

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090421\
 Data File : BF125371.D
 Acq On : 4 Sep 2021 16:12
 Operator : JU/CG
 Sample : M3648-07
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20211057-SI-COMP-2-MODIFIED-EL

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: BF125371.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	13	23	34	rVB	2973187	4247410	96.84%	13.838%
2	5.122	512	516	525	rVB	85270	104949	2.39%	0.342%
3	5.522	580	584	600	rBV	2743609	2455894	56.00%	8.001%
4	6.522	750	754	766	rBV	2132997	1974292	45.01%	6.432%
5	6.898	814	818	821	rBV	1100667	868543	19.80%	2.830%
6	7.463	906	914	917	rBV	2645336	2634631	60.07%	8.583%
7	8.086	1016	1020	1032	rBV	58172	122656	2.80%	0.400%
8	8.181	1032	1036	1044	rBV	1237469	1094774	24.96%	3.567%
9	9.257	1214	1219	1222	rBV	4744382	4385872	100.00%	14.289%
10	9.933	1330	1334	1337	rBV	1293633	1141439	26.03%	3.719%
11	9.969	1337	1340	1345	rVB	181773	157480	3.59%	0.513%
12	10.727	1464	1469	1472	rBV	2776056	2574165	58.69%	8.386%
13	11.421	1583	1587	1594	rBV	1230127	1062812	24.23%	3.463%
14	11.580	1611	1614	1618	rBV	1681558	1393436	31.77%	4.540%
15	11.804	1649	1652	1655	rVB	114128	85719	1.95%	0.279%
16	11.939	1671	1675	1679	rBV	240095	227257	5.18%	0.740%
17	11.980	1679	1682	1689	rVB	52929	70159	1.60%	0.229%
18	12.633	1790	1793	1799	rVB	100241	97776	2.23%	0.319%
19	12.727	1803	1809	1818	rBV	70957	92801	2.12%	0.302%
20	12.868	1827	1833	1835	rVB	47553	49378	1.13%	0.161%
21	13.010	1852	1857	1860	rBV	4205313	3718807	84.79%	12.116%
22	13.927	2009	2013	2028	rVB2	135120	264145	6.02%	0.861%
23	14.062	2033	2036	2040	rVB	891104	764956	17.44%	2.492%
24	15.557	2285	2290	2301	rVB2	700558	931722	21.24%	3.035%
25	16.015	2362	2368	2373	rBV	39482	60764	1.39%	0.198%
26	16.533	2451	2456	2463	rVB3	32511	59603	1.36%	0.194%
27	17.139	2554	2559	2569	rVB2	27083	53043	1.21%	0.173%

