

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031424\
 Data File : BF137599.D
 Acq On : 14 Mar 2024 19:29
 Operator : CG\JU
 Sample : P1746-04
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-01-7.0-9.5

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-BF022924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137599.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.334	548	552	576	rBV	3720431	3733650	86.65%	12.328%
2	6.363	722	727	746	rBV	3727857	3778100	87.68%	12.474%
3	6.722	785	788	802	rBV	844231	853730	19.81%	2.819%
4	7.287	881	884	898	rBV	2332409	2400372	55.71%	7.925%
5	8.004	1003	1006	1012	rBV	1222536	1079268	25.05%	3.563%
6	9.081	1185	1189	1201	rBV	4588541	4308864	100.00%	14.227%
7	9.757	1300	1304	1316	rBV	1499162	1260762	29.26%	4.163%
8	10.545	1434	1438	1455	rBV	2272416	2193669	50.91%	7.243%
9	10.663	1455	1458	1467	rVB2	30965	52026	1.21%	0.172%
10	11.239	1552	1556	1559	rBV	1280300	1124281	26.09%	3.712%
11	11.263	1559	1560	1565	rVB	124366	91523	2.12%	0.302%
12	11.774	1644	1647	1651	rBV2	188224	222245	5.16%	0.734%
13	12.451	1758	1762	1768	rBV	234379	264926	6.15%	0.875%
14	12.674	1793	1800	1803	rBV	241474	237912	5.52%	0.786%
15	12.763	1812	1815	1818	rVB	61999	48035	1.11%	0.159%
16	12.827	1821	1826	1829	rBV	3616642	3505660	81.36%	11.575%
17	12.898	1834	1838	1843	rVB4	27469	47302	1.10%	0.156%
18	13.057	1861	1865	1870	rBV2	37541	59563	1.38%	0.197%
19	13.627	1956	1962	1964	rBV3	31574	45985	1.07%	0.152%
20	13.727	1976	1979	1996	rBV	192628	310438	7.20%	1.025%
21	13.874	1997	2004	2007	rBV2	957921	1194454	27.72%	3.944%
22	13.898	2007	2008	2015	rVB	170603	130906	3.04%	0.432%
