

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010424\
 Data File : BF136951.D
 Acq On : 04 Jan 2024 20:46
 Operator : CG\JU
 Sample : 06031-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MR-321-0-2

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-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136951.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	12	rVB3	11382	13202	1.26%	0.156%
2	5.004	492	496	508	rVB	70613	82240	7.85%	0.971%
3	5.422	564	567	579	rBV	925320	871371	83.15%	10.292%
4	6.434	735	739	755	rBV	889297	908330	86.67%	10.729%
5	6.781	795	798	802	rBV	384644	287685	27.45%	3.398%
6	7.345	890	894	897	rBV	651028	571901	54.57%	6.755%
7	8.057	1012	1015	1022	rBV	463071	361072	34.45%	4.265%
8	9.133	1194	1198	1201	rBV	1336530	1047980	100.00%	12.379%
9	9.816	1310	1314	1318	rBV	453525	391046	37.31%	4.619%
10	10.610	1445	1449	1460	rBV	619281	585496	55.87%	6.916%
11	11.310	1564	1568	1570	rBV	457482	405208	38.67%	4.786%
12	11.327	1570	1571	1575	rVV	65307	53359	5.09%	0.630%
13	11.380	1576	1580	1584	rVB	15603	18579	1.77%	0.219%
14	11.839	1655	1658	1662	rBV	117685	111929	10.68%	1.322%
15	11.921	1670	1672	1675	rBV2	14401	15192	1.45%	0.179%
16	12.092	1697	1701	1703	rBV	13978	13098	1.25%	0.155%
17	12.527	1771	1775	1780	rBV	145384	122306	11.67%	1.445%
18	12.627	1789	1792	1797	rBV5	17147	22734	2.17%	0.269%
19	12.757	1808	1814	1819	rVB	128309	122399	11.68%	1.446%
20	12.904	1835	1839	1842	rBV	1104513	941350	89.83%	11.119%
21	12.986	1847	1853	1856	rVB3	7738	13318	1.27%	0.157%
22	13.092	1863	1871	1874	rBV	16925	24990	2.38%	0.295%
23	13.380	1917	1920	1923	rBV	17164	17301	1.65%	0.204%
24	13.474	1932	1936	1938	rBV4	10297	14413	1.38%	0.170%
25	13.810	1990	1993	1996	rBV2	14228	14450	1.38%	0.171%
26	13.863	1996	2002	2004	rBV5	20350	39964	3.81%	0.472%
27	13.963	2012	2019	2022	rBV2	383176	439295	41.92%	5.189%
28	13.992	2022	2024	2031	rVB	79786	73742	7.04%	0.871%
