

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092222\
 Data File : BF130376.D
 Acq On : 22 Sep 2022 15:10
 Operator : CG\JU
 Sample : N4732-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-1

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-BF091422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130376.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.863	469	472	482	rVB	76854	115202	2.56%	0.390%
2	5.269	535	541	544	rBV	3709911	3929716	87.34%	13.287%
3	6.298	710	716	719	rBV	3387490	3953194	87.86%	13.366%
4	6.651	772	776	780	rBV	1148903	917117	20.38%	3.101%
5	7.222	867	873	876	rBV	2535779	2634344	58.55%	8.907%
6	7.933	989	994	998	rBV	1403657	1243686	27.64%	4.205%
7	9.016	1172	1178	1181	rBV	5002102	4499245	100.00%	15.213%
8	9.686	1284	1292	1295	rBV	1643951	1298393	28.86%	4.390%
9	10.474	1420	1426	1429	rBV	2976198	2567073	57.06%	8.680%
10	10.598	1444	1447	1455	rVB2	34428	51497	1.14%	0.174%
11	11.168	1540	1544	1546	rBV	1155474	1061678	23.60%	3.590%
12	11.186	1546	1547	1551	rVB	188667	131678	2.93%	0.445%
13	11.239	1551	1556	1560	rVB	64159	55649	1.24%	0.188%
14	11.704	1630	1635	1639	rBV2	205784	252421	5.61%	0.853%
15	12.374	1745	1749	1752	rVB	318385	265093	5.89%	0.896%
16	12.492	1763	1769	1772	rBV4	43469	71587	1.59%	0.242%
17	12.598	1782	1787	1791	rBV	261172	271198	6.03%	0.917%
