

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012023\
 Data File : BF132181.D
 Acq On : 21 Jan 2023 02:00
 Operator : CG\JU
 Sample : 01233-09
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-P38B

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-BF011923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132181.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.343	421	426	434	rVB	1568508	2039502	36.97%	5.126%
2	5.719	484	490	493	rBV	4442300	4843037	87.79%	12.173%
3	6.701	649	657	660	rBV	4100132	4936752	89.49%	12.408%
4	6.913	690	693	697	rBV	79819	69604	1.26%	0.175%
5	7.090	719	723	726	rVB	1316939	1066915	19.34%	2.682%
6	7.401	774	776	782	rVB2	43765	57793	1.05%	0.145%
7	7.654	808	819	822	rBV	3300795	3304240	59.90%	8.305%
8	8.372	938	941	945	rBV	1427277	1301704	23.60%	3.272%
9	9.454	1119	1125	1128	rBV	5802014	5220834	94.64%	13.122%
10	10.136	1238	1241	1245	rVB	1636105	1505042	27.28%	3.783%
11	10.854	1360	1363	1366	rBV	606620	444667	8.06%	1.118%
12	10.936	1372	1377	1380	rBV	3845985	3906821	70.82%	9.819%
13	11.031	1389	1393	1398	rVB	63637	55752	1.01%	0.140%
14	11.636	1492	1496	1500	rBV	1898232	1611171	29.21%	4.050%
15	12.148	1579	1583	1588	rBV	327144	321205	5.82%	0.807%
16	12.807	1691	1695	1698	rBV	1006245	749918	13.59%	1.885%
17	12.936	1714	1717	1725	rBV	88790	87689	1.59%	0.220%
18	13.236	1763	1768	1771	rBV	5692779	5516472	100.00%	13.865%
19	14.124	1915	1919	1940	rBV	94197	320805	5.82%	0.806%
20	14.301	1945	1949	1952	rBV	1338665	1223405	22.18%	3.075%
21	15.189	2096	2100	2108	rVB	166282	173779	3.15%	0.437%
22	15.895	2214	2220	2231	rVB	762500	1029325	18.66%	2.587%

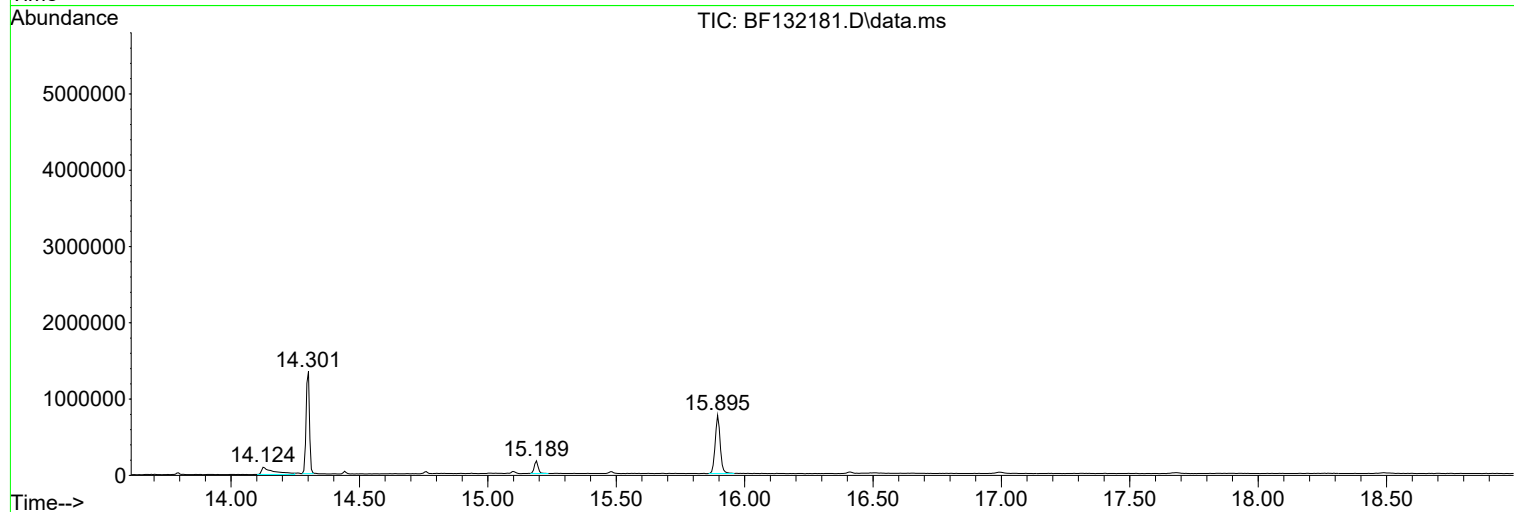
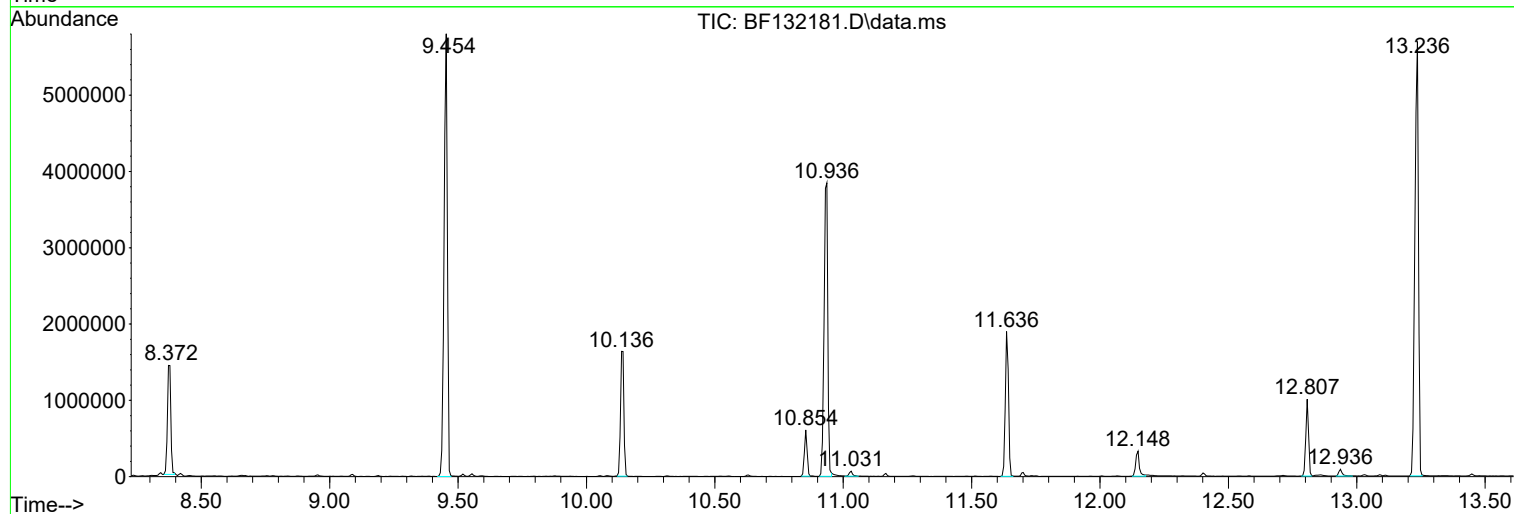
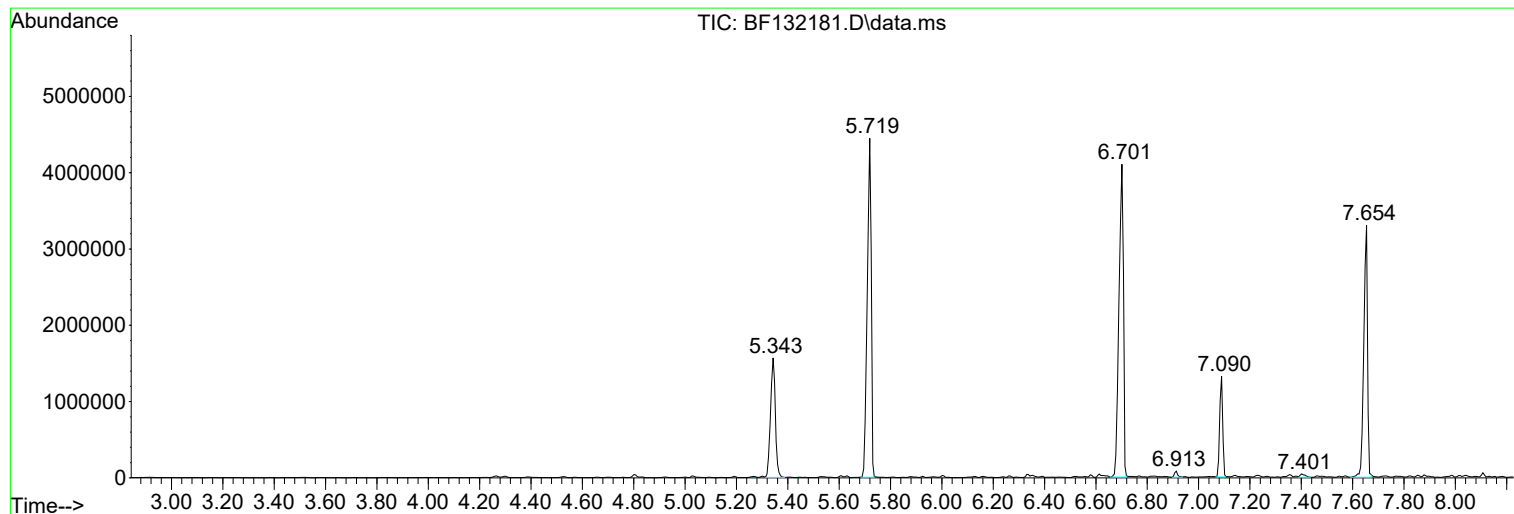
