

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
 Data File : BF136862.D
 Acq On : 30 Dec 2023 09:26
 Operator : CG\JU
 Sample : 05897-19
 Misc :
 ALS Vial : 44 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GHL-SS-23

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: BF136862.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.022	494	499	505	rVB	22291	30557	1.87%	0.262%
2	5.381	555	560	563	rBV	23311	24128	1.48%	0.207%
3	5.422	563	567	583	rVB	1616470	1400561	85.82%	12.028%
4	5.634	600	603	607	rBV	31809	29416	1.80%	0.253%
5	6.428	733	738	741	rBV	1535113	1408003	86.27%	12.092%
6	6.604	765	768	772	rBV2	33164	33224	2.04%	0.285%
7	6.781	794	798	801	rBV	525967	410245	25.14%	3.523%
8	7.345	889	894	897	rBV	939712	925717	56.72%	7.950%
9	8.057	1008	1015	1017	rBV	670818	555535	34.04%	4.771%
10	8.075	1017	1018	1021	rVB	59488	41930	2.57%	0.360%
11	8.769	1133	1136	1140	rBV	61944	50402	3.09%	0.433%
12	8.869	1150	1153	1156	rVB	45196	33268	2.04%	0.286%
13	9.133	1194	1198	1201	rBV	1990254	1632022	100.00%	14.016%
14	9.469	1249	1255	1258	rBV	23970	26496	1.62%	0.228%