23	14.045	2028	2033	2036	rBV3	36196	45838	1.06%	0.151%
24	14.351	2082	2085	2087	rBV	70580	72085	1.67%	0.238%
25	14.504	2109	2111	2115	rVB	52923	51956	1.21%	0.172%
26	14.715	2144	2147	2155	rVB3	79340	92389	2.14%	0.305%
27	14.786	2156	2159	2166	rVB	159042	163778	3.80%	0.541%
28	14.886	2172	2176	2180	rBV	173723	275314	6.39%	0.909%
29	14.968	2186	2190	2193	rBV	144611	173497	4.03%	0.573%
30	15.010	2193	2197	2207	rVB5	75540	181094	4.20%	0.598%
31	15.174	2221	2225	2231	rVB	107099	129661	3.01%	0.428%
32	15.233	2231	2235	2241	rBV	134677	173291	4.02%	0.572%
33	15.292	2241	2245	2260	rVB	838088	1061003	24.62%	3.503%
34	15.521	2280	2284	2292	rVB2	65631	88586	2.06%	0.292%
35	15.739	2316	2321	2328	rBV	126296	193596	4.49%	0.639%
36	16.492	2443	2449	2463	rBV8	72077	178212	4.14%	0.588%

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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-BF022924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.680	2476	2481	2491	rVB2	57676	138493	3.21%	0.457%
38	16.774	2493	2497	2502	rVV3	33748	57874	1.34%	0.191%
39	17.092	2546	2551	2559	rBV2	45275	93199	2.16%	0.308%
40	17.239	2570	2576	2586	rBV2	59218	173548	4.03%	0.573%

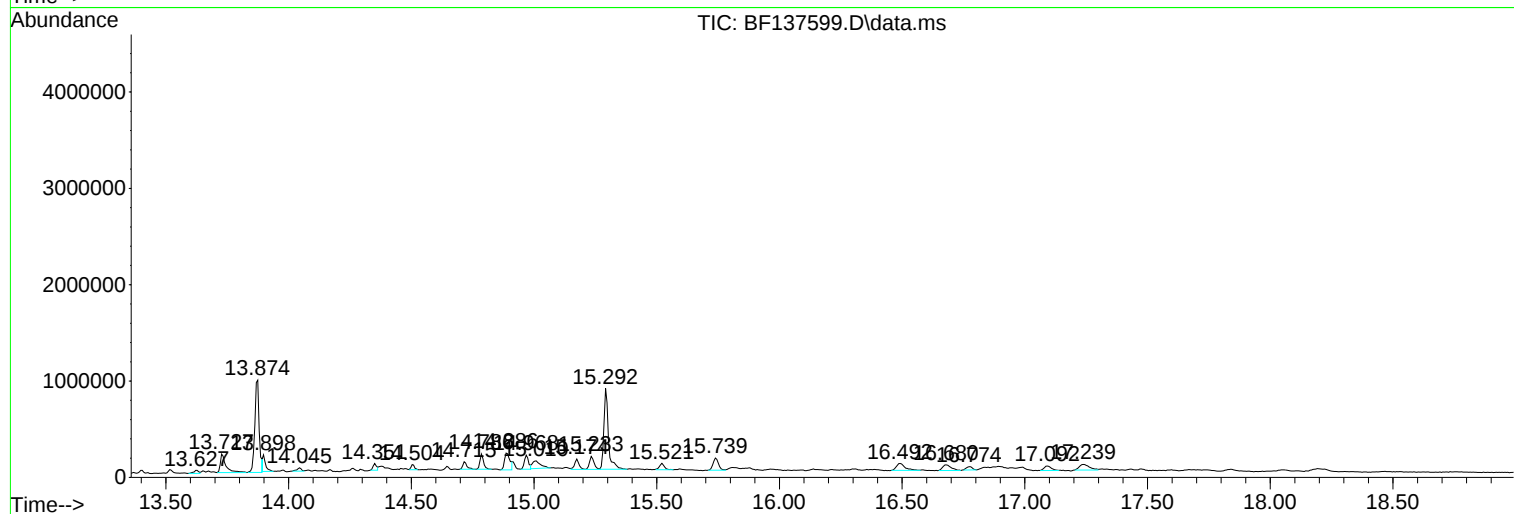
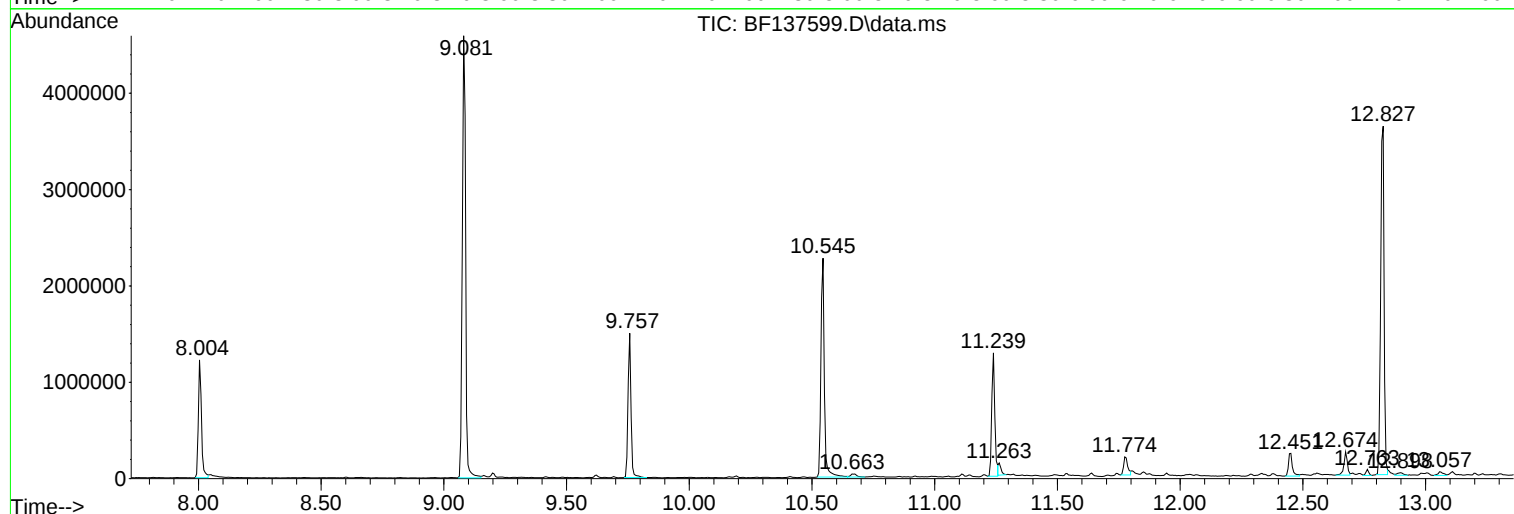
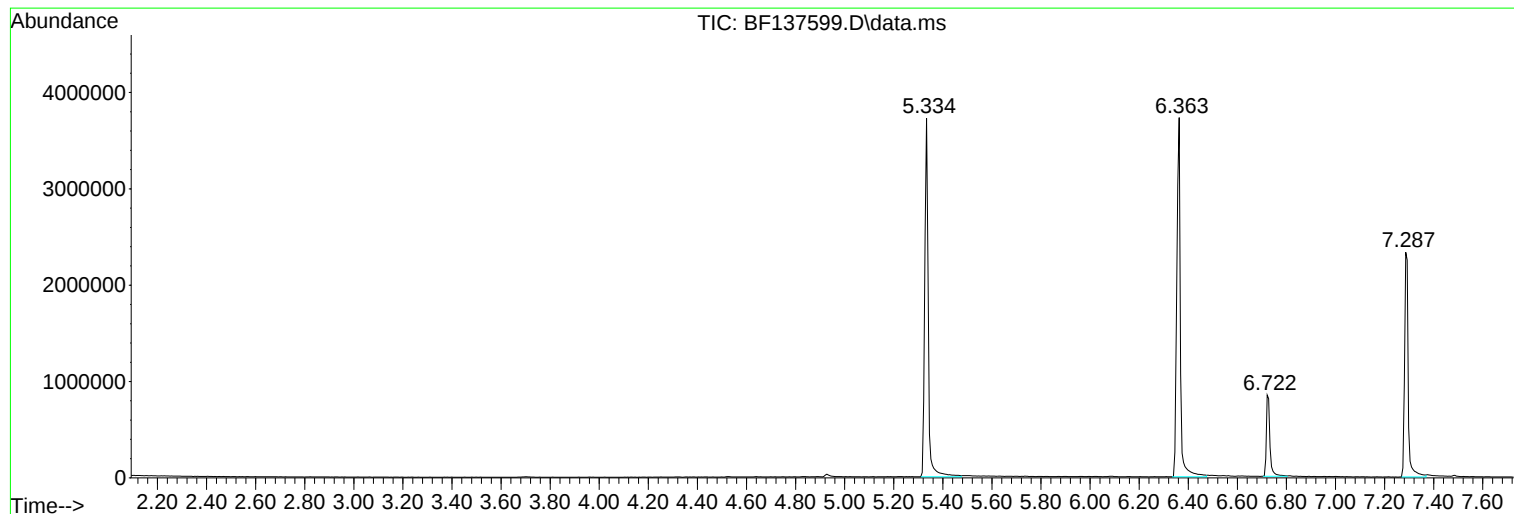
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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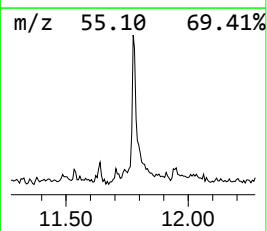
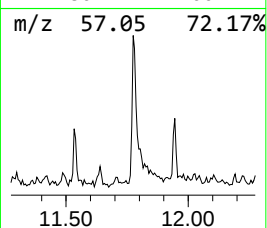
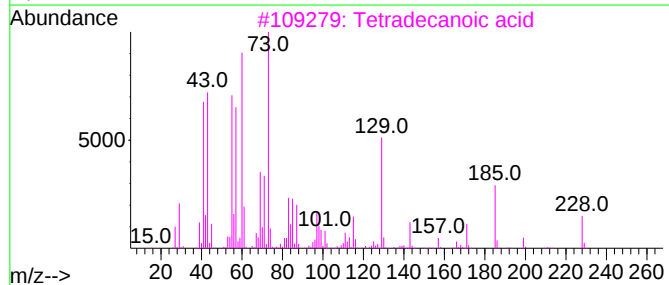
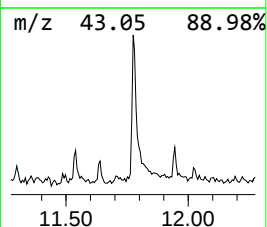
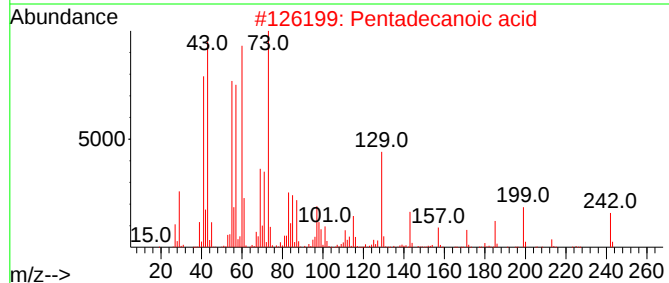
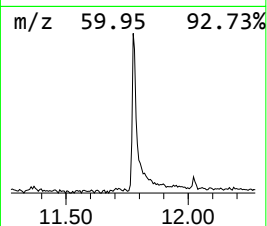