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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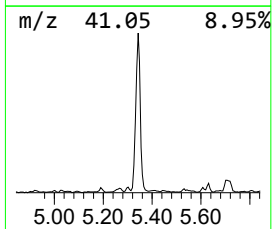
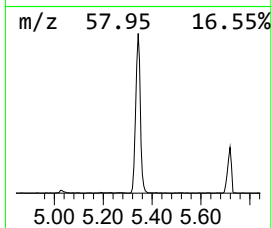
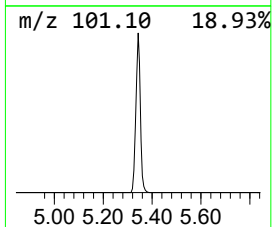
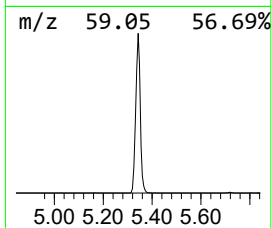
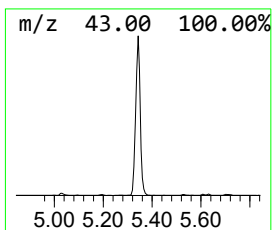
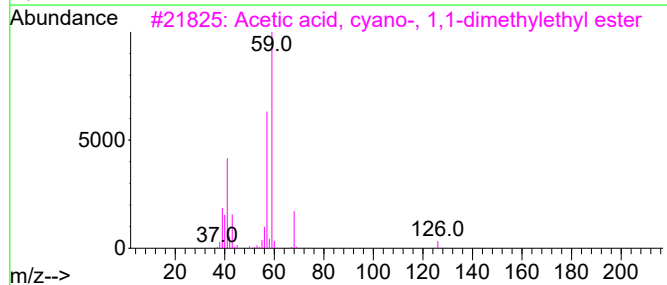
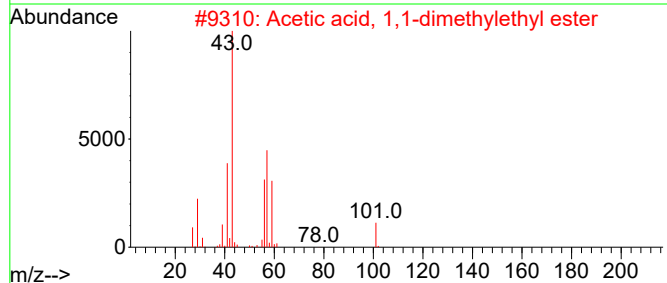
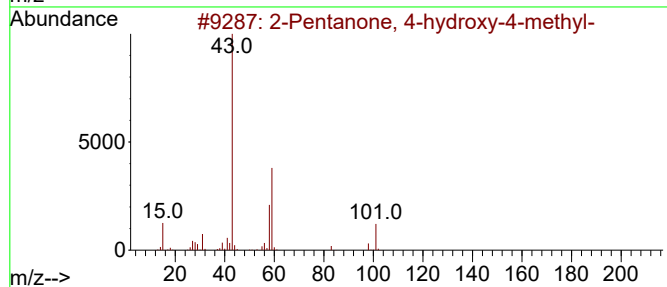
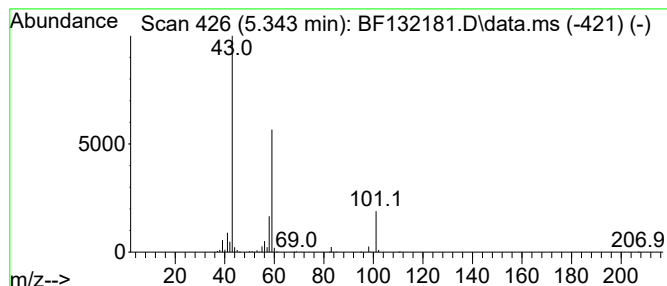
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.343	38.23 ng	2039500	1,4-Dichlorobenzene-d4	7.090

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
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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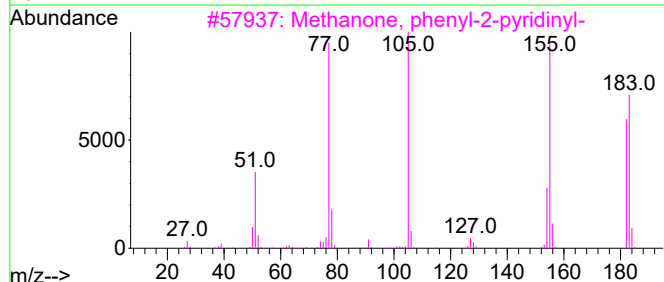
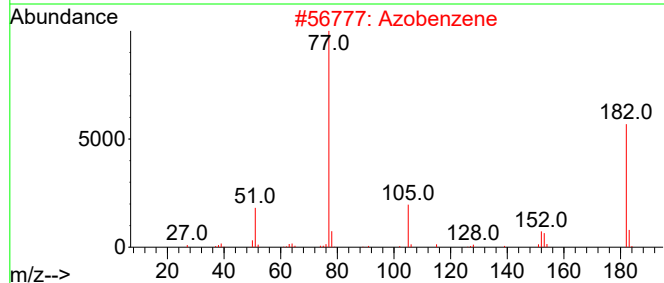
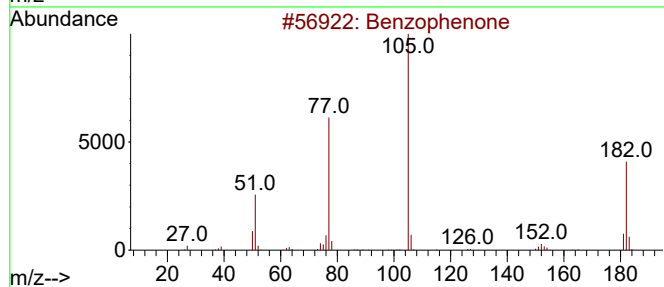
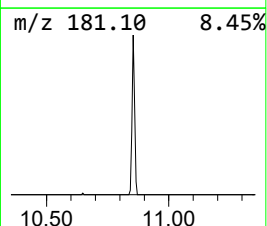
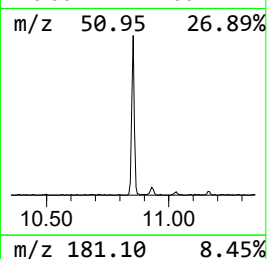
