

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100923\
 Data File : BF135664.D
 Acq On : 09 Oct 2023 22:12
 Operator : CG\JU
 Sample : 04656-10
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-103I

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-BF091123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135664.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.963	486	489	496	rBV	30357	44349	1.46%	0.287%
2	5.369	556	558	580	rBV	982168	1207580	39.66%	7.804%
3	6.387	728	731	748	rBV	632558	715882	23.51%	4.626%
4	6.740	787	791	800	rVB	649900	608955	20.00%	3.935%
5	7.304	883	887	903	rBV	1881382	1920424	63.07%	12.410%
6	8.016	1005	1008	1016	rBV	936347	790891	25.97%	5.111%
7	9.098	1187	1192	1195	rBV	3494372	3044889	100.00%	19.677%
8	9.775	1303	1307	1315	rVB	1046777	833404	27.37%	5.386%
9	10.575	1439	1443	1457	rBV	1648828	1732981	56.91%	11.199%
10	11.269	1558	1561	1569	rBV	897175	769716	25.28%	4.974%
11	11.804	1649	1652	1660	rBV3	137589	169988	5.58%	1.099%
12	12.375	1747	1749	1754	rVB2	50232	38919	1.28%	0.252%
13	12.598	1784	1787	1801	rBV4	29184	56654	1.86%	0.366%
14	12.869	1828	1833	1836	rBV	2495140	2239296	73.54%	14.471%
15	13.869	1993	2003	2008	rBV7	22414	76355	2.51%	0.493%
16	13.933	2010	2014	2019	rVB	551796	531193	17.45%	3.433%
17	14.769	2152	2156	2162	rBV	76651	83173	2.73%	0.537%
18	15.398	2258	2263	2272	rBV	385769	558283	18.34%	3.608%
19	15.845	2335	2339	2348	rVB2	30178	51301	1.68%	0.332%

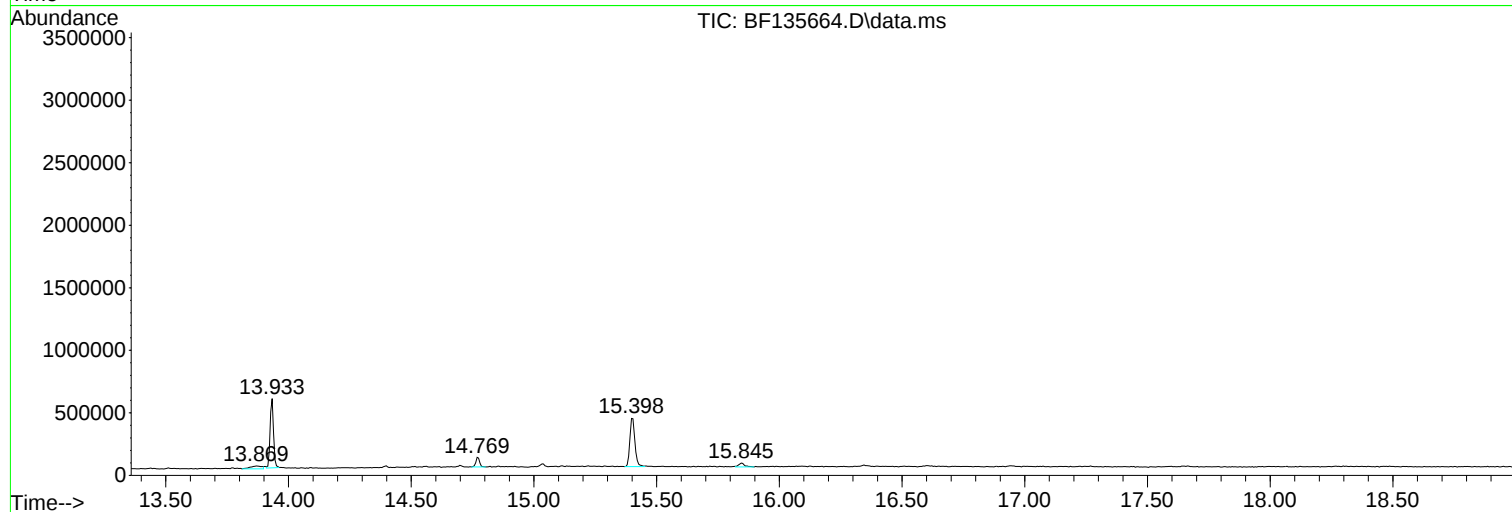
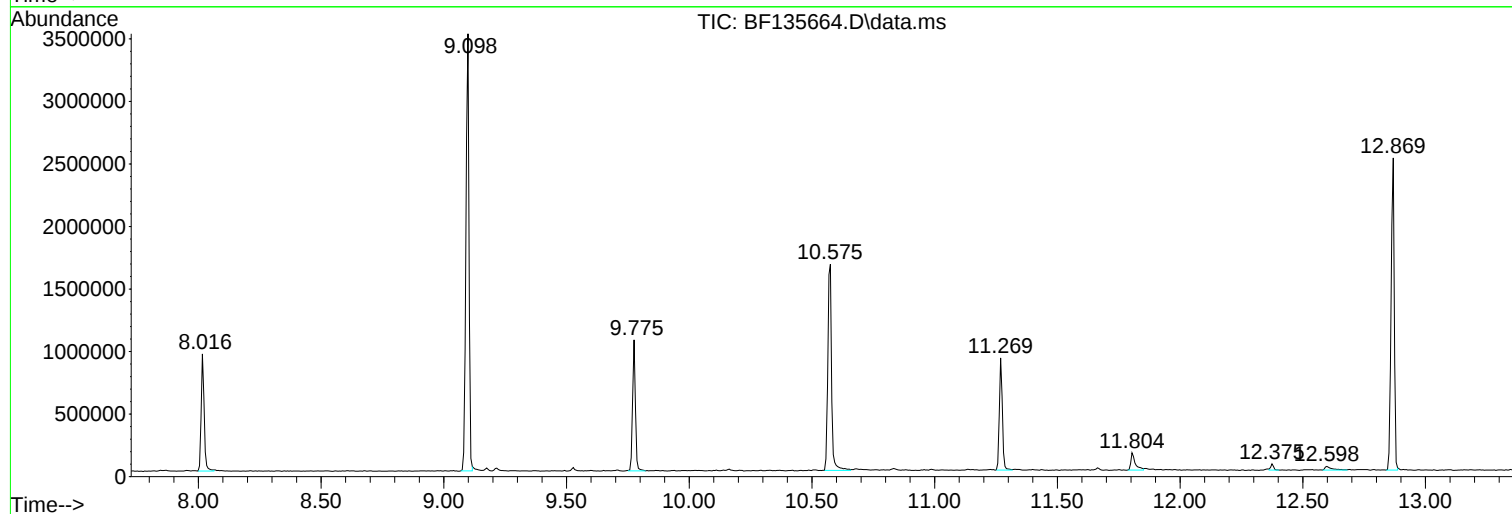
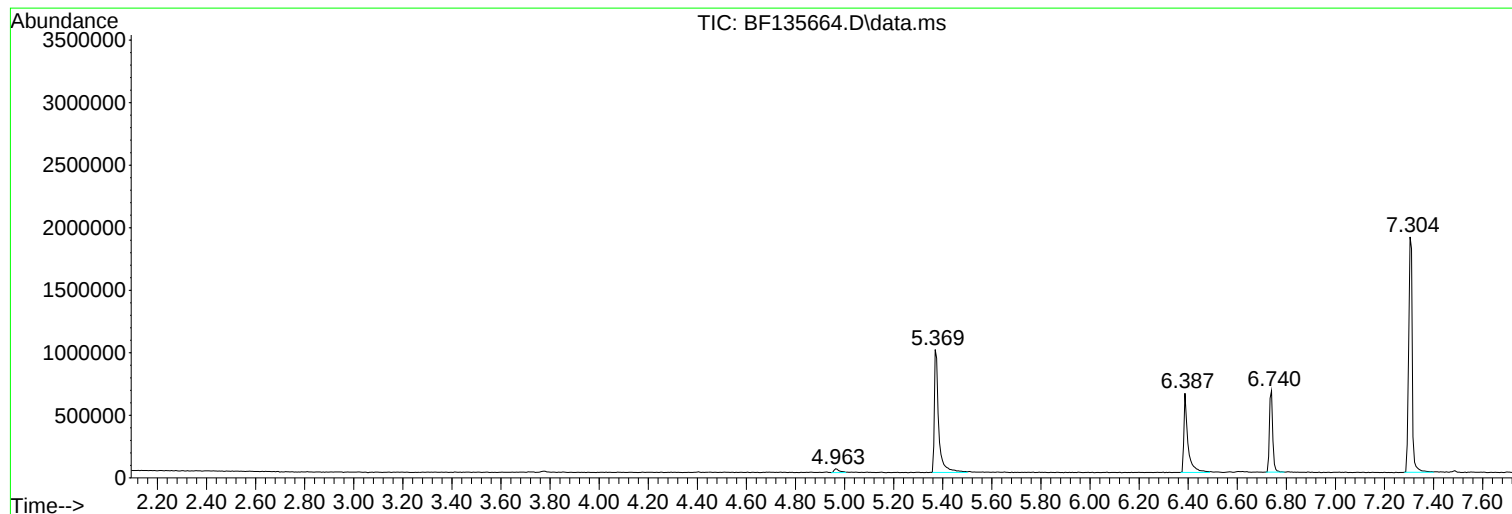
Sum of corrected areas: 15474233