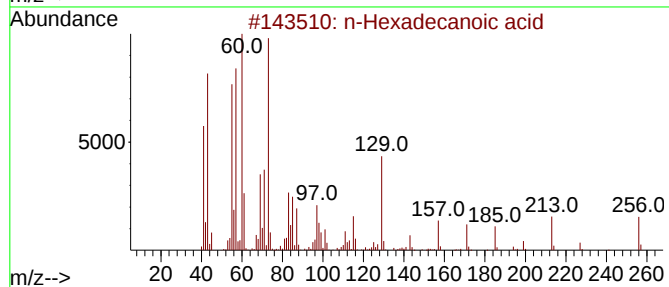
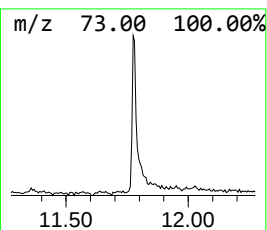
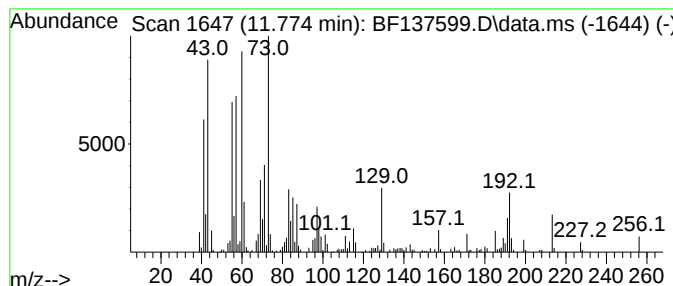
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.775	3.95 ng	222245	Phenanthrene-d10	11.239

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	78
5			Tridecanoic acid	214	C13H26O2	000638-53-9	64



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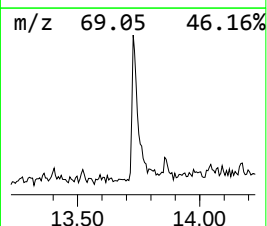
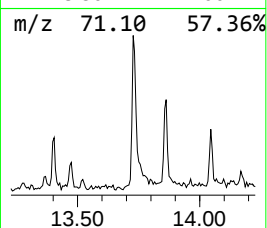
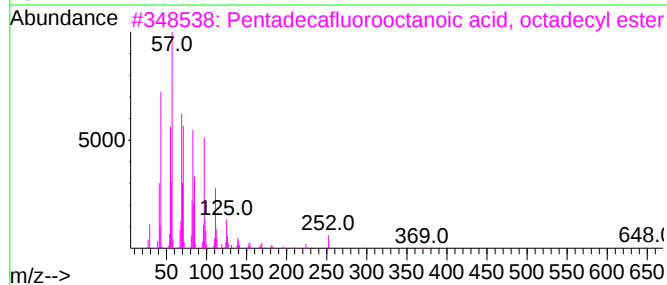
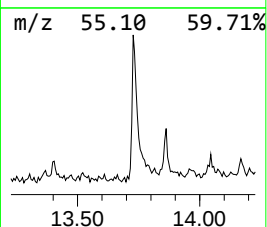
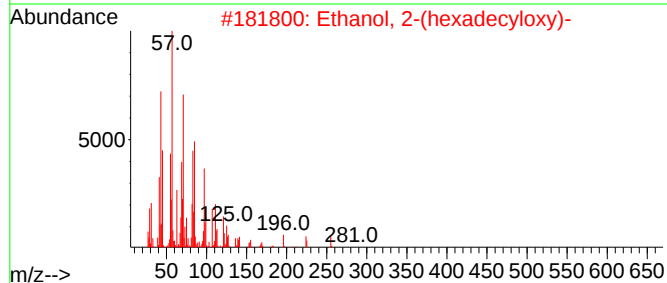
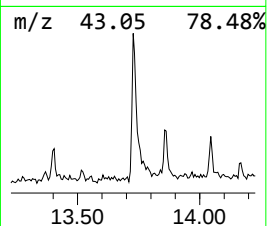
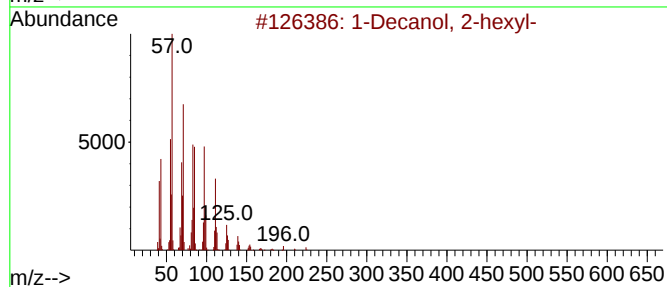
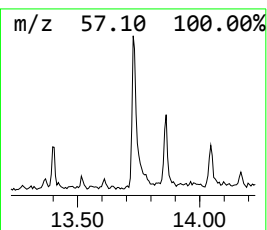
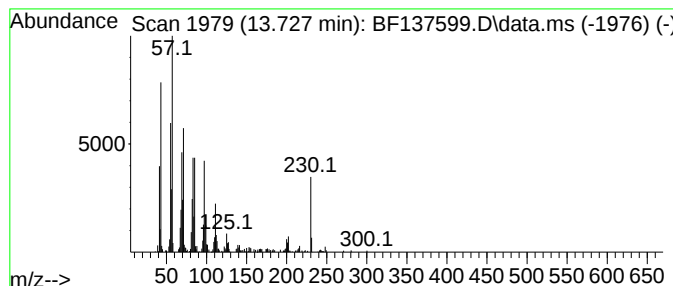
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Decanol, 2-hexyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.727	5.20 ng	310438	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol, 2-hexyl-			242	C16H34O	002425-77-6	90
2	Ethanol, 2-(hexadecyloxy)-			286	C18H38O2	002136-71-2	83
3	Pentadecafluorooctanoic acid, oc...			666	C26H37F15O2	1000406-04-8	81
4	Ethanol, 2-(tetradecyloxy)-			258	C16H34O2	002136-70-1	74
5	Docosyl pentafluoropropionate			472	C25H45F5O2	1000351-80-9	74



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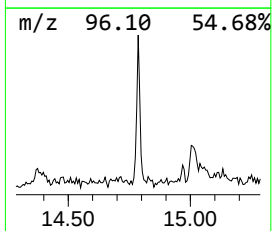
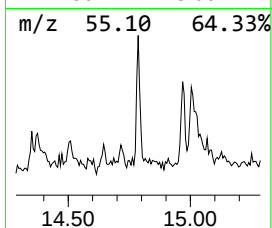
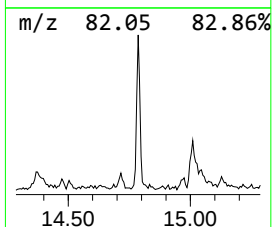
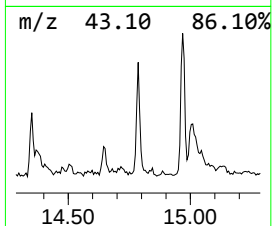
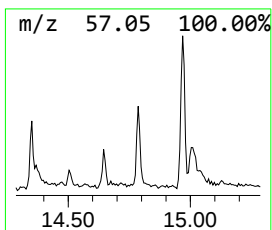
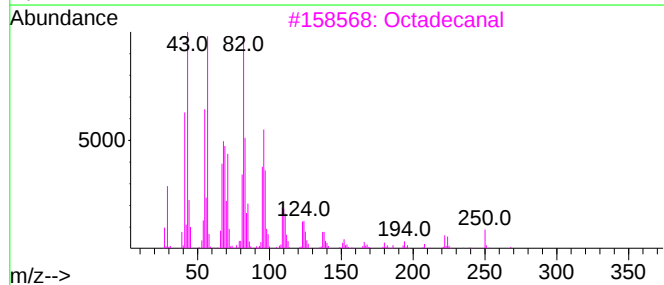
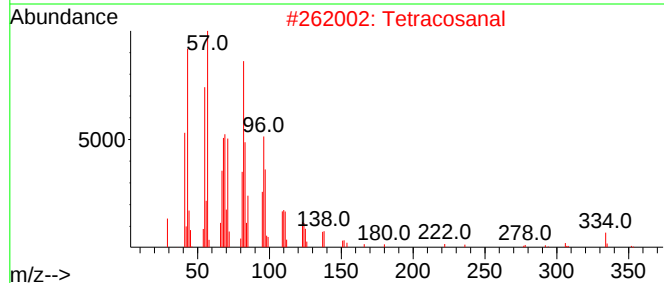
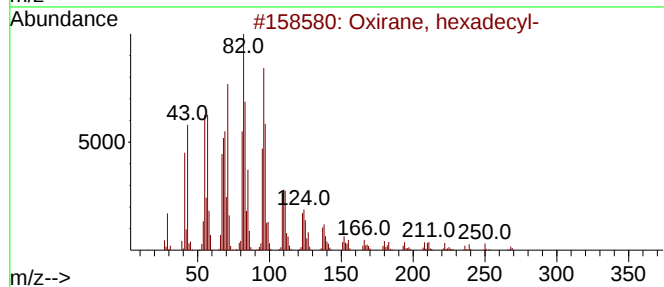
