

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090721\
 Data File : BF125387.D
 Acq On : 7 Sep 2021 14:47
 Operator : JU/CG
 Sample : M3657-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TFI-358

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: BF125387.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	12	18	28	rVB	960204	1235573	51.53%	5.240%
2	3.999	321	325	330	rVB	21384	26110	1.09%	0.111%
3	5.522	580	584	587	rBV	2615802	2397547	100.00%	10.168%
4	6.528	750	755	765	rBV	2511778	2333964	97.35%	9.899%
5	6.898	814	818	821	rBV	972855	780866	32.57%	3.312%
6	7.457	909	913	924	rBV	1622063	1496393	62.41%	6.346%
7	8.081	1016	1019	1032	rBV	221295	486516	20.29%	2.063%
8	8.181	1032	1036	1049	rVB	1120763	973798	40.62%	4.130%
9	8.869	1149	1153	1163	rBV	18113	33454	1.40%	0.142%
10	9.251	1214	1218	1235	rBV	2294117	2335105	97.40%	9.903%
11	9.369	1235	1238	1250	rVB	44509	56715	2.37%	0.241%
12	9.933	1331	1334	1346	rVB	941684	888310	37.05%	3.767%
13	10.722	1465	1468	1479	rBV	1379684	1337113	55.77%	5.671%
