484%
8	8.204	1036	1040	1043	rVB	1526405	1254973	32.73%	4.284%
9	9.281	1218	1223	1226	rBV	4466819	3834714	100.00%	13.092%
10	9.386	1238	1241	1246	rBV	106520	98732	2.57%	0.337%
11	9.957	1334	1338	1342	rVB	1592714	1359644	35.46%	4.642%
12	10.745	1468	1472	1475	rBV	2712837	2383993	62.17%	8.139%
13	11.445	1587	1591	1594	rBV	1535017	1277582	33.32%	4.362%
14	11.833	1654	1657	1660	rVB	67310	49114	1.28%	0.168%
15	11.963	1672	1679	1685	rBV2	283084	315876	8.24%	1.078%
16	12.539	1772	1777	1782	rVB2	175736	196679	5.13%	0.671%
17	12.627	1789	1792	1794	rBV	57647	44796	1.17%	0.153%
18	12.657	1794	1797	1802	rVV	118940	112132	2.92%	0.383%
19	12.751	1810	1813	1818	rBV	116813	122848	3.20%	0.419%
20	12.886	1831	1836	1841	rBV	117351	142916	3.73%	0.488%
21	13.033	1856	1861	1864	rBV	3602043	3203276	83.53%	10.936%
22	13.927	2011	2013	2015	rBV2	42826	43020	1.12%	0.147%
23	14.086	2036	2040	2043	rBV	1023073	928049	24.20%	3.168%
24	14.110	2043	2044	2050	rVB	63463	53297	1.39%	0.182%