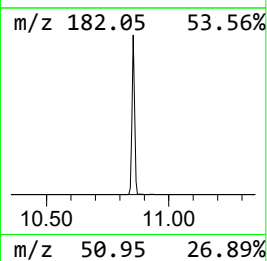
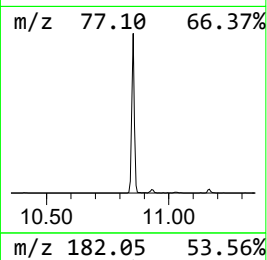
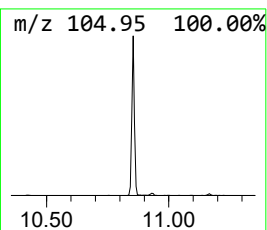
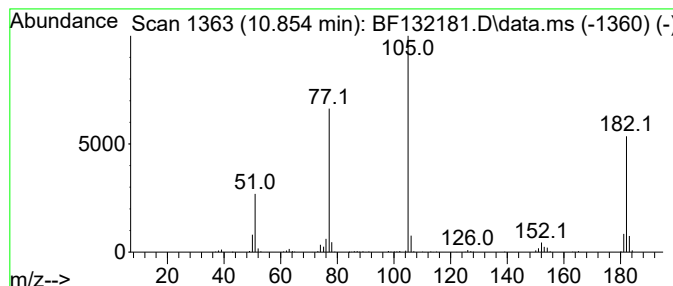
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Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.854	5.91 ng	444667	Acenaphthene-d10	10.142

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	72
3			Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	72
4			Azobenzene, (E)-	182	C12H10N2	017082-12-1	50
5			N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	47



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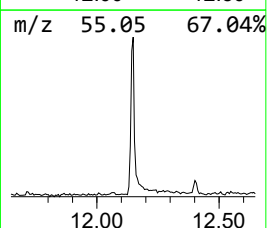
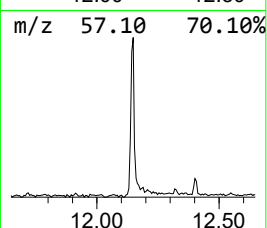
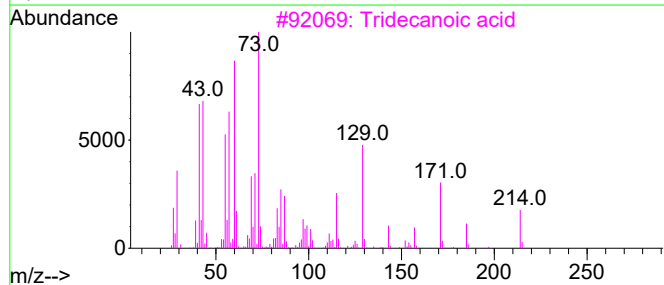
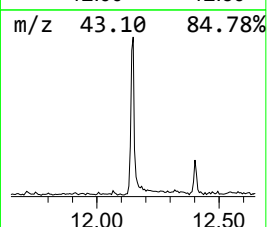
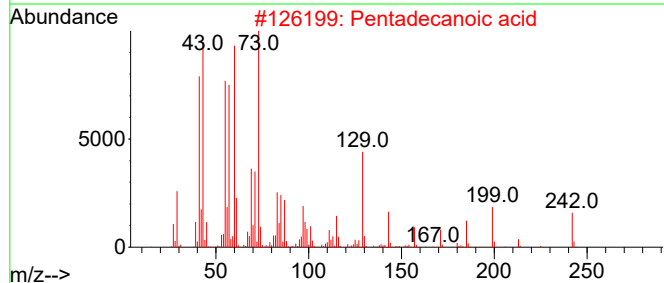
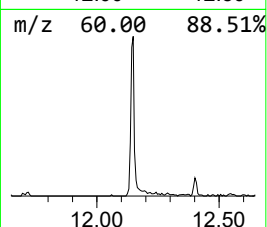
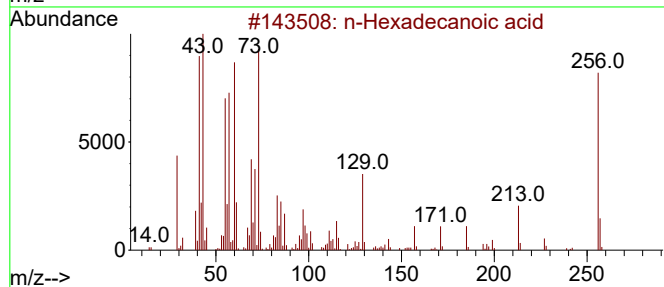