15	9.586	1272	1275	1281	rBV2	16347	19808	1.21%	0.170%
16	9.816	1310	1314	1317	rBV	624241	573063	35.11%	4.921%
17	10.022	1344	1349	1351	rBV2	15693	20225	1.24%	0.174%
18	10.357	1403	1406	1408	rBV	27073	23851	1.46%	0.205%
19	10.604	1444	1448	1460	rVV	943664	850961	52.14%	7.308%
20	10.733	1464	1470	1475	rVB	53950	62834	3.85%	0.540%
21	11.045	1519	1523	1528	rVB3	19484	21829	1.34%	0.187%
22	11.169	1538	1544	1548	rBV4	14461	19531	1.20%	0.168%
23	11.304	1563	1567	1570	rBV	663444	543958	33.33%	4.672%
24	11.598	1611	1617	1622	rBV	25440	40912	2.51%	0.351%
25	11.839	1655	1658	1670	rBV	276073	333639	20.44%	2.865%
26	12.092	1699	1701	1703	rVB	36209	26085	1.60%	0.224%
27	12.398	1751	1753	1759	rBV4	15903	19148	1.17%	0.164%
28	12.557	1776	1780	1789	rVB6	38337	74487	4.56%	0.640%
29	12.633	1789	1793	1803	rBV	102669	134981	8.27%	1.159%
30	12.904	1835	1839	1842	rBV	1252651	1153386	70.67%	9.905%
31	13.763	1982	1985	1991	rBV6	17521	29661	1.82%	0.255%
32	13.810	1991	1993	1997	rVB2	25398	23434	1.44%	0.201%
33	13.880	2000	2005	2014	rBV9	41627	123967	7.60%	1.065%