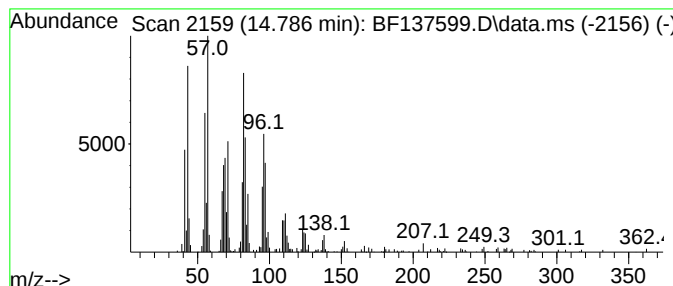
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Oxirane, hexadecyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.786	3.09 ng	163778	Perylene-d12	15.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	97
2			Tetracosanal	352	C24H48O	057866-08-7	94
3			Octadecanal	268	C18H36O	000638-66-4	93
4			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91
5			Eicosanal-	296	C20H40O	002400-66-0	87



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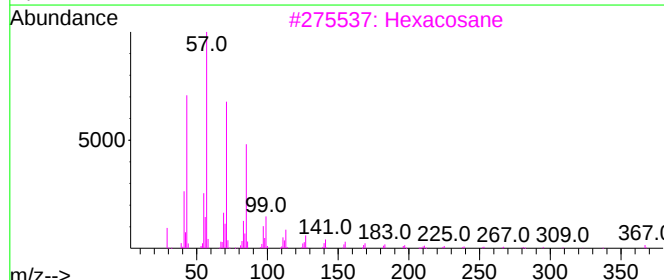
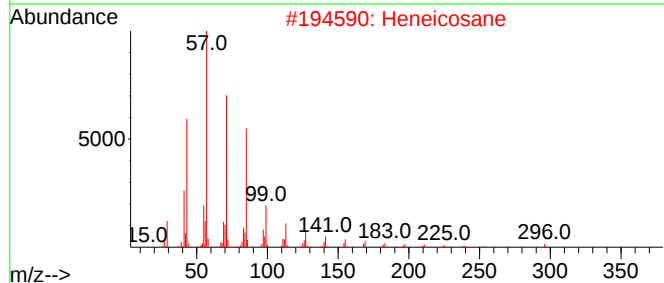
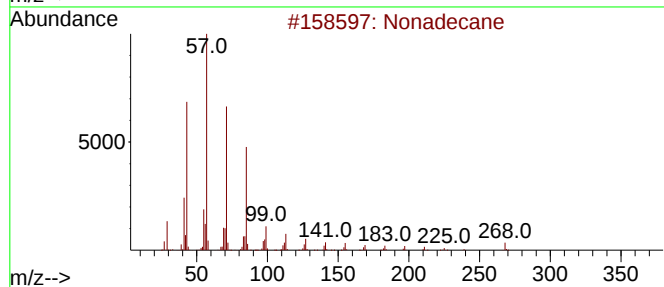
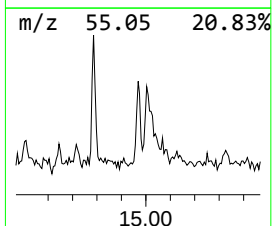
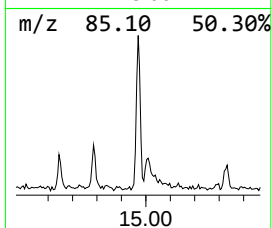
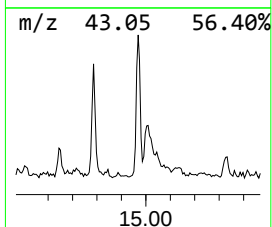
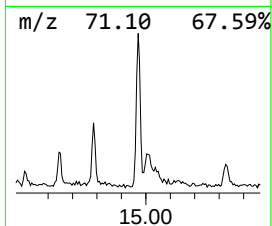
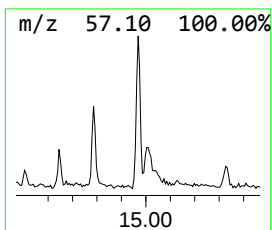
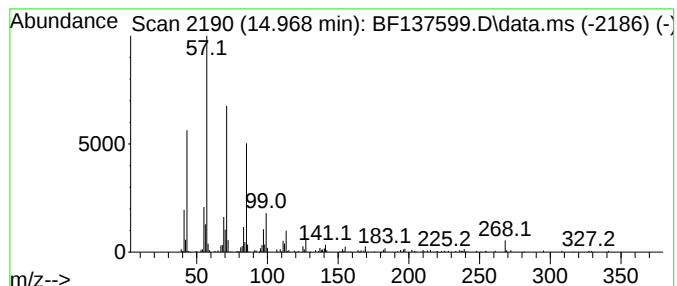
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.968	3.27 ng	173497	Perylene-d12	15.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	94
2			Heneicosane	296	C21H44	000629-94-7	91
3			Hexacosane	366	C26H54	000630-01-3	91
4			Octacosane	394	C28H58	000630-02-4	91
5			Tetracosane	338	C24H50	000646-31-1	90



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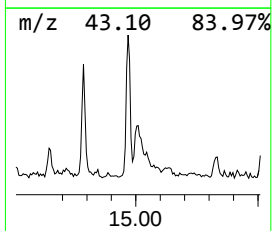
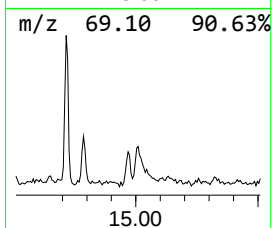
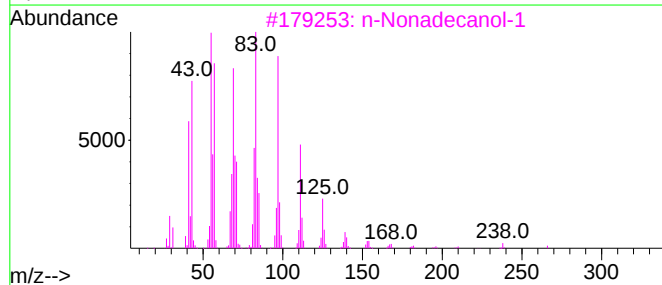
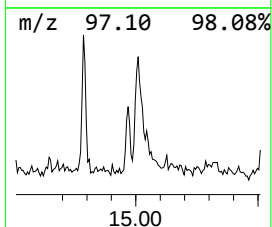
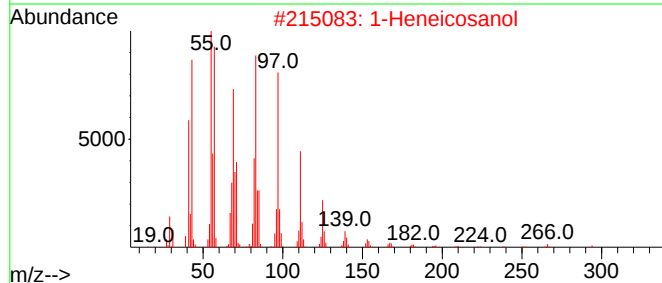
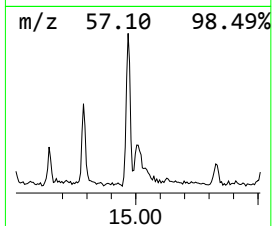
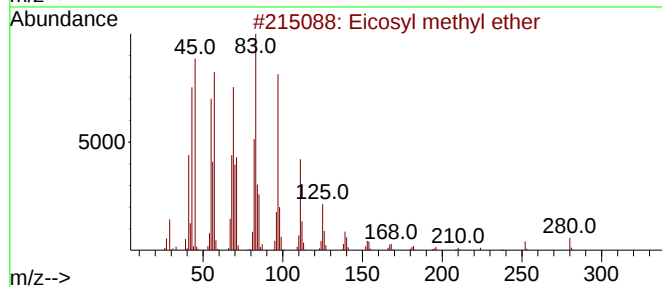
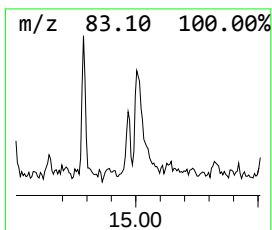
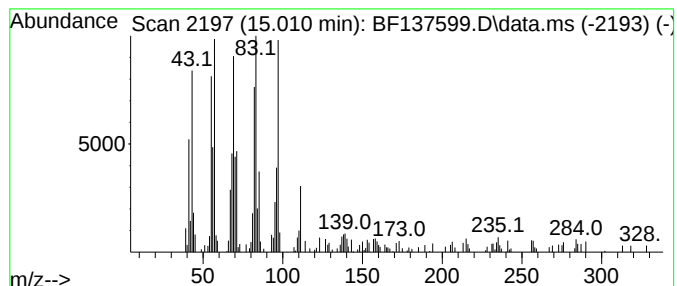
