

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111820\
 Data File : BF122366.D
 Acq On : 18 Nov 2020 14:24
 Operator : JU/CG
 Sample : L4771-03
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CD-BH-01-2-3

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-BF110920.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122366.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	5	10	16	rVB	962882	1268887	15.09%	2.213%
2	3.945	311	316	322	rVB	76654	105081	1.25%	0.183%
3	5.087	501	510	518	rVB	59884	87048	1.04%	0.152%
4	5.481	571	577	580	rBV	5989926	6340639	75.41%	11.059%
5	6.339	720	723	736	rBV	84823	133072	1.58%	0.232%
6	6.486	742	748	751	rBV	5738414	6687037	79.53%	11.664%
7	6.686	779	782	789	rBV	189706	176211	2.10%	0.307%
8	6.863	809	812	816	rVB	1678417	1315256	15.64%	2.294%
9	7.428	902	908	911	rBV	4480231	4279253	50.90%	7.464%
10	8.151	1026	1031	1034	rBV	1825848	1736759	20.66%	3.029%
11	9.227	1209	1214	1217	rBV	7724490	7067803	84.06%	12.328%
12	9.616	1276	1280	1290	rVB	1480178	1257847	14.96%	2.194%
13	9.904	1324	1329	1340	rVB	2535614	2135813	25.40%	3.725%
14	10.692	1458	1463	1466	rBV	5680716	5384289	64.04%	9.391%
15	11.386	1577	1581	1585	rBV	2577556	2261660	26.90%	3.945%
16	11.915	1664	1671	1685	rBV	564674	825446	9.82%	1.440%
17	12.374	1745	1749	1752	rVB	235433	211942	2.52%	0.370%
18	12.704	1801	1805	1815	rBV	488697	646677	7.69%	1.128%
19	12.980	1847	1852	1855	rBV	8498549	8407978	100.00%	14.665%
20	13.880	2001	2005	2024	rBV	922586	1712615	20.37%	2.987%
21	14.027	2026	2030	2033	rBV	2782014	2397544	28.52%	4.182%
22	15.156	2218	2222	2225	rBV2	78317	88962	1.06%	0.155%
23	15.498	2274	2280	2285	rBV	1871944	2301881	27.38%	4.015%
24	15.980	2358	2362	2367	rVB2	60911	88560	1.05%	0.154%