34	13.962	2015	2019	2027	rVB	393875	385919	23.65%	3.314%
35	14.133	2045	2048	2050	rBV	18898	20110	1.23%	0.173%
36	14.433	2097	2099	2103	rBV2	28006	27441	1.68%	0.236%

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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	15.004	2194	2196	2200	rBV3	22420	30288	1.86%	0.260%
38	15.445	2266	2271	2275	rBV	323837	415713	25.47%	3.570%
39	15.921	2349	2352	2358	rBV7	15427	24342	1.49%	0.209%
40	17.568	2627	2632	2639	rVB7	19327	43101	2.64%	0.370%

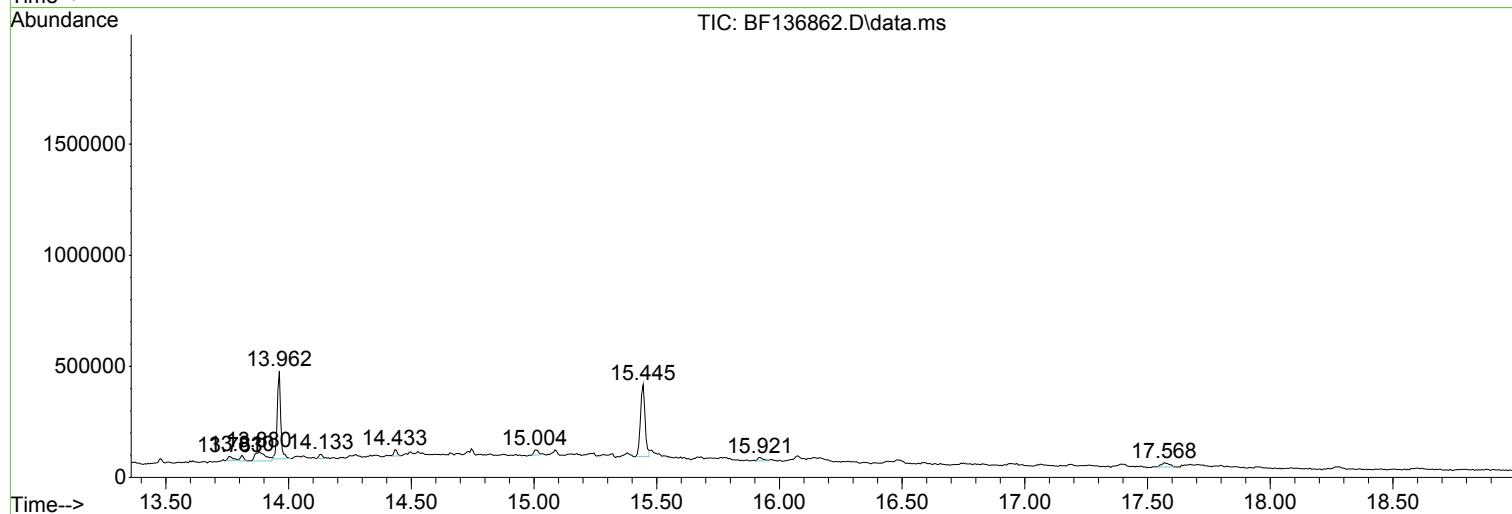
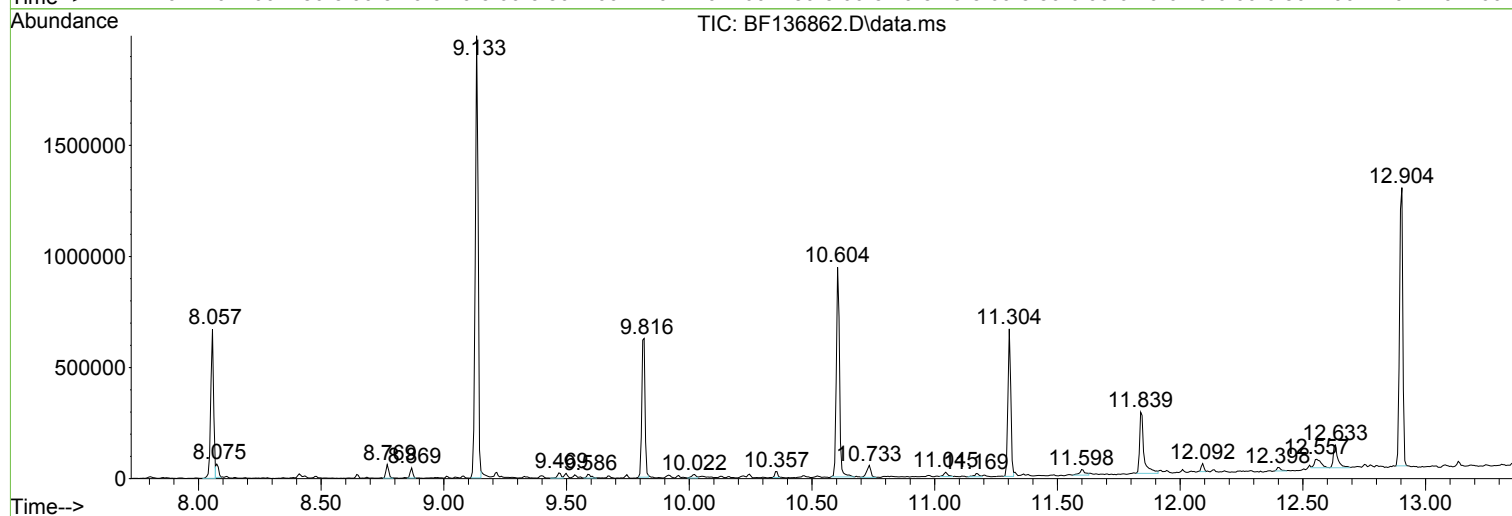
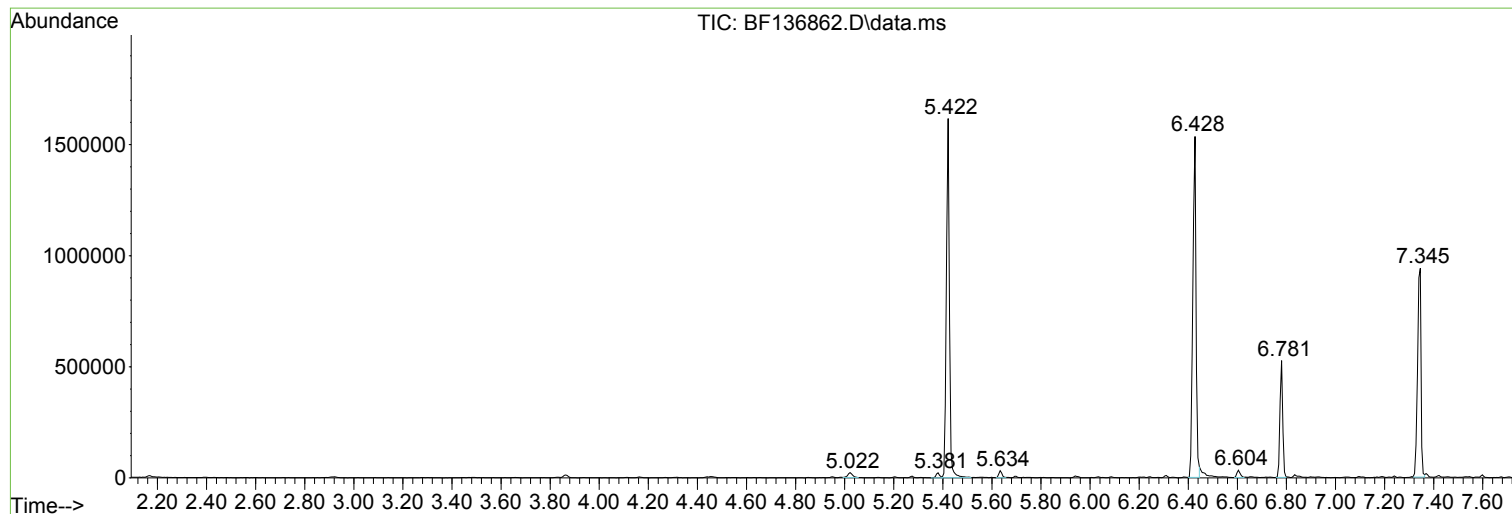
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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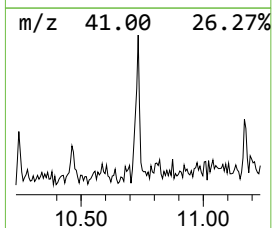
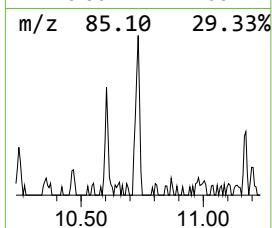
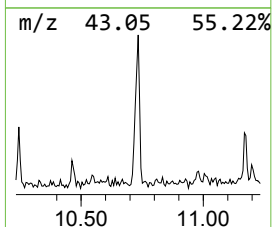
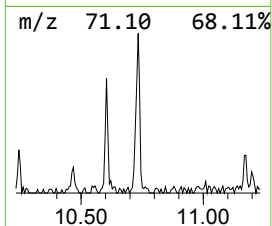
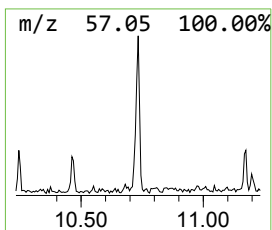
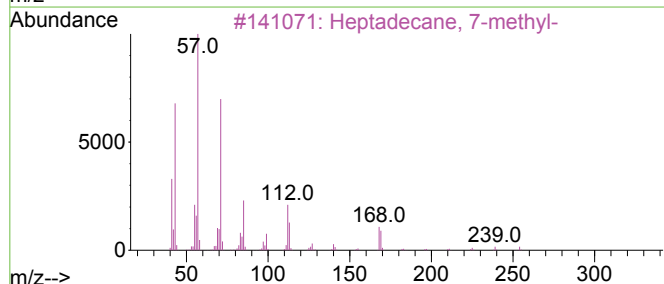
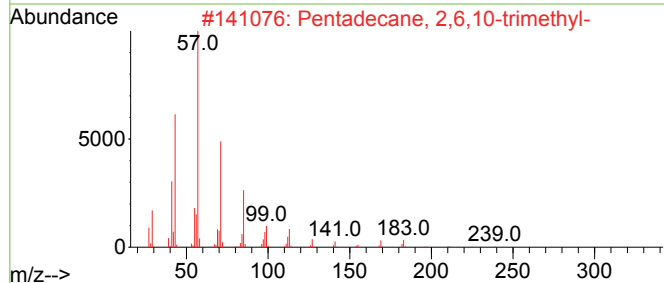
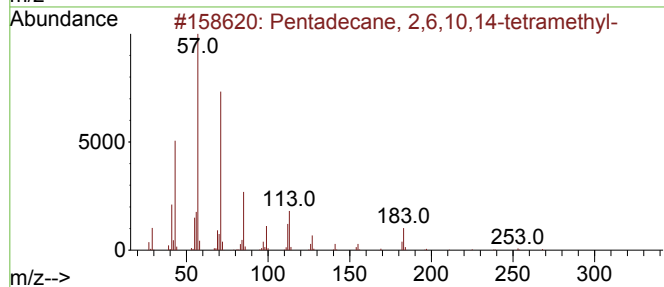