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Eicosyl methyl ether Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.009	3.41 ng	181094	Perylene-d12	15.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosyl methyl ether	312	C21H44O	1000406-29-4	72
2			1-Heneicosanol	312	C21H44O	015594-90-8	62
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	58
4			13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	49
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031424\
Data File : BF137599.D
Acq On : 14 Mar 2024 19:29
Operator : CG\JU
Sample : P1746-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-01-7.0-9.5

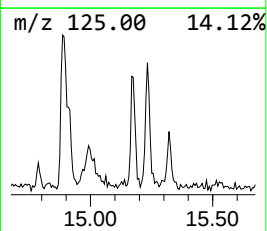
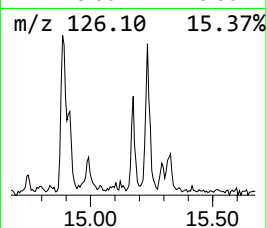
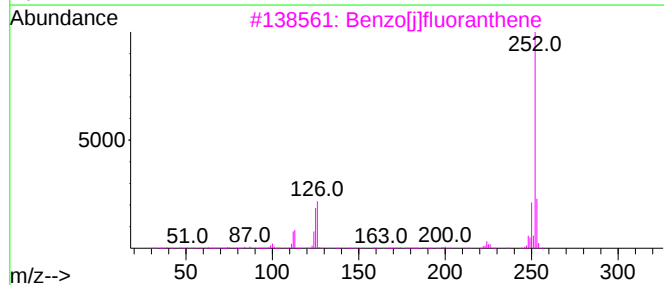
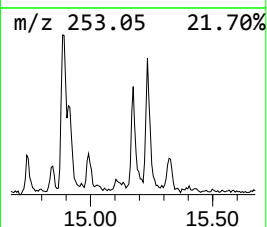
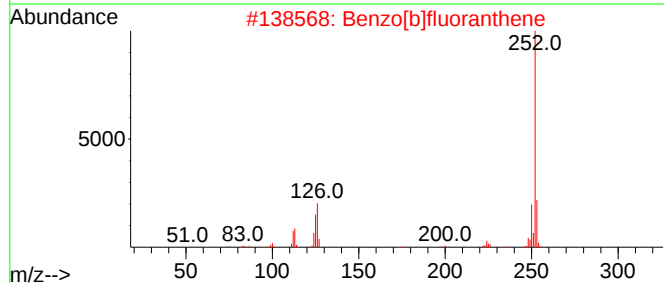
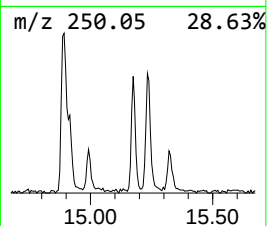
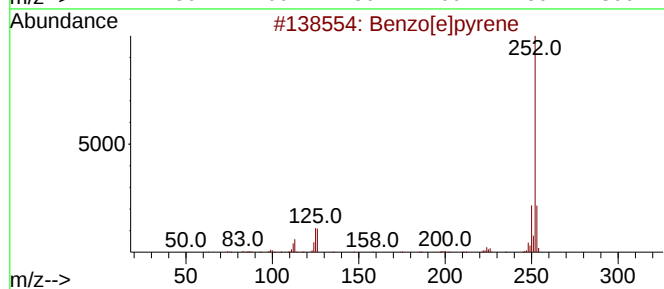
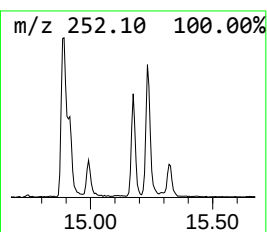
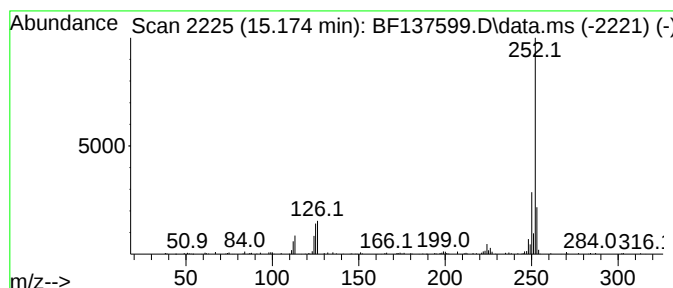
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzo[e]pyrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.174	2.44 ng	129661	Perylene-d12	15.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	98
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
3			Benzo[j]fluoranthene	252	C20H12	000205-82-3	96
4			Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
5			Perylene	252	C20H12	000198-55-0	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031424\
Data File : BF137599.D
Acq On : 14 Mar 2024 19:29
Operator : CG\JU
Sample : P1746-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-01-7.0-9.5

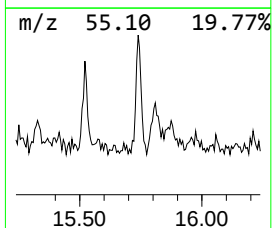