29	14.068	2034	2037	2040	rVB3	11804	13197	1.26%	0.156%
30	14.127	2043	2047	2050	rBV5	11557	16606	1.58%	0.196%
31	14.433	2096	2099	2105	rBV6	11732	20656	1.97%	0.244%
32	14.492	2105	2109	2115	rVV3	35207	60652	5.79%	0.716%
33	14.557	2117	2120	2124	rVB2	18222	18998	1.81%	0.224%
34	14.815	2161	2164	2168	rBV	54067	53245	5.08%	0.629%
35	15.009	2194	2197	2201	rBV	59660	85327	8.14%	1.008%
36	15.127	2214	2217	2221	rVB	15347	16438	1.57%	0.194%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010424\
Data File : BF136951.D
Acq On : 04 Jan 2024 20:46
Operator : CG\JU
Sample : 06031-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-321-0-2

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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.321	2246	2250	2257	rBV	34422	49403	4.71%	0.584%
38	15.386	2257	2261	2265	rVB	53470	64923	6.20%	0.767%
39	15.451	2267	2272	2285	rVB	281775	388707	37.09%	4.591%
40	16.962	2525	2529	2539	rVB3	25338	59148	5.64%	0.699%
41	17.415	2603	2606	2615	rVB2	15718	34873	3.33%	0.412%

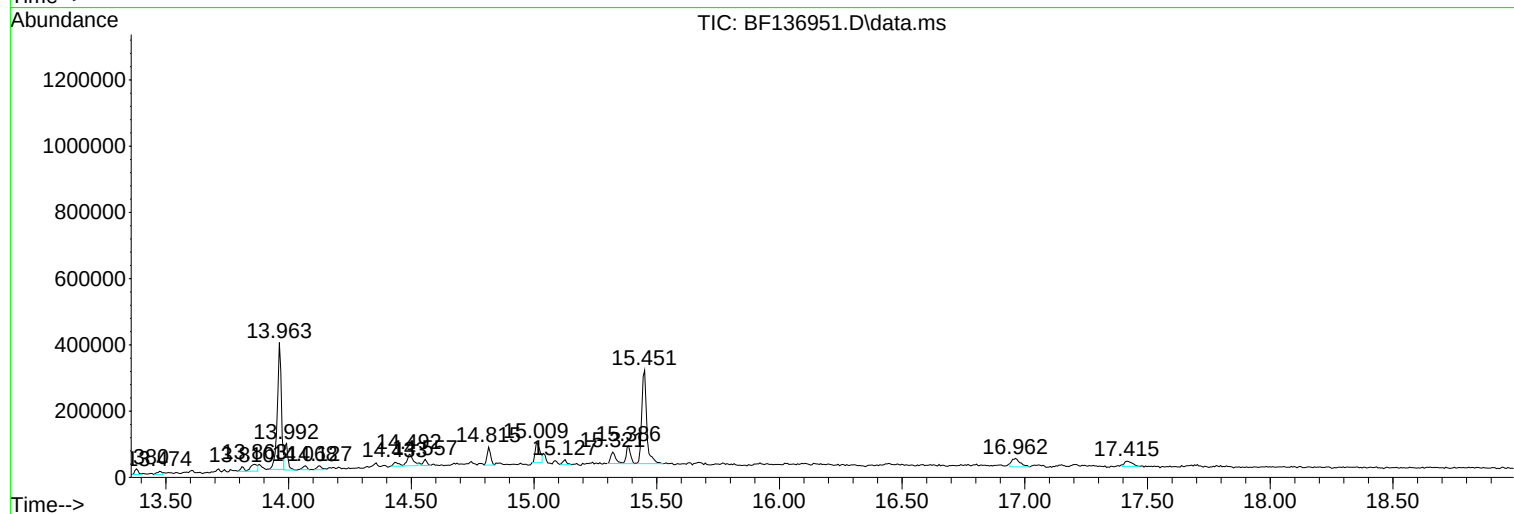
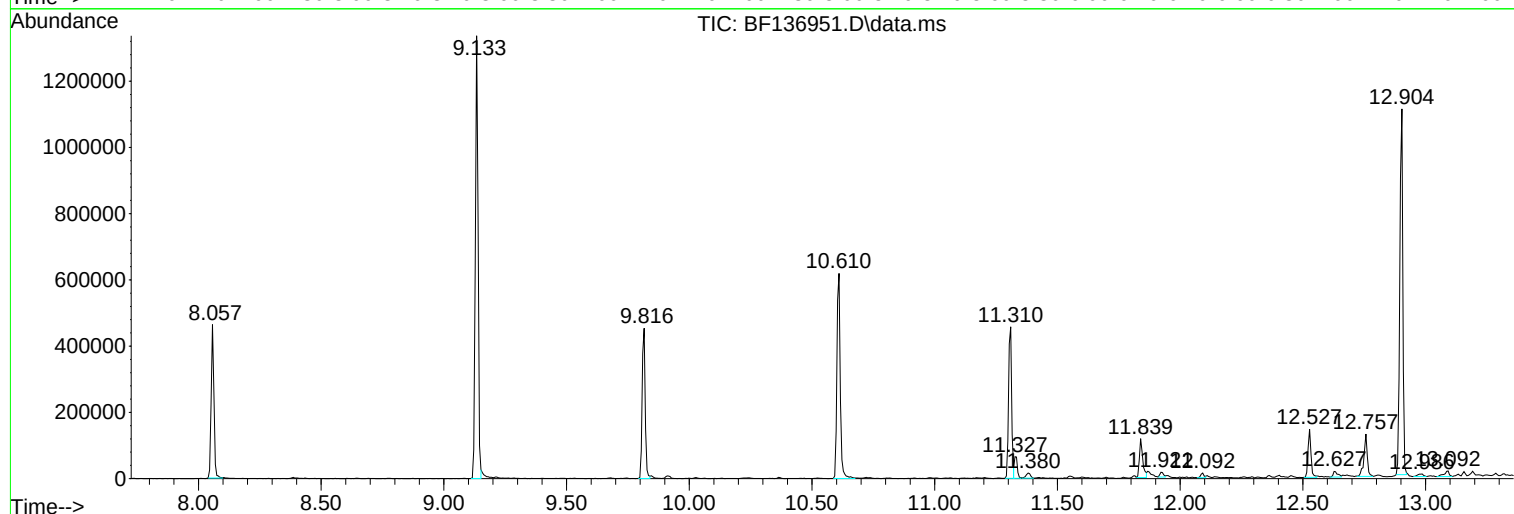
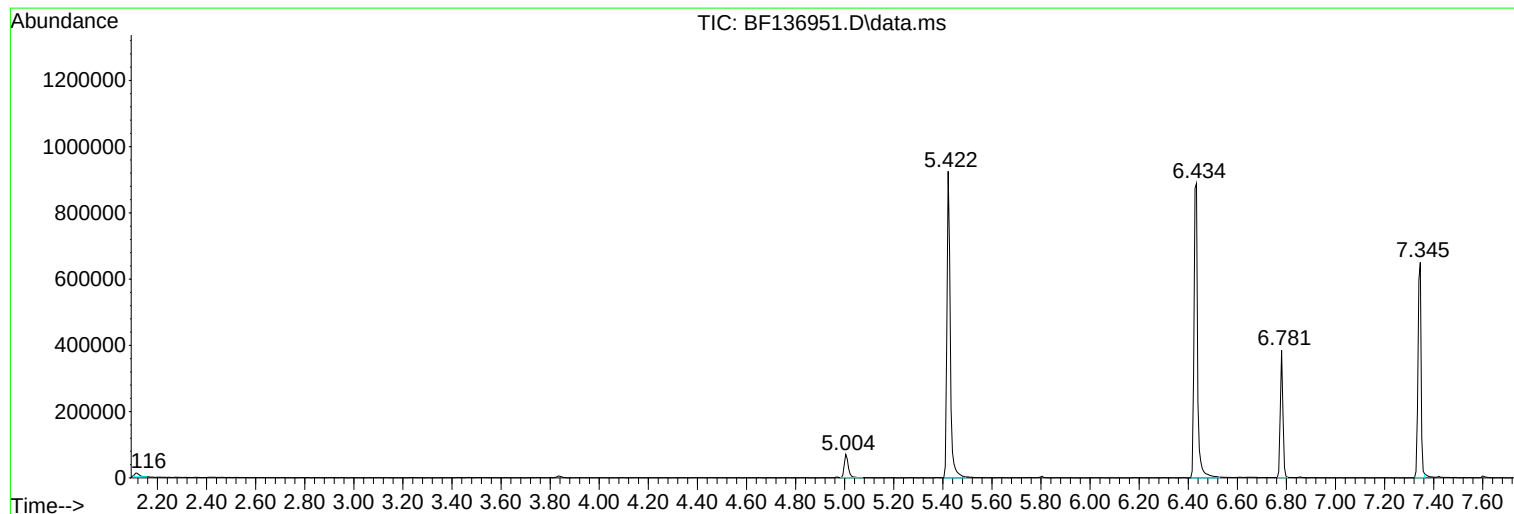
Sum of corrected areas: 8466123

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010424\
Data File : BF136951.D
Acq On : 04 Jan 2024 20:46
Operator : CG\JU
Sample : 06031-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-321-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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\BF010424\
Data File : BF136951.D
Acq On : 04 Jan 2024 20:46
Operator : CG\JU
Sample : 06031-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-321-0-2

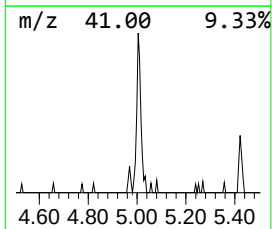
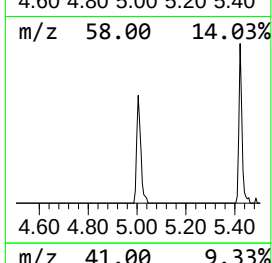
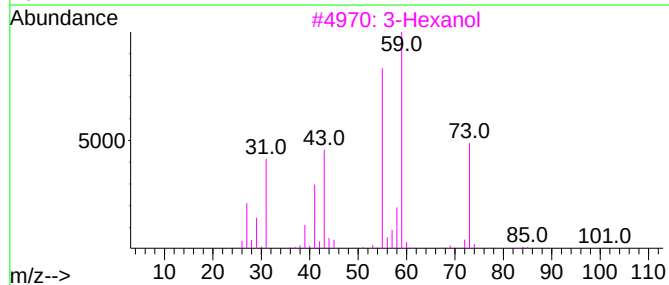
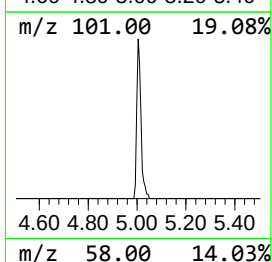
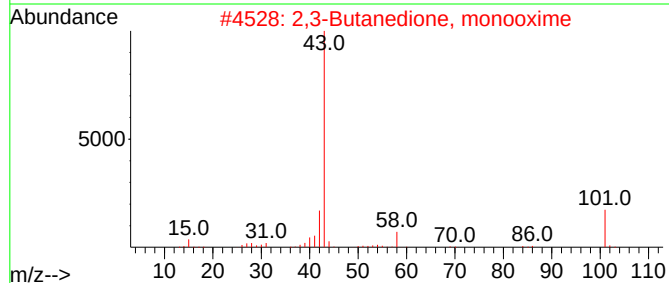
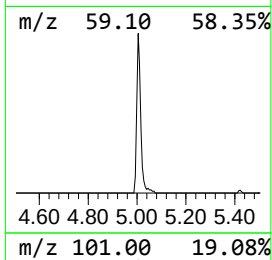
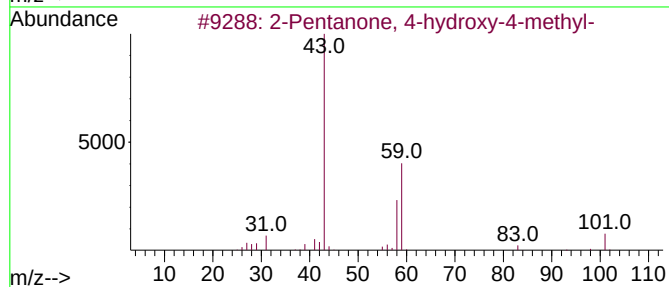