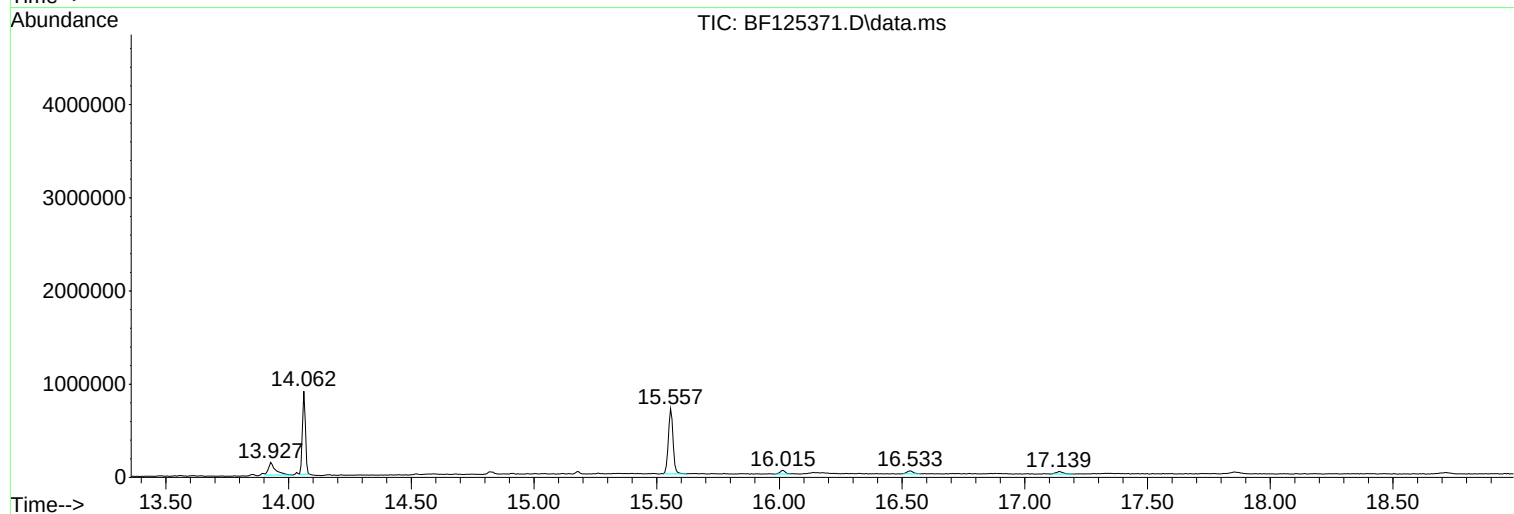
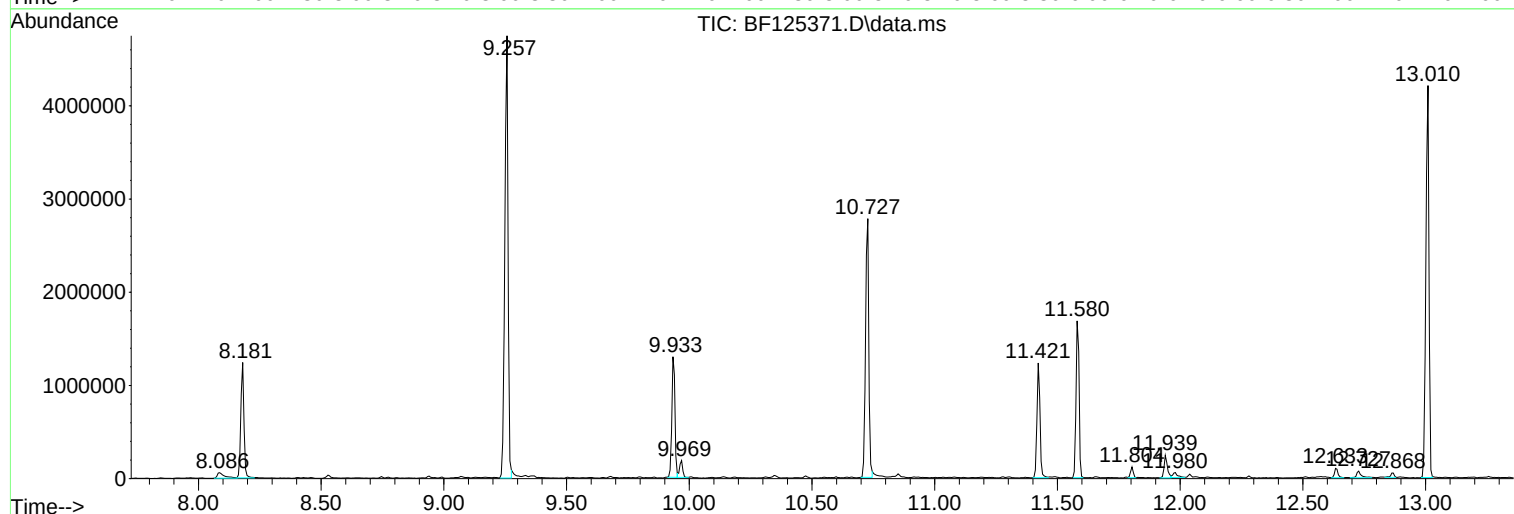
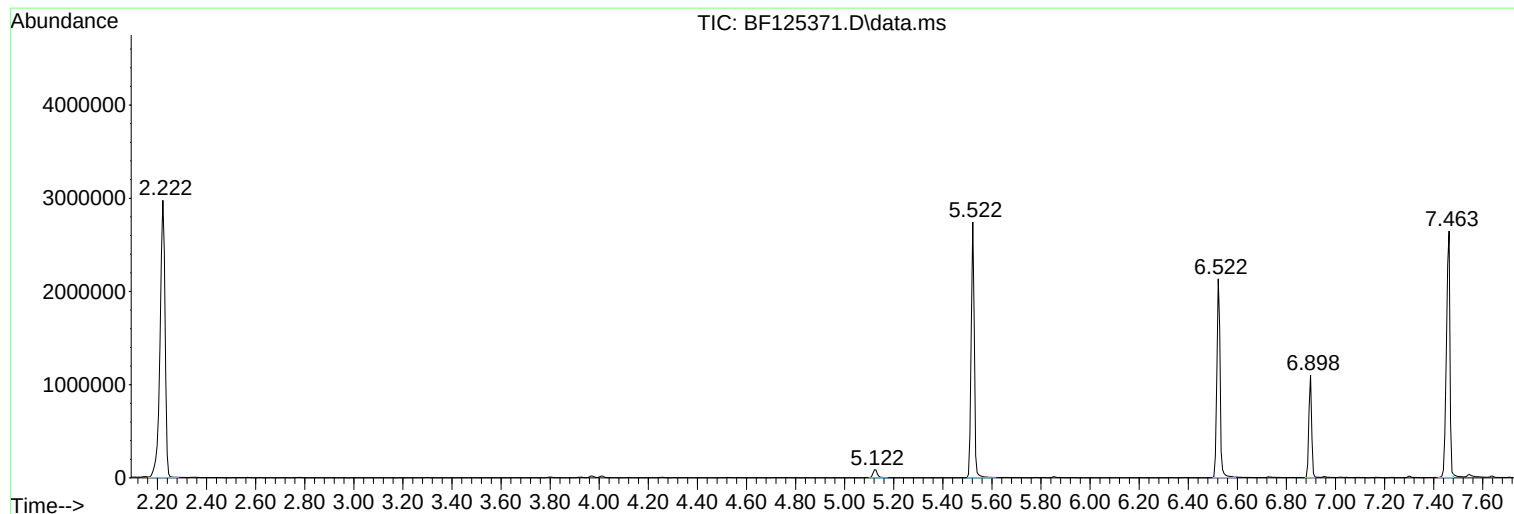
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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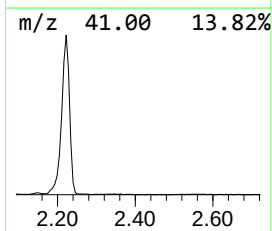
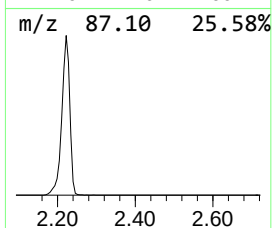
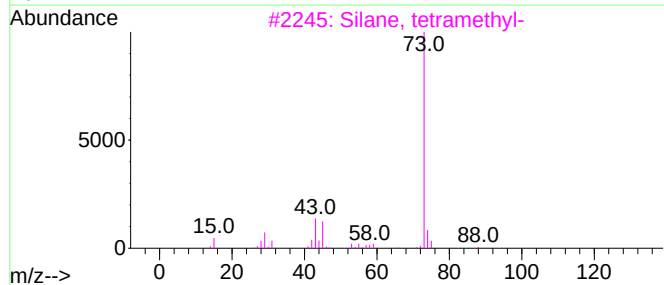
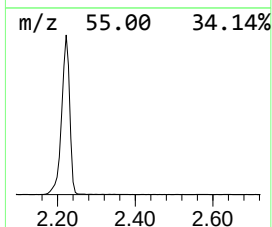
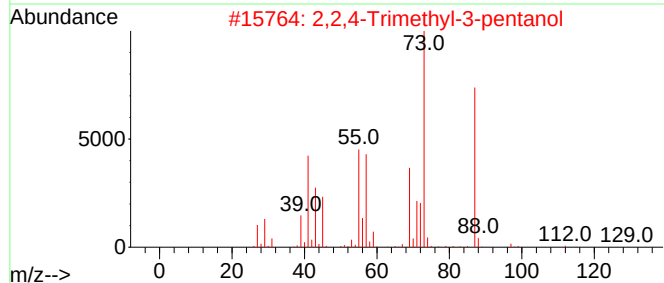
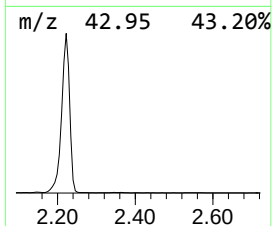
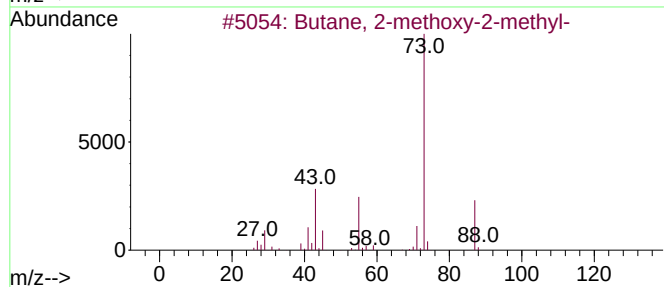
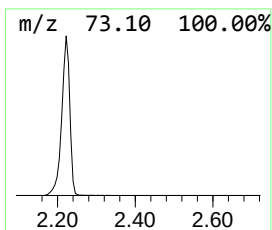
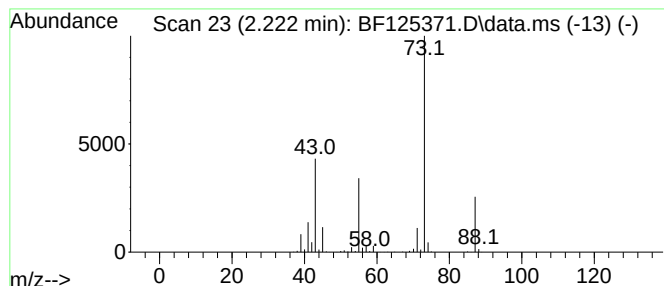
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.222	97.81 ng	4247410	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			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	23
5			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23



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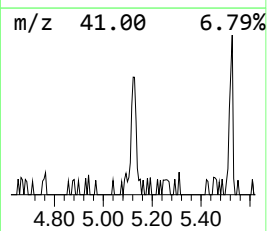