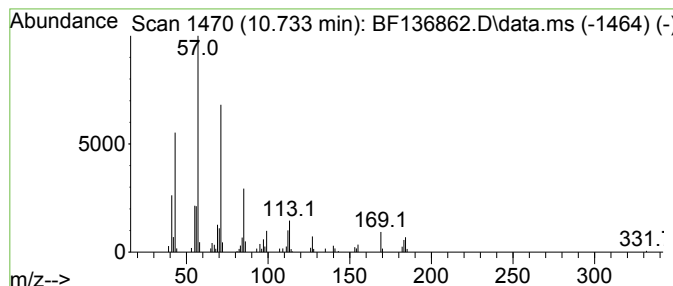
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Pentadecane, 2,6,10,14-tetr... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.733	2.31 ng	62834	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	87
2			Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	86
3			Heptadecane, 7-methyl-	254	C18H38	020959-33-5	80
4			Octadecane, 2,6-dimethyl-	282	C20H42	075163-97-2	80
5			Hexadecane, 2,6,11,15-tetramethyl-	282	C20H42	000504-44-9	80



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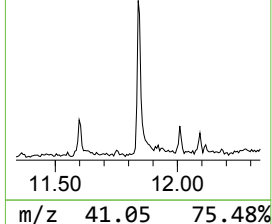
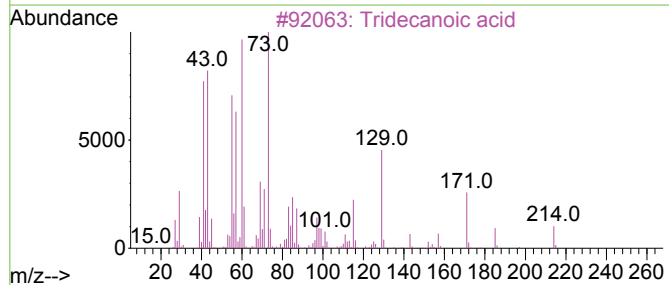
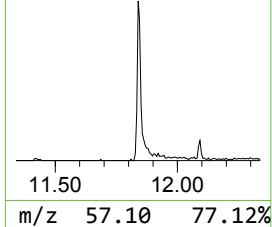
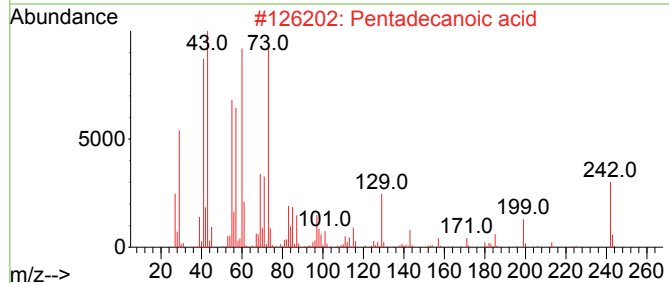
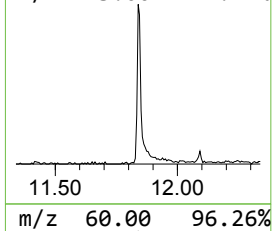
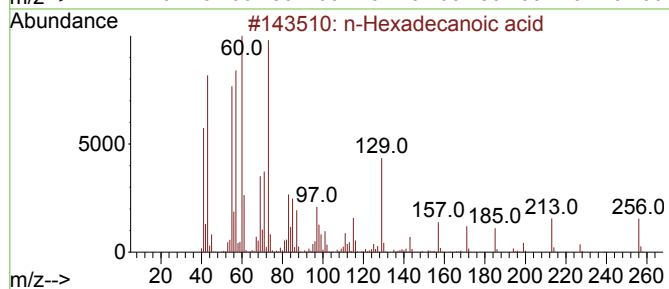
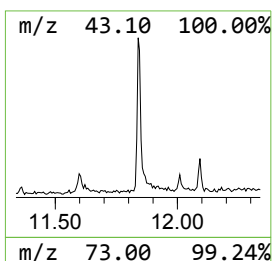
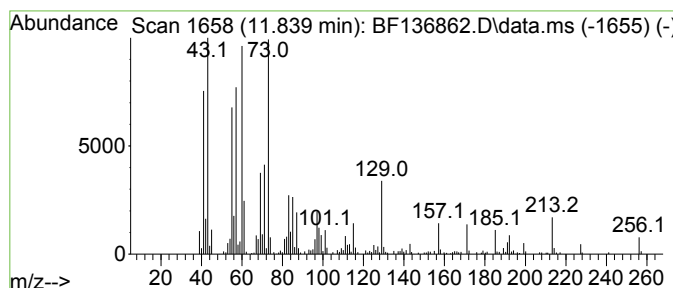
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	12.27 ng	333639	Phenanthrene-d10	11.304

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	91