18	12.757	1809	1814	1817	rBV	3432307	2960069	65.79%	10.009%
19	13.233	1891	1895	1898	rBV	239661	203793	4.53%	0.689%
20	13.798	1986	1991	1994	rBV2	927088	969115	21.54%	3.277%
21	13.821	1994	1995	1998	rVV	133806	79148	1.76%	0.268%
22	13.886	2002	2006	2013	rBV2	119675	194418	4.32%	0.657%
23	14.562	2118	2121	2129	rBV5	30741	74232	1.65%	0.251%
24	14.798	2158	2161	2168	rVB	152029	255281	5.67%	0.863%
25	15.074	2205	2208	2213	rVB	83647	97920	2.18%	0.331%
26	15.127	2214	2217	2221	rBV	105339	124794	2.77%	0.422%
27	15.192	2223	2228	2231	rBV	612116	702689	15.62%	2.376%
28	16.215	2399	2402	2410	rVB4	40936	73174	1.63%	0.247%
29	16.509	2449	2452	2461	rVB2	52570	96360	2.14%	0.326%
30	16.909	2516	2520	2529	rVB2	39619	70774	1.57%	0.239%
31	18.915	2852	2861	2870	rVB6	123689	354877	7.89%	1.200%

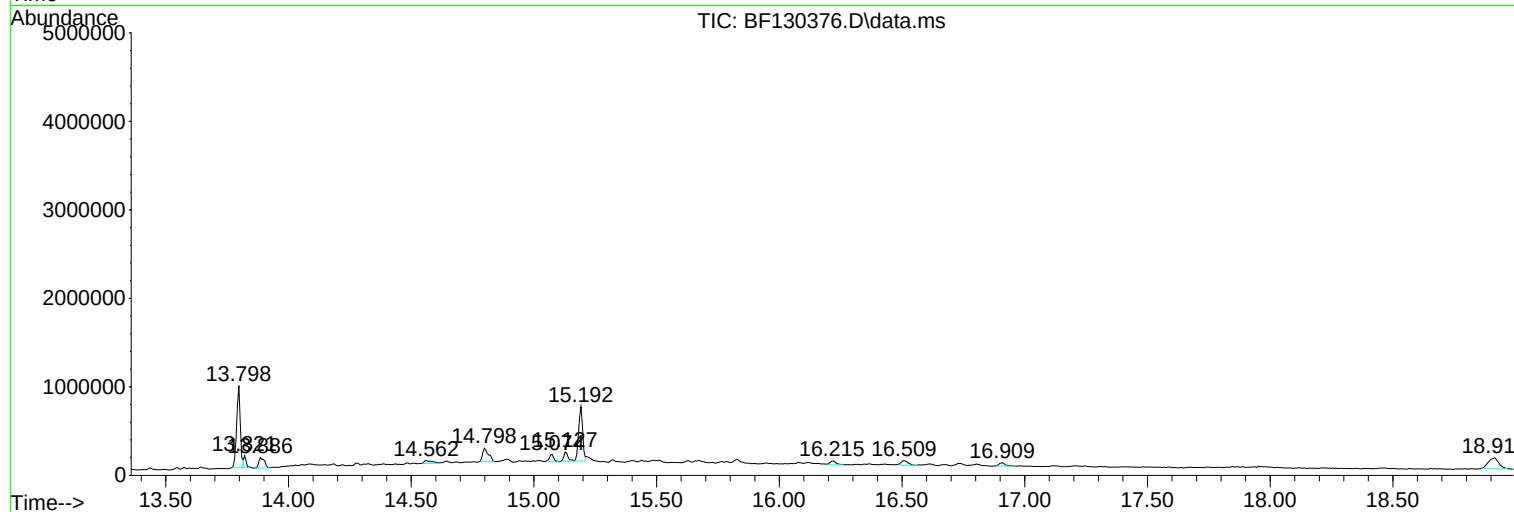
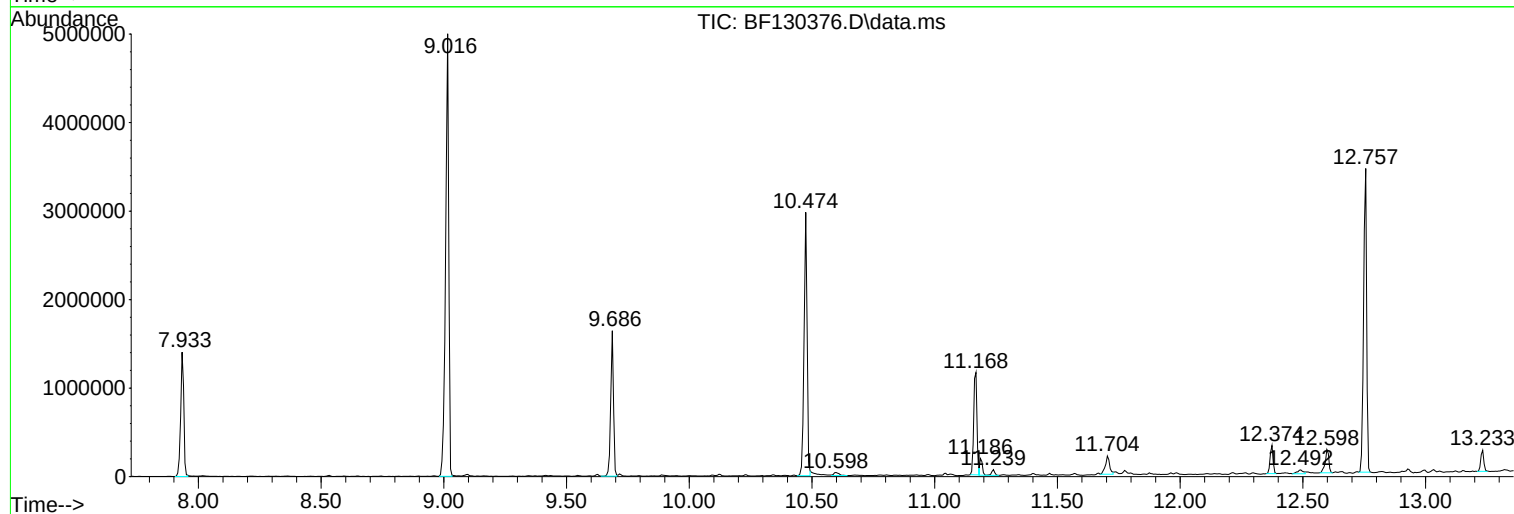
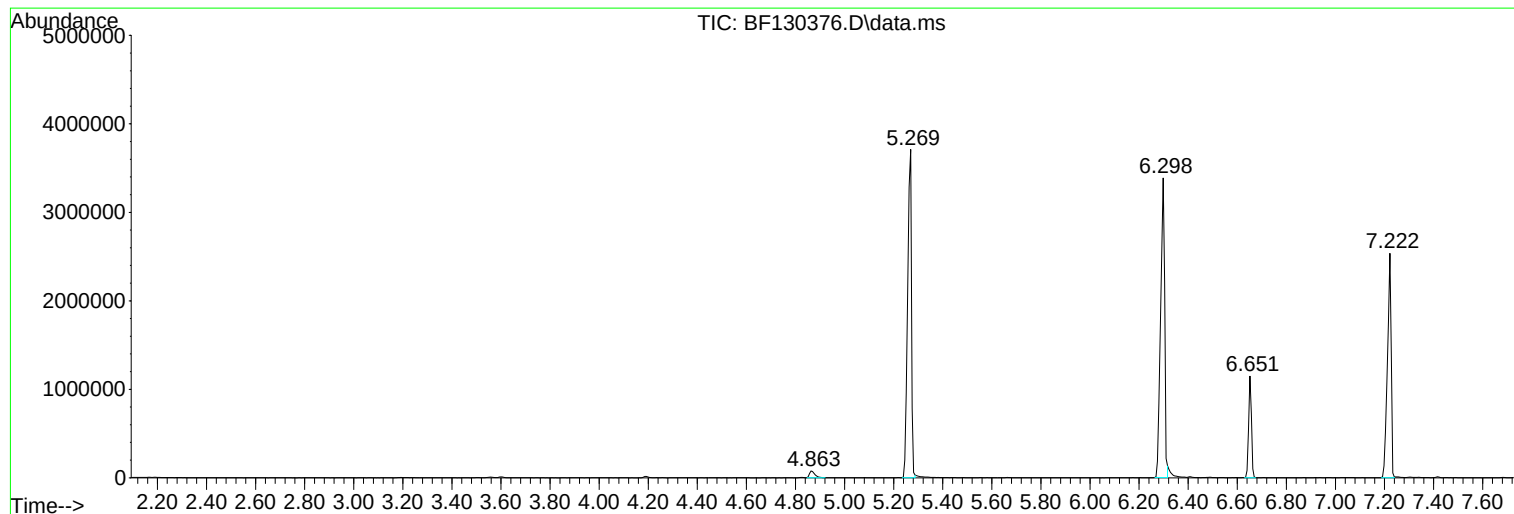
Sum of corrected areas: 29575415

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092222\
Data File : BF130376.D
Acq On : 22 Sep 2022 15:10
Operator : CG\JU
Sample : N4732-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092222\
Data File : BF130376.D
Acq On : 22 Sep 2022 15:10
Operator : CG\JU
Sample : N4732-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

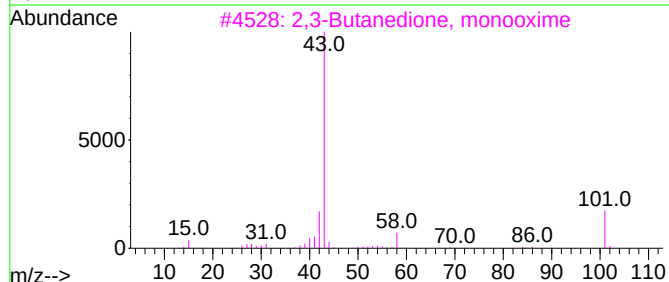