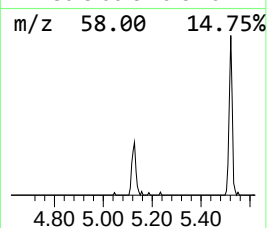
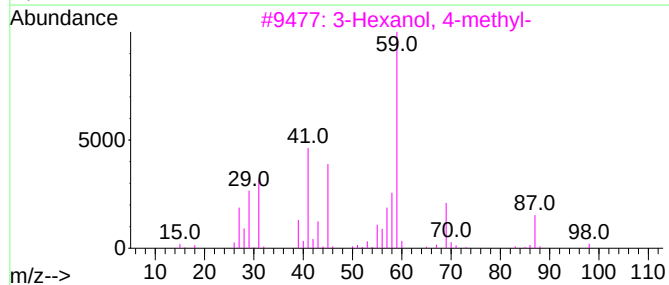
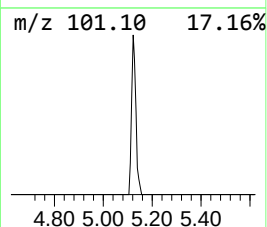
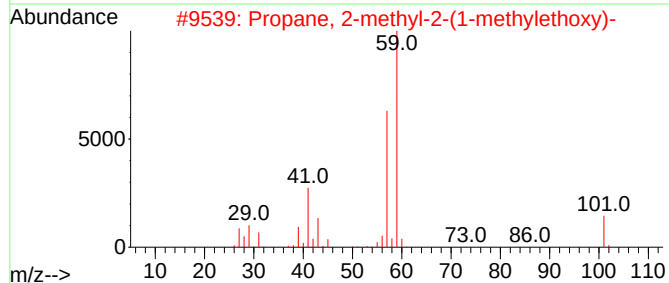
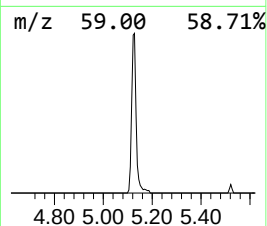
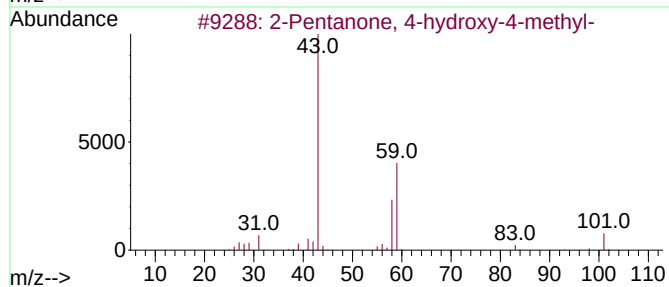
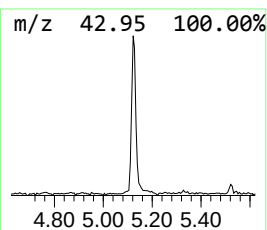
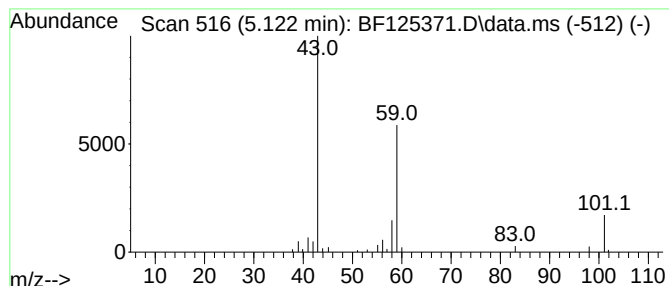
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.122	2.42 ng	104949	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	23
5			Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	23



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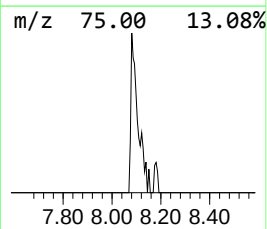
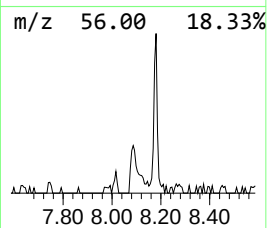
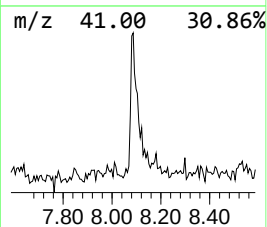
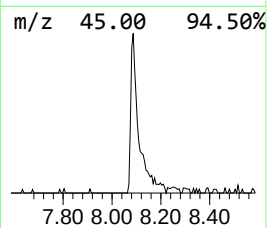
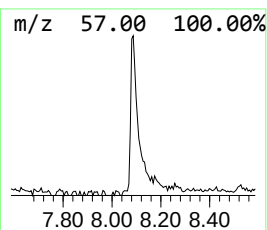
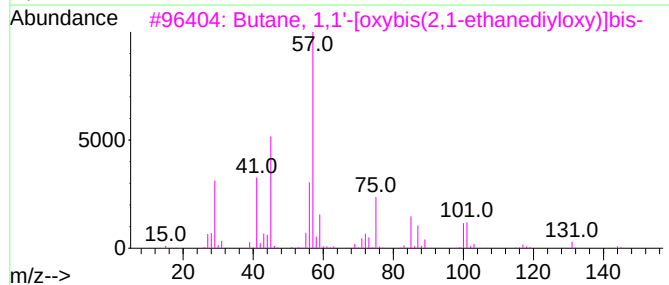
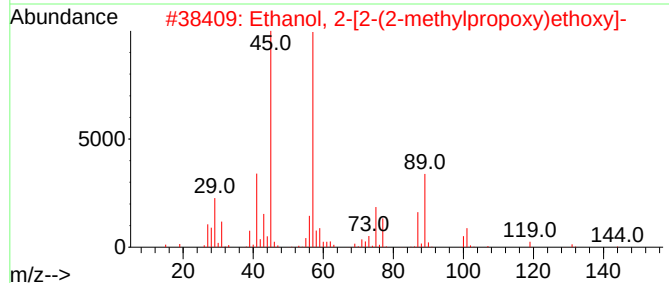