14	11.422	1584	1587	1590	rBV	929151	823372	34.34%	3.492%
15	11.804	1648	1652	1657	rVB	48276	42867	1.79%	0.182%
16	11.939	1671	1675	1680	rBV2	224966	258391	10.78%	1.096%
17	12.474	1760	1766	1768	rBV	18318	24955	1.04%	0.106%
18	12.510	1768	1772	1775	rVV2	67085	68019	2.84%	0.288%
19	12.639	1790	1794	1800	rBV	133125	136879	5.71%	0.581%
20	12.727	1806	1809	1814	rBV3	45789	54002	2.25%	0.229%
21	12.869	1826	1833	1838	rVB	151718	178452	7.44%	0.757%
22	13.004	1852	1856	1860	rBV	2433201	2144280	89.44%	9.094%
23	13.433	1925	1929	1933	rBV5	15220	28969	1.21%	0.123%
24	13.474	1933	1936	1939	rBV4	21380	27706	1.16%	0.118%
25	13.851	1997	2000	2004	rBV2	57137	88499	3.69%	0.375%
26	13.892	2004	2007	2010	rBV2	95820	106568	4.44%	0.452%
27	13.927	2010	2013	2018	rBV	355746	353503	14.74%	1.499%
28	14.033	2028	2031	2034	rBV	2128374	1985262	82.80%	8.420%
29	14.063	2034	2036	2039	rVV	1017748	907458	37.85%	3.849%
30	14.086	2039	2040	2046	rVB	112083	93347	3.89%	0.396%
31	14.216	2059	2062	2065	rVB2	34881	31011	1.29%	0.132%