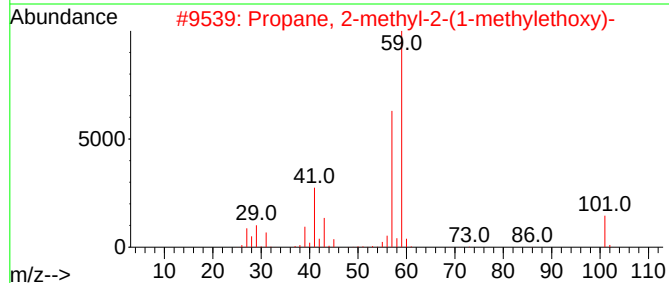
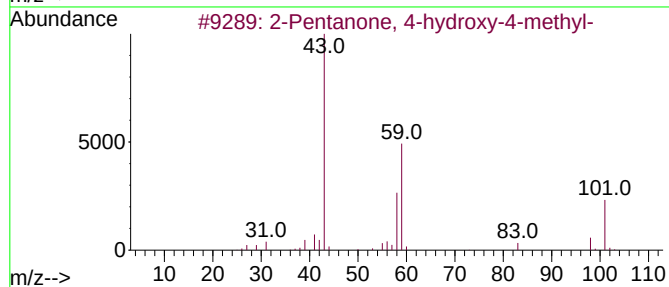
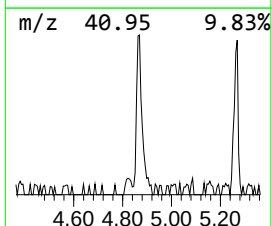
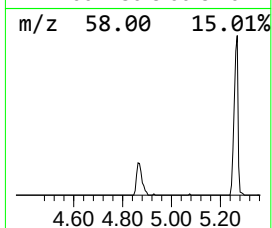
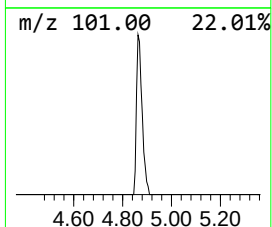
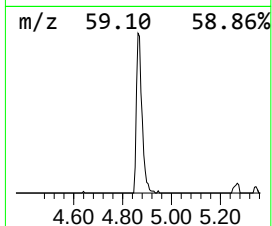
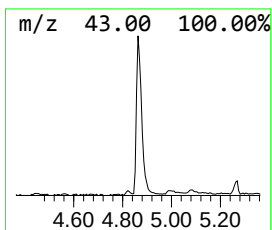
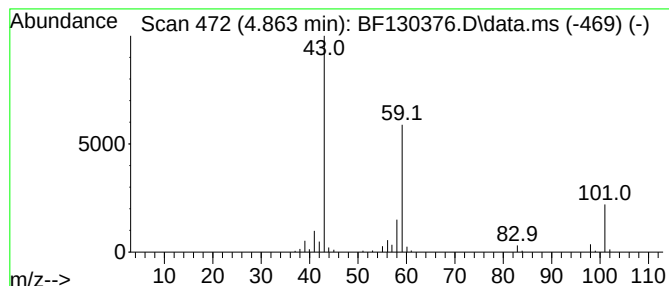
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.863	2.51 ng	115202	1,4-Dichlorobenzene-d4	6.651

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	40
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092222\
Data File : BF130376.D
Acq On : 22 Sep 2022 15:10
Operator : CG\JU
Sample : N4732-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

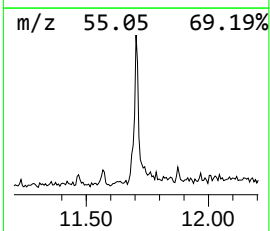
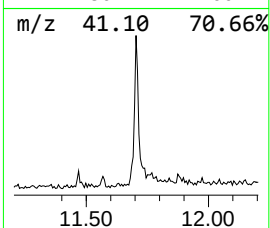
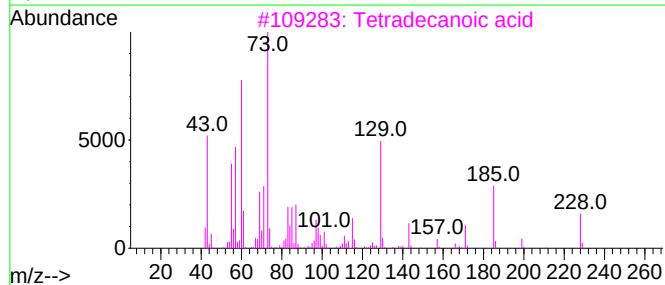
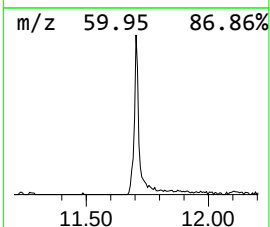
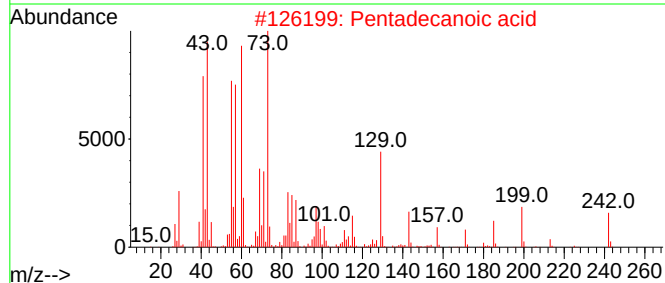
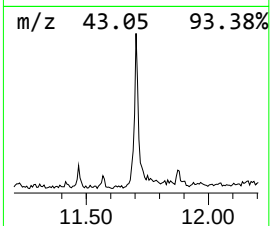
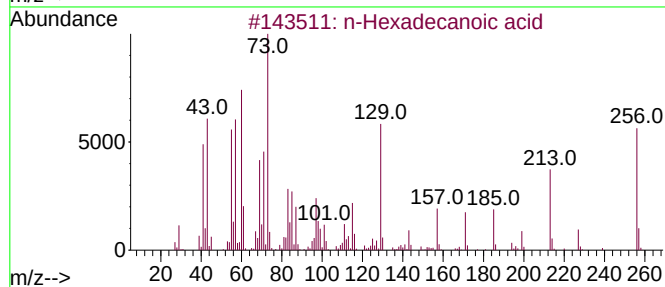
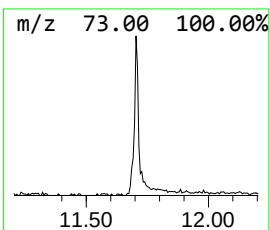
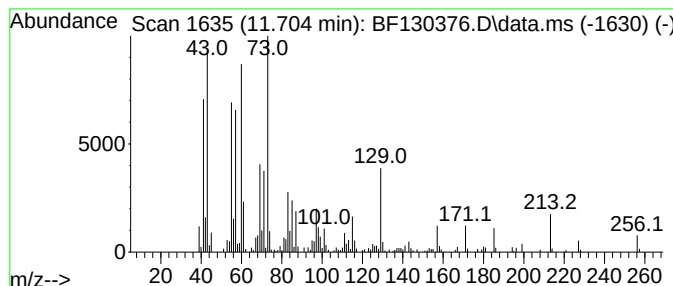
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.704	4.76 ng	252421	Phenanthrene-d10	11.168

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			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4			Tridecanoic acid	214	C13H26O2	000638-53-9	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092222\
