

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122222\
 Data File : BF131782.D
 Acq On : 22 Dec 2022 18:00
 Operator : CG\JU
 Sample : N6157-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20221418-COMPOSITE-A

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-BF122022.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131782.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.063	501	506	516	rVB	631544	752753	38.36%	4.950%
2	5.469	570	575	578	rBV	1900937	1806612	92.07%	11.881%
3	6.487	742	748	757	rBV	1798891	1863324	94.96%	12.254%
4	6.851	807	810	814	rBV	623701	480281	24.48%	3.158%
5	7.422	902	907	910	rBV	1301866	1169025	59.57%	7.688%
6	8.140	1025	1029	1033	rBV	654928	609915	31.08%	4.011%
7	9.222	1208	1213	1216	rBV	2338132	1962279	100.00%	12.905%
8	9.904	1325	1329	1332	rBV	925705	736246	37.52%	4.842%
9	10.622	1448	1451	1455	rBV	44799	34837	1.78%	0.229%
10	10.698	1459	1464	1467	rBV	1682906	1514562	77.18%	9.960%
11	11.398	1579	1583	1586	rBV	916516	798354	40.69%	5.250%
12	11.922	1668	1672	1676	rBV	102034	91856	4.68%	0.604%
13	12.986	1849	1853	1856	rBV	2295923	1947536	99.25%	12.808%
14	13.892	2001	2007	2023	rBV4	46648	169672	8.65%	1.116%
15	14.045	2029	2033	2037	rVB	803157	677822	34.54%	4.458%
16	14.139	2045	2049	2054	rVB	40191	37196	1.90%	0.245%
17	14.892	2174	2177	2184	rVB	39060	46575	2.37%	0.306%
18	15.533	2281	2286	2297	rVB	410019	507269	25.85%	3.336%