32	14.686	2139	2142	2145	rBV	120307	119366	4.98%	0.506%
33	14.910	2178	2180	2183	rBV	43627	36284	1.51%	0.154%
34	15.115	2212	2215	2222	rBV	126265	229581	9.58%	0.974%
35	15.174	2223	2225	2231	rVB2	66365	86528	3.61%	0.367%
36	15.427	2265	2268	2275	rVB	65921	89231	3.72%	0.378%

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37	15.492	2276	2279	2283	rVB	85037	105457	4.40%	0.447%
38	15.557	2285	2290	2302	rBV2	764442	1090408	45.48%	4.625%
39	16.015	2364	2368	2372	rVB2	63785	87025	3.63%	0.369%

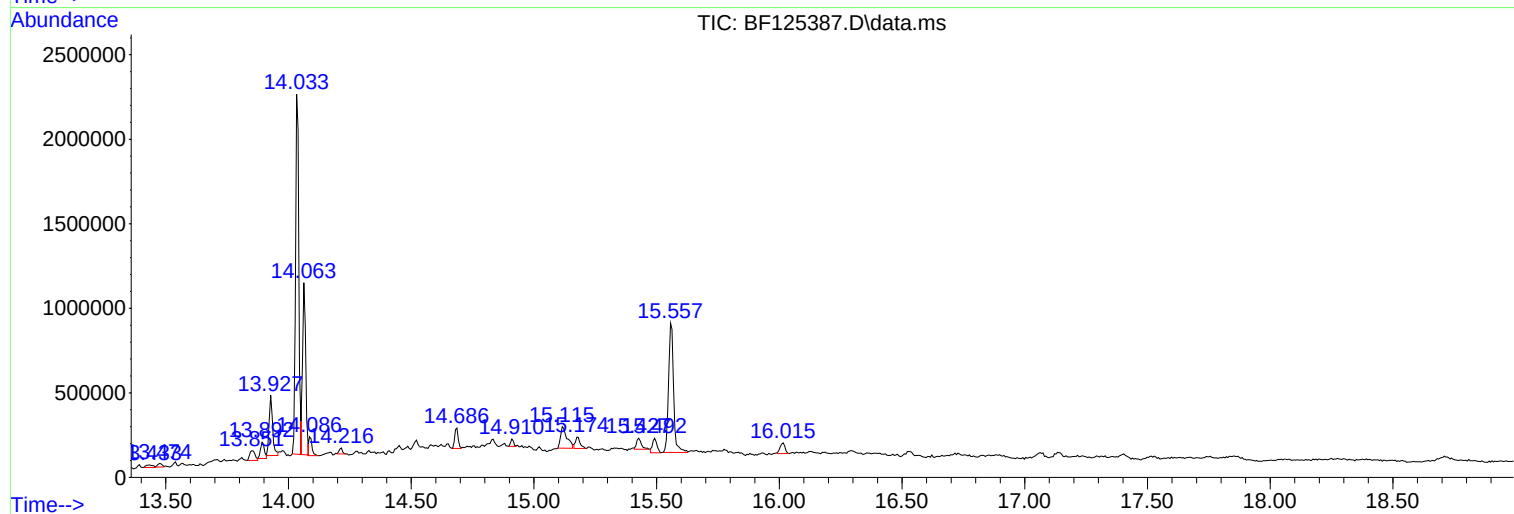
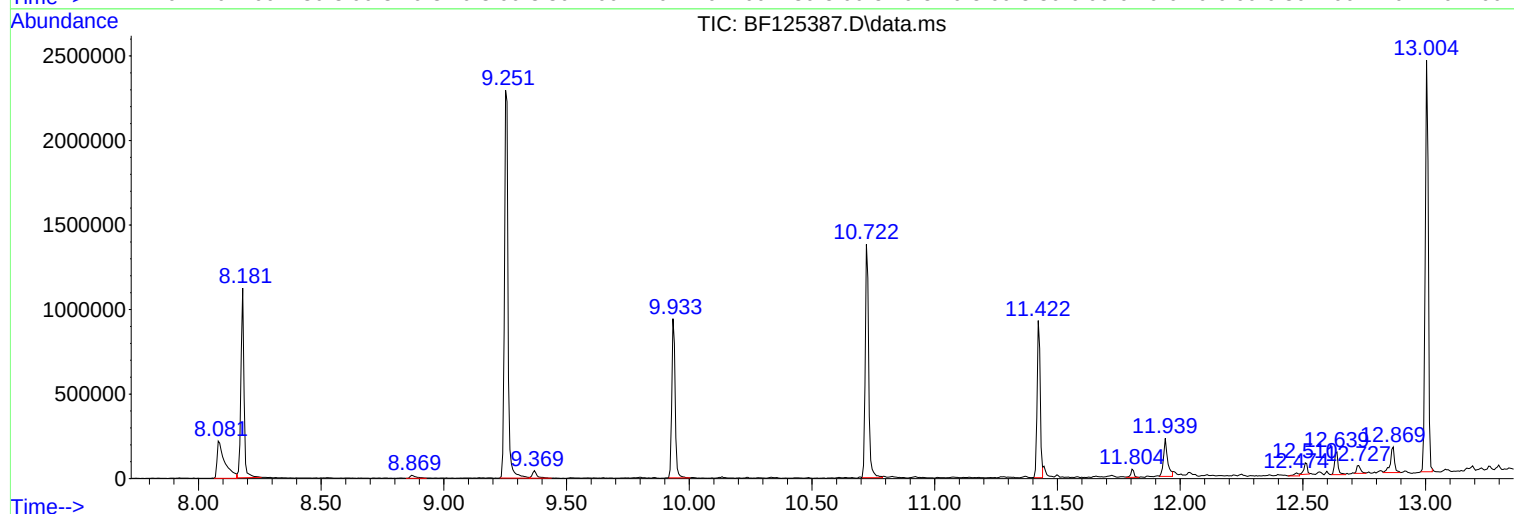
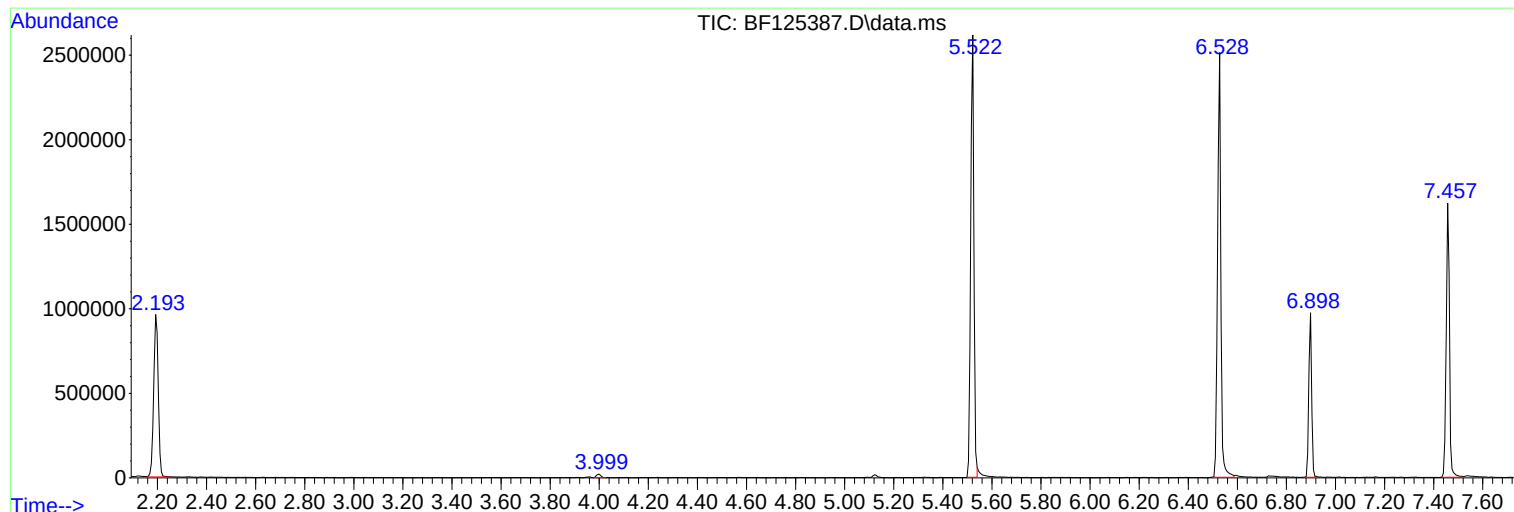
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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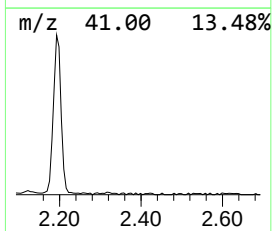
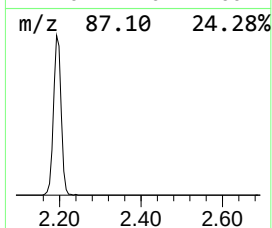
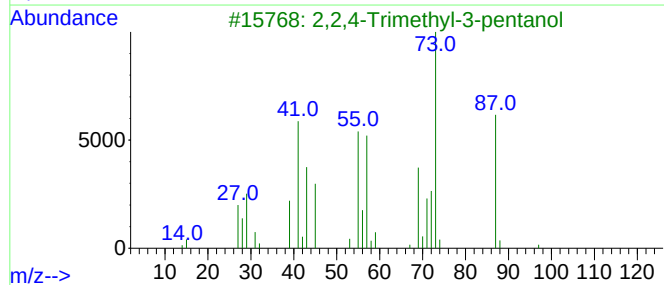
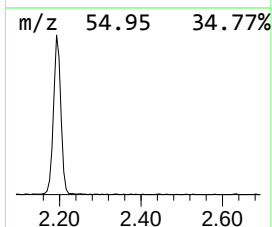
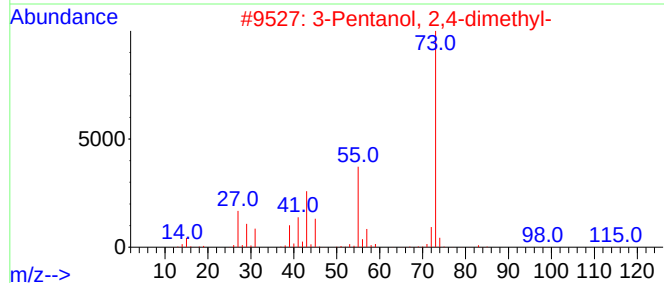
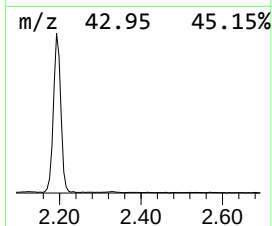
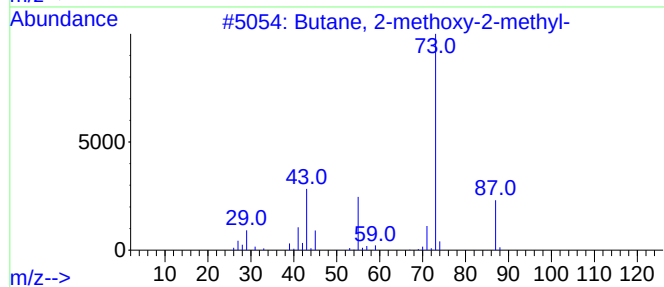