Data File : BF130376.D
Acq On : 22 Sep 2022 15:10
Operator : CG\JU
Sample : N4732-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

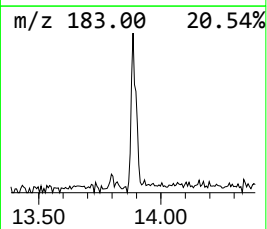
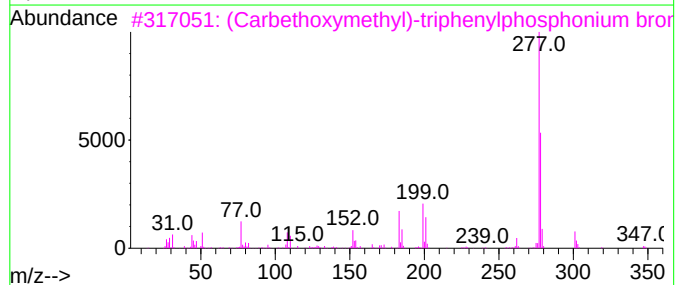
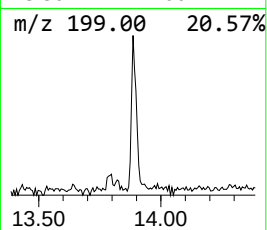
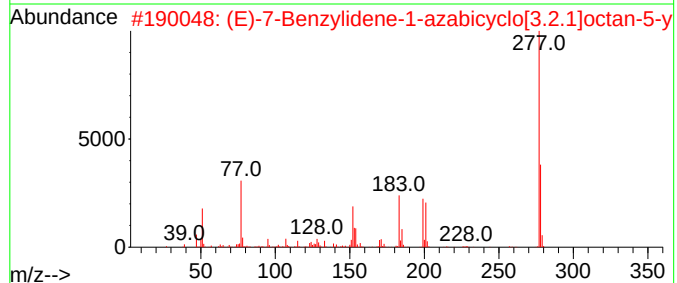
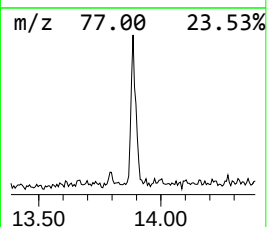
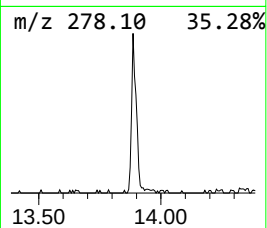
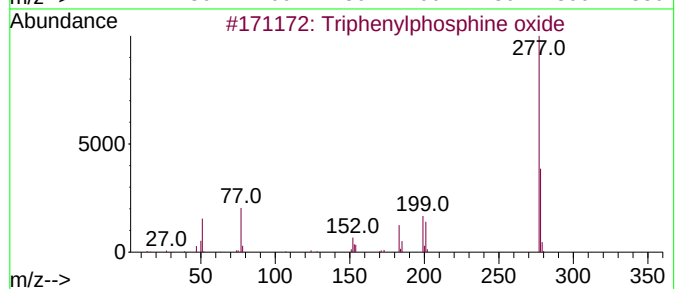
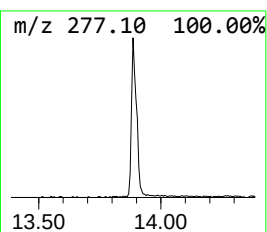
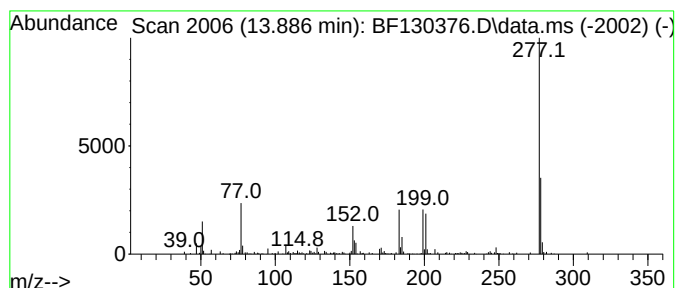
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	4.01 ng	194418	Chrysene-d12	13.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	91
3			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	40
4			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	32
5			1H-Indole-3-acetic acid, 5-[(tri...	277	C14H19N03Si	072101-35-0	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092222\
Data File : BF130376.D
Acq On : 22 Sep 2022 15:10
Operator : CG\JU
Sample : N4732-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

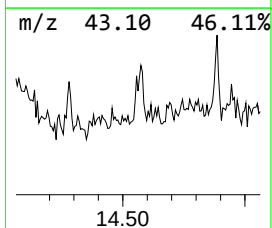
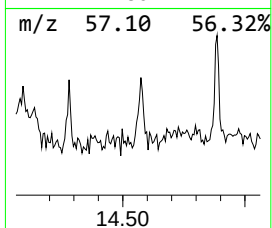
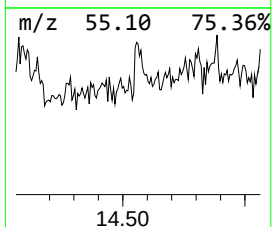
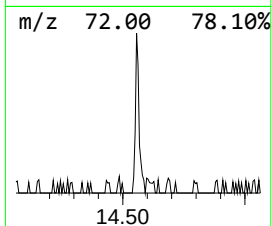
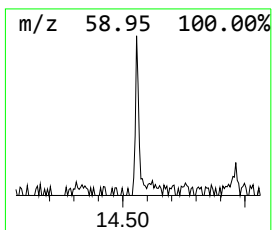
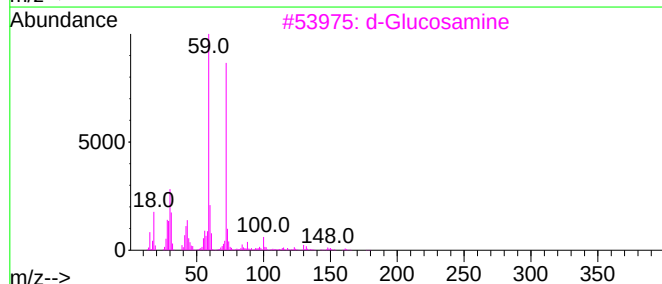