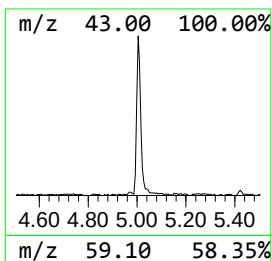
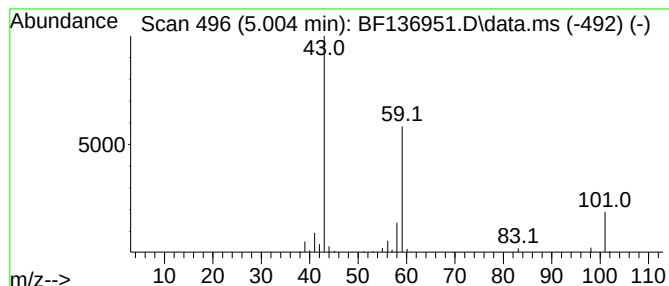
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.004	5.72 ng	82240	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35		
3	3-Hexanol	102	C6H14O	000623-37-0	28		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010424\
Data File : BF136951.D
Acq On : 04 Jan 2024 20:46
Operator : CG\JU
Sample : 06031-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

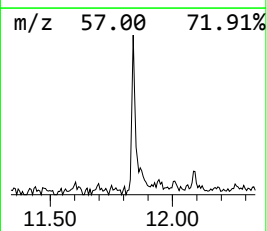
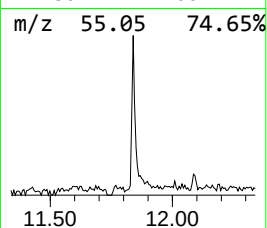
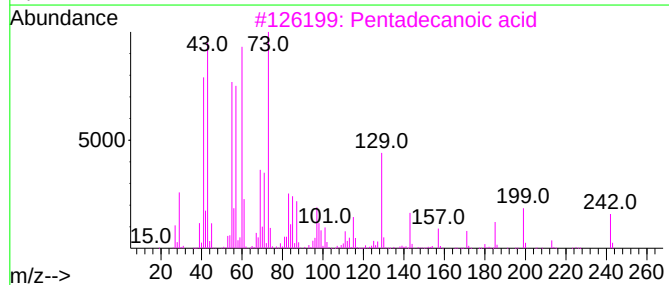
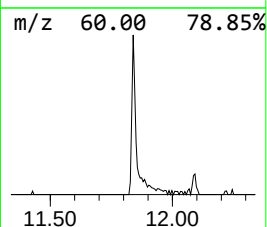
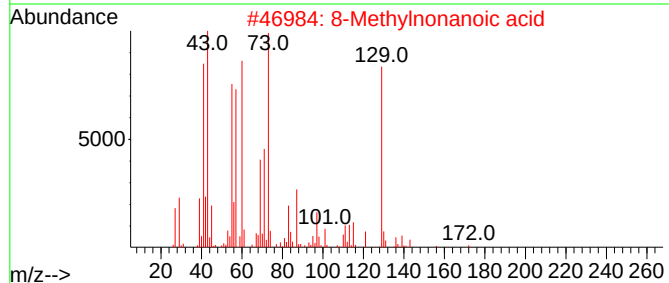
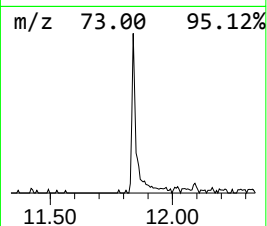
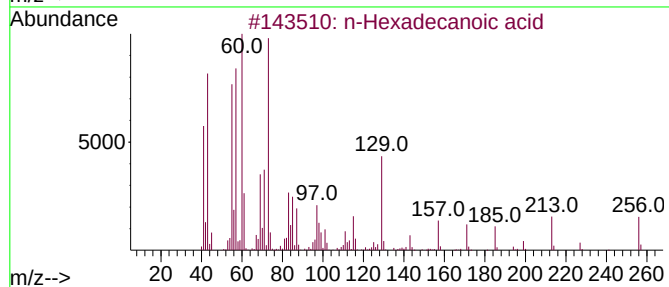
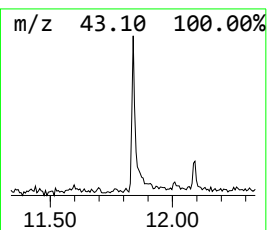
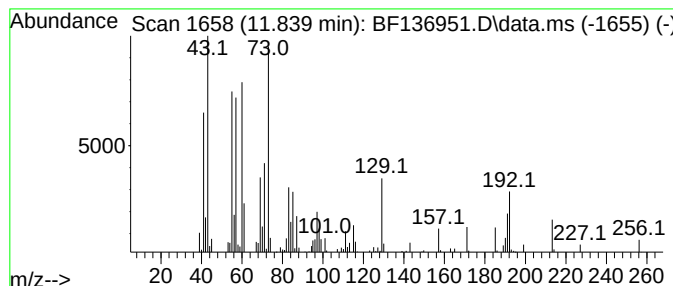
Instrument :
BNA_F
ClientSampleId :
MR-321-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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.	