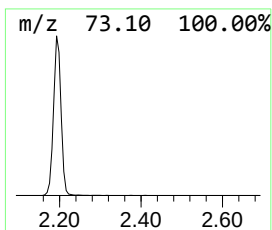
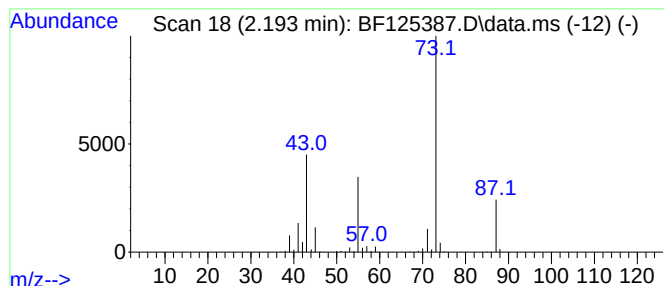
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.193	31.65 ng	1235570	1,4-Dichlorobenzene-d4	6.898

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	40
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23



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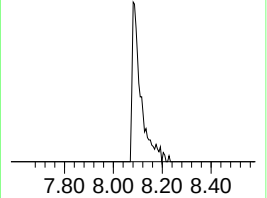
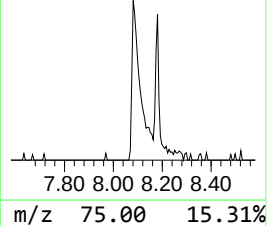
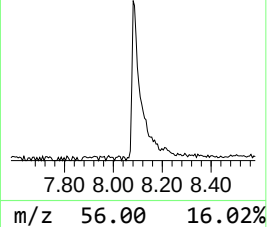
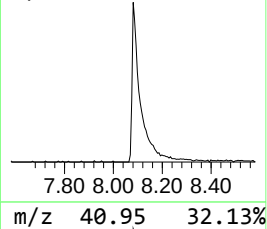
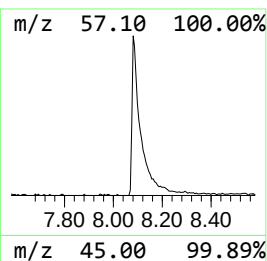
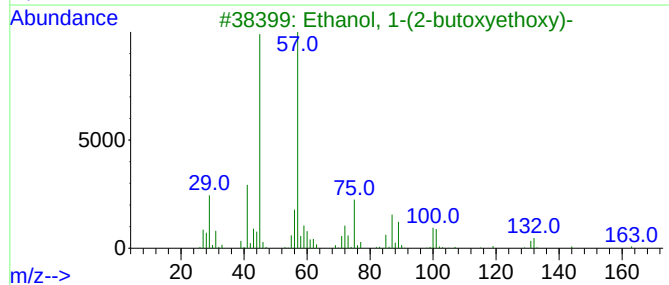
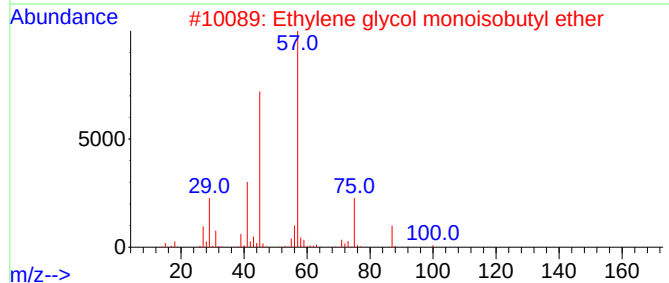
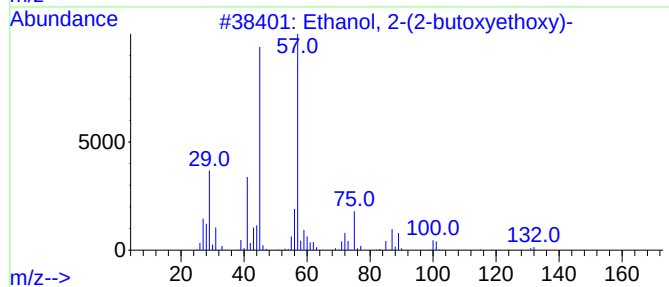
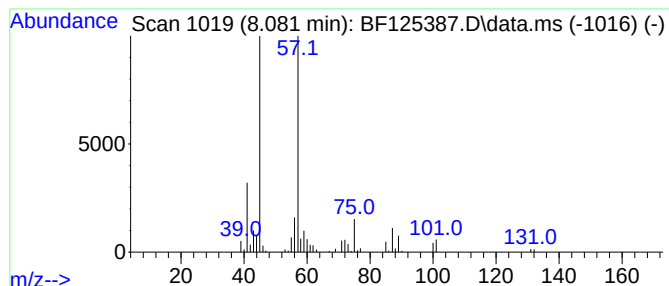
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.081	9.99 ng	486516	Naphthalene-d8	8.181

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, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
5			Ethanol, 2-[2-(2-propenyloxy)eth...	146	C7H14O3	015075-50-0	50