25	16.039	2367	2372	2380	rBV3	108217	322951	3.84%	0.563%
26	16.486	2442	2448	2453	rBV5	45943	91708	1.09%	0.160%

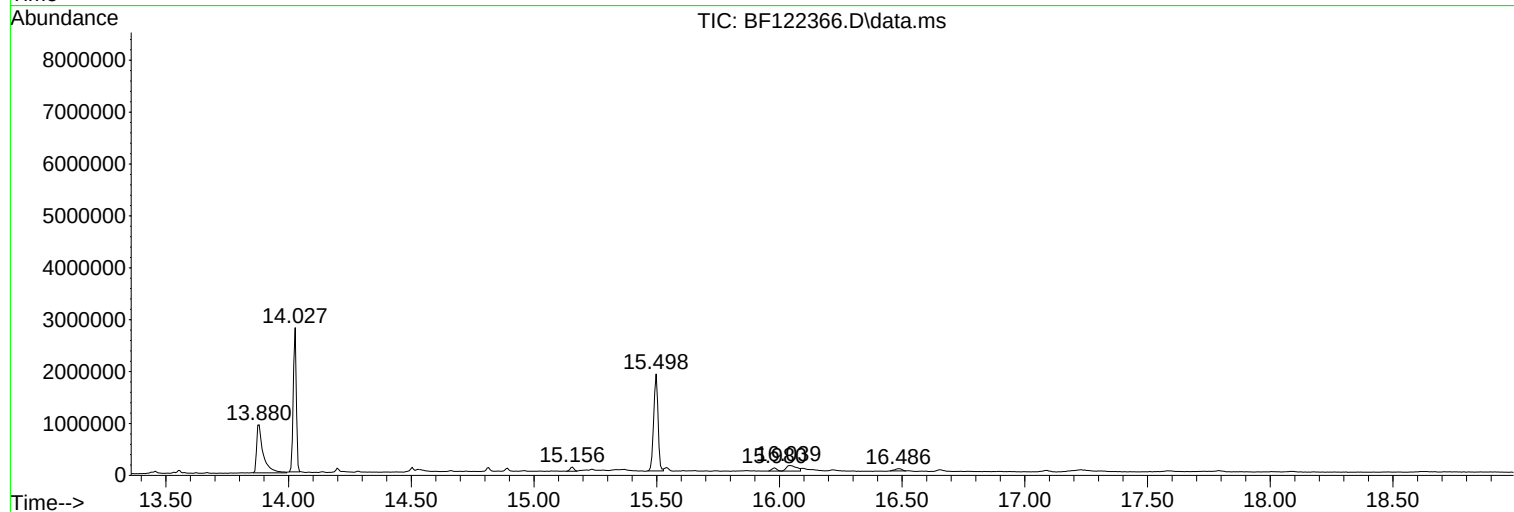
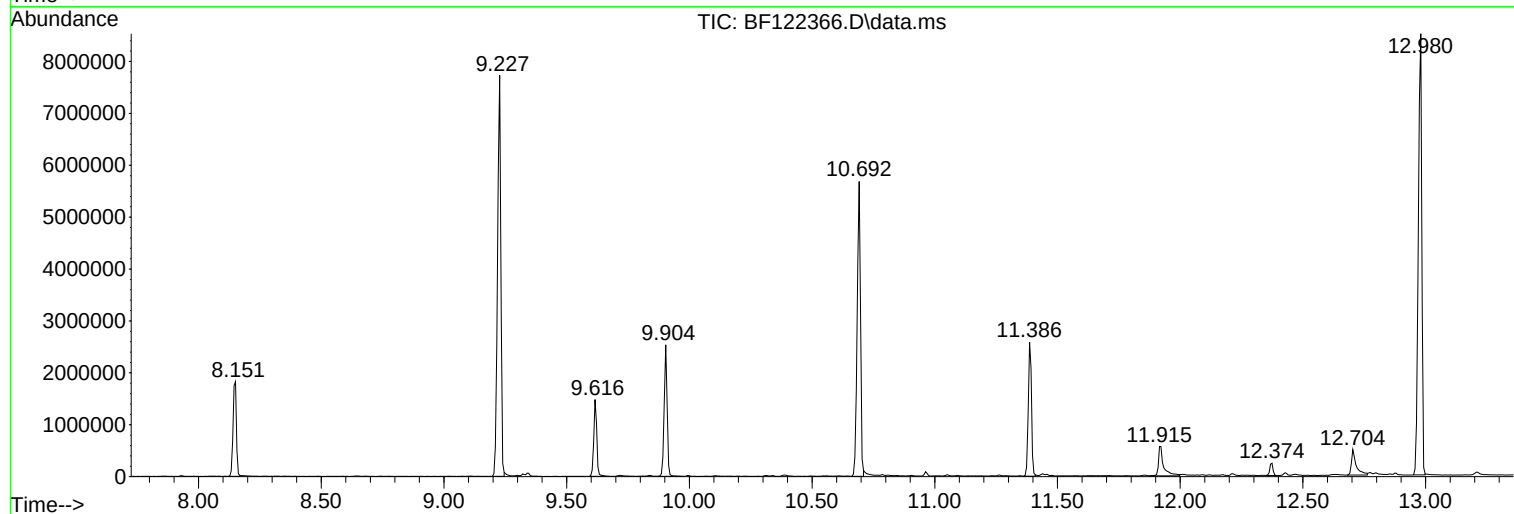
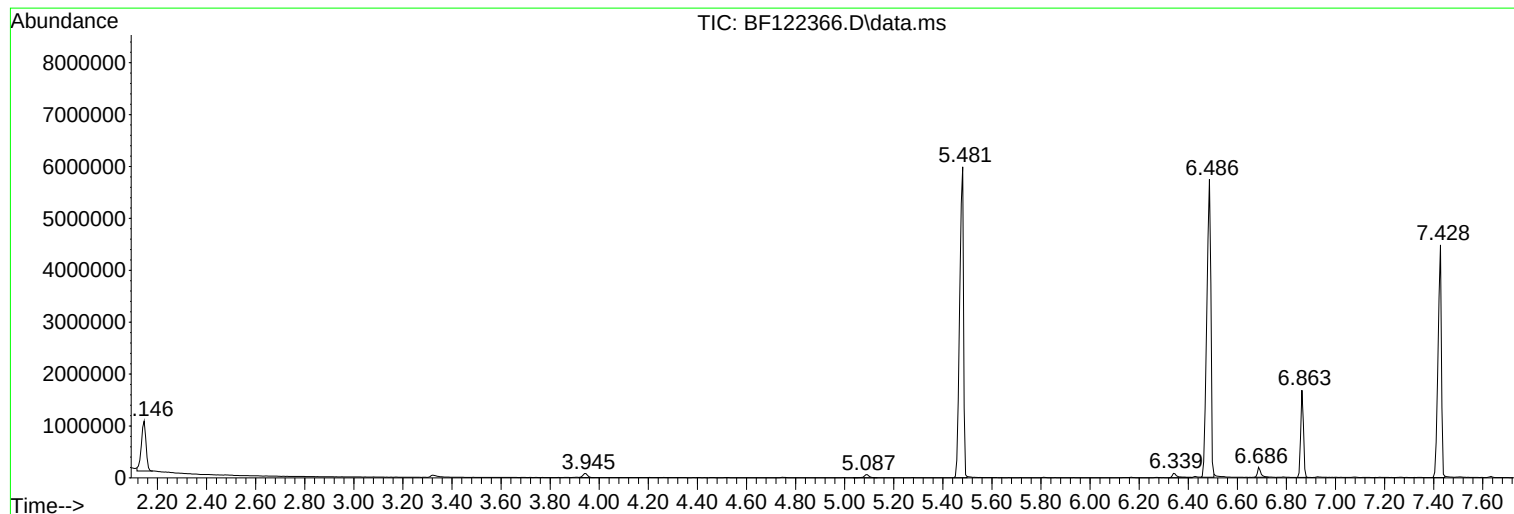
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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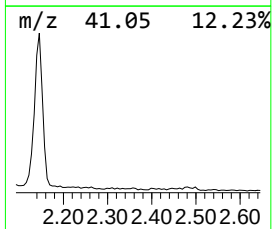
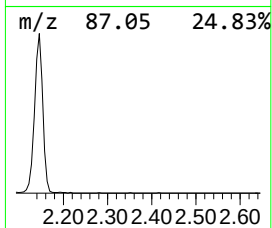
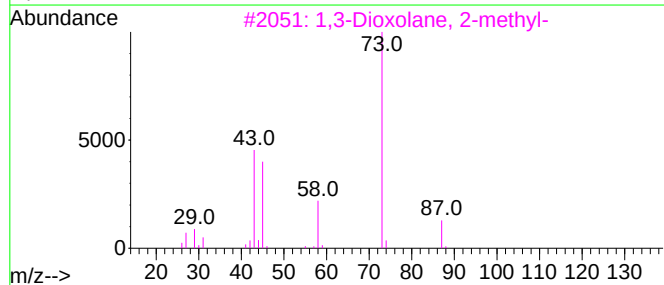
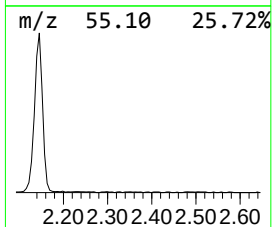
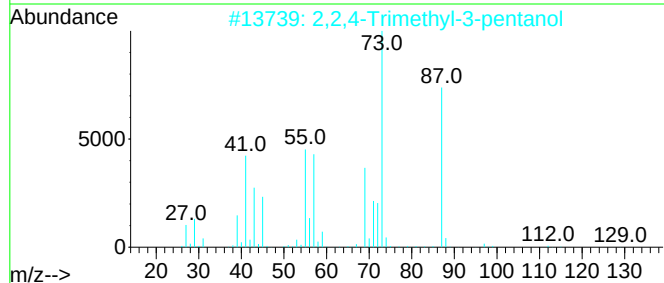
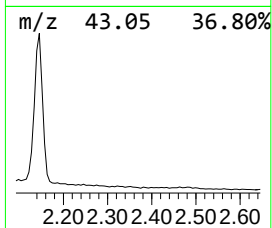
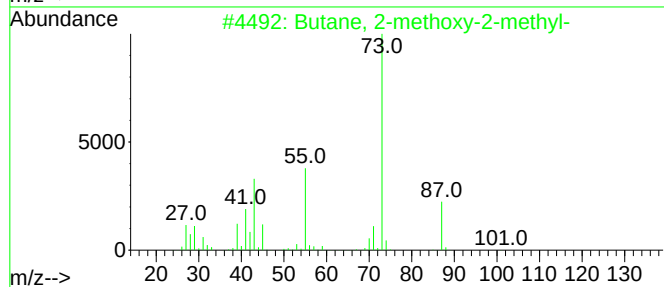
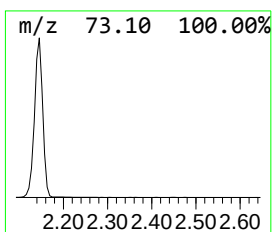
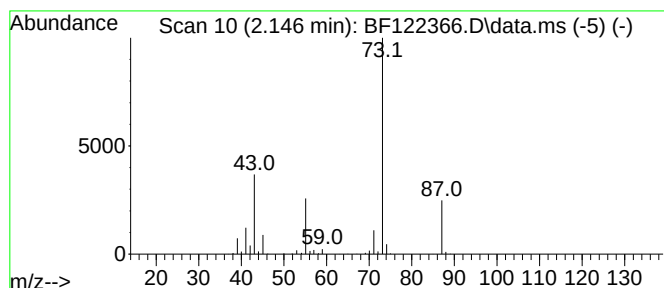
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.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.