11.839	5.52 ng	111929	Phenanthrene-d10	11.310	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	78
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010424\
Data File : BF136951.D
Acq On : 04 Jan 2024 20:46
Operator : CG\JU
Sample : 06031-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-321-0-2

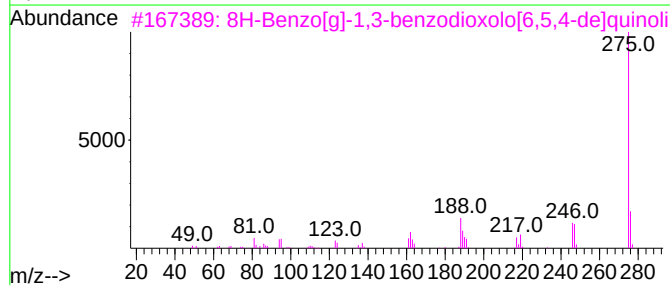
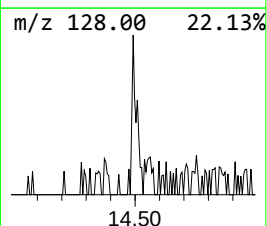
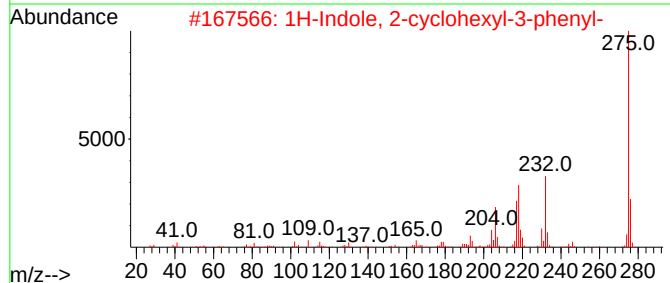
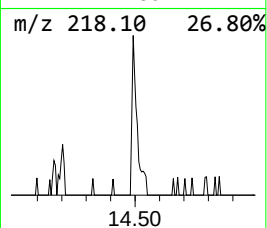
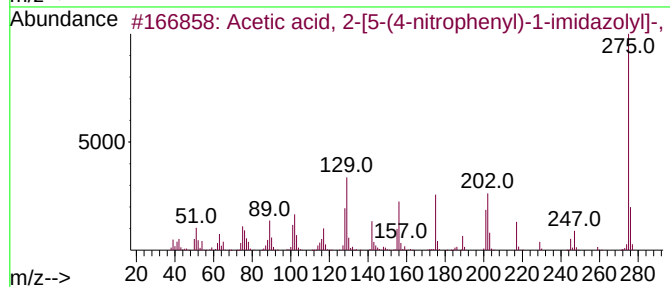
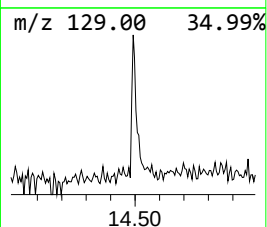
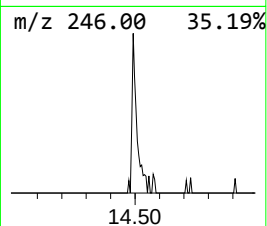
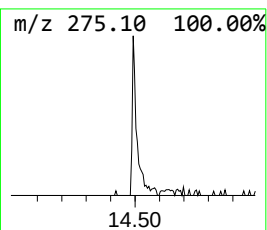
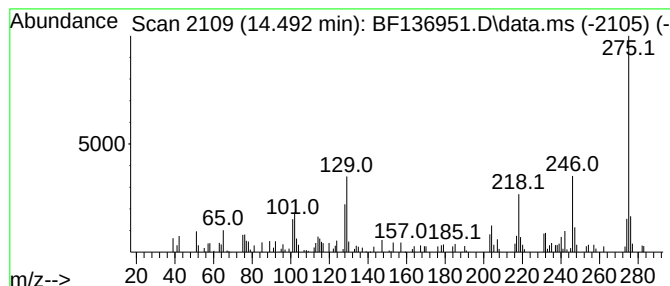
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Acetic acid, 2-[5-(4-nitrop... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.492	2.76 ng	60652	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, 2-[5-(4-nitrophenyl)...	275	C13H13N3O4	351064-45-4	52
2			1H-Indole, 2-cyclohexyl-3-phenyl-	275	C20H21N	1010163-87-0	49
3			8H-Benzo[g]-1,3-benzodioxolo[6,5...	275	C17H9NO3	000475-75-2	46
4			Ethyl 2-ethoxy-6-methoxy-4-quino...	275	C15H17NO4	015432-29-8	43
5			5-(Adamantan-1-yl)-4-(prop-2-en-...	275	C15H21N3S	345987-96-4	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010424\