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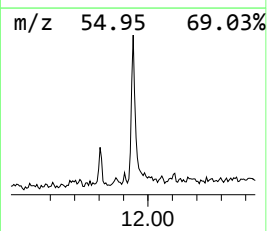
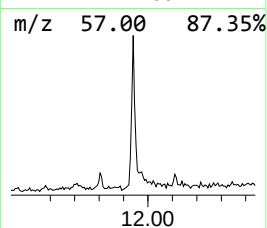
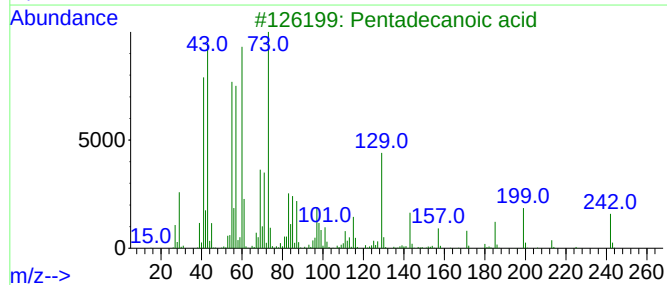
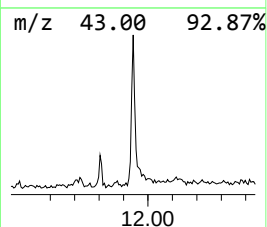
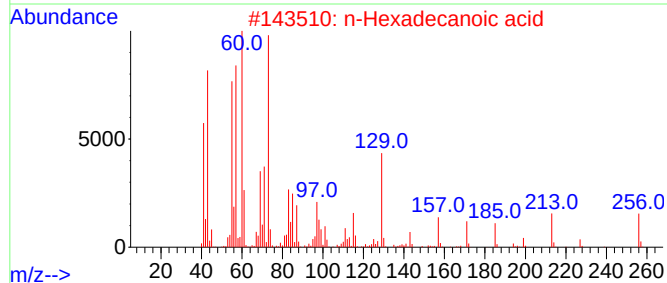
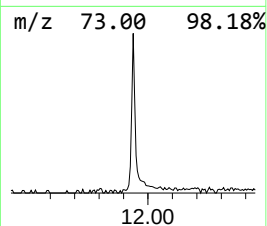
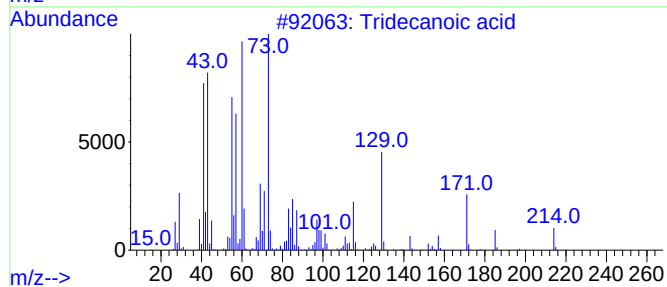
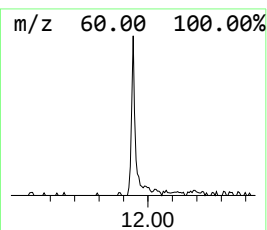
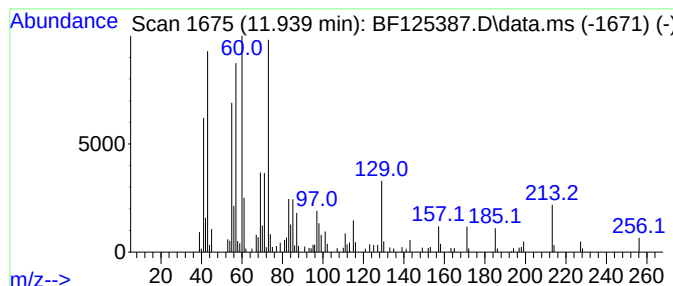
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.939	6.28 ng	258391	Phenanthrene-d10	11.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	94
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



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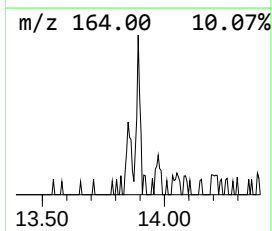
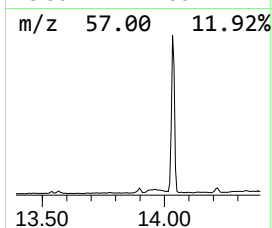
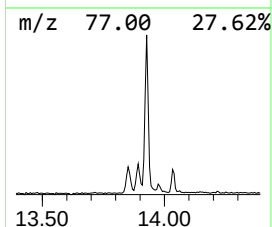
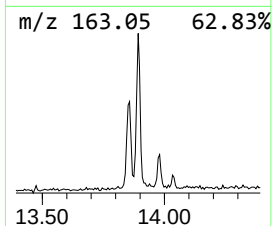
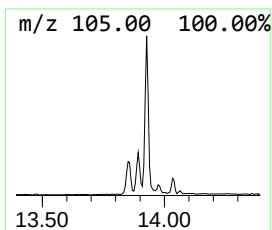
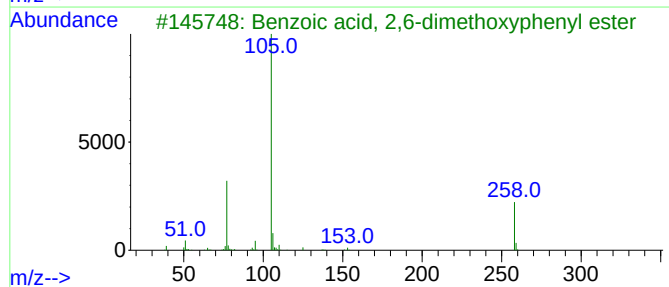
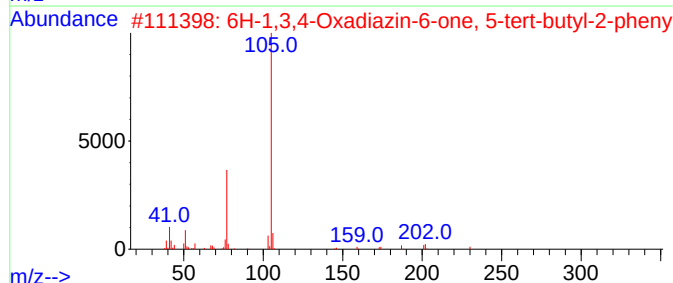
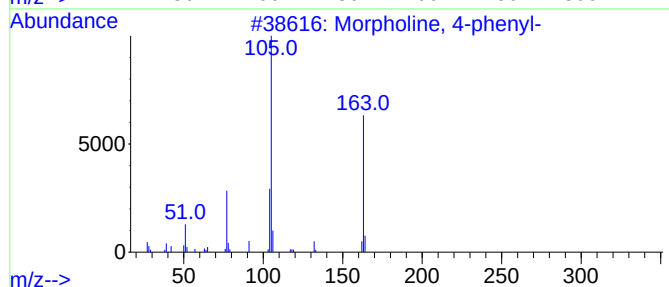