2.146	19.29 ng	1268890	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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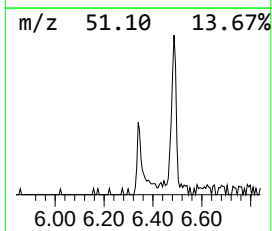
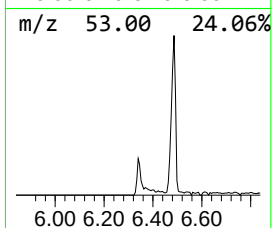
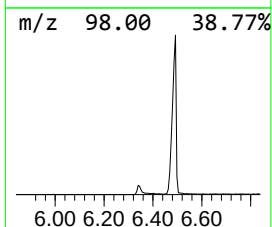
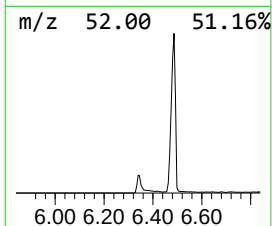
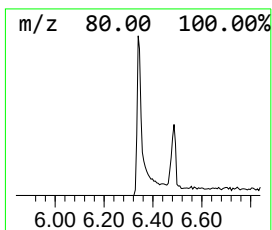
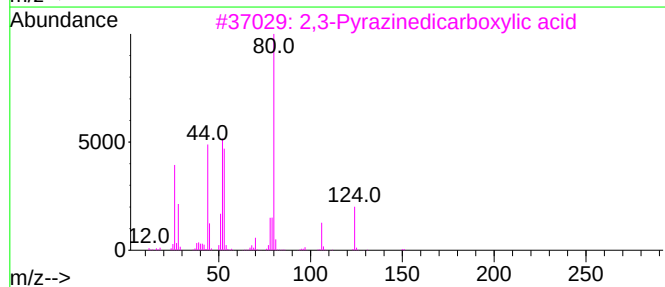
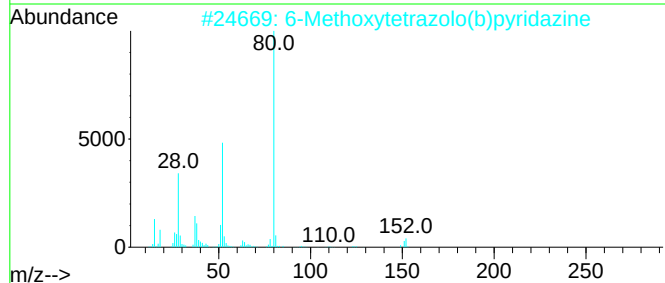
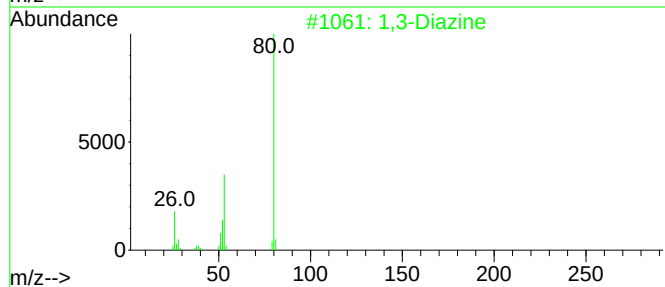
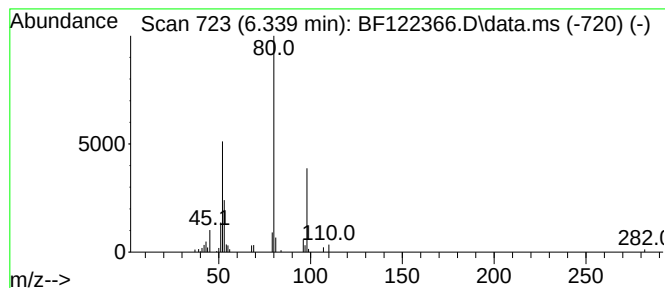
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.33 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.339	2.02 ng	133072	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Diazine	80	C4H4N2	000289-95-2	47
2			6-Methoxytetrazolo(b)pyridazine	151	C5H5N5O	027062-50-6	40
3			2,3-Pyrazinedicarboxylic acid	168	C6H4N2O4	000089-01-0	40
4			Pyridazine	80	C4H4N2	000289-80-5	39
5			2,3-Dicyanopropionamide	123	C5H5N3O	098024-59-0	28



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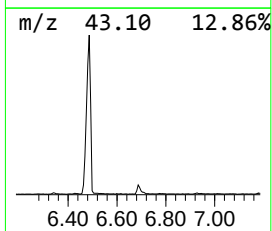
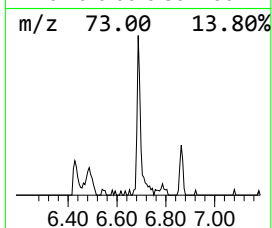