25	14.245	2065	2067	2072	rBV6	30724	46085	1.20%	0.157%
26	14.951	2184	2187	2195	rVB	67875	122282	3.19%	0.417%
27	15.139	2216	2219	2226	rVB	58343	107839	2.81%	0.368%
28	15.586	2290	2295	2307	rBV	712367	937437	24.45%	3.200%

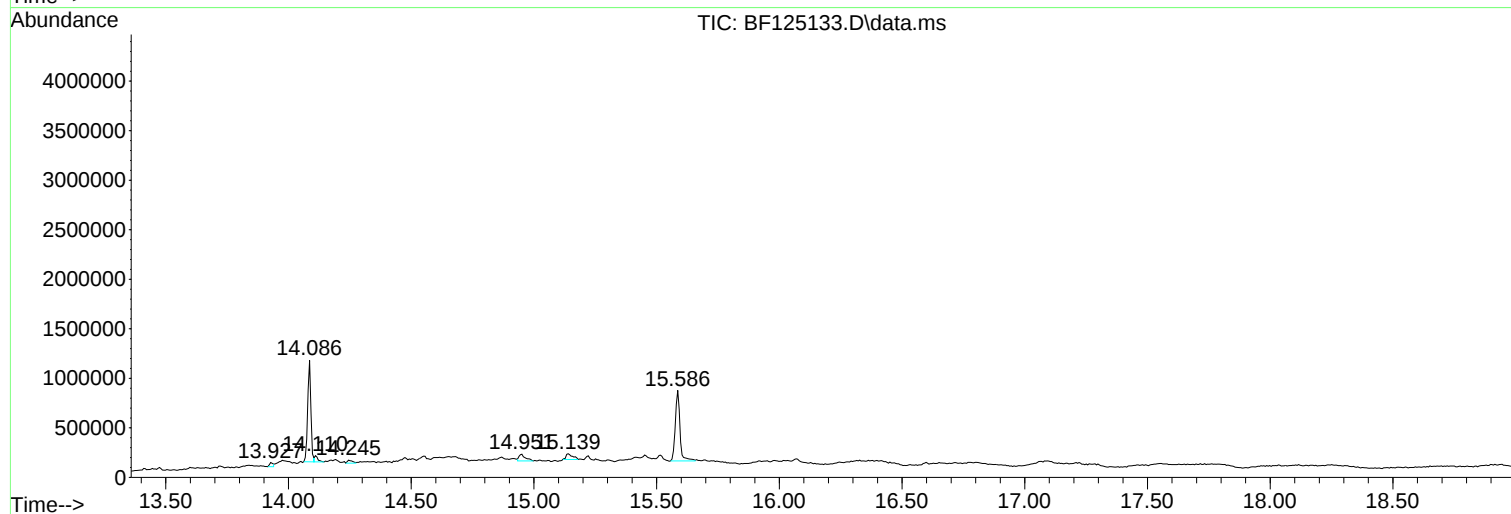
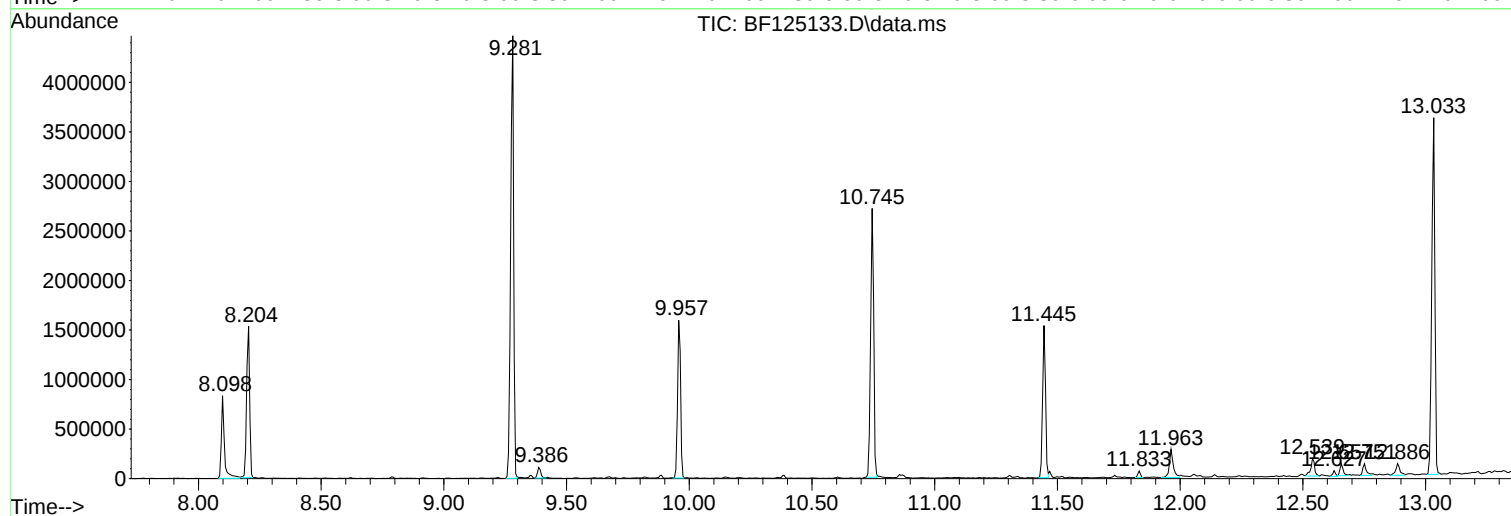
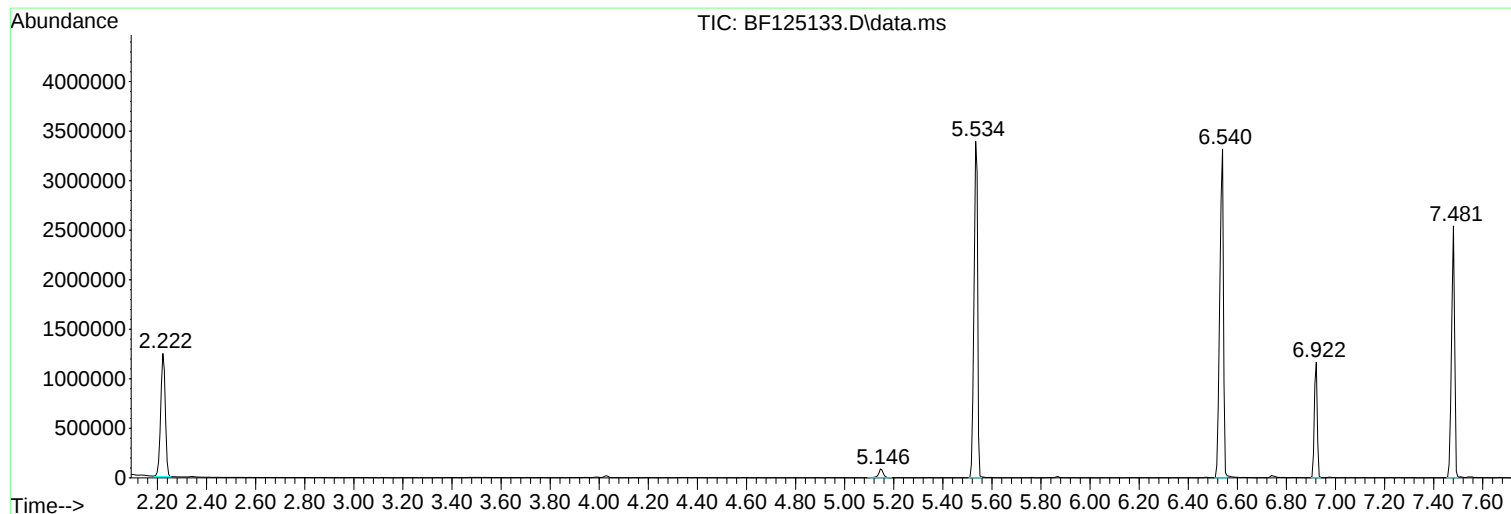
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Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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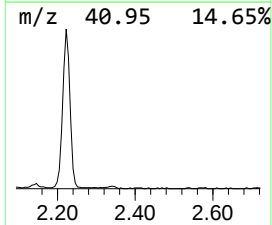
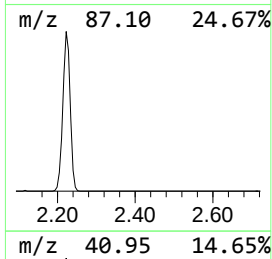
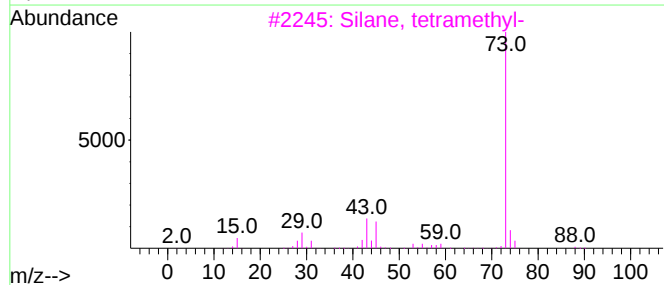
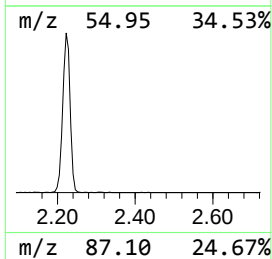
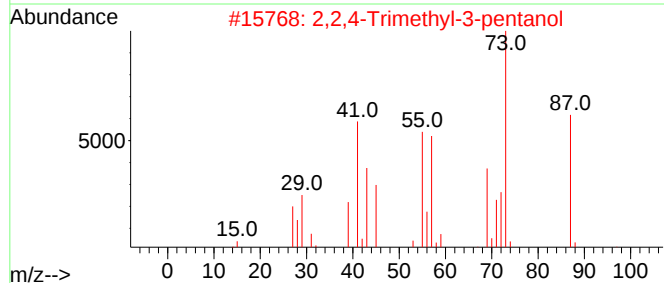
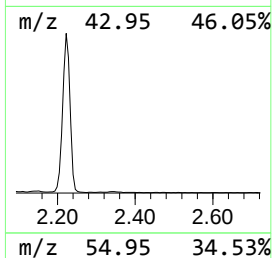
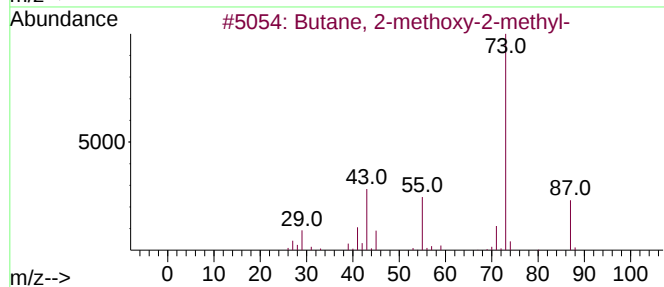
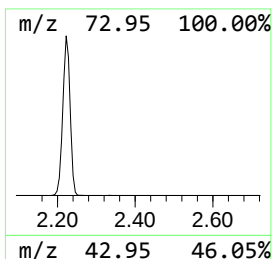
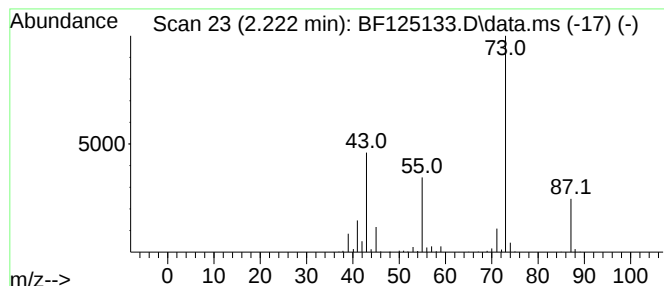
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.222	33.68 ng	1623820	1,4-Dichlorobenzene-d4	6.922