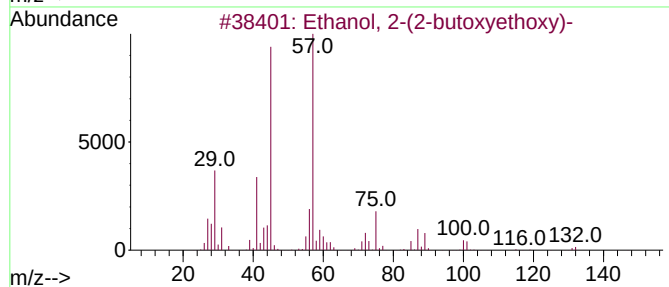
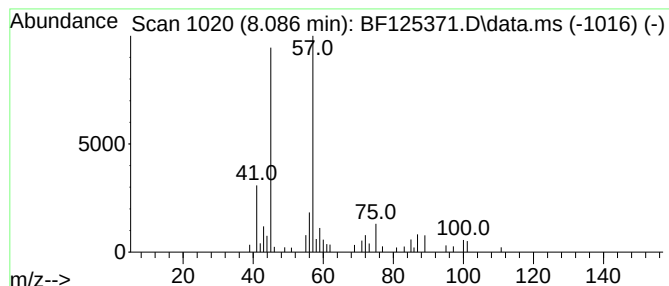
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.086	2.24 ng	122656	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			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
3			Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	56
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
5			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	50



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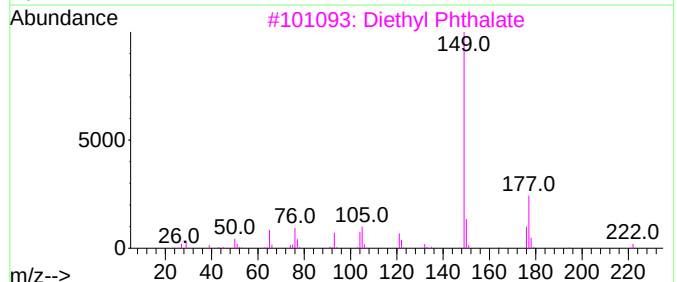
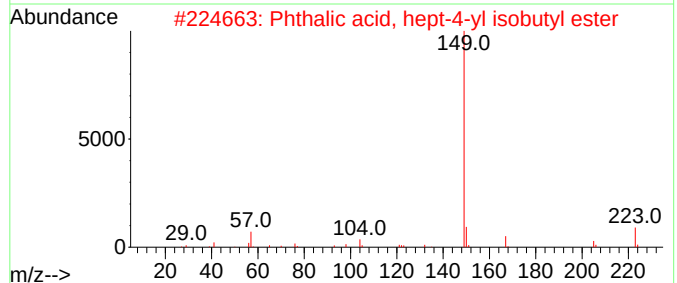
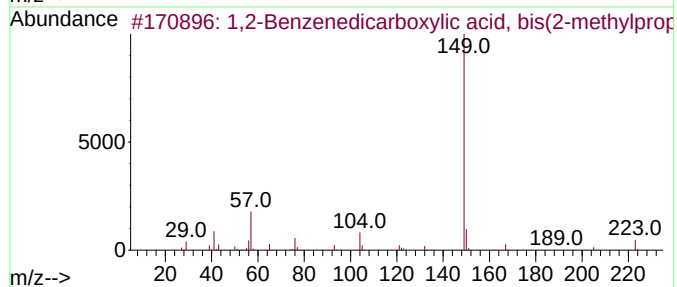
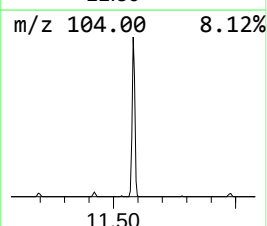
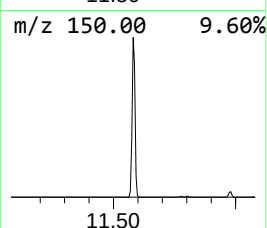
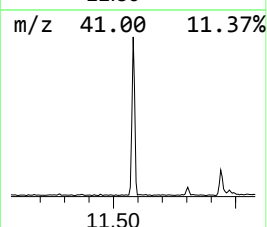
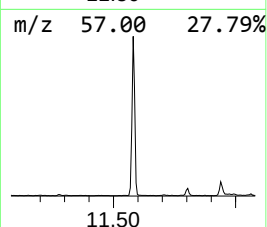
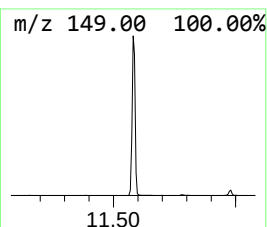
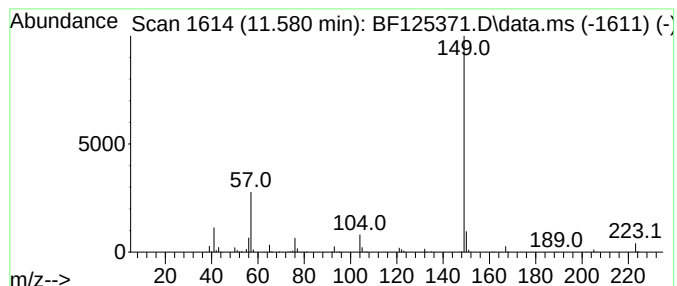