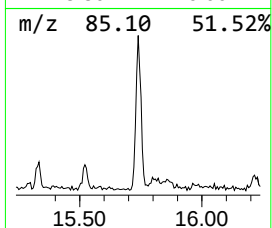
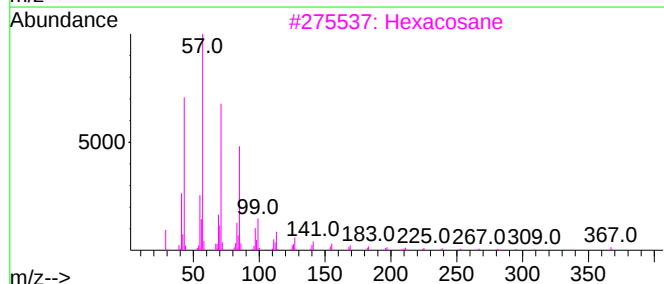
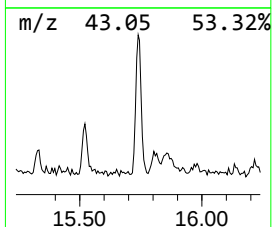
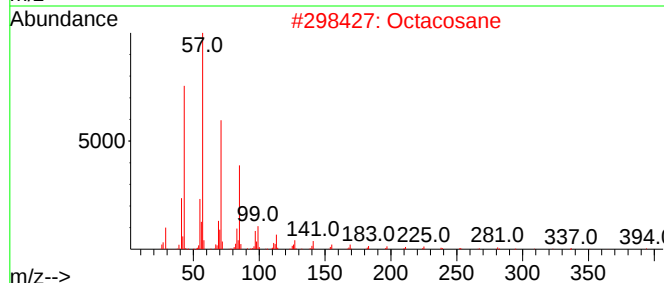
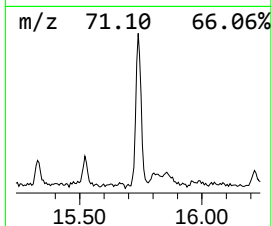
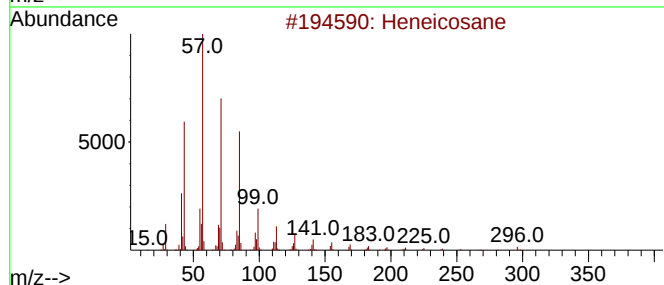
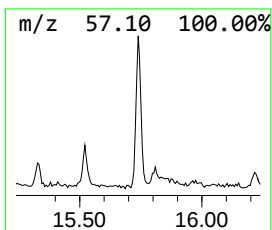
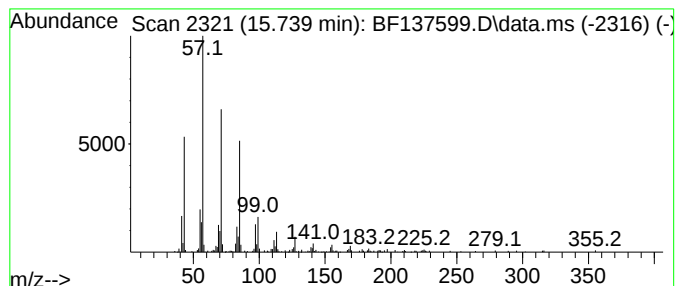
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.739	3.65 ng	193596	Perylene-d12	15.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Octacosane	394	C28H58	000630-02-4	91
3			Hexacosane	366	C26H54	000630-01-3	91
4			Tetracosane	338	C24H50	000646-31-1	91
5			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031424\
Data File : BF137599.D
Acq On : 14 Mar 2024 19:29
Operator : CG\JU
Sample : P1746-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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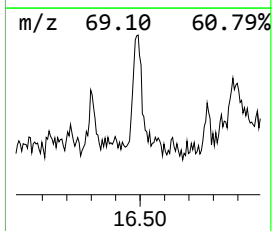
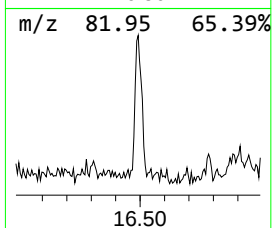
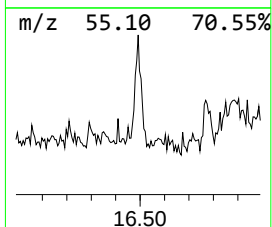
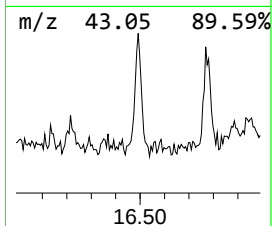
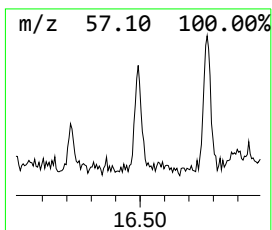
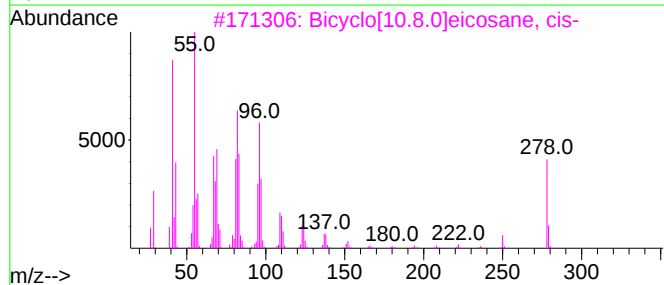
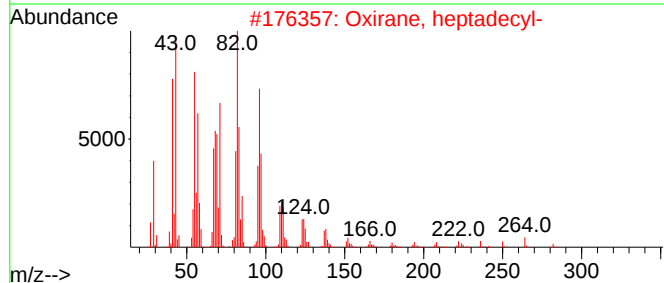
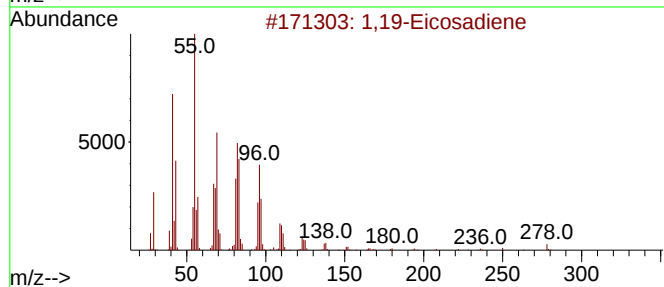
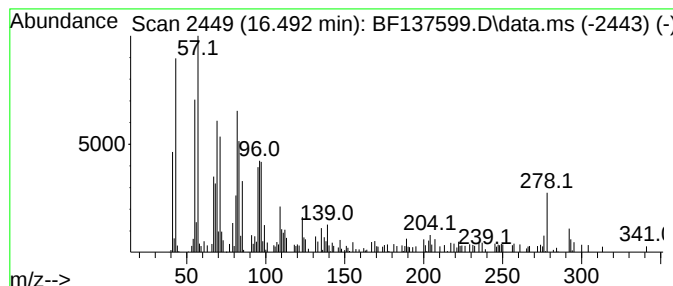
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1,19-Eicosadiene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.492	3.36 ng	178212	Perylene-d12	15.292

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene		278	C20H38	014811-95-1	64
2	Oxirane, heptadecyl-		282	C19H38O	067860-04-2	55
3	Bicyclo[10.8.0]eicosane, cis-		278	C20H38	1000155-82-2	50
4	Hexadecane, 1,1-bis(dodecyloxy)-		595	C40H82O2	056554-64-4	46