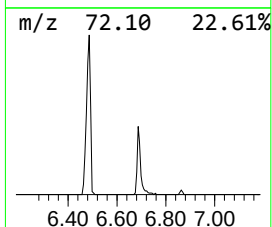
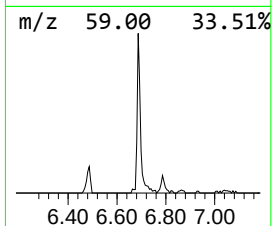
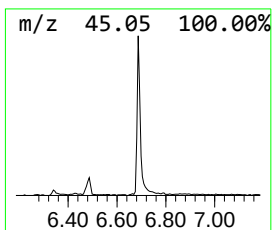
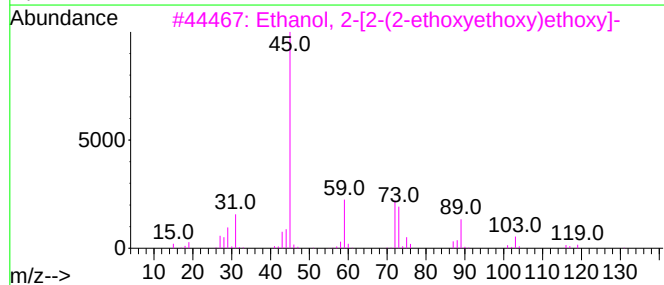
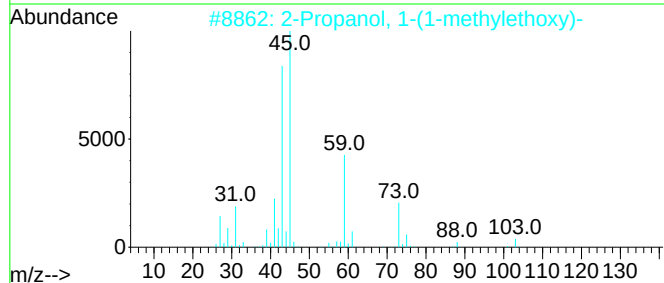
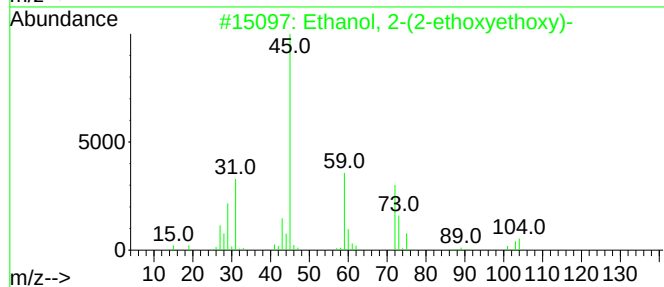
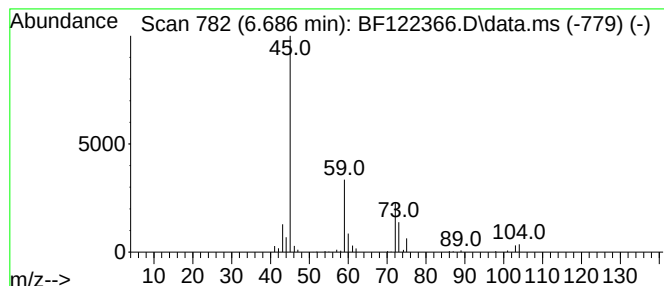
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.686	2.68 ng	176211	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	50
3			Ethanol, 2-[2-(2-ethoxyethoxy)et...]	178	C8H18O4	000112-50-5	39
4			Ethanol, 2-[2-(2-propenyloxy)eth...]	146	C7H14O3	015075-50-0	33
5			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	25



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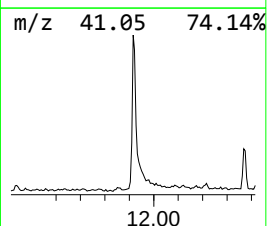
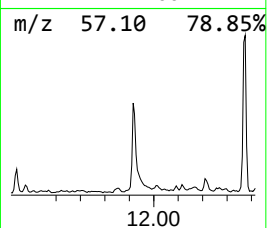
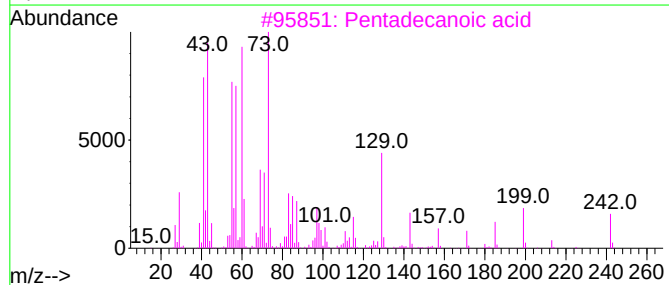
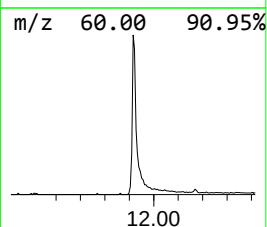
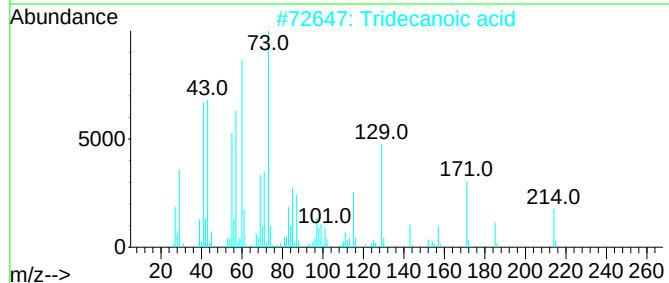
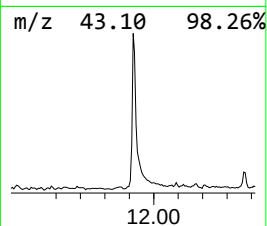
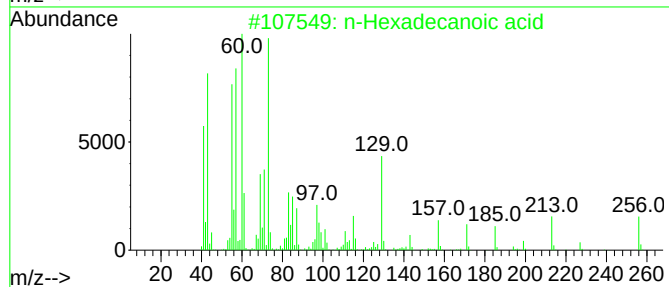
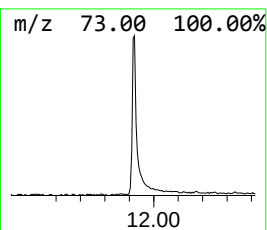
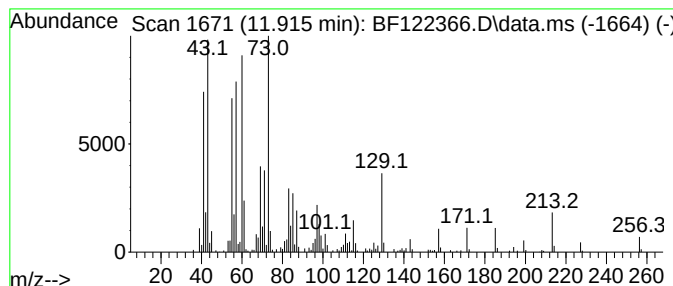