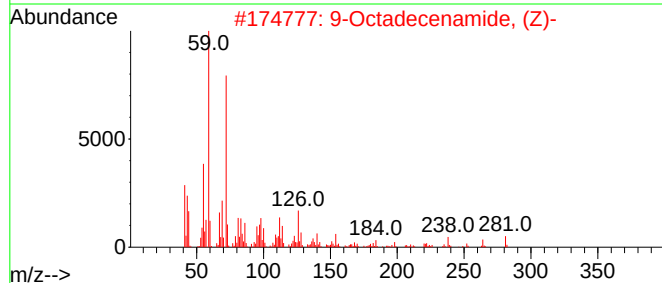
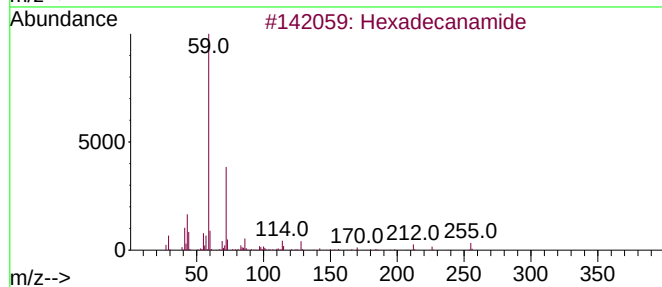
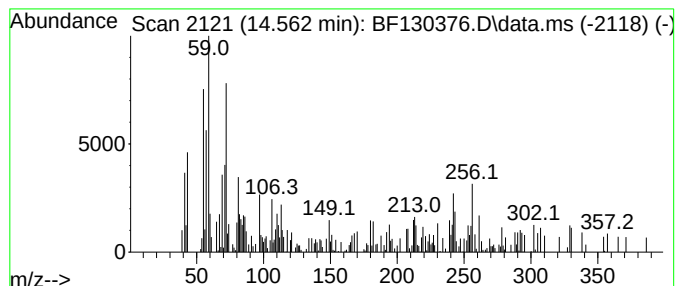
Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexadecanamide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.562	2.11 ng	74232	Perylene-d12	15.192	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanamide	255	C16H33NO	000629-54-9	58
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	52
3	d-Glucosamine	179	C6H13NO5	000090-77-7	50
4	Pentanamide	101	C5H11NO	000626-97-1	43
5	Decanamide-	171	C10H21NO	002319-29-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092222\
Data File : BF130376.D
Acq On : 22 Sep 2022 15:10
Operator : CG\JU
Sample : N4732-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

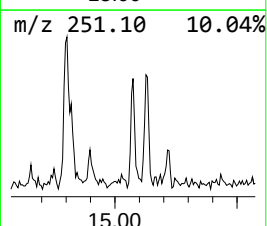
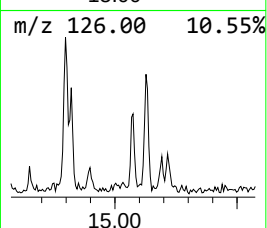
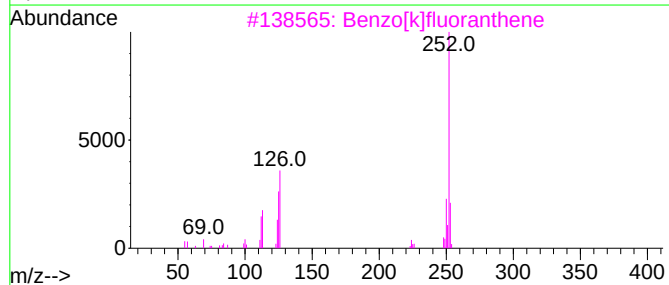
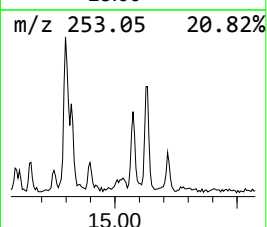
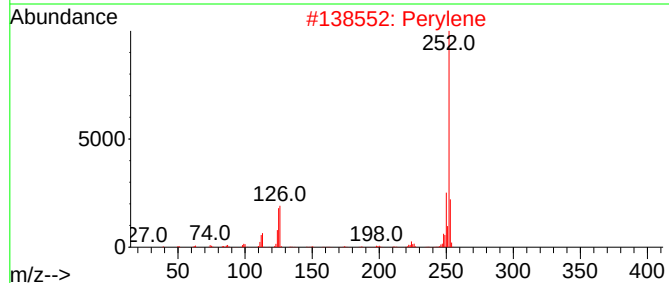
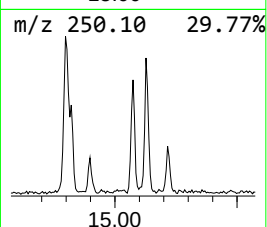
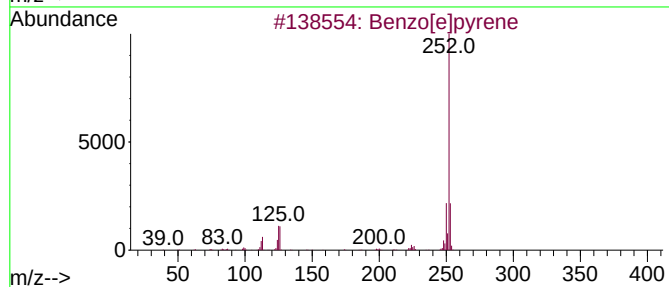
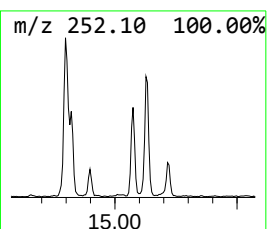
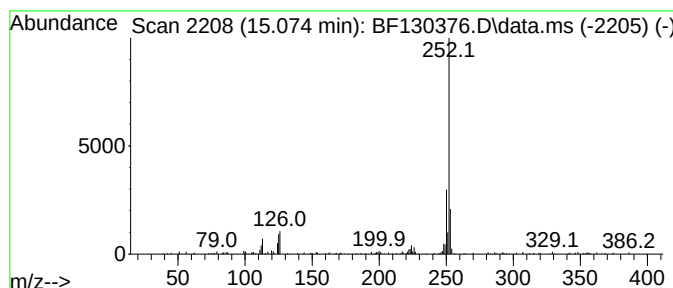
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.074	2.79 ng	97920	Perylene-d12	15.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	98
2			Perylene	252	C20H12	000198-55-0	94