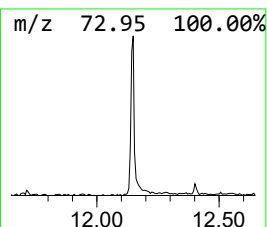
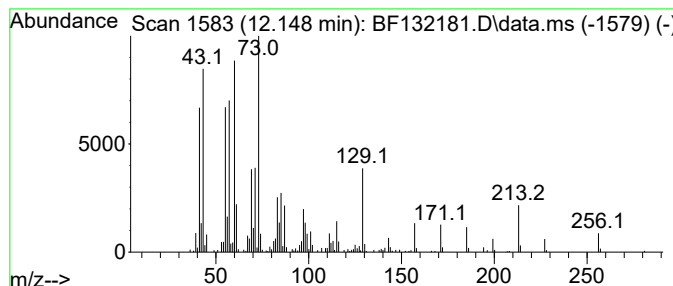
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.148	3.99 ng	321205	Phenanthrene-d10	11.636

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	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5			n-Decanoic acid	172	C10H20O2	000334-48-5	68



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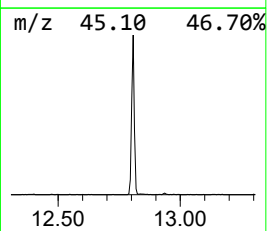
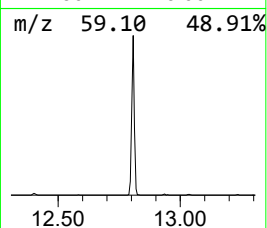
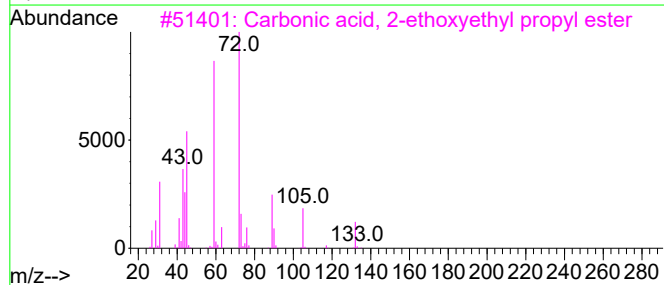
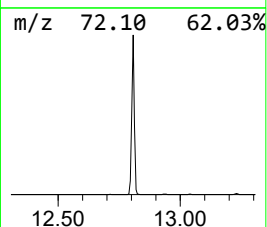
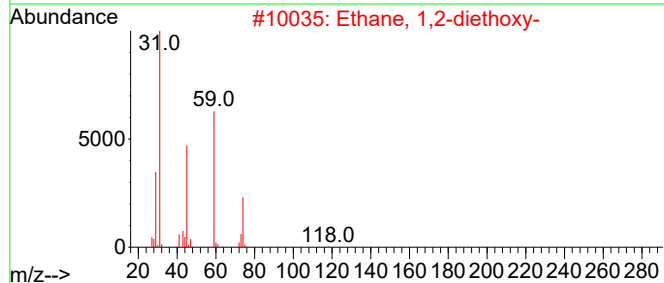
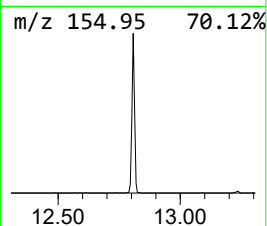
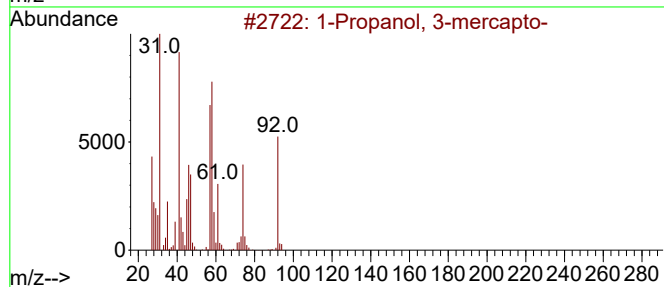
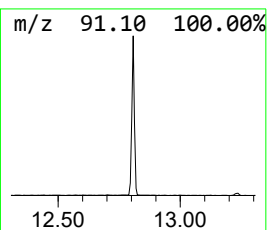
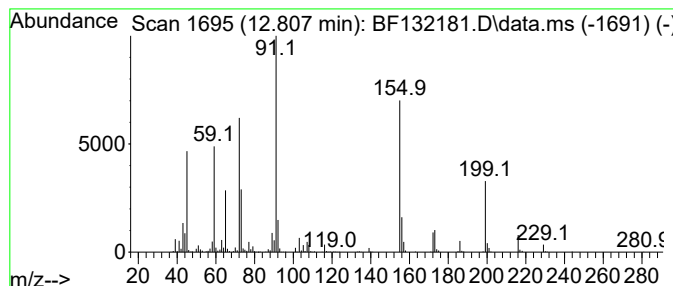
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Peak Number 4 unknown12.807 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.807	9.31 ng	749918	Phenanthrene-d10	11.636