3		Tridecanoic acid	214	C13H26O2	000638-53-9	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5		Dodecanoic acid	200	C12H24O2	000143-07-7	76



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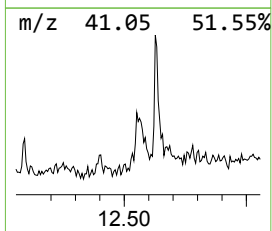
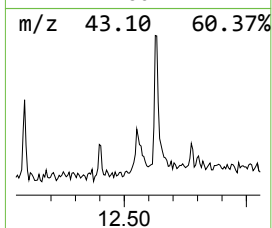
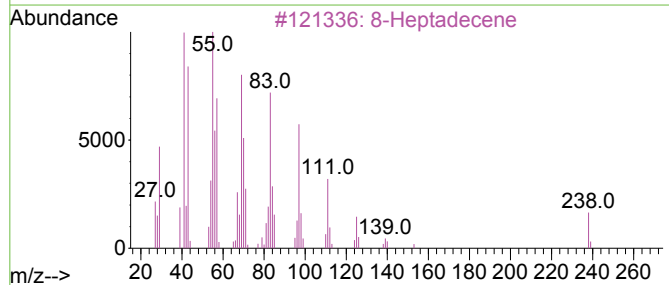
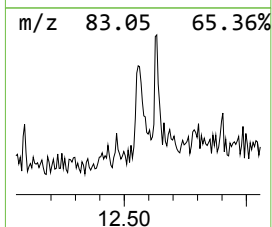
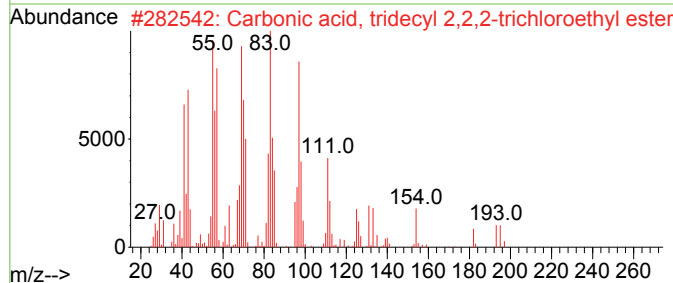
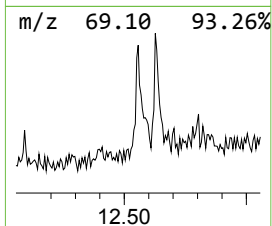
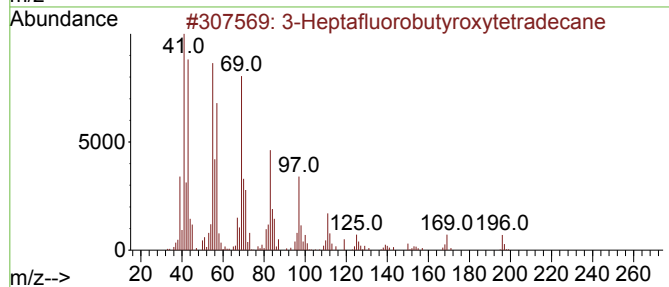
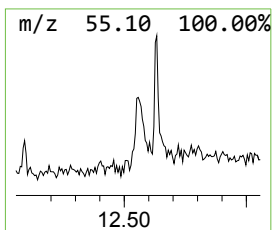
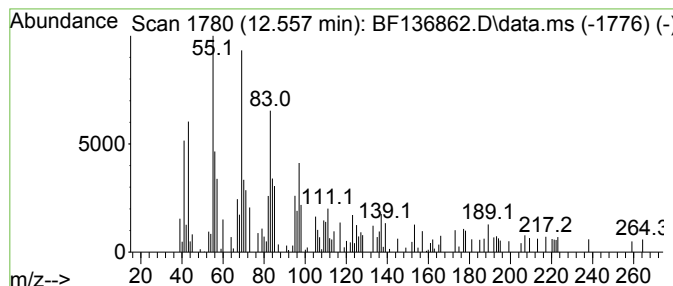
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 3-Heptafluorobutyroxytetrad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.557	2.74 ng	74487	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Heptafluorobutyroxytetradecane	410	C18H29F7O2	1000245-49-8	64
2			Carbonic acid, tridecyl 2,2,2-tr...	374	C16H29Cl3O3	1000314-55-9	64
3			8-Heptadecene	238	C17H34	002579-04-6	50
4			Carbonic acid, dodecyl 2,2,2-tri...	360	C15H27Cl3O3	1000314-55-8	49
5			cis-Vaccenic acid	282	C18H34O2	000506-17-2	49