5	Octadecanal		268	C18H36O	000638-66-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031424\
Data File : BF137599.D
Acq On : 14 Mar 2024 19:29
Operator : CG\JU
Sample : P1746-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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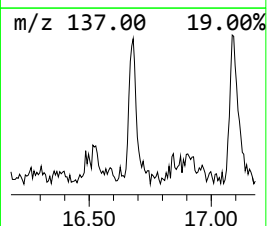
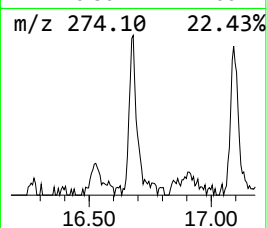
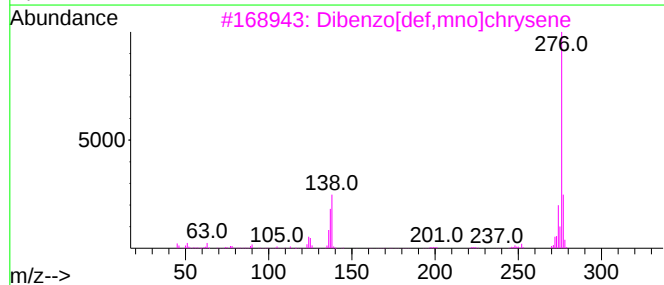
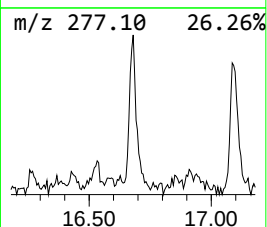
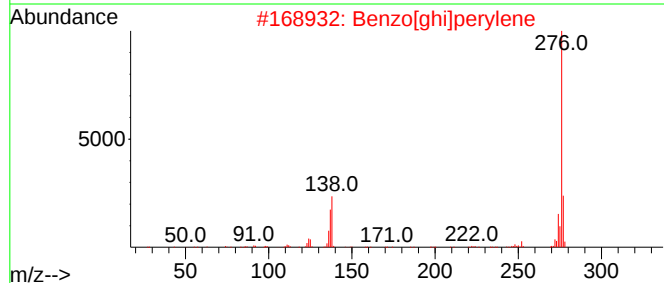
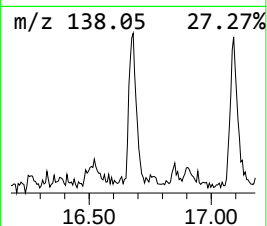
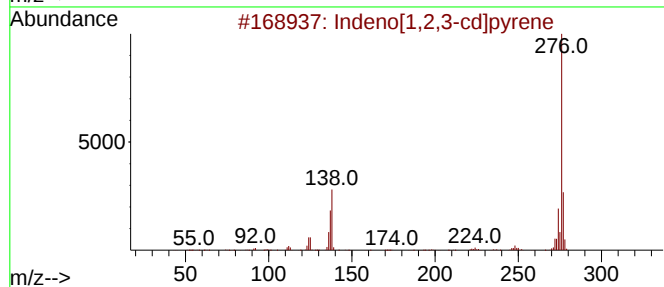
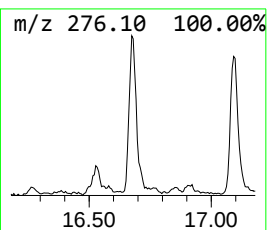
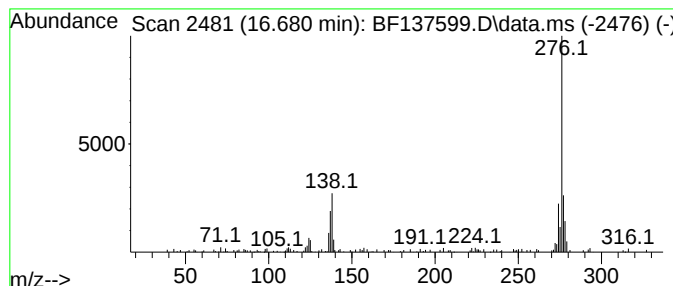
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Dibenzo[def,mno]chrysene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.680	2.61 ng	138493	Perylene-d12	15.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	93
2			Benzo[ghi]perylene	276	C22H12	000191-24-2	93
3			Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	90
4			Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	68
5			1,3,5-Triazin-2-amine, N-isoprop...	276	C14H24N6	1000276-80-0	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031424\
Data File : BF137599.D
Acq On : 14 Mar 2024 19:29
Operator : CG\JU
Sample : P1746-04
Misc :
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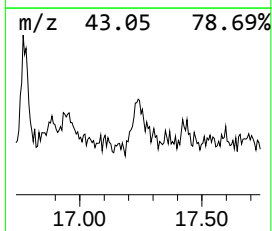
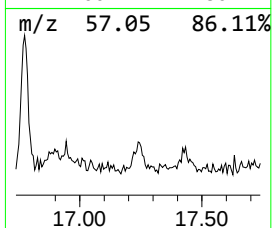
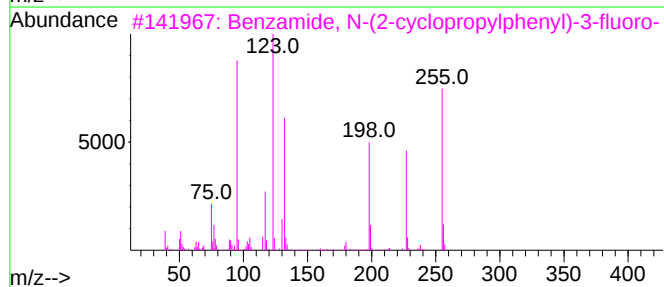
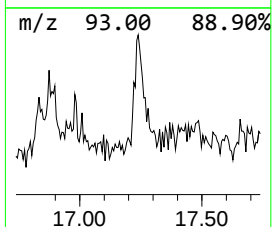
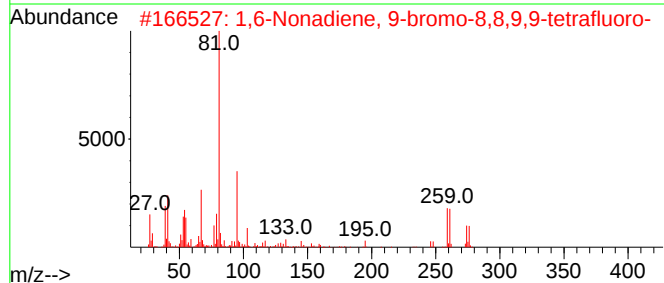
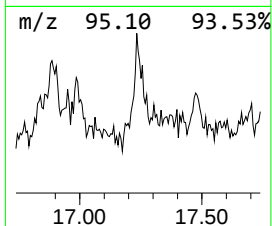
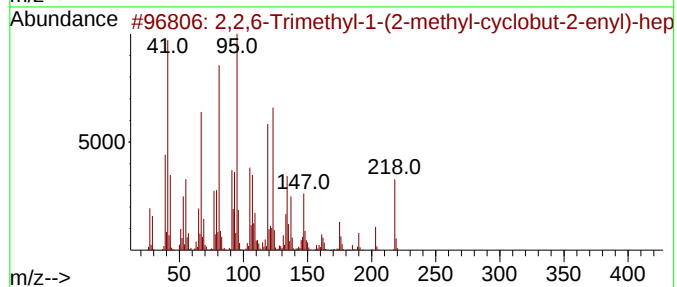