Data File : BF136951.D
Acq On : 04 Jan 2024 20:46
Operator : CG\JU
Sample : 06031-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-321-0-2

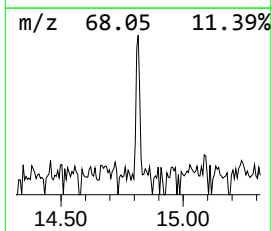
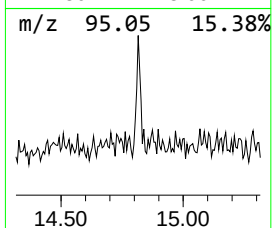
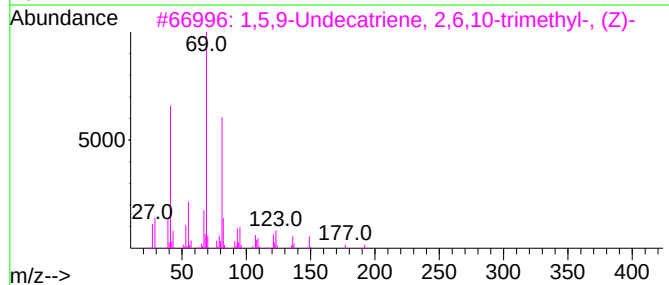
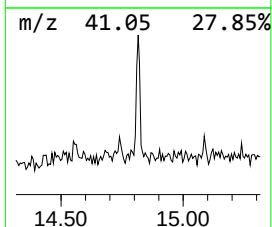
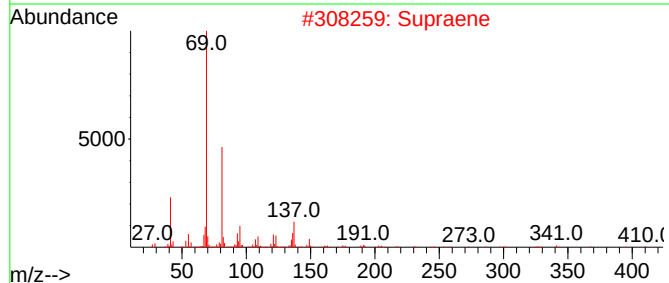
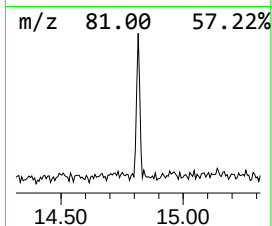
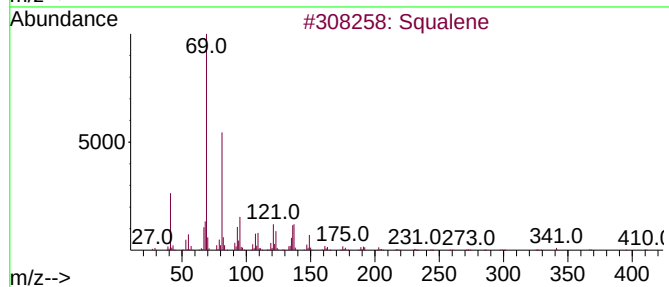
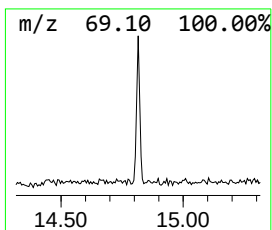
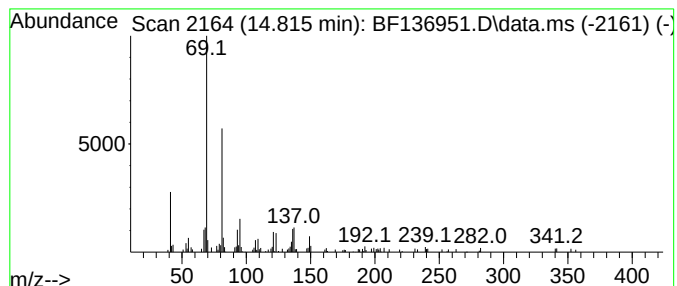
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.815	2.74 ng	53245	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	90
2			Supraene	410	C30H50	007683-64-9	87
3			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	81
4			4,8,12-Tetradecatrienenitrile, 5...	245	C17H27N	005981-31-7	64
5			3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010424\
Data File : BF136951.D
Acq On : 04 Jan 2024 20:46
Operator : CG\JU
Sample : 06031-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-321-0-2

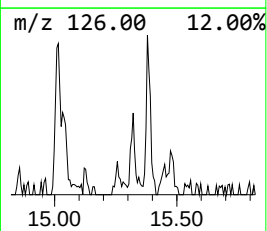
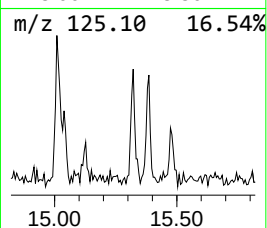
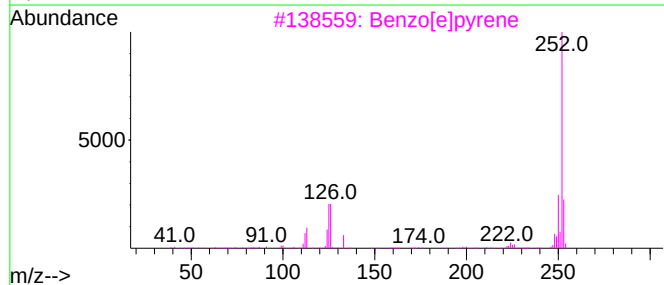