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Propanol, 3-mercapto-	92	C3H8OS	019721-22-3	22
2			Ethane, 1,2-diethoxy-	118	C6H14O2	000629-14-1	22
3			Carbonic acid, 2-ethoxyethyl pro...	176	C8H16O4	1000331-38-4	14
4			Urea, N,N-dimethyl-N'-octyl-	200	C11H24N2O	1000419-88-6	14
5			(2S)-Glycidyl tosylate	228	C10H12O4S	070987-78-9	11



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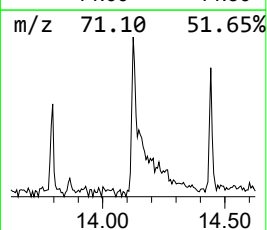
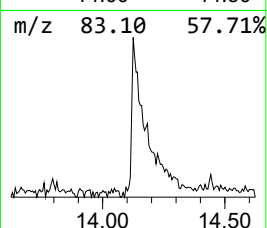
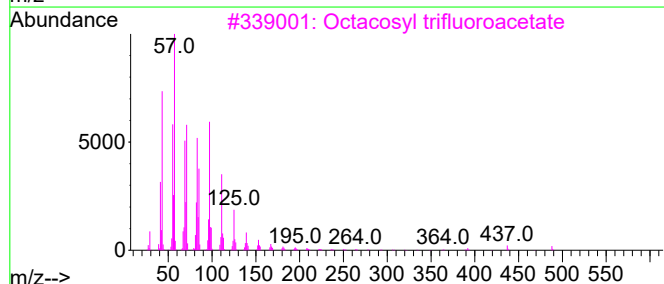
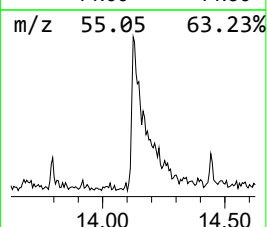
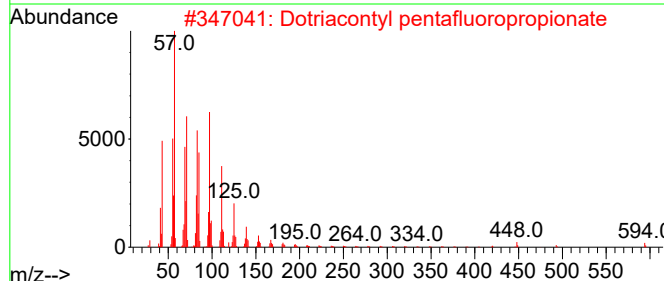
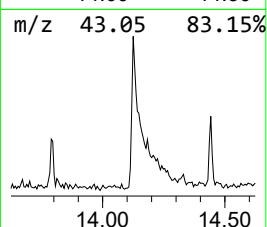
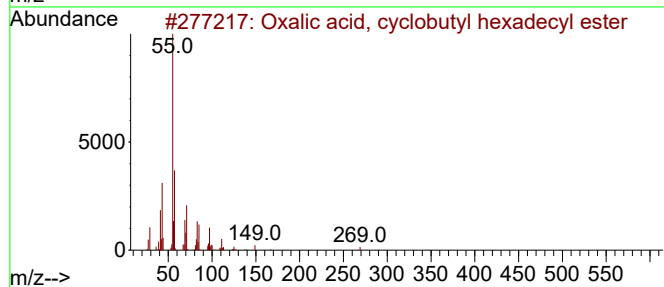
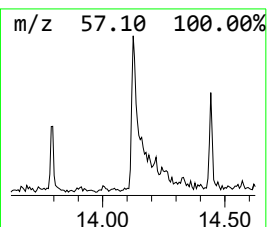
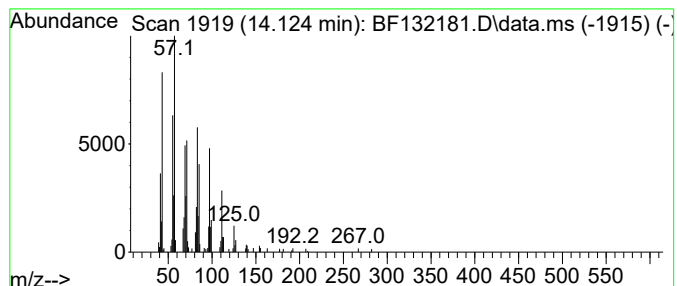
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Peak Number 5 Oxalic acid, cyclobutyl hex... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.124	5.24 ng	320805	Chrysene-d12	14.301