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	40
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23



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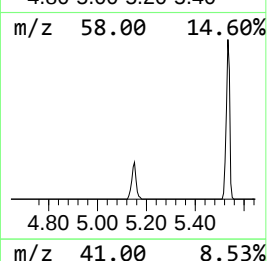
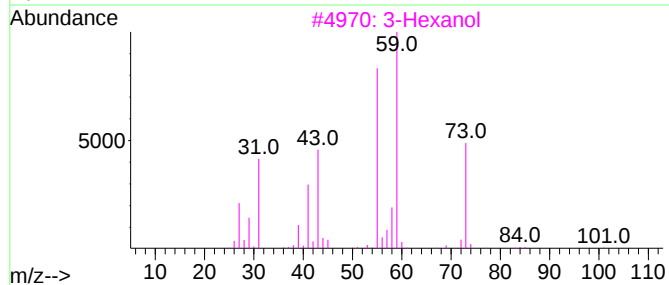
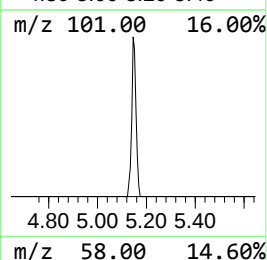
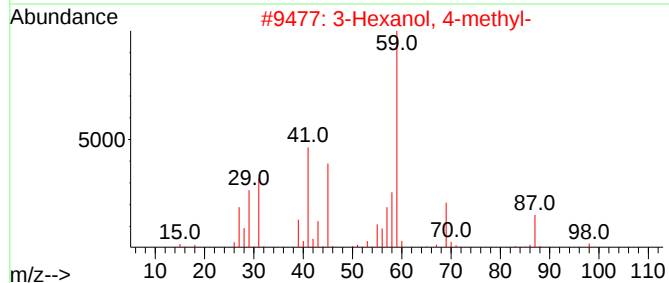
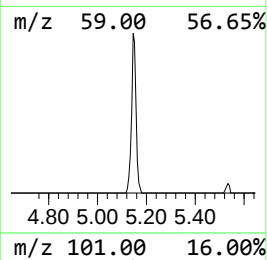
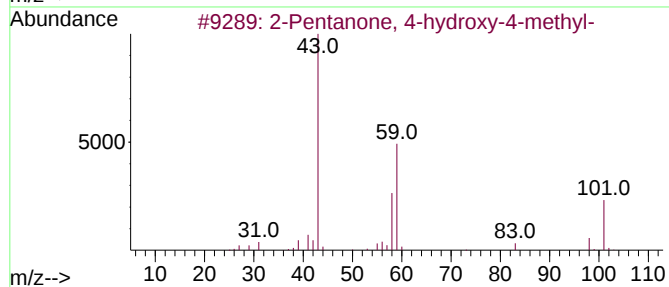
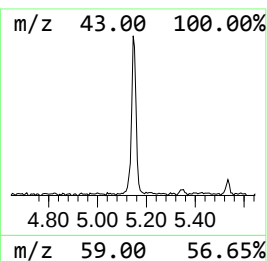
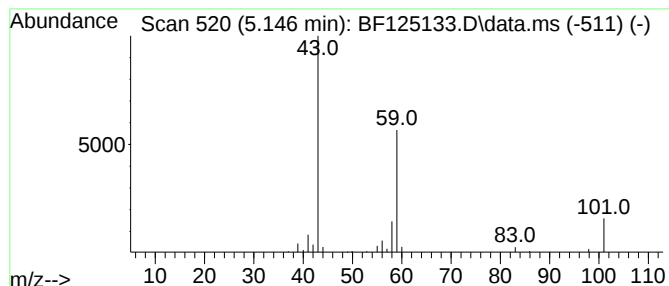
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.146	2.39 ng	115406	1,4-Dichlorobenzene-d4	6.922

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59	
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	40	
3	3-Hexanol	102	C6H14O	000623-37-0	33	
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28	
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25	



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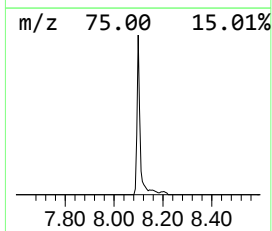