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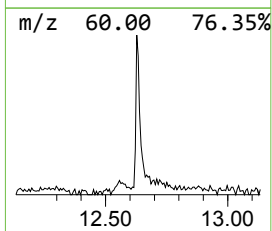
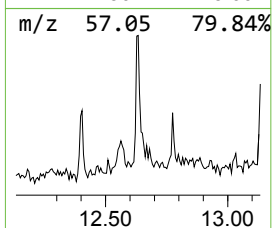
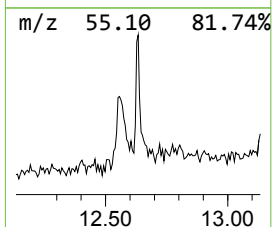
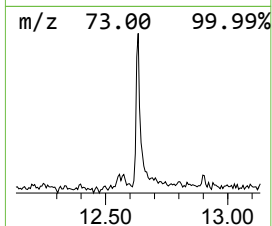
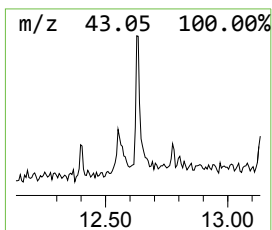
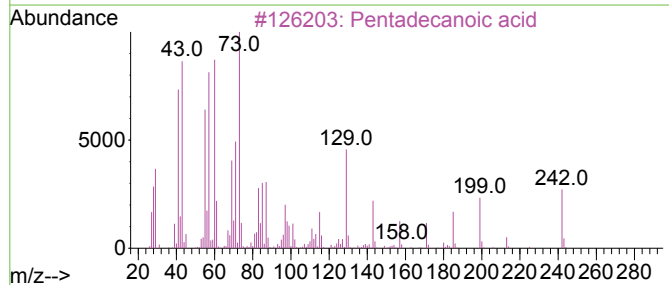
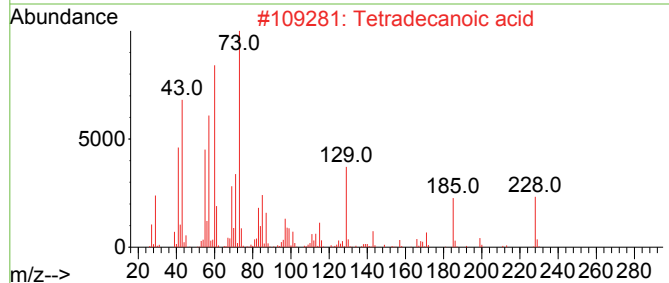
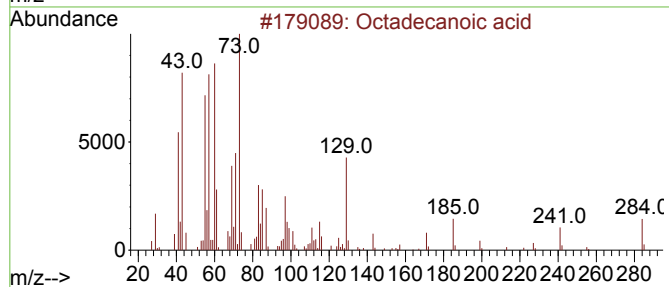
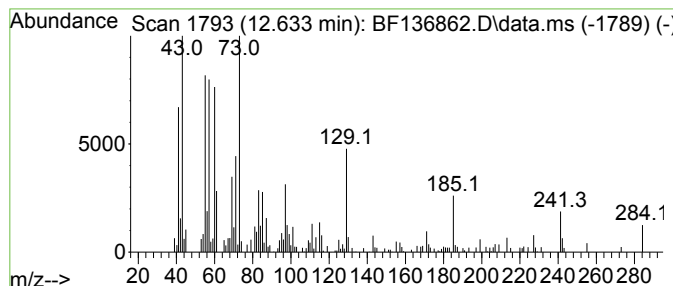
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.633	4.96 ng	134981	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4			n-Decanoic acid	172	C10H20O2	000334-48-5	70
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68



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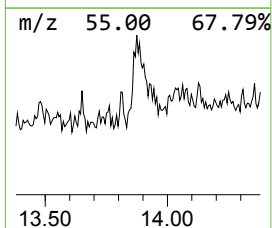
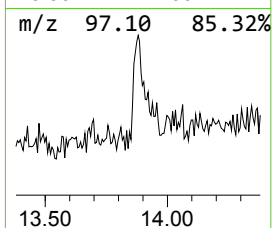
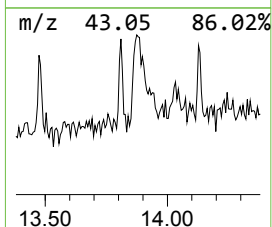
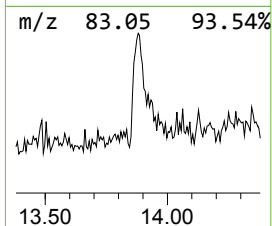
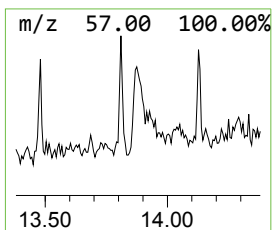
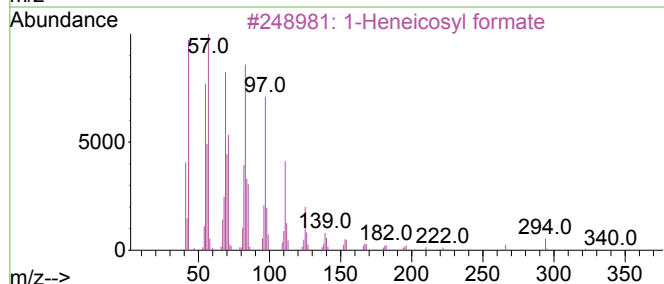
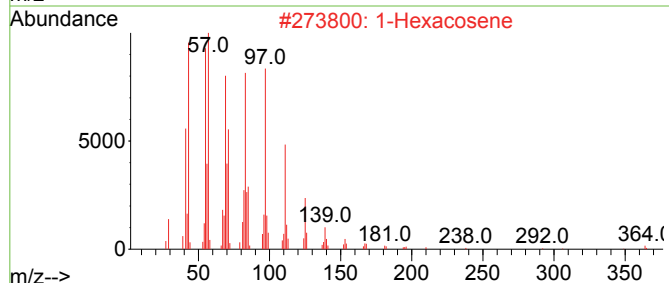
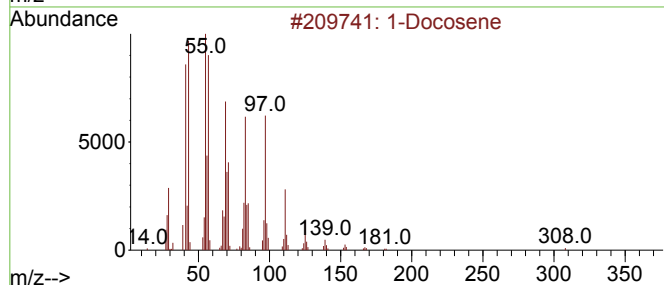
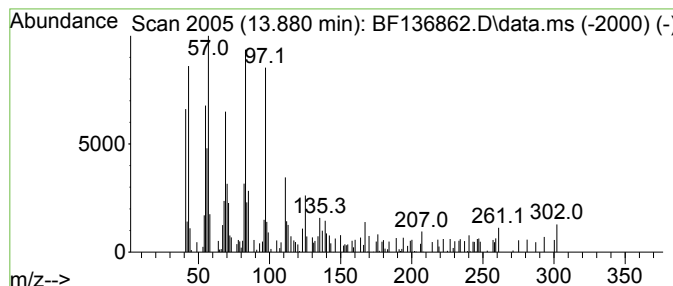
