

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041923\
 Data File : BF132921.D
 Acq On : 19 Apr 2023 20:09
 Operator : CG\JU
 Sample : 02366-07
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20230335-COMP-13

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-BF041723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132921.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.116	173	175	187	rBV	68244	159291	1.54%	0.239%
2	4.957	479	488	497	rBV	2068367	3098976	29.90%	4.659%
3	5.369	552	558	561	rBV	7057715	8343182	80.50%	12.544%
4	5.769	623	626	630	rBV	256288	209038	2.02%	0.314%
5	6.393	726	732	735	rBV	7202755	8546811	82.47%	12.850%
6	6.763	791	795	798	rBV	1856975	1468981	14.17%	2.209%
7	7.328	886	891	894	rBV	6017773	5420606	52.30%	8.150%
8	8.045	1009	1013	1016	rBV	2709105	2007792	19.37%	3.019%
9	9.128	1192	1197	1200	rBV	10009685	8833433	85.23%	13.281%
10	9.798	1307	1311	1314	rBV	3144294	2352584	22.70%	3.537%
11	10.510	1429	1432	1436	rBV	434568	381434	3.68%	0.573%
12	10.586	1440	1445	1448	rBV	6655350	6620431	63.88%	9.954%
13	11.280	1559	1563	1566	rBV	3271158	2557652	24.68%	3.845%
14	11.816	1650	1654	1658	rBV	656964	700606	6.76%	1.053%
15	12.604	1784	1788	1800	rBV	116312	158702	1.53%	0.239%
16	12.874	1828	1834	1837	rBV	10281343	10364111	100.00%	15.583%
17	13.457	1930	1933	1935	rBV	136314	125304	1.21%	0.188%
18	13.774	1983	1987	2003	rBV2	540007	906664	8.75%	1.363%
19	13.916	2007	2011	2014	rBV	2288621	2073732	20.01%	3.118%
20	14.098	2039	2042	2046	rBV	183524	158690	1.53%	0.239%
21	14.404	2090	2094	2099	rBV	187480	186344	1.80%	0.280%
22	14.704	2142	2145	2152	rBV	128764	119468	1.15%	0.180%
23	15.033	2197	2201	2205	rBV	110622	116923	1.13%	0.176%
24	15.345	2248	2254	2260	rBV	1326417	1599682	15.43%	2.405%

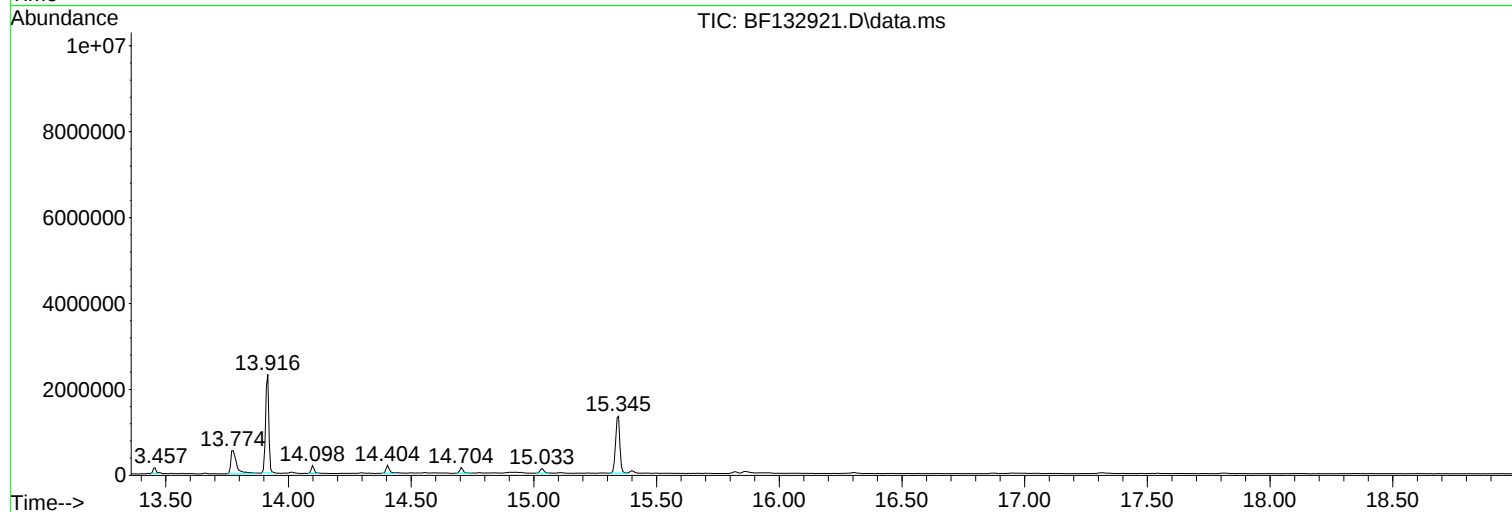
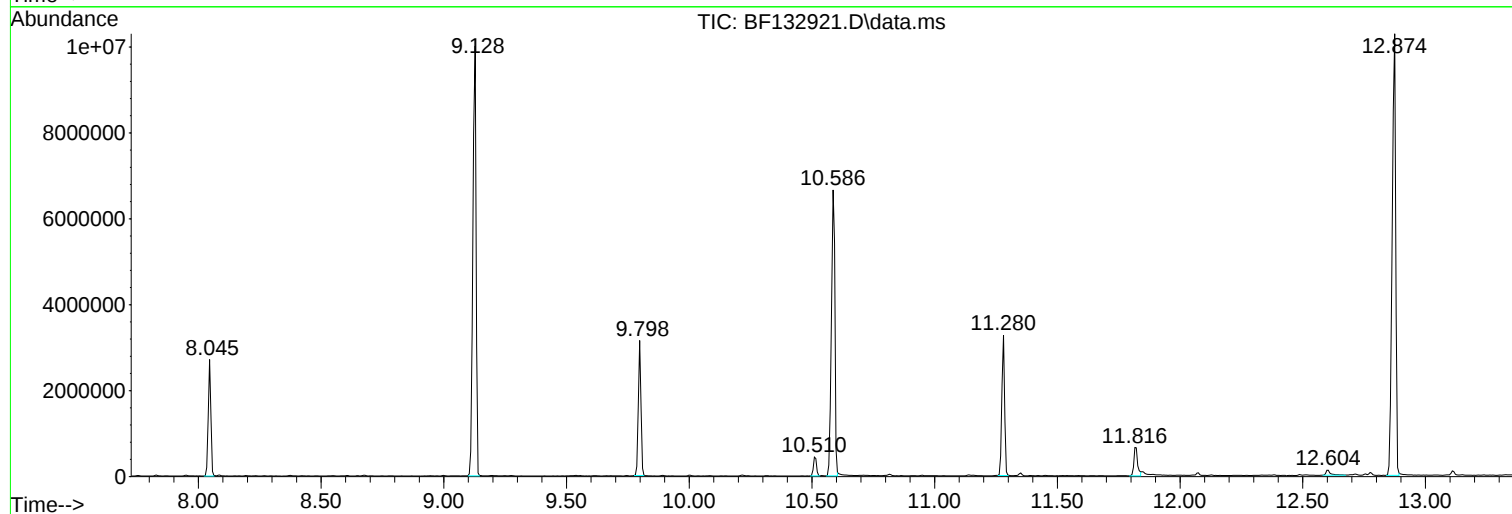