Sum of corrected areas: 15206114

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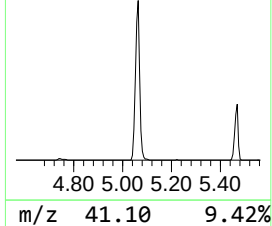
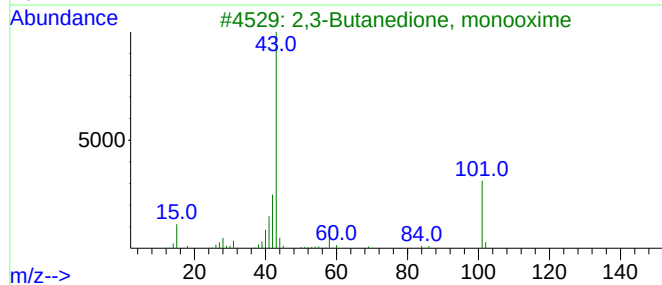
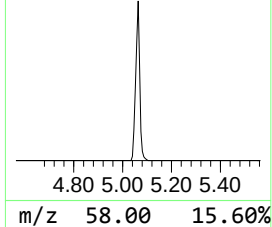
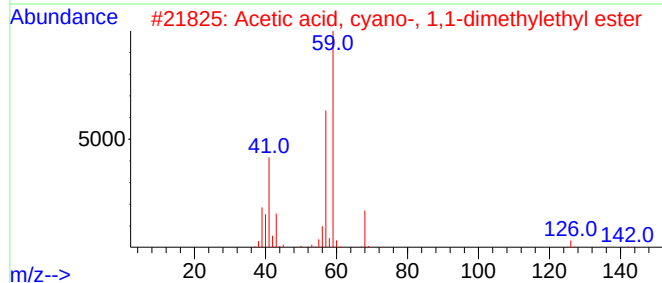
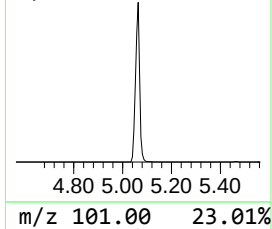
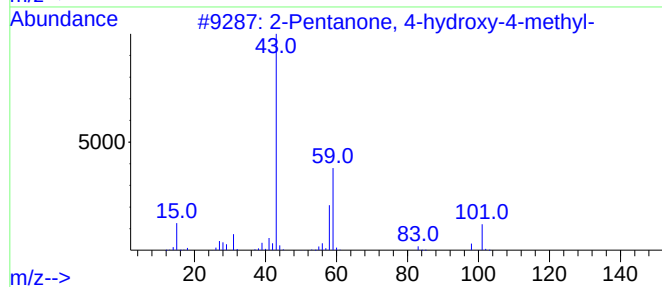
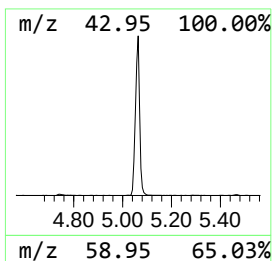
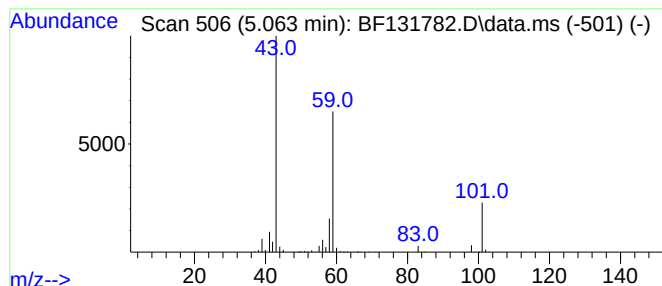
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	31.35 ng	752753	1,4-Dichlorobenzene-d4	6.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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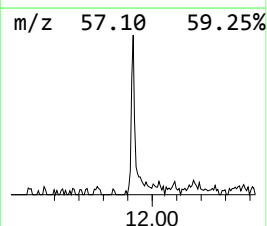
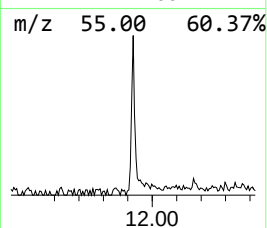
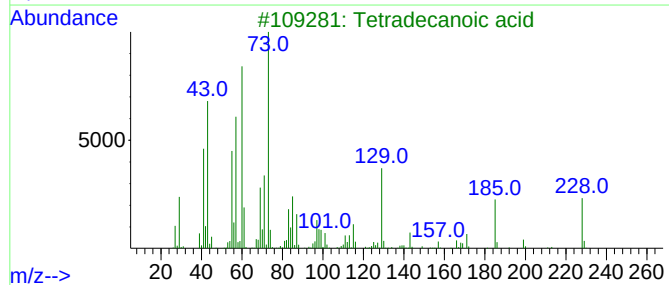
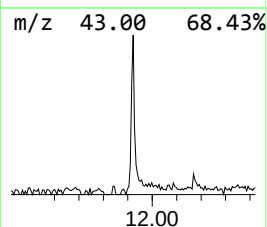
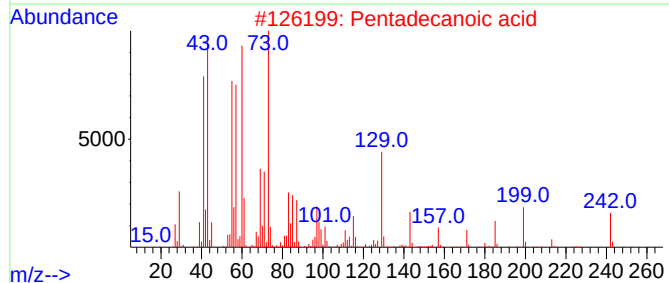
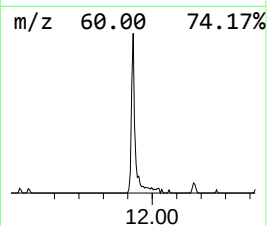
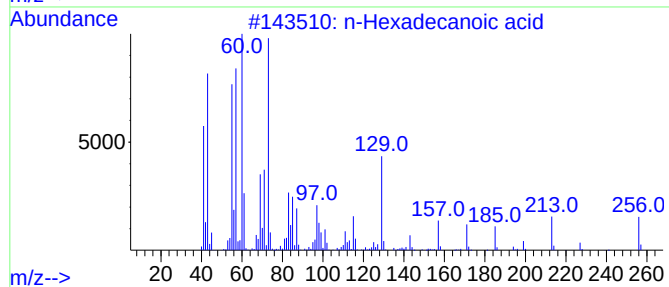
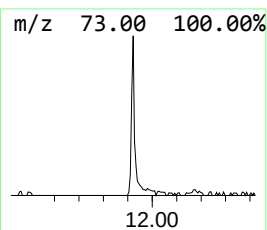
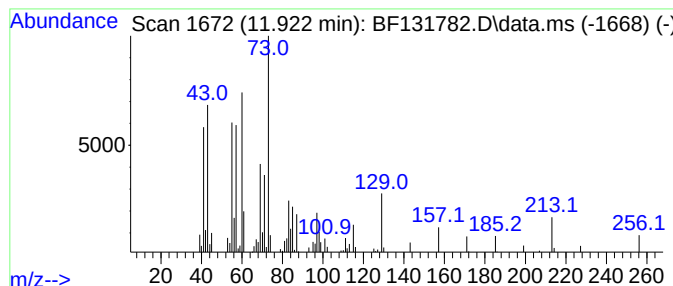
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	2.30 ng	91856	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			Tridecanoic acid	214	C13H26O2	000638-53-9	70
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	43