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Peak Number 4 1,2-Benzenedicarboxylic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.580	26.22 ng	1393440	Phenanthrene-d10	11.422	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	90
2	Phthalic acid, hept-4-yl isobuty...	320	C19H28O4	1000356-78-3	83
3	Diethyl Phthalate	222	C12H14O4	000084-66-2	78
4	Phthalic acid, cyclohexylmethyl ...	318	C19H26O4	1000309-08-6	78
5	Phthalic acid, 2,4-dimethylpent-...	320	C19H28O4	1000356-84-3	78



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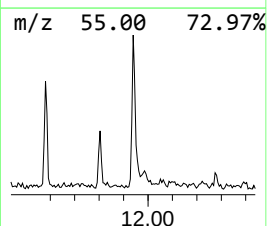
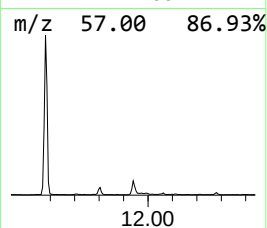
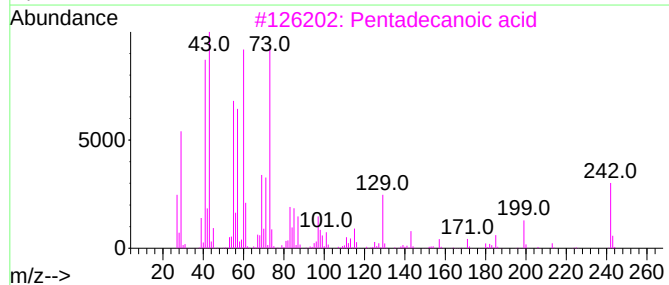
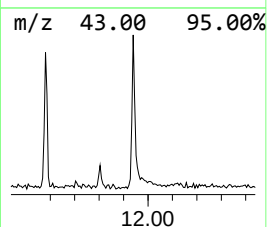
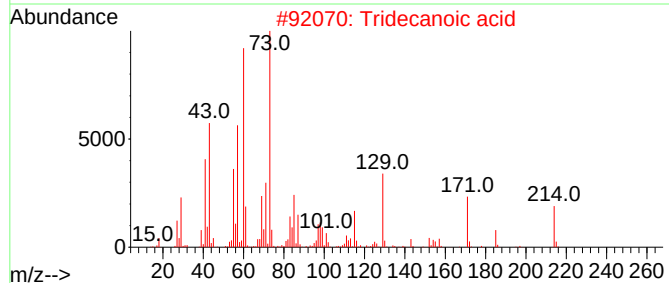
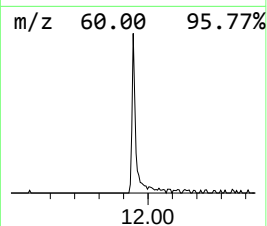
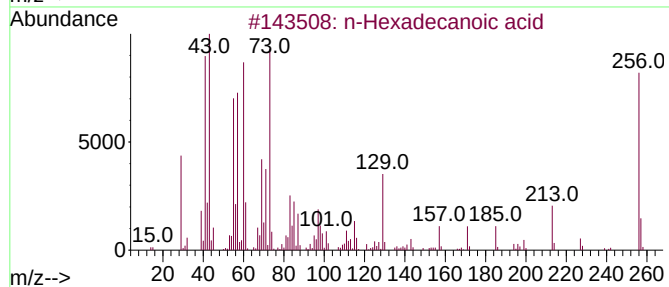
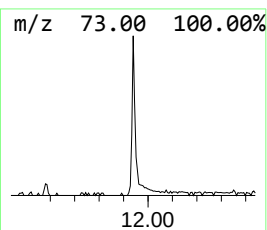
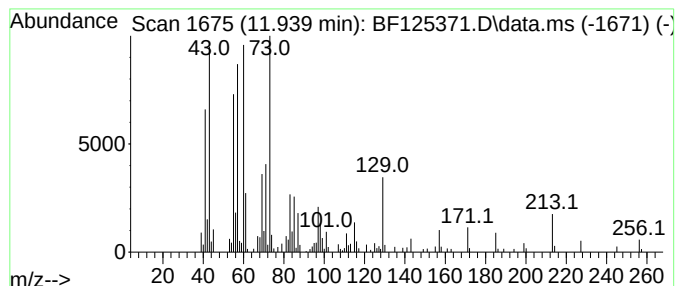
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.939	4.28 ng	227257	Phenanthrene-d10	11.422