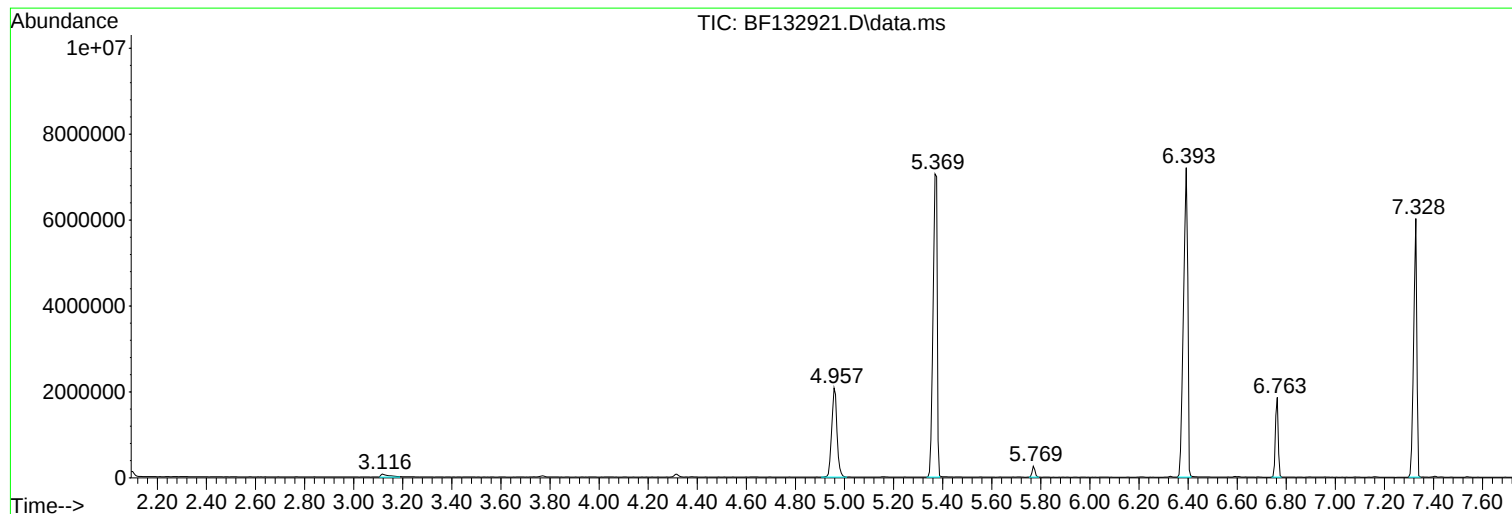
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BNA_F
ClientSampleId :
20230335-COMP-13

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF041723.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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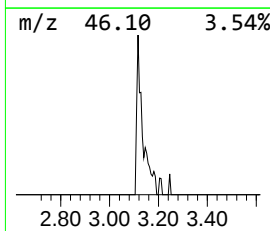
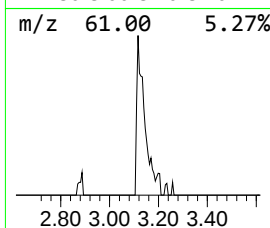
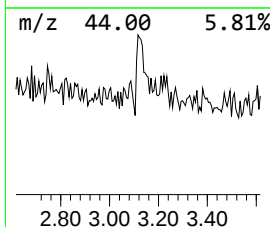
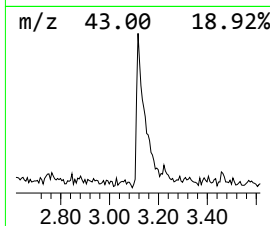
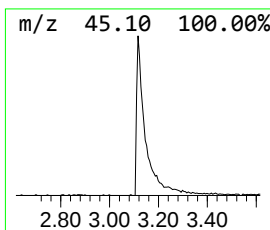
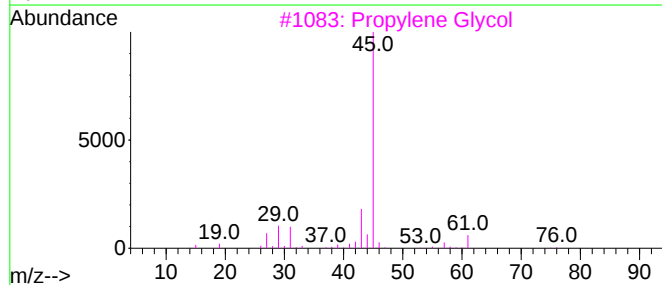
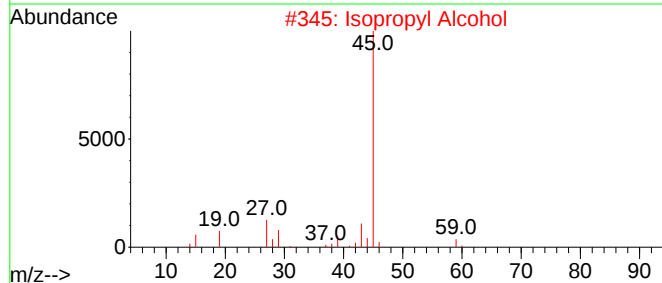
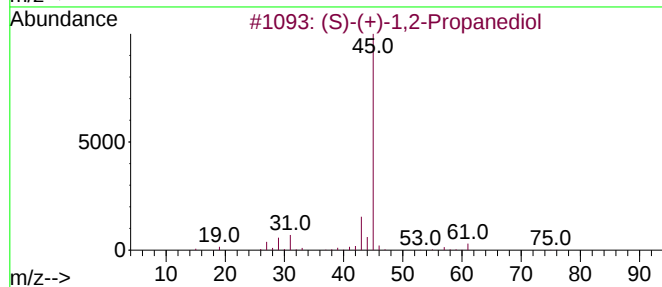
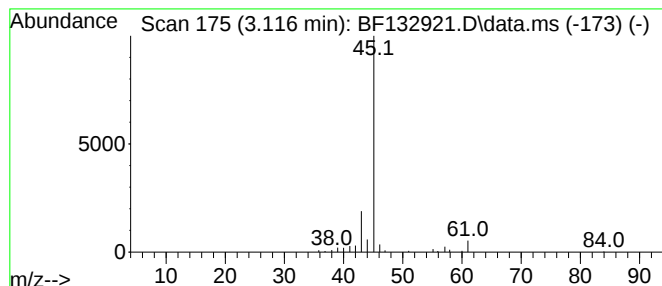
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.116	2.17 ng	159291	1,4-Dichlorobenzene-d4	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol			76	C3H8O2	004254-15-3	56
2	Isopropyl Alcohol			60	C3H8O	000067-63-0	56
3	Propylene Glycol			76	C3H8O2	000057-55-6	43