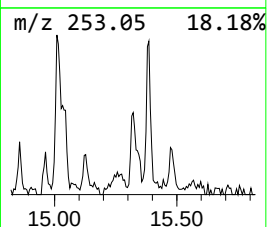
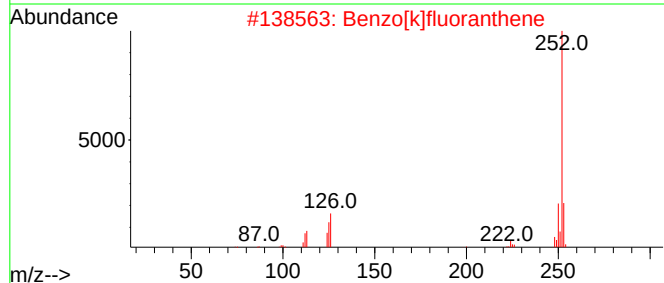
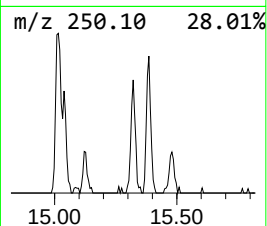
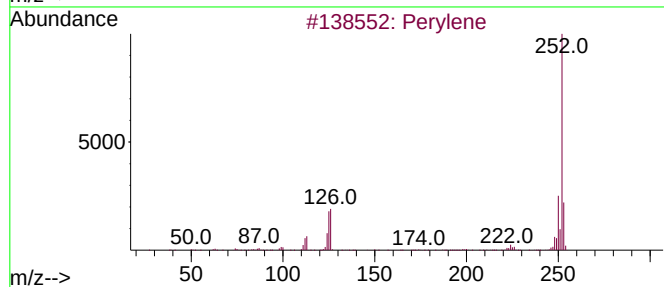
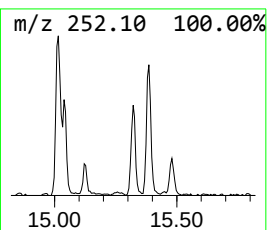
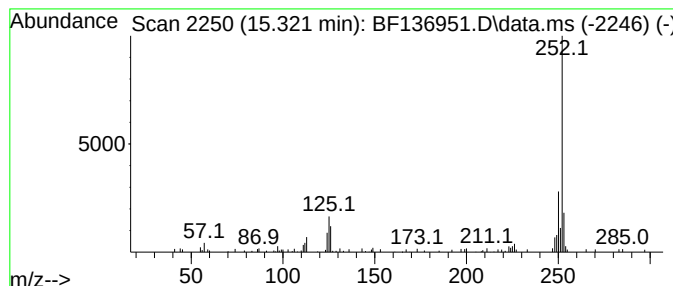
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Perylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.321	2.54 ng	49403	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Perylene	252	C20H12	000198-55-0	95
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
3			Benzo[e]pyrene	252	C20H12	000192-97-2	90
4			Benzo[a]pyrene	252	C20H12	000050-32-8	81
5			Benzo[b]fluoranthene	252	C20H12	000205-99-2	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010424\
Data File : BF136951.D
Acq On : 04 Jan 2024 20:46
Operator : CG\JU
Sample : 06031-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-321-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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-...	5.004	5.7	ng	82240	1	6.781	287685	20.0
n-Hexadecanoic ...	11.839	5.5	ng	111929	4	11.310	405208	20.0
Acetic acid, 2-...	14.492	2.8	ng	60652	5	13.963	439295	20.0
Squalene	14.815	2.7	ng	53245	6	15.451	388707	20.0
Perylene	15.321	2.5	ng	49403	6	15.451	388707	20.0