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	7.30 ng	825446	Phenanthrene-d10	11.386

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	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



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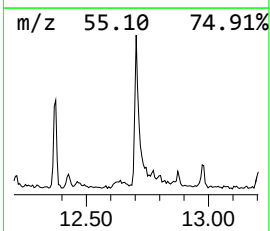
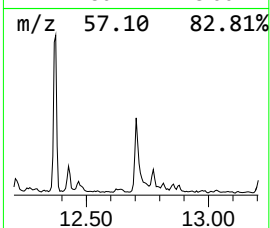
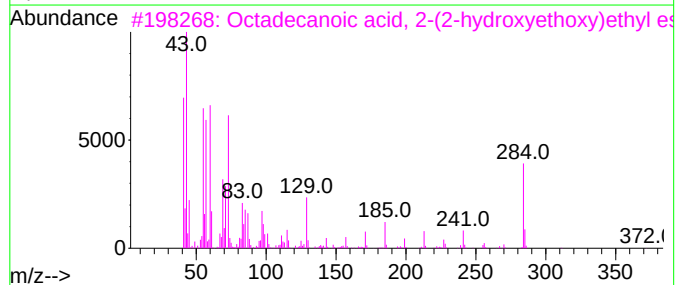
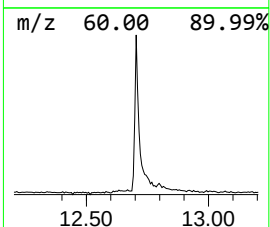
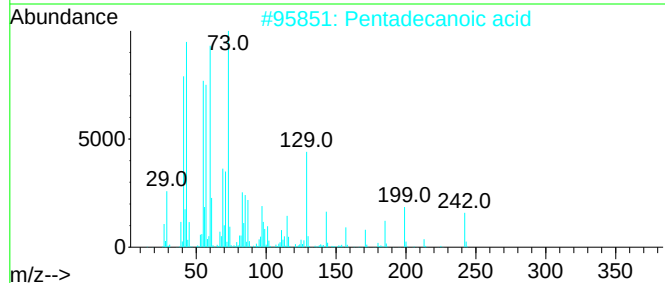
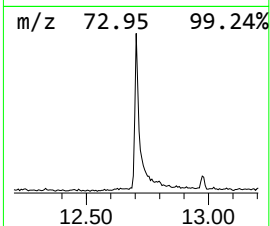
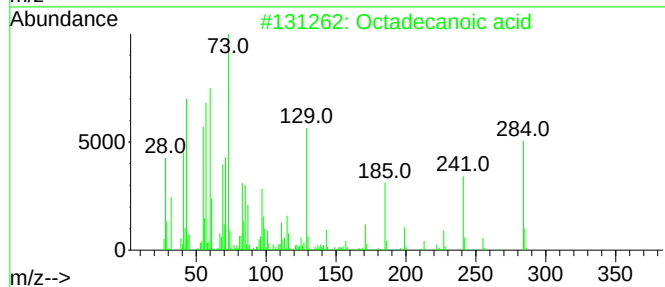
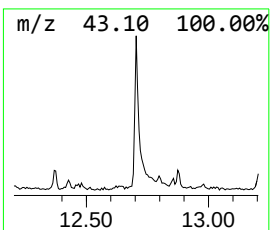
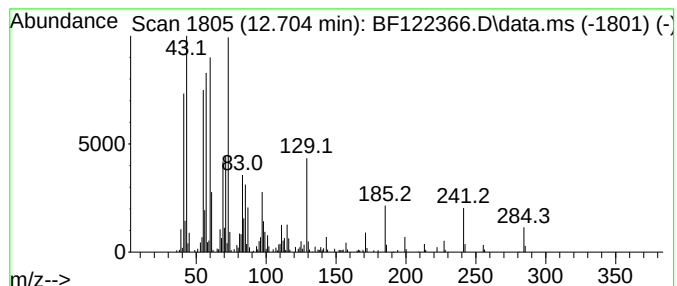
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.704	5.72 ng	646677	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Tridecanoic acid	214	C13H26O2	000638-53-9	76



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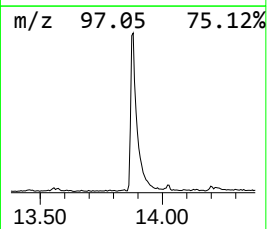
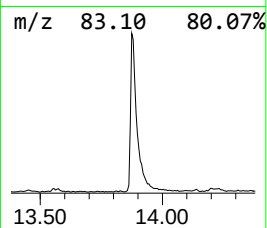
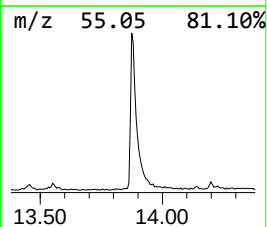
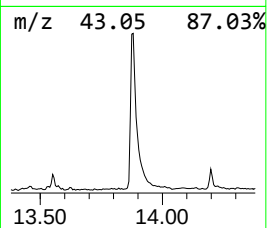
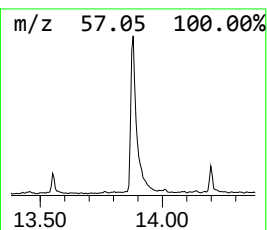
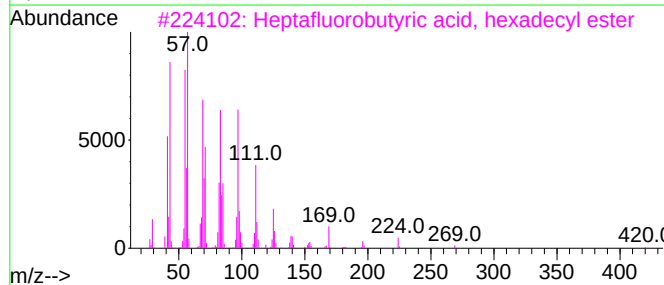