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



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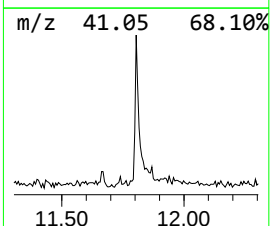
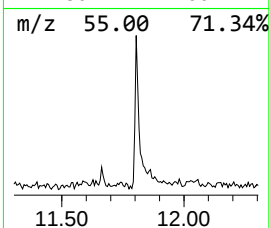
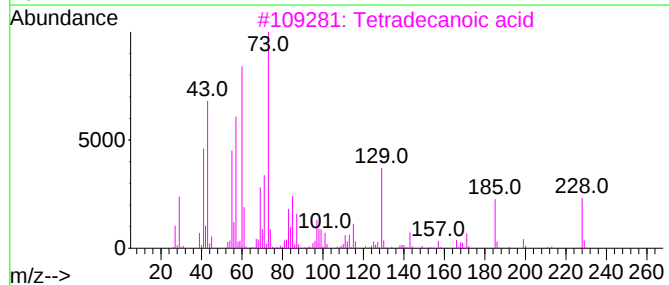
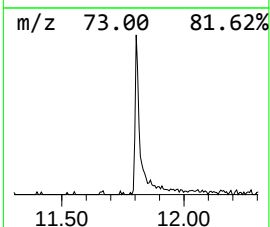
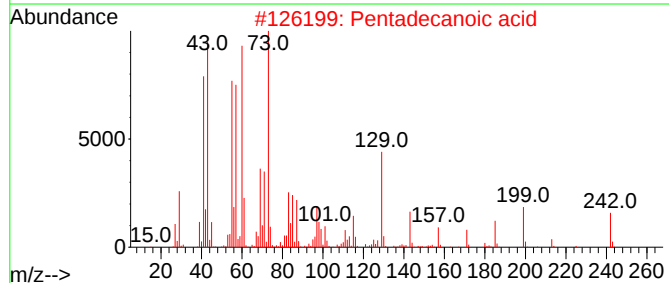
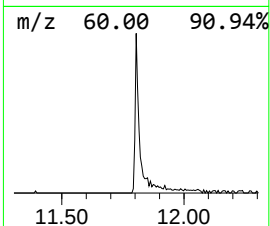
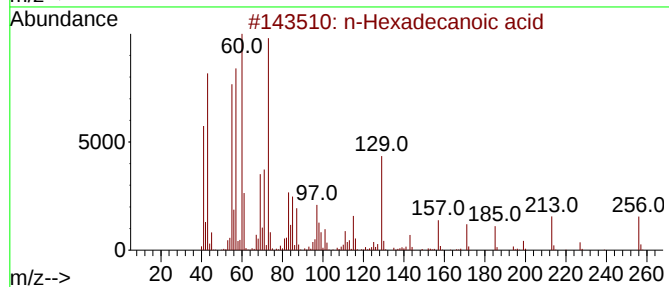
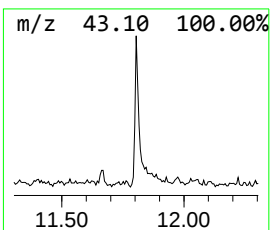
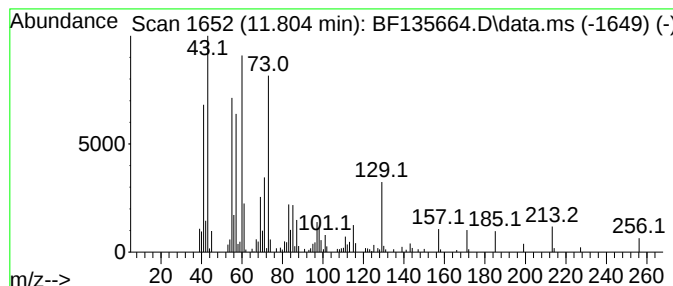
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	4.42 ng	169988	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4			Tridecanoic acid	214	C13H26O2	000638-53-9	64
5			Octanoic acid	144	C8H16O2	000124-07-2	60



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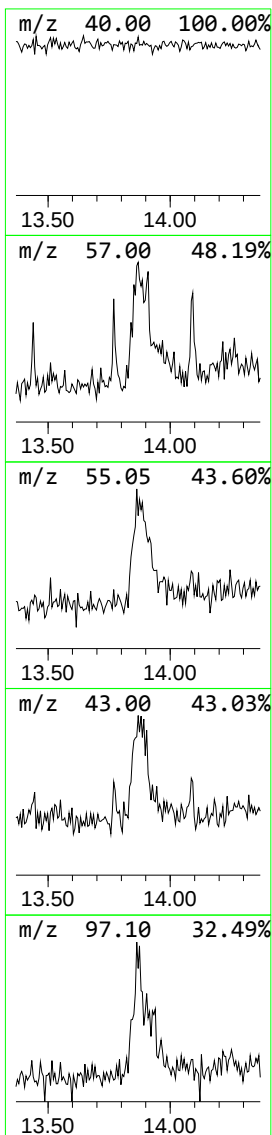
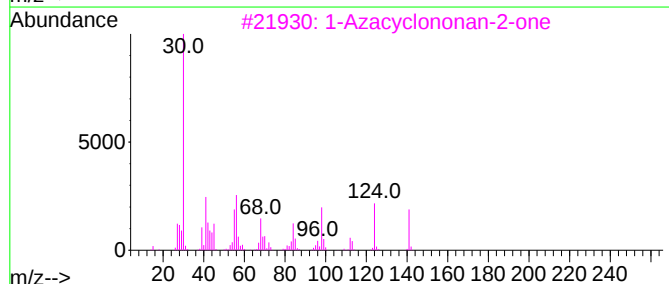
