

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082522\
 Data File : BF129999.D
 Acq On : 25 Aug 2022 14:58
 Operator : CG\JU
 Sample : N4292-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TR-04-082222

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-BF081422.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129999.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.969	453	456	470	rBV	247562	321433	13.76%	1.640%
2	5.393	525	528	555	rBV	2084558	2215560	94.85%	11.303%
3	6.416	699	702	719	rBV	2319074	2106778	90.19%	10.748%
4	6.757	756	760	768	rBV	718259	650031	27.83%	3.316%
5	7.328	853	857	869	rBV	1472490	1373454	58.80%	7.007%
6	8.040	974	978	981	rBV	881105	795439	34.05%	4.058%
7	8.751	1097	1099	1105	rVB	36586	33471	1.43%	0.171%
8	9.110	1156	1160	1163	rBV	2967274	2335842	100.00%	11.917%
9	9.787	1272	1275	1279	rBV	892858	725904	31.08%	3.703%
10	9.822	1279	1281	1284	rVB	53924	43868	1.88%	0.224%
11	9.998	1306	1311	1315	rBV	34976	33158	1.42%	0.169%
12	10.339	1366	1369	1375	rVB	35789	36113	1.55%	0.184%
13	10.581	1407	1410	1423	rBV	1266815	1156661	49.52%	5.901%
14	10.686	1423	1428	1434	rVV3	22096	34452	1.47%	0.176%
15	11.281	1525	1529	1531	rBV	705286	640759	27.43%	3.269%
16	11.304	1531	1533	1538	rVB	128917	118726	5.08%	0.606%
17	11.798	1612	1617	1624	rBV3	100684	171687	7.35%	0.876%
18	11.892	1631	1633	1636	rBV3	29427	34969	1.50%	0.178%
19	12.510	1732	1738	1748	rBV2	463157	876379	37.52%	4.471%
20	12.586	1748	1751	1755	rVV2	78947	86748	3.71%	0.443%
21	12.727	1770	1775	1781	rBV	193285	223873	9.58%	1.142%
22	12.863	1794	1798	1801	rBV	2304864	2104278	90.09%	10.736%
23	13.810	1954	1959	1968	rBV7	55134	199672	8.55%	1.019%
24	13.880	1968	1971	1975	rVV	322212	296843	12.71%	1.514%
25	13.927	1975	1979	1982	rVV2	810715	842439	36.07%	4.298%
26	13.951	1982	1983	1988	rVB	99669	91932	3.94%	0.469%
27	14.010	1991	1993	1996	rVB	82889	71341	3.05%	0.364%
28	14.363	2051	2053	2055	rBV	53474	40909	1.75%	0.209%
29	14.392	2056	2058	2063	rBV2	82017	85536	3.66%	0.436%
30	14.469	2065	2071	2073	rBV6	88389	181496	7.77%	0.926%
31	14.804	2126	2128	2133	rVB4	86822	80315	3.44%	0.410%
32	14.980	2152	2158	2164	rVB2	268713	452599	19.38%	2.309%
33	15.257	2203	2205	2211	rVB	64914	72258	3.09%	0.369%
34	15.321	2213	2216	2218	rVV	82834	101006	4.32%	0.515%
35	15.374	2221	2225	2234	rVB	553564	713130	30.53%	3.638%
36	15.751	2286	2289	2294	rVB	189450	251877	10.78%	1.285%

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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-BF081422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