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Docosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	6.42 ng	123967	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene			308	C22H44	001599-67-3	87
2	1-Hexacosene			364	C26H52	018835-33-1	64
3	1-Heneicosyl formate			340	C22H44O2	077899-03-7	60
4	Pentafluoropropionic acid, octad...			416	C21H37F5O2	959261-25-7	60
5	Heptafluorobutyric acid, n-octad...			466	C22H37F7O2	000400-57-7	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136862.D
Acq On : 30 Dec 2023 09:26
Operator : CG\JU
Sample : 05897-19
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-23

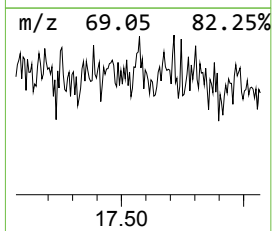
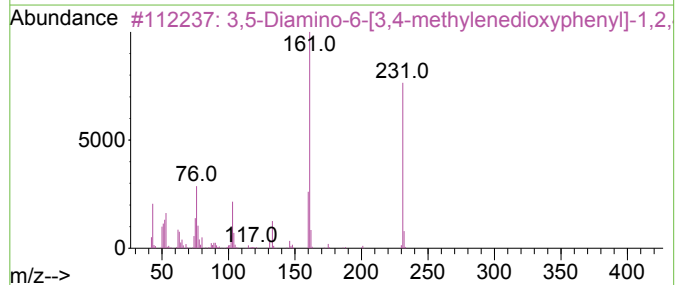
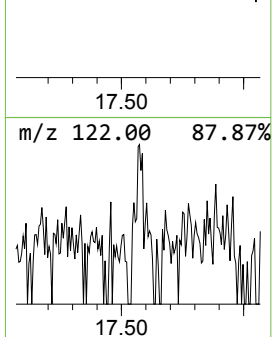
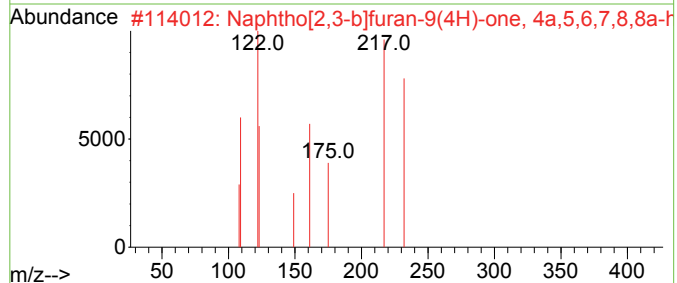
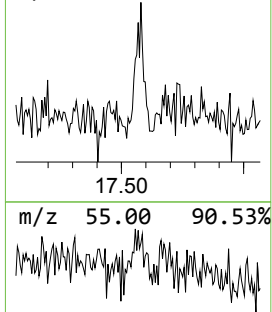
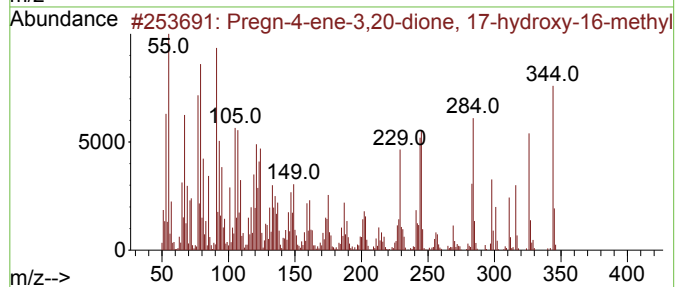
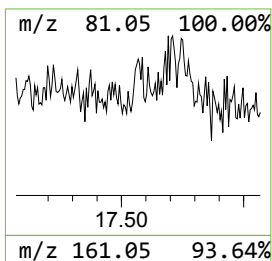
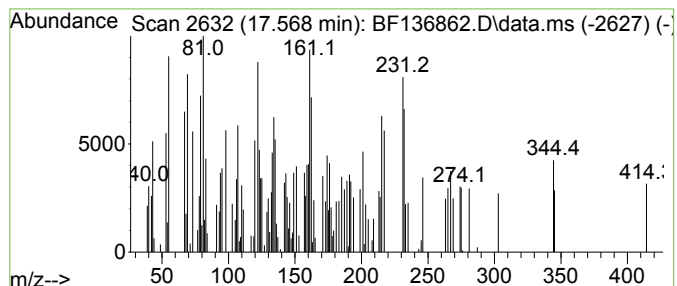