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	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Dodecanoic acid	200	C12H24O2	000143-07-7	74
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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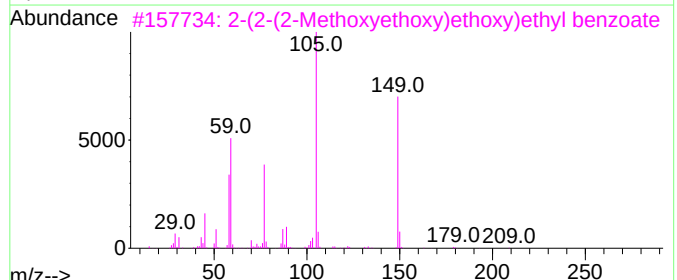
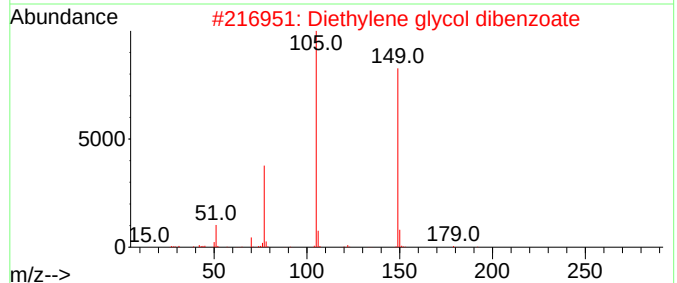
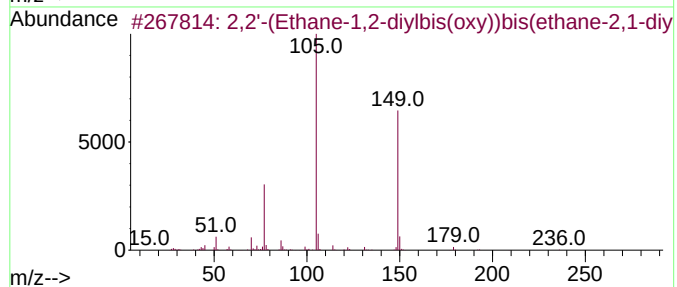
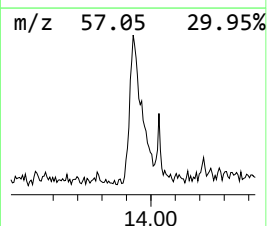
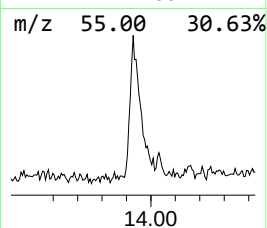
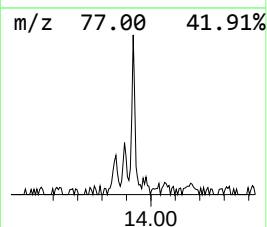
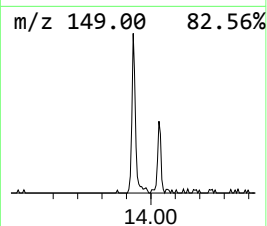
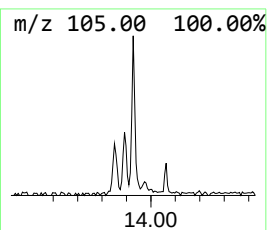
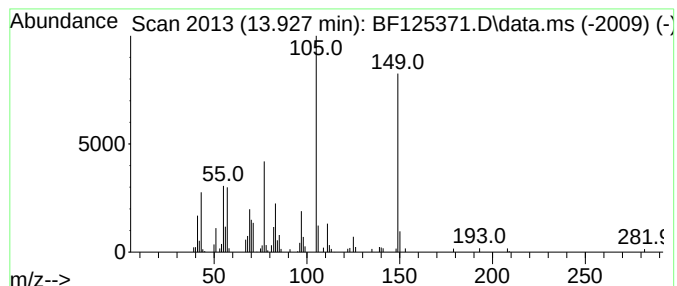
Instrument :
BNA_F
ClientSampleId :
20211057-SI-COMP-2-MODIFIED-EL

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 6 2,2'-(Ethane-1,2-diylbis(ox... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.927	6.91 ng	264145	Chrysene-d12	14.063	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	59
2	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	59
3	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	59
4	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	59
5	Phthalic acid, 5-methoxy-3-methy...	350	C20H30O5	1000314-88-6	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090421\
Data File : BF125371.D
Acq On : 4 Sep 2021 16:12
Operator : JU/CG
Sample : M3648-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20211057-SI-COMP-2-MODIFIED-EL

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.222	97.8	ng	4247410	1	6.898	868543	20.0
2-Pentanone, 4-...	5.122	2.4	ng	104949	1	6.898	868543	20.0
Ethanol, 2-(2-b...	8.086	2.2	ng	122656	2	8.181	1094770	20.0
1,2-Benzenedica...	11.580	26.2	ng	1393440	4	11.422	1062810	20.0
n-Hexadecanoic ...	11.939	4.3	ng	227257	4	11.422	1062810	20.0
2,2'-(Ethane-1,...	13.927	6.9	ng	264145	5	14.063	764956	20.0