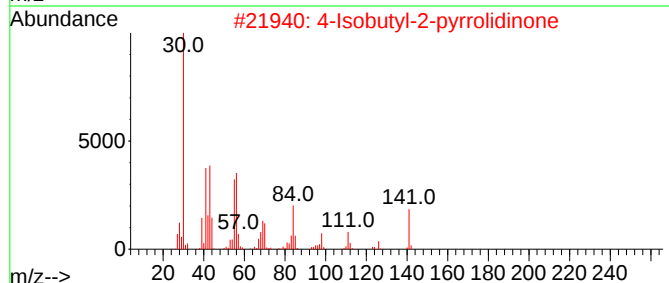
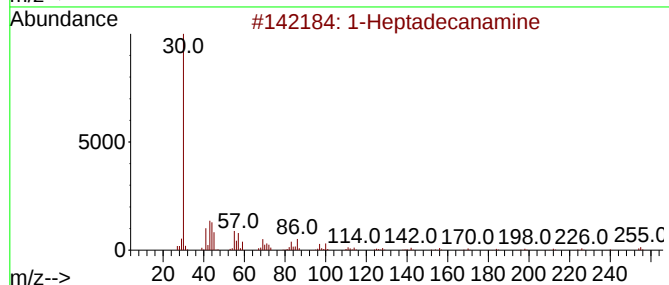
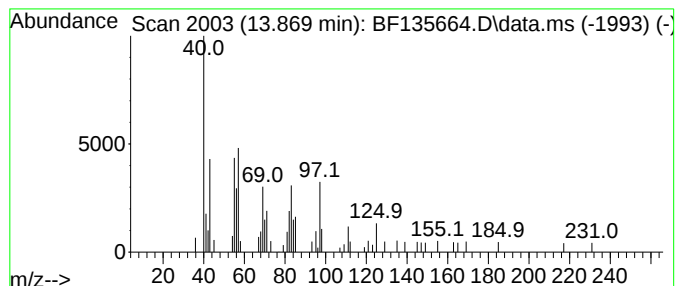
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Peak Number 2 unknown13.869 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.869	2.87 ng	76355	Chrysene-d12	13.933	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptadecanamine	255	C17H37N	004200-95-7	25
2	4-Isobutyl-2-pyrrolidinone	141	C8H15NO	061312-87-6	9
3	1-Azacyclononan-2-one	141	C8H15NO	000935-30-8	9
4	(2-Piperidin-3-ylethyl)amine	128	C7H16N2	089850-94-2	9
5	Spermine	202	C10H26N4	000071-44-3	9



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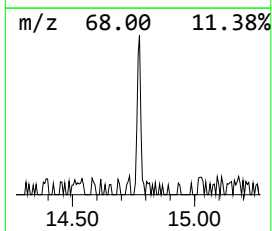
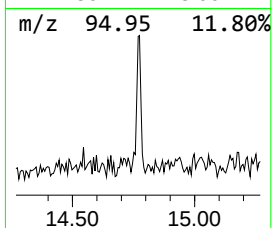
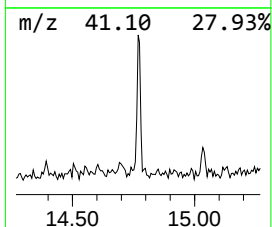