4	R-(-)-1,2-propanediol			76	C3H8O2	004254-14-2	40
5	L-Lactic acid			90	C3H6O3	000079-33-4	9



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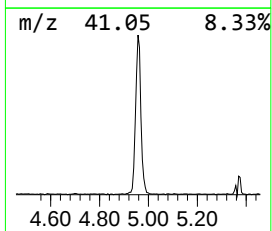
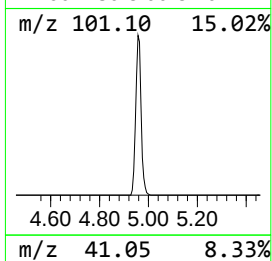
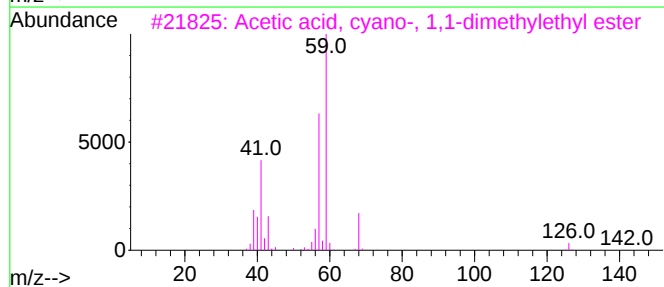
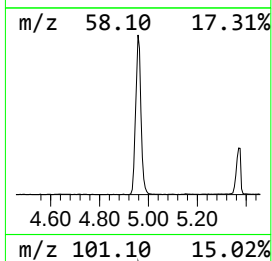
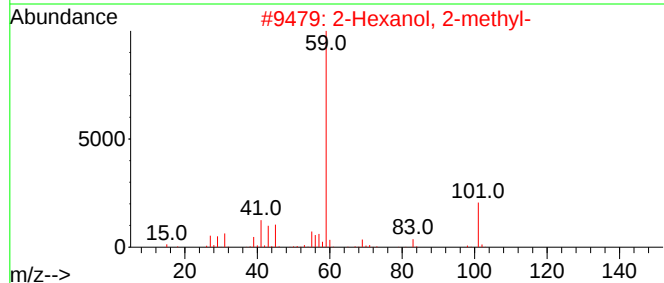
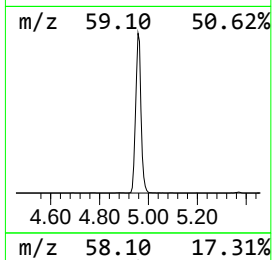
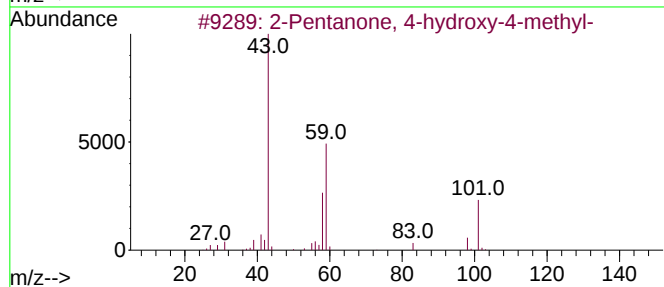
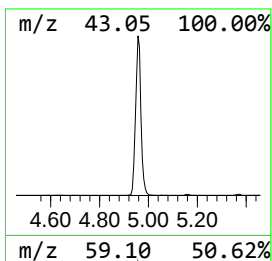
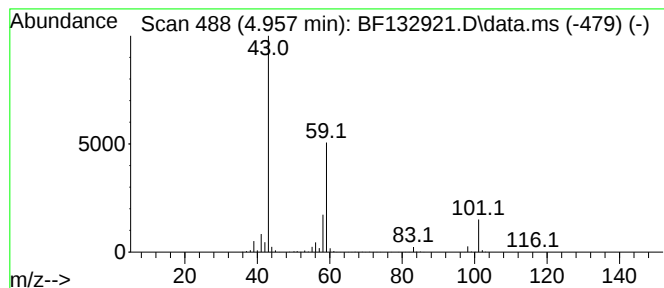
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.957	42.19 ng	3098980	1,4-Dichlorobenzene-d4	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		



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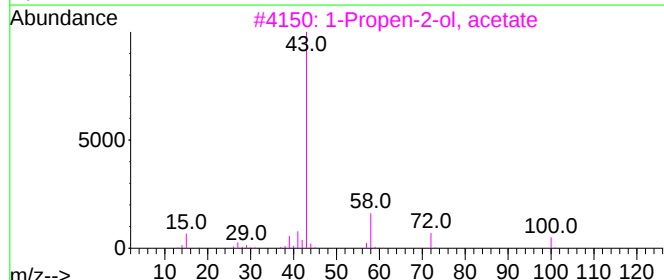
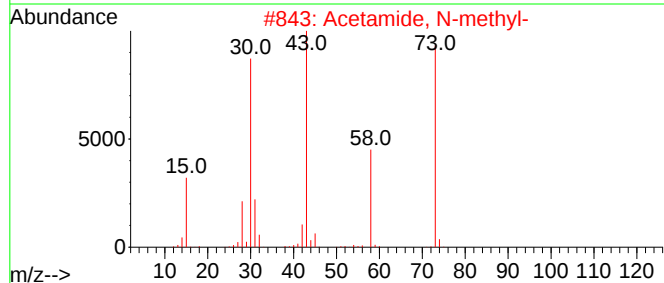
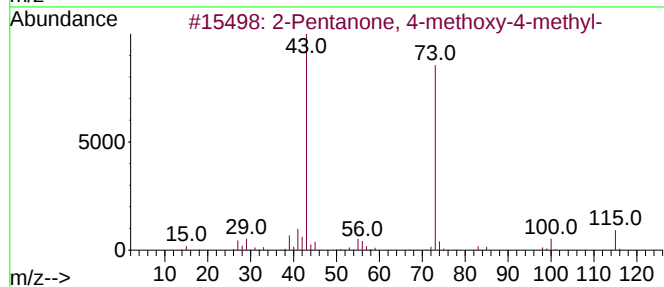
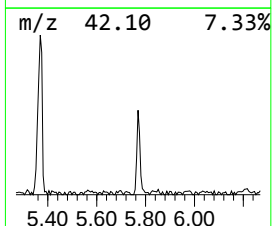
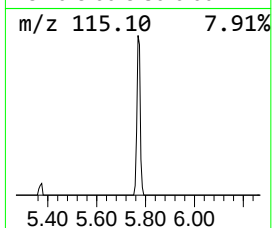