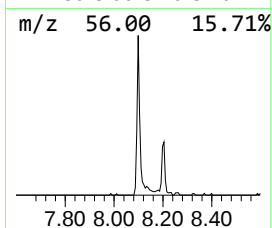
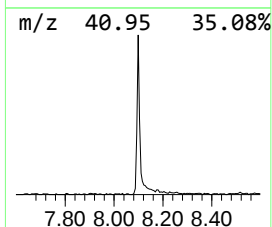
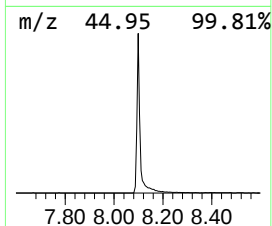
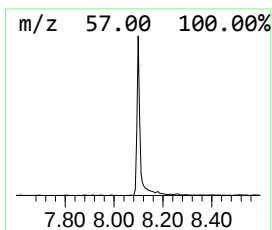
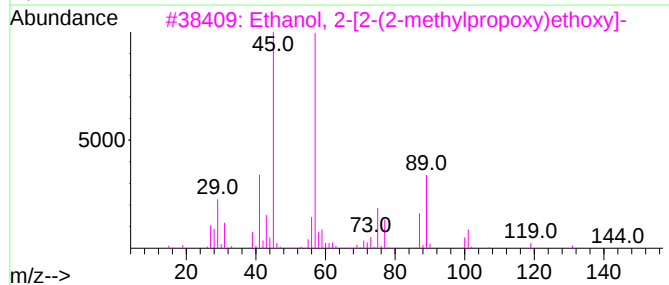
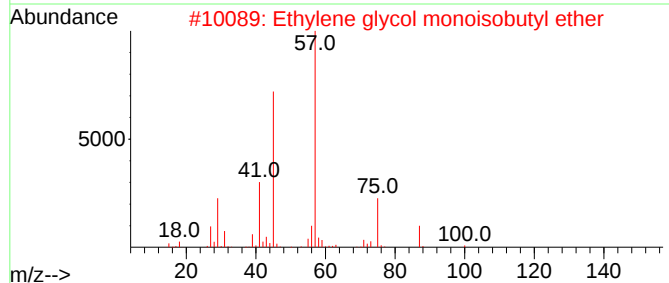
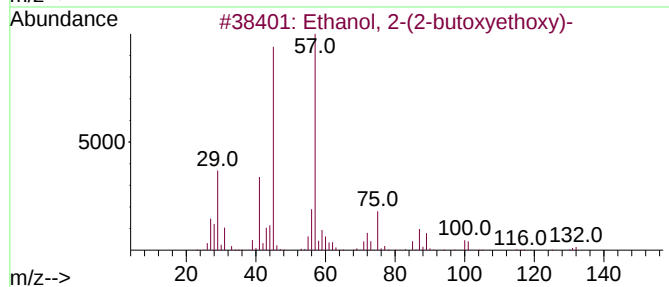
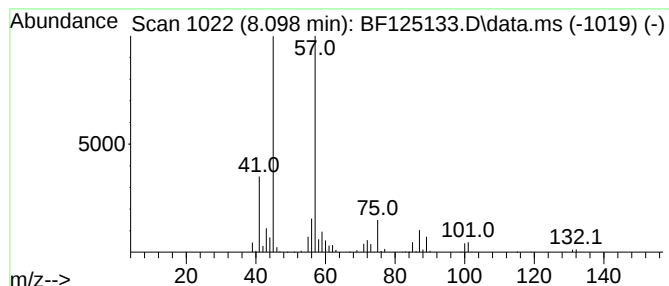
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.098	11.59 ng	727533	Naphthalene-d8	8.204

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	59
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
5			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	52



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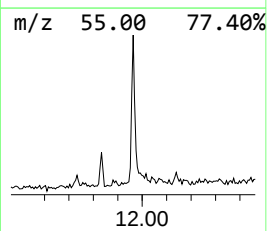
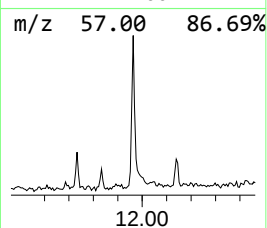
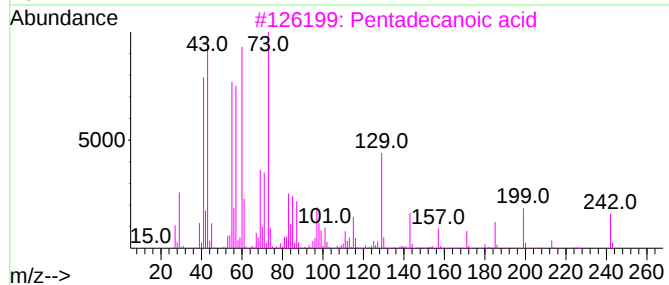
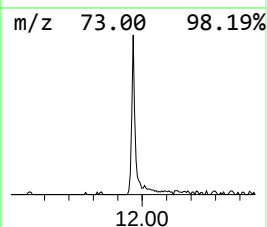
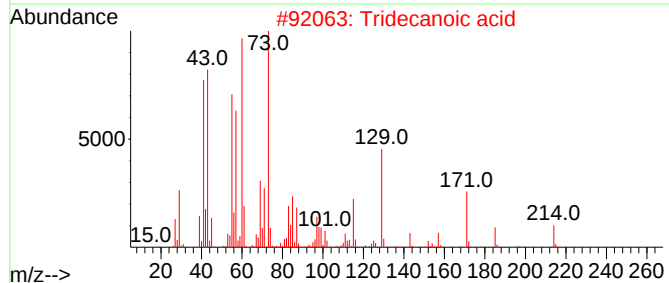
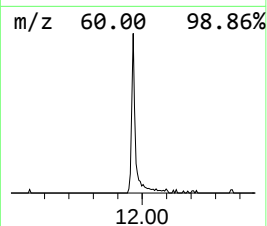
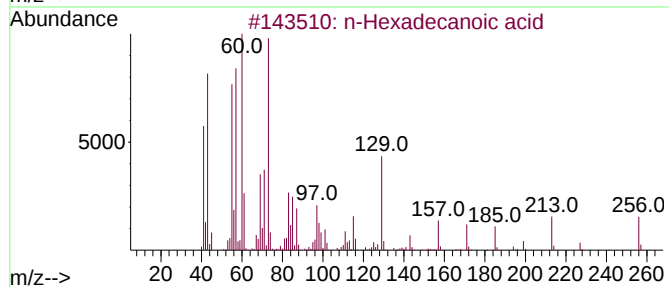
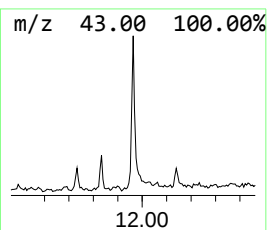