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
4			Benzo[j]fluoranthene	252	C20H12	000205-82-3	94
5			Benzo[b]fluoranthene	252	C20H12	000205-99-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092222\
Data File : BF130376.D
Acq On : 22 Sep 2022 15:10
Operator : CG\JU
Sample : N4732-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

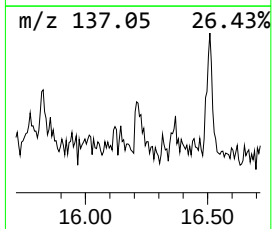
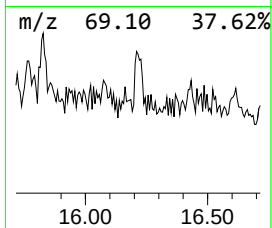
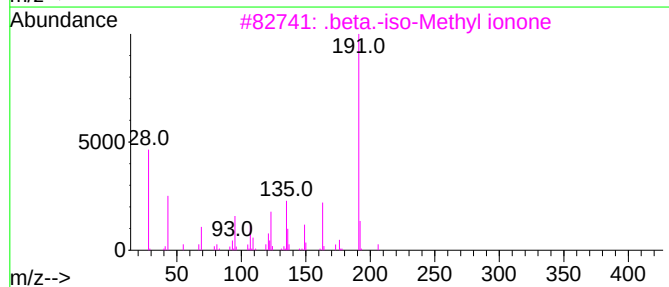
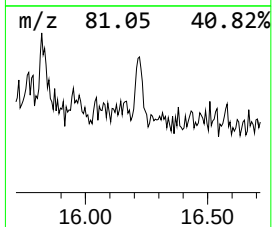
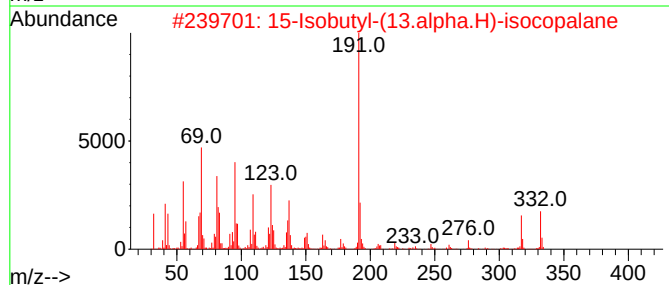
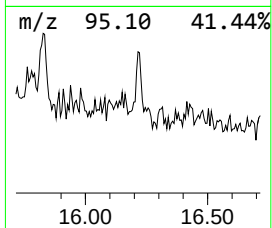
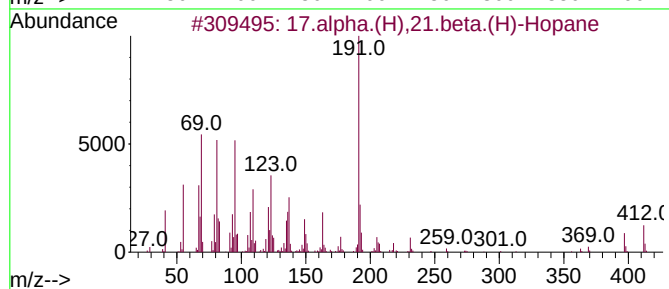
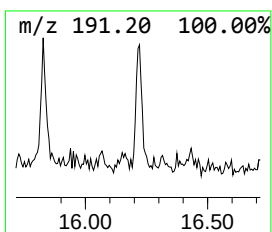
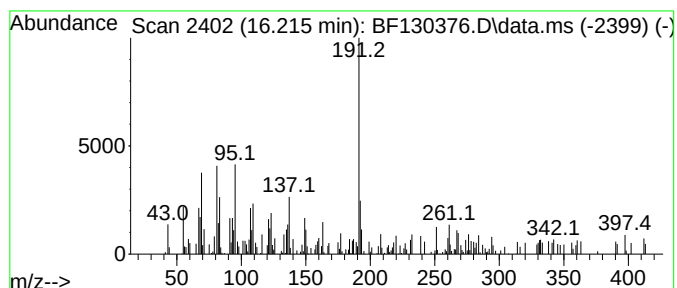
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 17.alpha.(H),21.beta.(H)-Ho... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.215	2.08 ng	73174	Perylene-d12	15.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17.alpha.(H),21.beta.(H)-Hopane	412	C30H52	013849-96-2	80
2			15-Isobutyl-(13.alpha.H)-isocopa...	332	C24H44	087953-47-7	76
3			.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	58
4			5-Amino-1,3,6-trimethyl-1,3-dihy...	191	C10H13N3O	073778-94-6	52
5			1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092222\
Data File : BF130376.D
Acq On : 22 Sep 2022 15:10
Operator : CG\JU