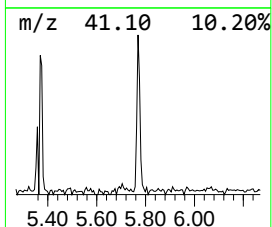
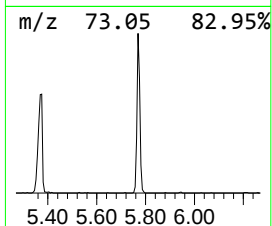
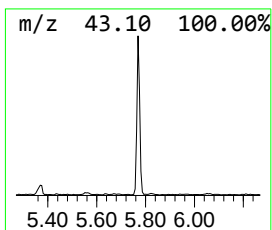
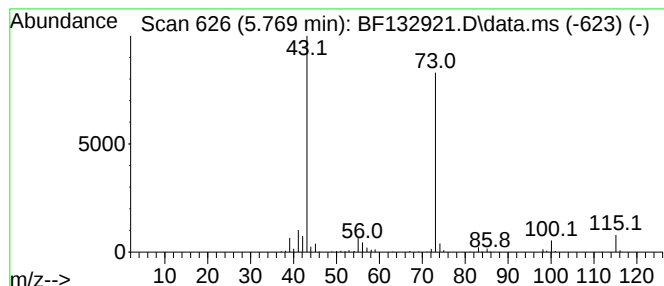
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.769	2.85 ng	209038	1,4-Dichlorobenzene-d4	6.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	40
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	27
4		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	23
5		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	12



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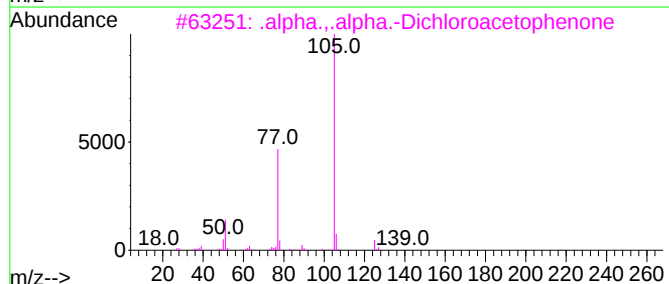
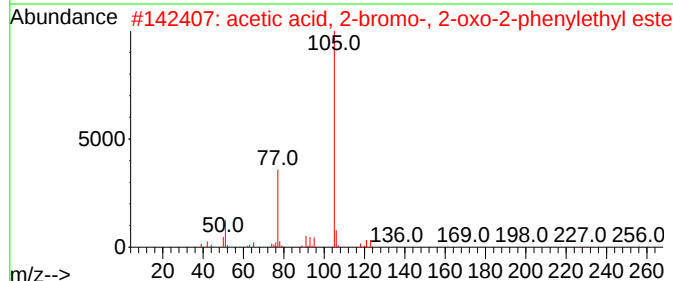
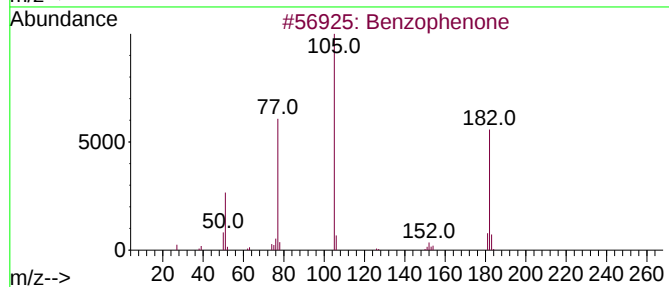
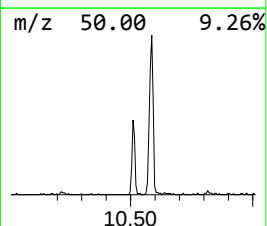
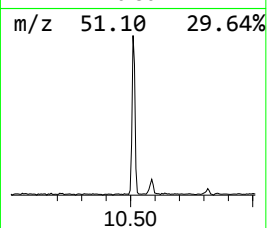
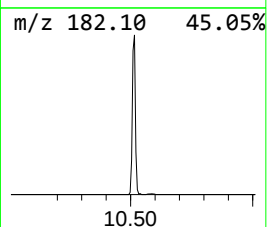
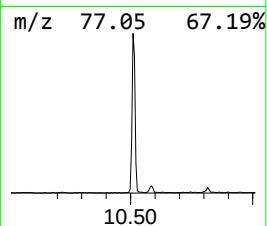
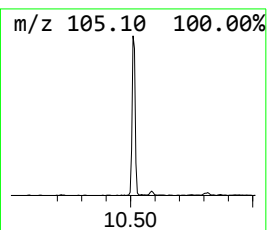
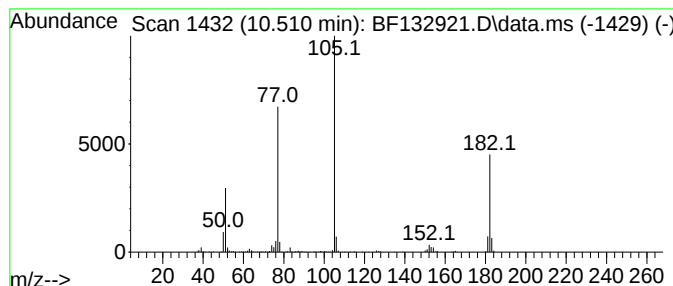