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown17.568 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.568	2.07 ng	43101	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pregn-4-ene-3,20-dione, 17-hydro...	344	C22H32O3	002868-02-2	38
2			Naphtho[2,3-b]furan-9(4H)-one, 4...	232	C15H20O2	006902-61-0	32
3			3,5-Diamino-6-[3,4-methylenedioxy...	231	C10H9N5O2	058848-65-0	14
4			Silane, diethyl(2-methylbutoxy)p...	260	C14H32O2Si	1000363-09-9	10
5			2-[4-Chloro-trans-styryl]-4-hydr...	232	C12H9ClN2O	1000251-23-8	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136862.D
Acq On : 30 Dec 2023 09:26
Operator : CG\JU
Sample : 05897-19
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-23

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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
Pentadecane, 2,...	10.733	2.3	ng	62834	4	11.304	543958	20.0
n-Hexadecanoic ...	11.839	12.3	ng	333639	4	11.304	543958	20.0
3-Heptafluorobu...	12.557	2.7	ng	74487	4	11.304	543958	20.0
Octadecanoic acid	12.633	5.0	ng	134981	4	11.304	543958	20.0
1-Docosene	13.880	6.4	ng	123967	5	13.963	385919	20.0
unknown17.568	17.568	2.1	ng	43101	6	15.445	415713	20.0