Sample : N4732-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

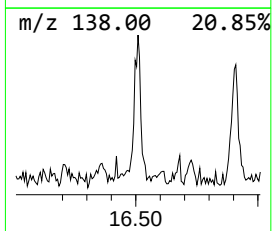
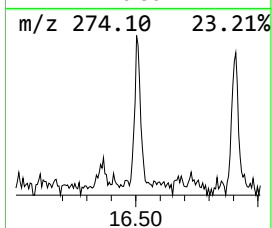
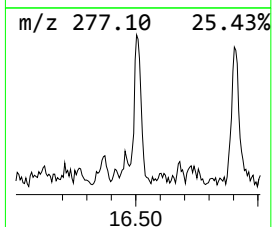
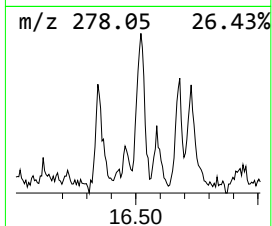
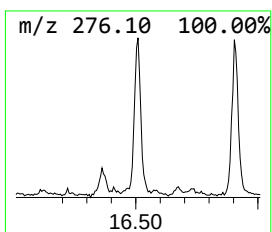
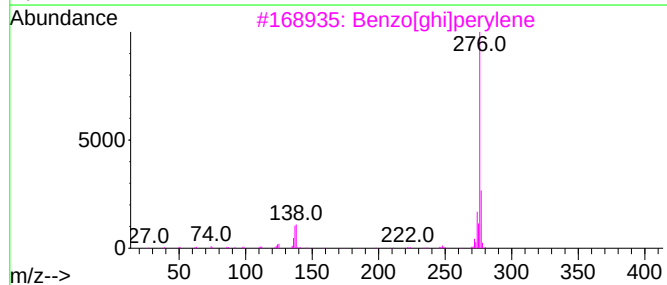
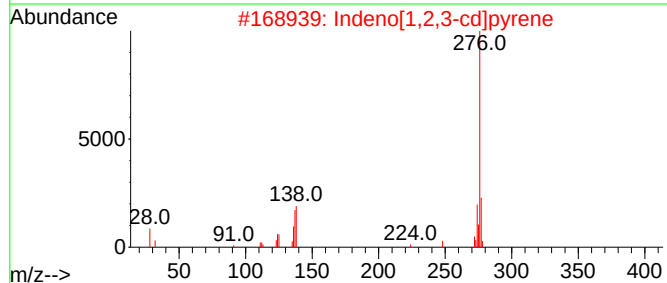
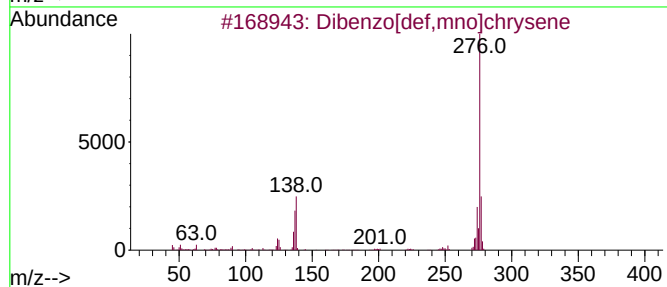
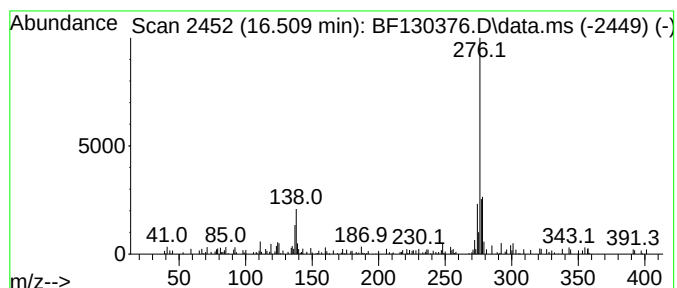
Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Dibenzo[def,mno]chrysene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.509	2.74 ng	96360	Perylene-d12	15.192	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	86
2	Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	86
3	Benzo[ghi]perylene	276	C22H12	000191-24-2	70
4	Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	62
5	Phenol, 2-(4-chlorophenyliminome...	276	C13H9ClN2O3	1000262-90-3	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092222\
Data File : BF130376.D
Acq On : 22 Sep 2022 15:10
Operator : CG\JU
Sample : N4732-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

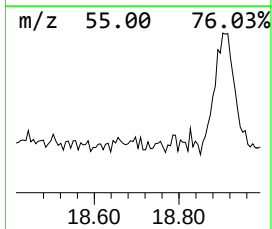
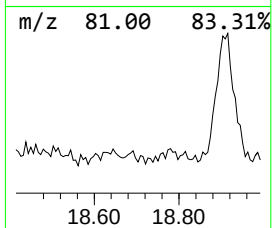
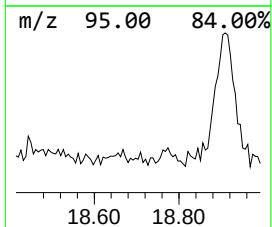
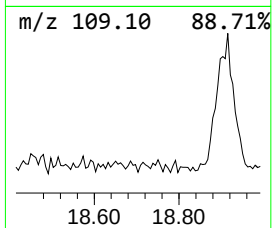
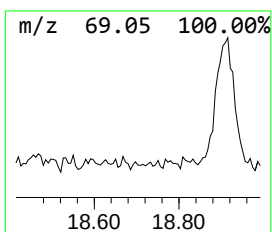