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, cyclobutyl hexadecy...	368	C22H40O4	1000309-70-6	91
2			Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1010351-81-4	91
3			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
4			Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
5			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87



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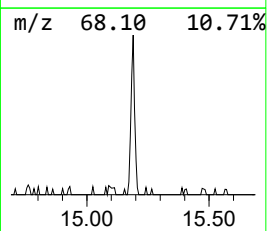
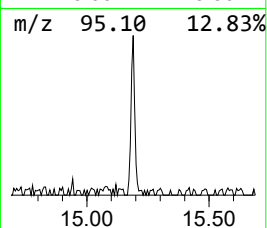
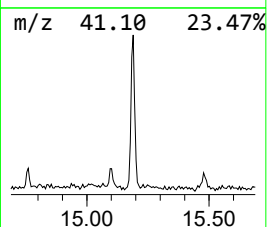
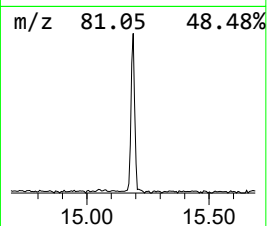
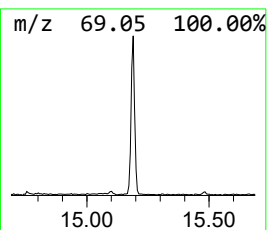
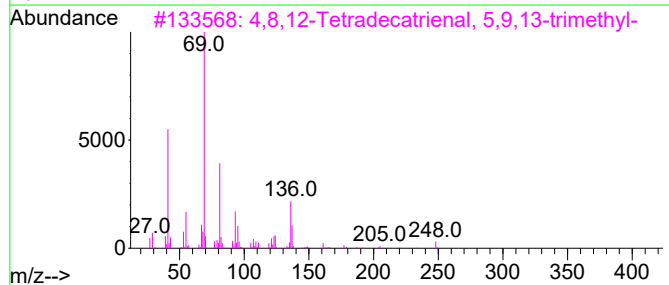
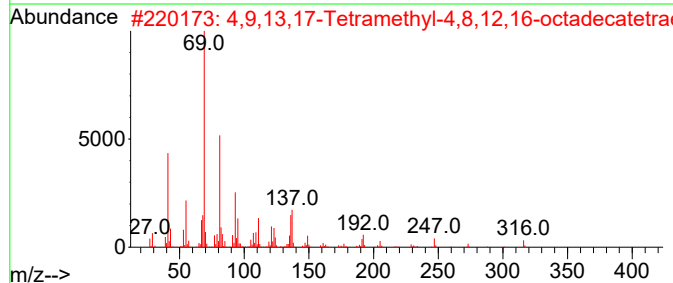
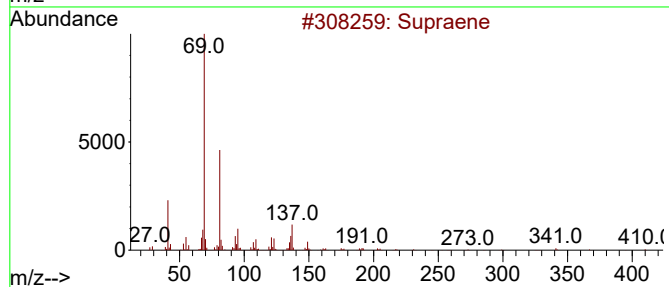
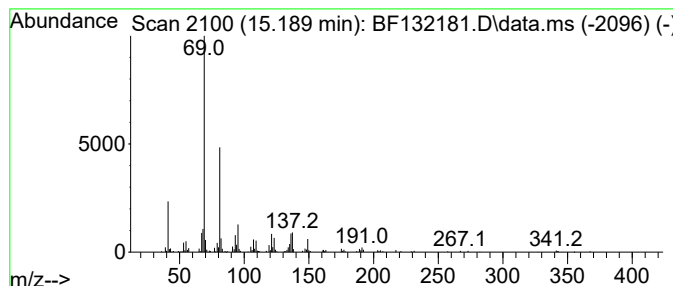
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.189	3.38 ng	173779	Perylene-d12	15.895

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	87
2			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
3			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
4			4,8,12-Tetradecatrienenitrile, 5-...	245	C17H27N	005981-31-7	64
5			1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012023\
Data File : BF132181.D
Acq On : 21 Jan 2023 02:00
Operator : CG\JU
Sample : 01233-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-P38B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.343	38.2	ng	2039500	1	7.090	1066920	20.0
Benzophenone	10.854	5.9	ng	444667	3	10.142	1505040	20.0
n-Hexadecanoic ...	12.148	4.0	ng	321205	4	11.636	1611170	20.0
unknown12.807	12.807	9.3	ng	749918	4	11.636	1611170	20.0
Oxalic acid, cy...	14.124	5.2	ng	320805	5	14.301	1223410	20.0
Supraene	15.189	3.4	ng	173779	6	15.895	1029330	20.0