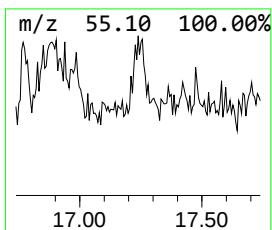
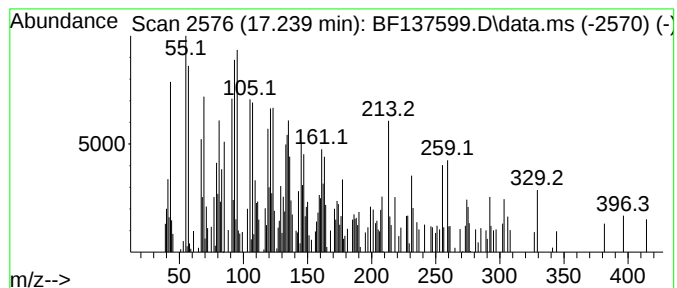
Instrument :
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ClientSampleId :
SB-01-7.0-9.5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2,2,6-Trimethyl-1-(2-methyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.239	3.27 ng	173548	Perylene-d12	15.292	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,6-Trimethyl-1-(2-methyl-cycl...	218	C15H22O	1000188-72-8	53
2	1,6-Nonadiene, 9-bromo-8,8,9,9-t...	274	C9H11BrF4	1010149-23-4	45
3	Benzamide, N-(2-cyclopropylpheny...	255	C16H14FNO	1000351-11-8	30
4	1-[p-Nitrophenyl]-3-[2-pyrimidyl...	259	C11H9N5O3	023656-31-7	27
5	Isobenzofuran-1(3H)-one, 3-(3-fu...	232	C14H16O3	1000260-36-9	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031424\
Data File : BF137599.D
Acq On : 14 Mar 2024 19:29
Operator : CG\JU
Sample : P1746-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-01-7.0-9.5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.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
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1-Decanol, 2-he...	13.727	5.2	ng	310438	5	13.874	1194450	20.0
Oxirane, hexade...	14.786	3.1	ng	163778	6	15.292	1061000	20.0
Nonadecane	14.968	3.3	ng	173497	6	15.292	1061000	20.0
Eicosyl methyl ...	15.009	3.4	ng	181094	6	15.292	1061000	20.0
Benzo[e]pyrene	15.174	2.4	ng	129661	6	15.292	1061000	20.0
Heneicosane	15.739	3.6	ng	193596	6	15.292	1061000	20.0
1,19-Eicosadiene	16.492	3.4	ng	178212	6	15.292	1061000	20.0
Dibenzo[def,mno...	16.680	2.6	ng	138493	6	15.292	1061000	20.0
2,2,6-Trimethyl...	17.239	3.3	ng	173548	6	15.292	1061000	20.0