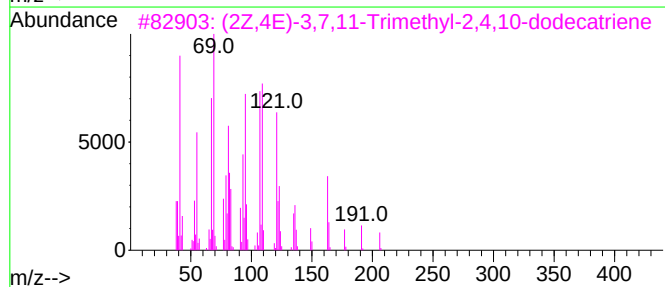
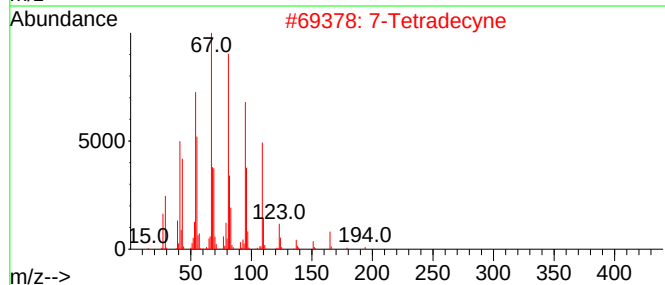
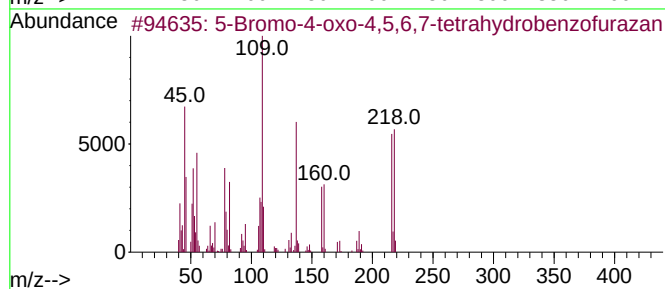
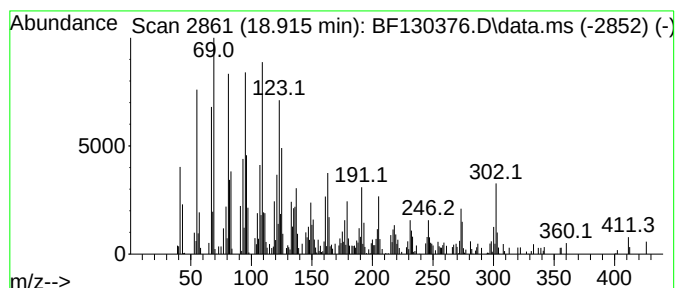
Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 5-Bromo-4-oxo-4,5,6,7-tetra... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.915	10.10 ng	354877	Perylene-d12	15.192	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	91
2	7-Tetradecyne	194	C14H26	035216-11-6	55
3	(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	50
4	Sesquirosefuran	218	C15H22O	039007-93-7	38
5	Methyl 2-octylcyclopropene-1-oct...	308	C20H36O2	003220-60-8	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092222\
Data File : BF130376.D
Acq On : 22 Sep 2022 15:10
Operator : CG\JU
Sample : N4732-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.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
2-Pentanone, 4-...	4.863	2.5	ng	115202	1	6.651	917117	20.0
n-Hexadecanoic ...	11.704	4.8	ng	252421	4	11.168	1061680	20.0
Triphenylphosph...	13.886	4.0	ng	194418	5	13.798	969115	20.0
Hexadecanamide	14.562	2.1	ng	74232	6	15.192	702689	20.0
Benzo[e]pyrene	15.074	2.8	ng	97920	6	15.192	702689	20.0
17.alpha.(H),21...	16.215	2.1	ng	73174	6	15.192	702689	20.0
Dibenzo[def,mno...	16.509	2.7	ng	96360	6	15.192	702689	20.0
5-Bromo-4-oxo-4...	18.915	10.1	ng	354877	6	15.192	702689	20.0