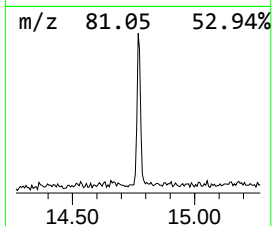
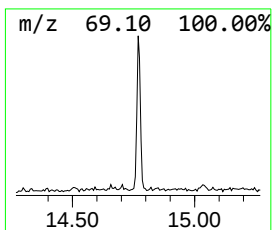
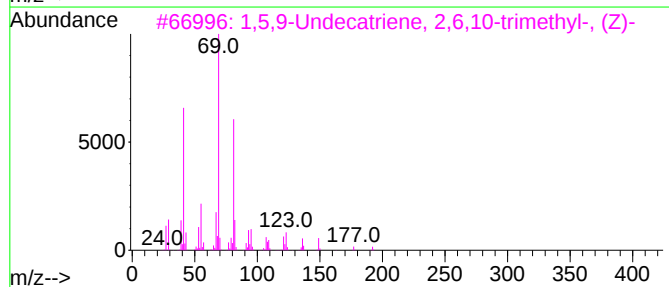
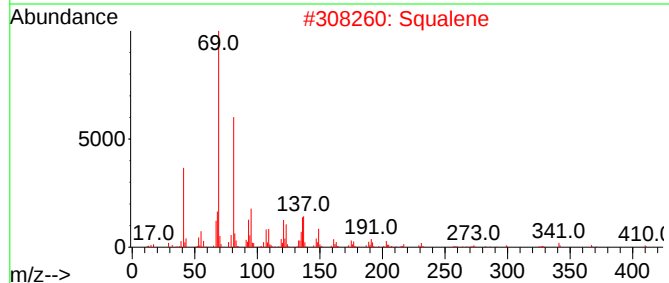
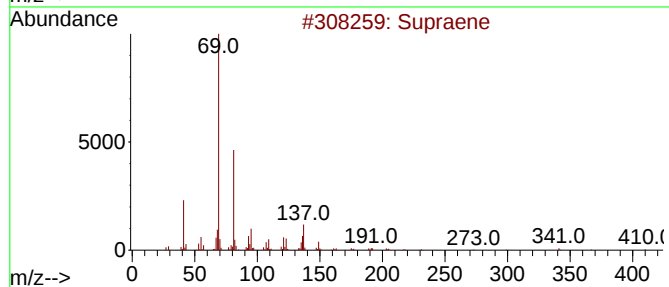
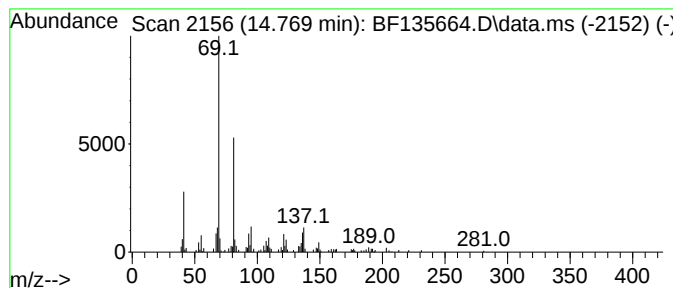
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Peak Number 3 Supraene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.769	2.98 ng	83173	Perylene-d12	15.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			Squalene	410	C30H50	000111-02-4	90
3			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	83
4			.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
5			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	11.804	4.4	ng	169988	4	11.269	769716	20.0
unknown13.869	13.869	2.9	ng	76355	5	13.933	531193	20.0
Supraene	14.769	3.0	ng	83173	6	15.398	558283	20.0