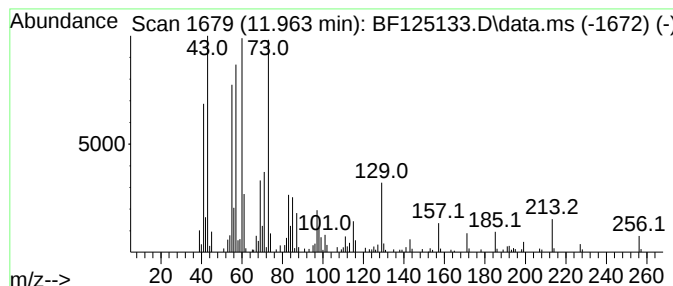
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.963	4.94 ng	315876	Phenanthrene-d10	11.445

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	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	76
5			n-Decanoic acid	172	C10H20O2	000334-48-5	60



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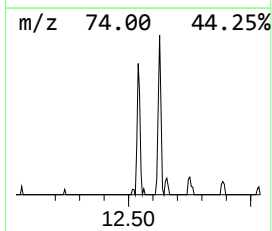
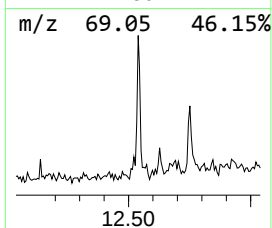
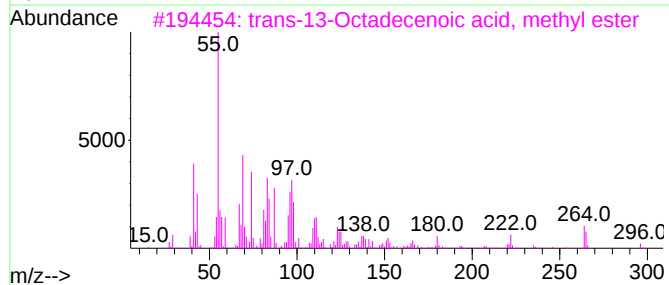
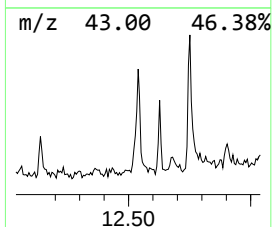
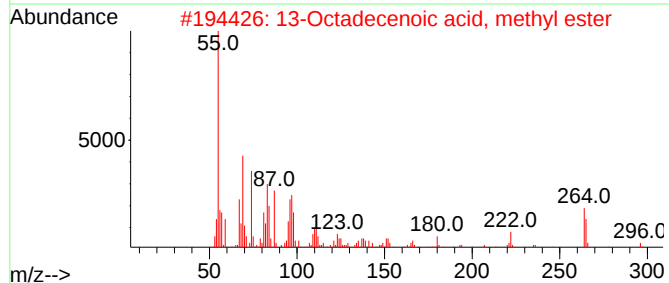
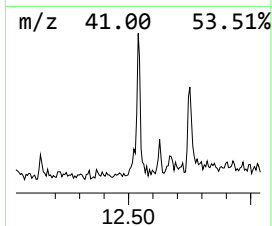
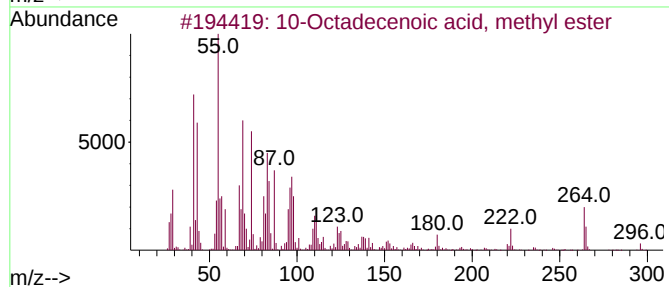
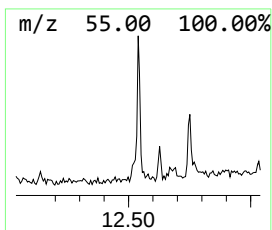
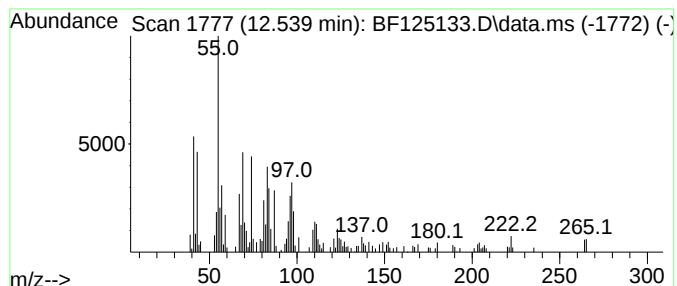
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 10-Octadecenoic acid, methyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.539	3.08 ng	196679	Phenanthrene-d10		11.445	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	10-Octadecenoic acid, methyl ester		296	C19H36O2	013481-95-3	94