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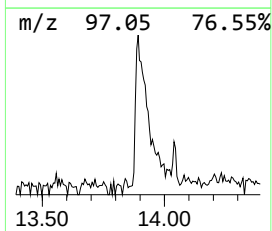
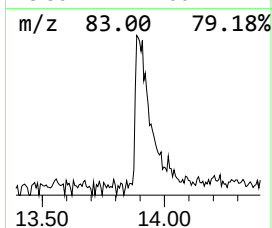
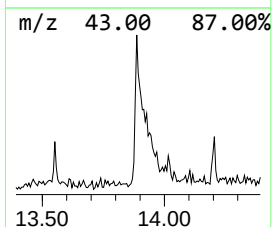
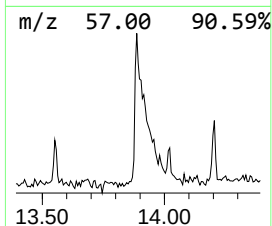
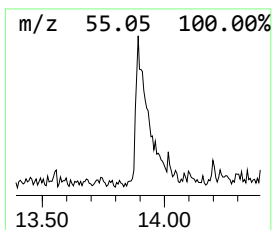
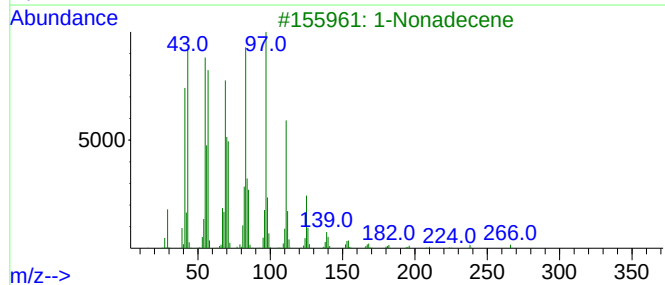
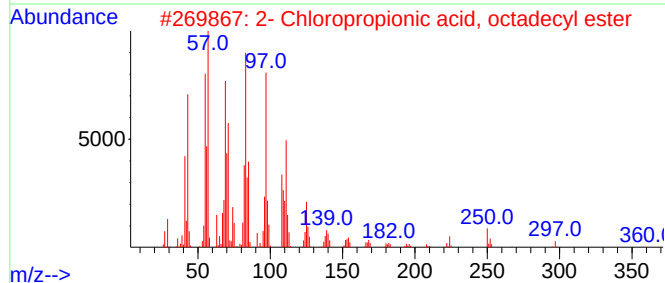
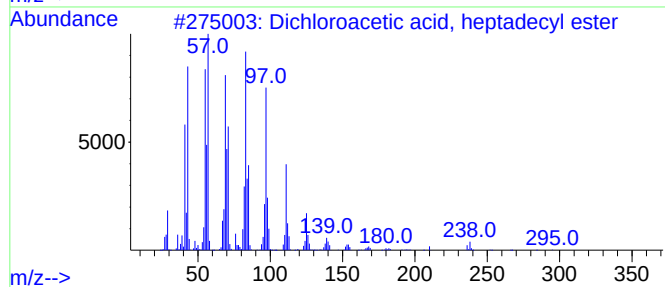
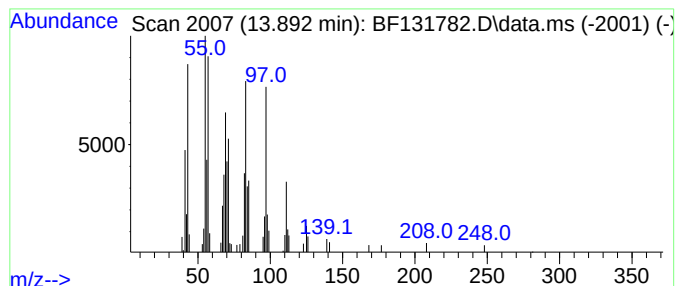
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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Dichloroacetic acid, heptad... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	5.01 ng	169672	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
2			2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
3			1-Nonadecene	266	C19H38	018435-45-5	91
4			Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	91



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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
2-Pentanone, 4-...	5.063	31.4	ng	752753	1	6.851	480281	20.0
n-Hexadecanoic ...	11.922	2.3	ng	91856	4	11.398	798354	20.0
Dichloroacetic ...	13.892	5.0	ng	169672	5	14.045	677822	20.0