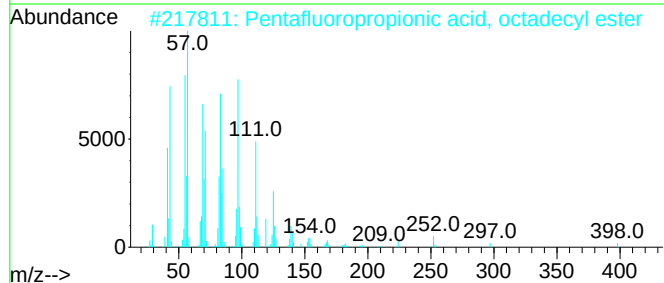
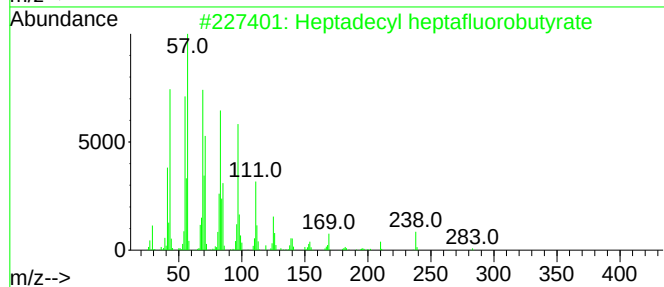
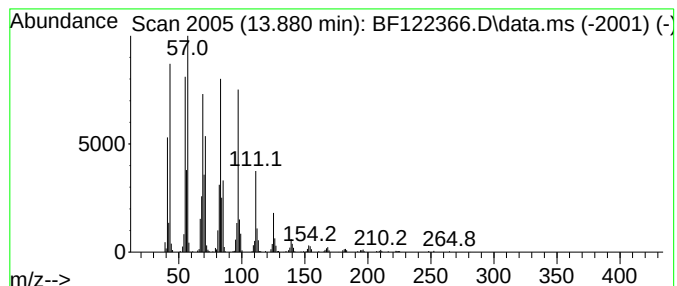
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	14.29 ng	1712620	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2			Pentafluoropropionic acid, octadecyl ester	416	C21H37F5O2	959261-25-7	94
3			Heptafluorobutyric acid, hexadecyl ester	438	C20H33F7O2	006385-15-5	94
4			Behenic alcohol	326	C22H46O	000661-19-8	93
5			1-Heneicosanol	312	C21H44O	015594-90-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111820\
Data File : BF122366.D
Acq On : 18 Nov 2020 14:24
Operator : JU/CG
Sample : L4771-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CD-BH-01-2-3

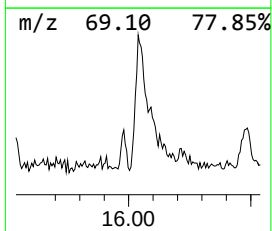
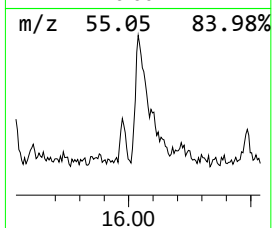
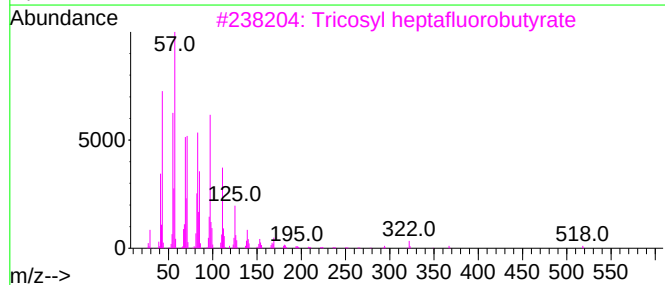
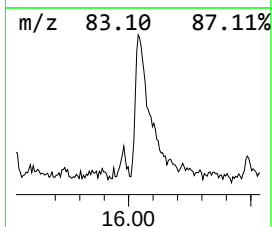
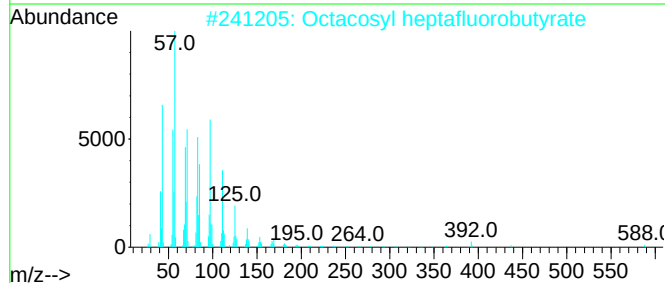
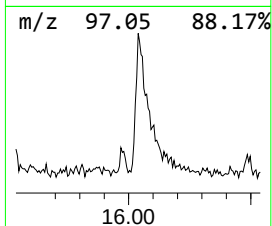
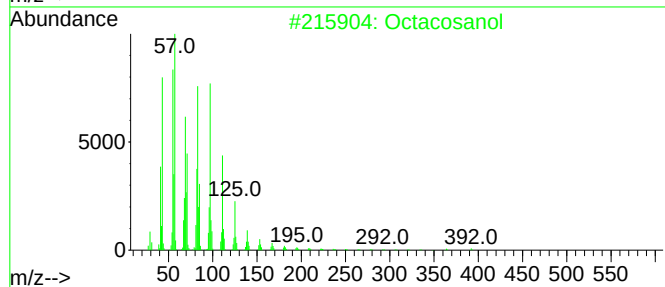
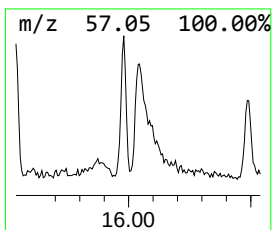
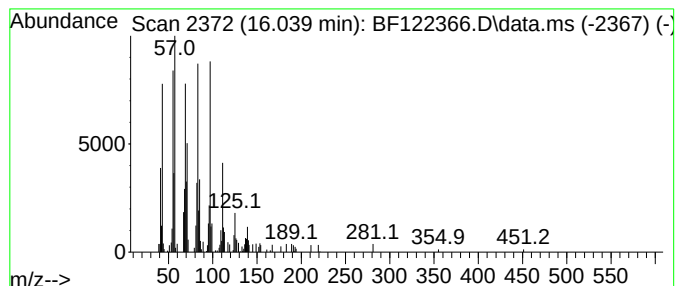
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Octacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.039	2.81 ng	322951	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosanol	410	C28H58O	000557-61-9	93
2			Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	55
3			Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	55
4			Triacontyl acetate	480	C32H64O2	041755-58-2	55
5			17-Pentatriacontene	491	C35H70	006971-40-0	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111820\
Data File : BF122366.D
Acq On : 18 Nov 2020 14:24
Operator : JU/CG
Sample : L4771-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CD-BH-01-2-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.146	19.3	ng	1268890	1	6.863	1315260	20.0
unknown6.33	6.339	2.0	ng	133072	1	6.863	1315260	20.0
Ethanol, 2-(2-e...	6.686	2.7	ng	176211	1	6.863	1315260	20.0
n-Hexadecanoic ...	11.916	7.3	ng	825446	4	11.386	2261660	20.0
Octadecanoic acid	12.704	5.7	ng	646677	4	11.386	2261660	20.0
Heptadecyl hept...	13.880	14.3	ng	1712620	5	14.027	2397540	20.0
Octacosanol	16.039	2.8	ng	322951	6	15.498	2301880	20.0