2	13-Octadecenoic acid, methyl ester		296	C19H36O2	056554-47-3	91
3	trans-13-Octadecenoic acid, meth...		296	C19H36O2	1000333-61-3	91
4	14-Octadecenoic acid, methyl ester		296	C19H36O2	056554-48-4	90
5	15-Octadecenoic acid, methyl ester		296	C19H36O2	004764-72-1	90



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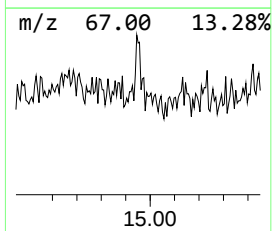
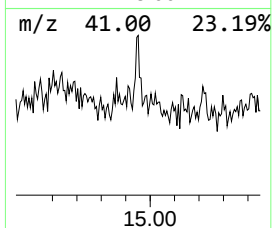
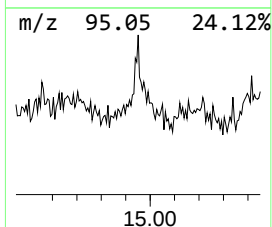
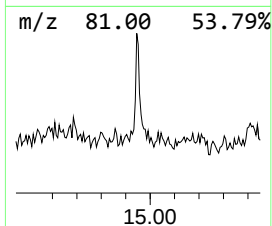
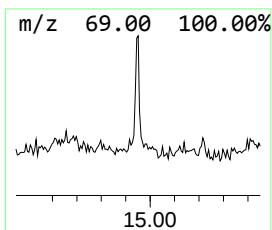
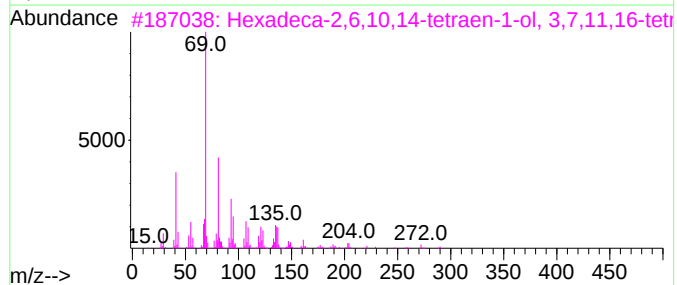
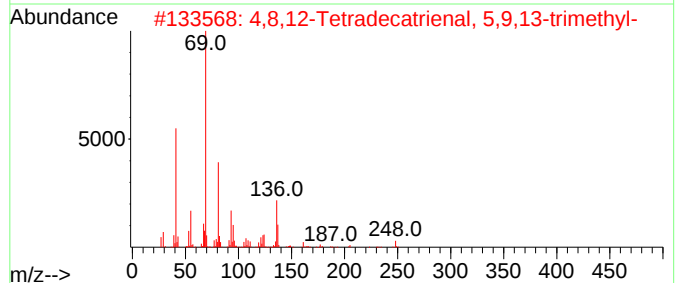
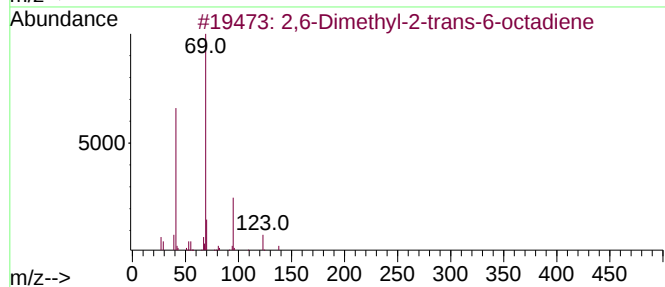
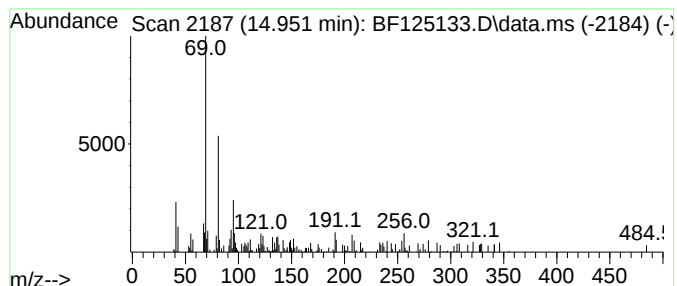
Instrument :
BNA_F
ClientSampleId :
PE-2D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2,6-Dimethyl-2-trans-6-octa... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.951	2.61 ng	122282	Perylene-d12	15.586	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Dimethyl-2-trans-6-octadiene	138	C10H18	002609-23-6	53