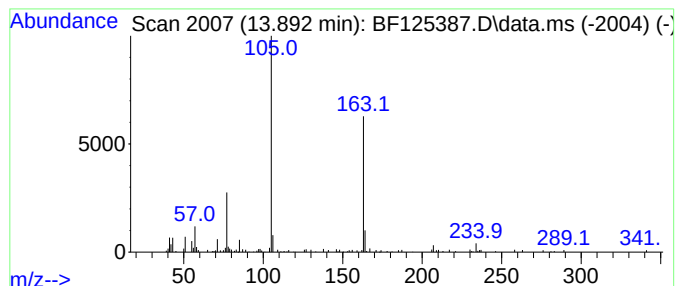
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Peak Number 4 Morpholine, 4-phenyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.892	2.35 ng	106568	Chrysene-d12	14.063	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	64
2	6H-1,3,4-Oxadiazin-6-one, 5-tert...	230	C13H14N2O2	1000142-96-3	30
3	Benzoic acid, 2,6-dimethoxypheny...	258	C15H14O4	1000368-91-2	27
4	Benzoic acid, 3,5-difluophenyl e...	234	C13H8F2O2	1000357-79-5	27
5	Benzoylcarbamic acid, 1,1-dioxot...	283	C12H13NO5S	1000303-97-1	27



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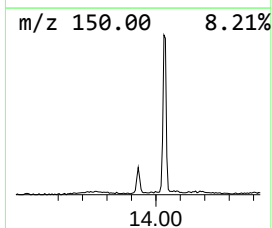
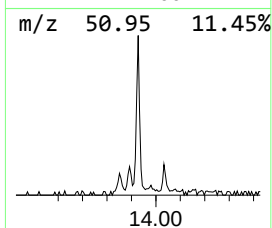
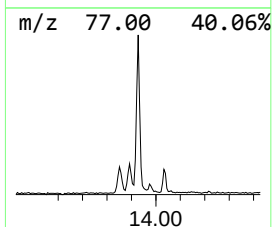
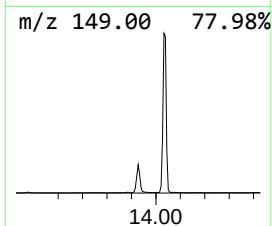
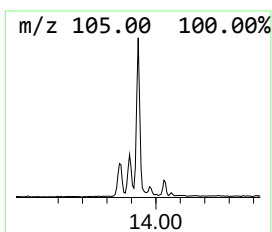
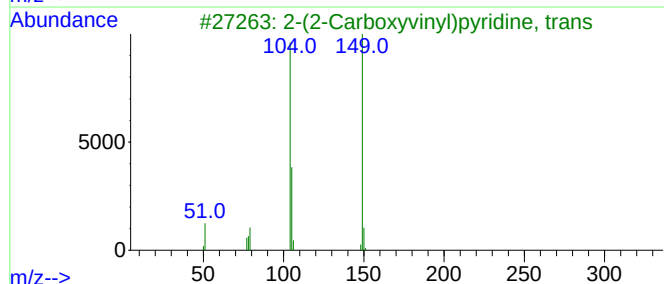
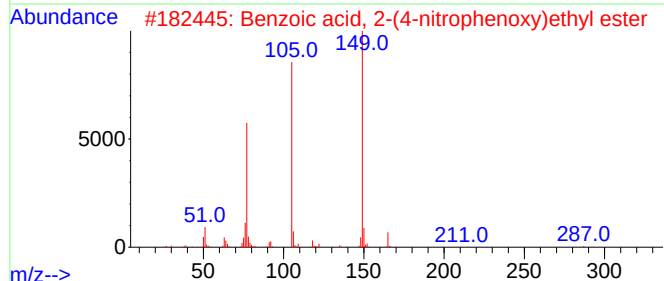
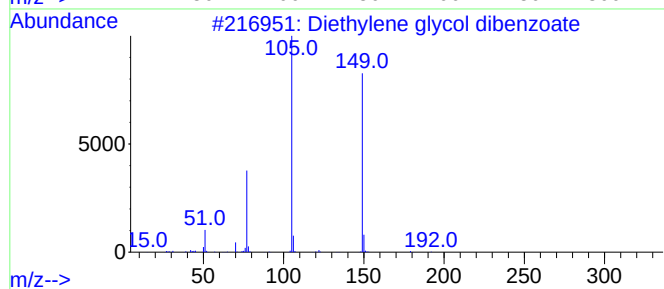
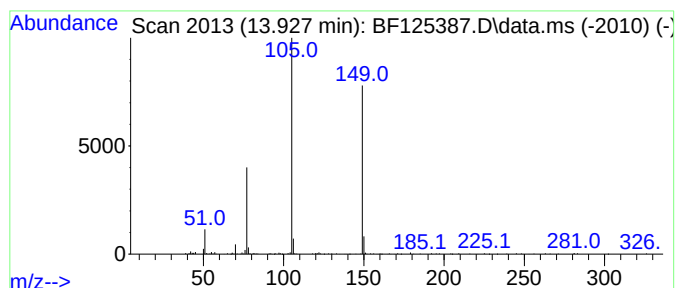