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Peak Number 4 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.510	3.24 ng	381434	Acenaphthene-d10	9.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			acetic acid, 2-bromo-, 2-oxo-2-p...	256	C10H9BrO3	1000401-50-0	50
3			.alpha.,.alpha.-Dichloroacetophe...	188	C8H6Cl2O	002648-61-5	50
4			Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	50
5			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	50



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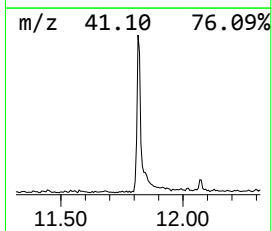
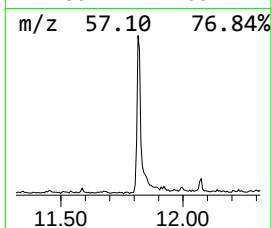
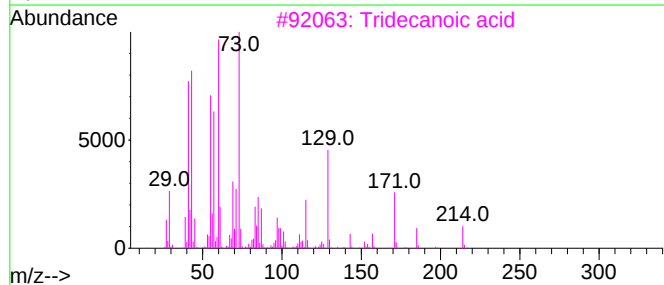
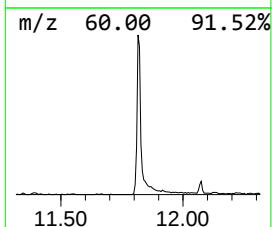
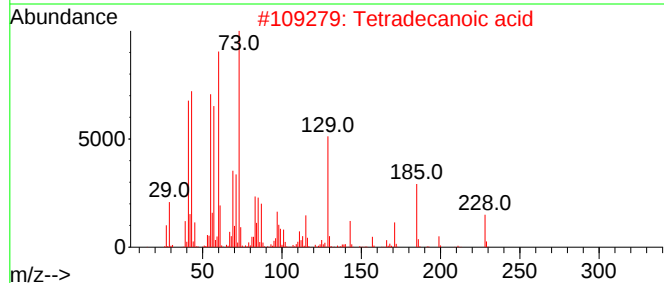
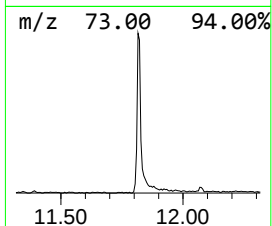
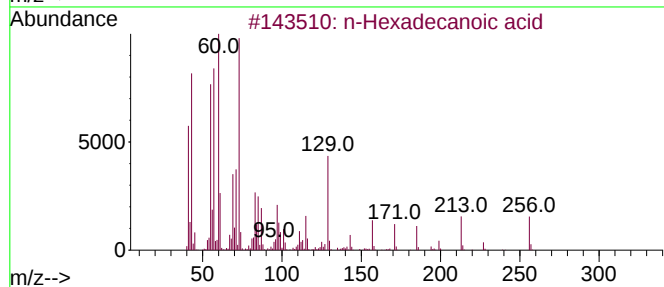
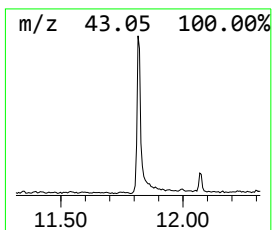
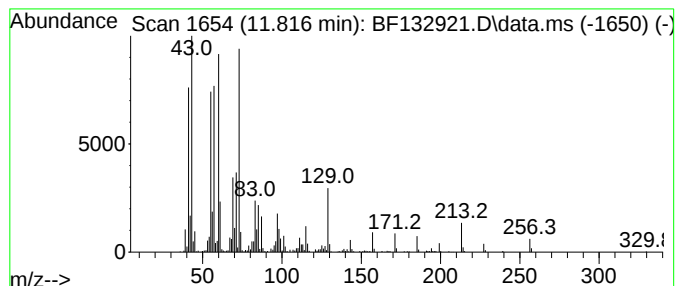