2	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	52
3	Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	50
4	3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	49
5	1,4-Hexadiene, 3,3,5-trimethyl-	124	C9H16	074753-00-7	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082021\
Data File : BF125133.D
Acq On : 20 Aug 2021 14:13
Operator : JU/CG
Sample : M3430-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PE-2D

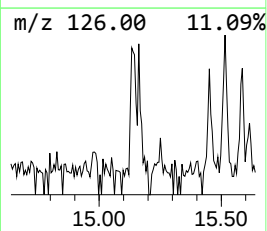
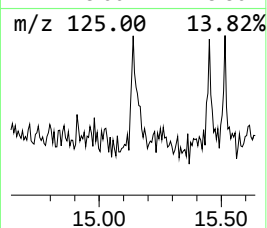
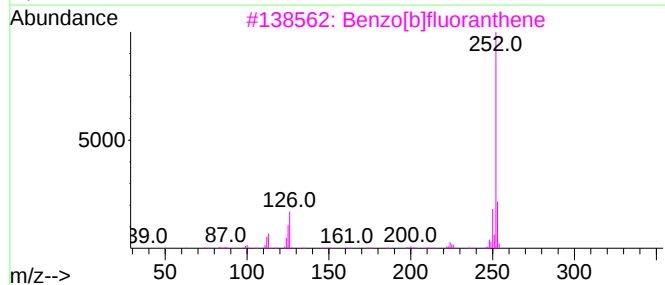
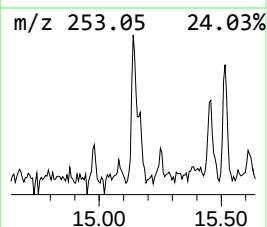
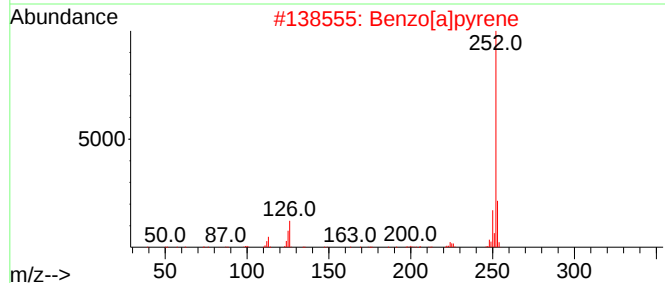
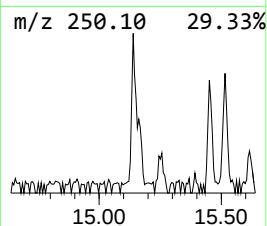
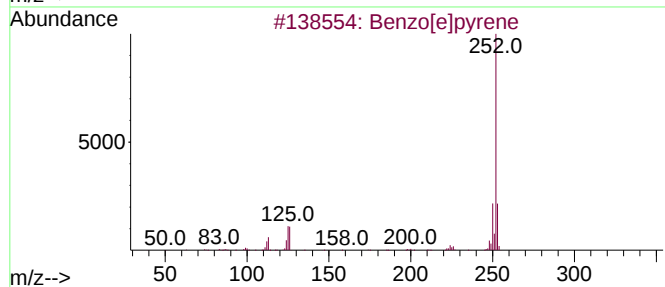
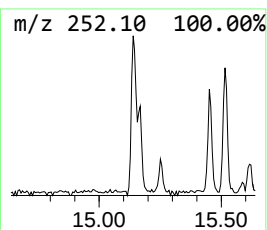
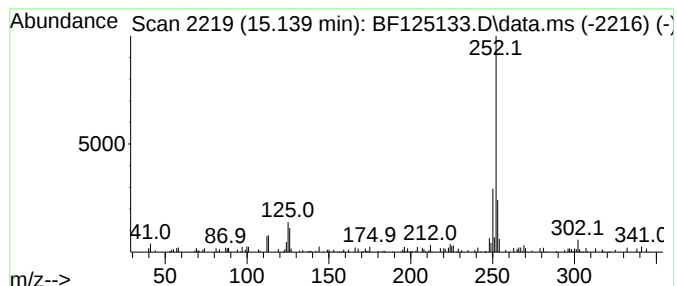
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzo[e]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.139	2.30 ng	107839	Perylene-d12	15.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	96
2			Benzo[a]pyrene	252	C20H12	000050-32-8	94
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
4			Benzo[k]fluoranthene	252	C20H12	000207-08-9	81
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082021\
Data File : BF125133.D
Acq On : 20 Aug 2021 14:13
Operator : JU/CG
Sample : M3430-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PE-2D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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...	2.222	33.7	ng	1623820	1	6.922	964209	20.0
2-Pentanone, 4-...	5.146	2.4	ng	115406	1	6.922	964209	20.0
Ethanol, 2-(2-b...	8.098	11.6	ng	727533	2	8.204	1254970	20.0
n-Hexadecanoic ...	11.963	4.9	ng	315876	4	11.445	1277580	20.0
10-Octadecenoic...	12.539	3.1	ng	196679	4	11.445	1277580	20.0
2,6-Dimethyl-2-...	14.951	2.6	ng	122282	6	15.586	937437	20.0
Benzo[e]pyrene	15.139	2.3	ng	107839	6	15.586	937437	20.0