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Peak Number 5 Diethylene glycol dibenzoate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.927	7.79 ng	353503	Chrysene-d12	14.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	90
2			Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	72
3			2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	52
4			Cyclobutyl phenyl ketone	160	C11H12O	005407-98-7	35
5			N-(2-Fluoro-5-nitrophenyl)benzamide	260	C13H9FN2O3	144205-37-8	35



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Data File : BF125387.D
Acq On : 7 Sep 2021 14:47
Operator : JU/CG
Sample : M3657-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

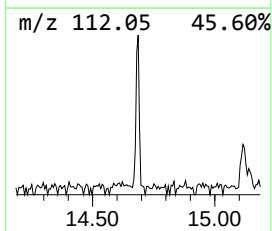
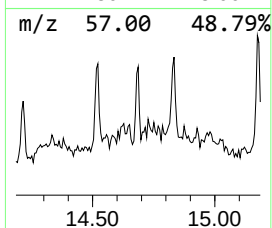
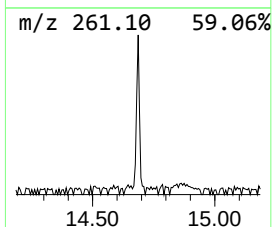
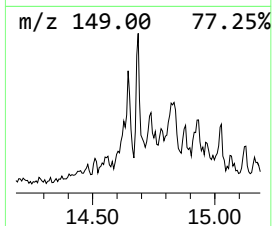
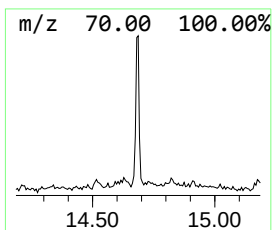
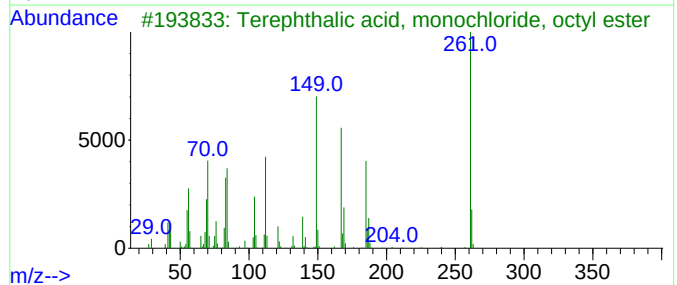
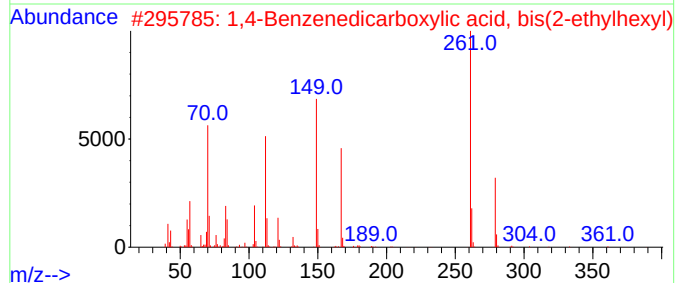
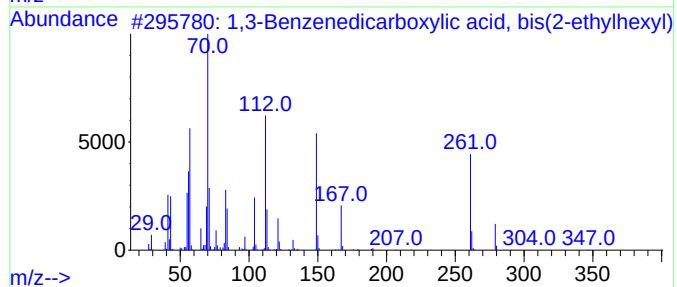
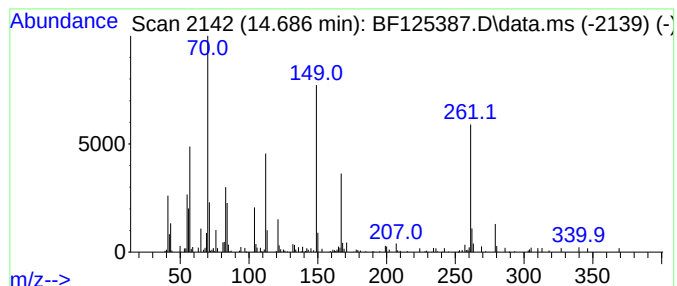
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1,3-Benzenedicarboxylic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.686	2.63 ng	119366	Chrysene-d12	14.063	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	72
2	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	58
3	Terephthalic acid, monochloride,...	296	C16H21ClO3	1000324-22-9	47
4	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	46
5	Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090721\
Data File : BF125387.D
Acq On : 7 Sep 2021 14:47
Operator : JU/CG
Sample : M3657-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TFI-358

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...	2.193	31.6	ng	1235570	1	6.898	780866	20.0
Ethanol, 2-(2-b...	8.081	10.0	ng	486516	2	8.181	973798	20.0
Tridecanoic acid	11.939	6.3	ng	258391	4	11.422	823372	20.0
Morpholine, 4-p...	13.892	2.4	ng	106568	5	14.063	907458	20.0
Diethylene glyc...	13.927	7.8	ng	353503	5	14.063	907458	20.0
1,3-Benzenedica...	14.686	2.6	ng	119366	5	14.063	907458	20.0