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.816	5.48 ng	700606	Phenanthrene-d10	11.281

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	96
3			Tridecanoic acid	214	C13H26O2	000638-53-9	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5			Octadecanoic acid	284	C18H36O2	000057-11-4	90



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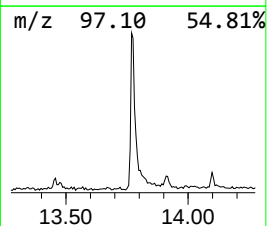
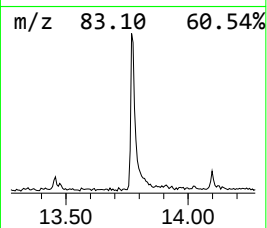
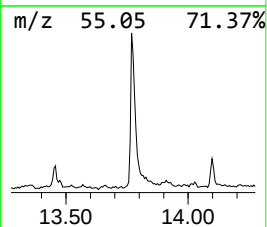
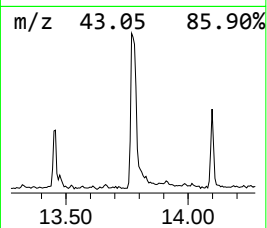
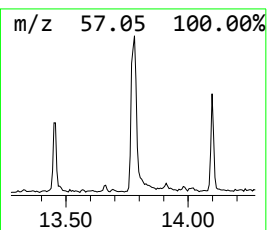
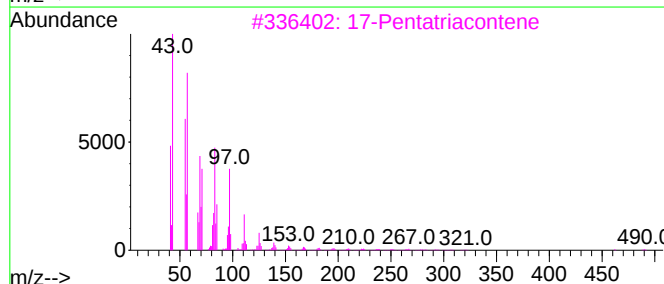
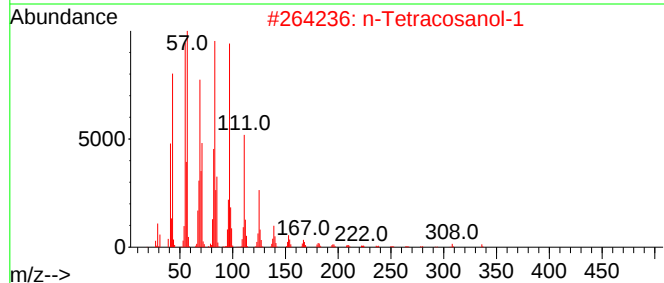
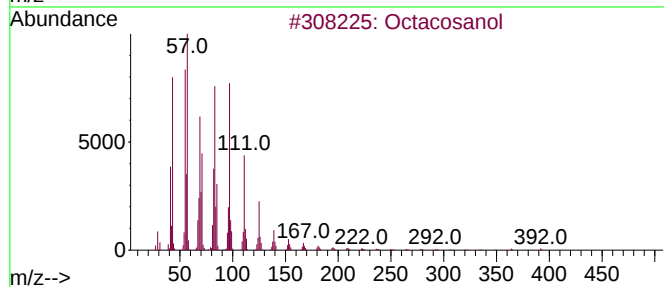
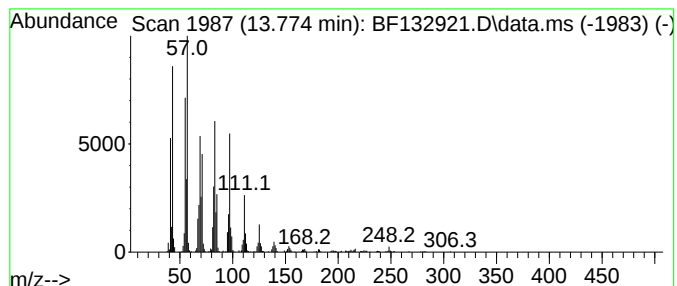
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF041723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octacosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	8.74 ng	906664	Chrysene-d12	13.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosanol	410	C28H58O	000557-61-9	94
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3			17-Pentatriacontene	491	C35H70	006971-40-0	94
4			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
5			Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041923\
Data File : BF132921.D
Acq On : 19 Apr 2023 20:09
Operator : CG\JU
Sample : 02366-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20230335-COMP-13

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF041723.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
(S)-(+)-1,2-Pro...	3.116	2.2	ng	159291	1	6.763	1468980	20.0
2-Pentanone, 4-...	4.957	42.2	ng	3098980	1	6.763	1468980	20.0
2-Pentanone, 4-...	5.769	2.9	ng	209038	1	6.763	1468980	20.0
Benzophenone	10.510	3.2	ng	381434	3	9.798	2352580	20.0
n-Hexadecanoic ...	11.816	5.5	ng	700606	4	11.281	2557650	20.0
Octacosanol	13.774	8.7	ng	906664	5	13.916	2073730	20.0