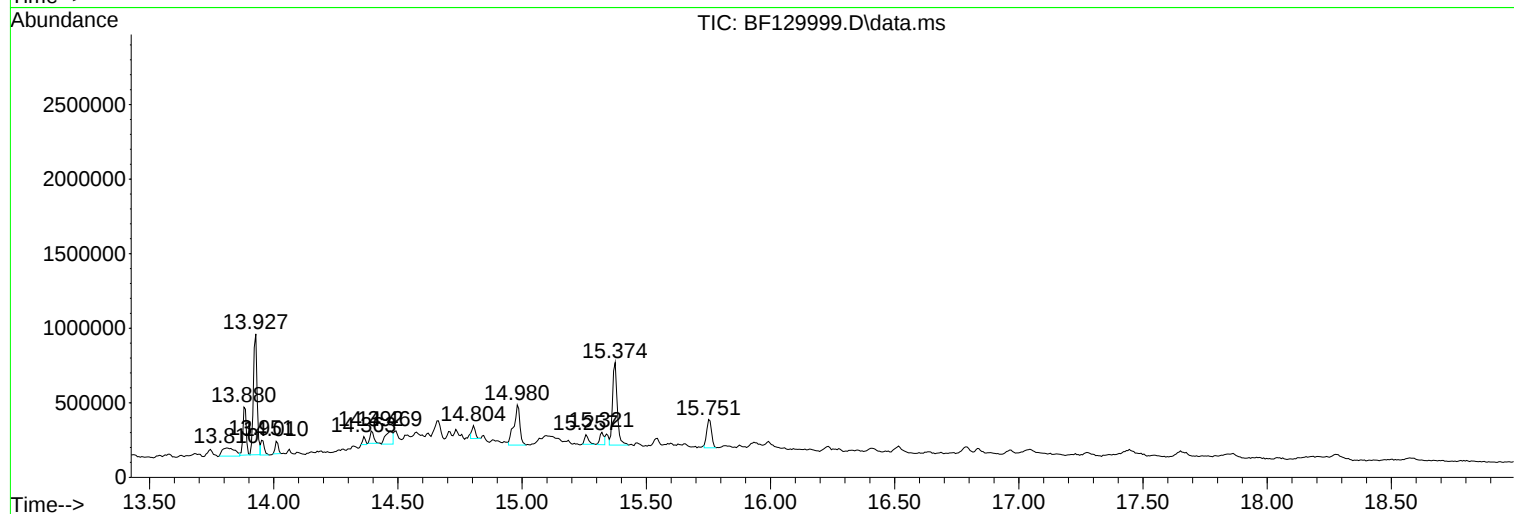
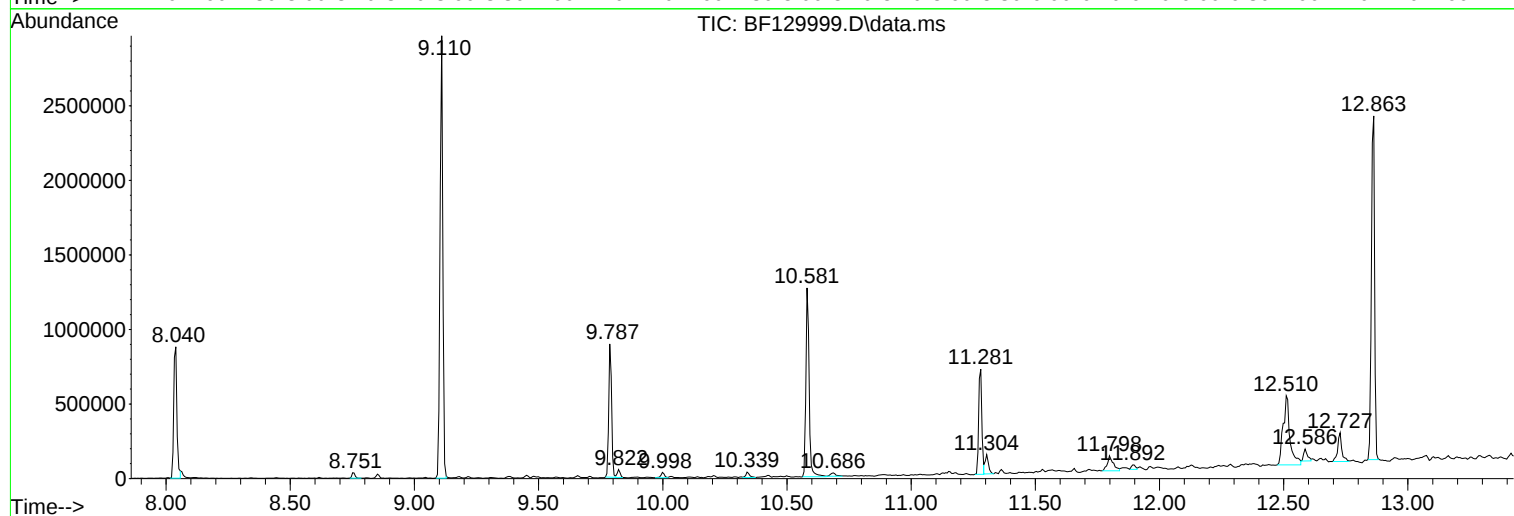
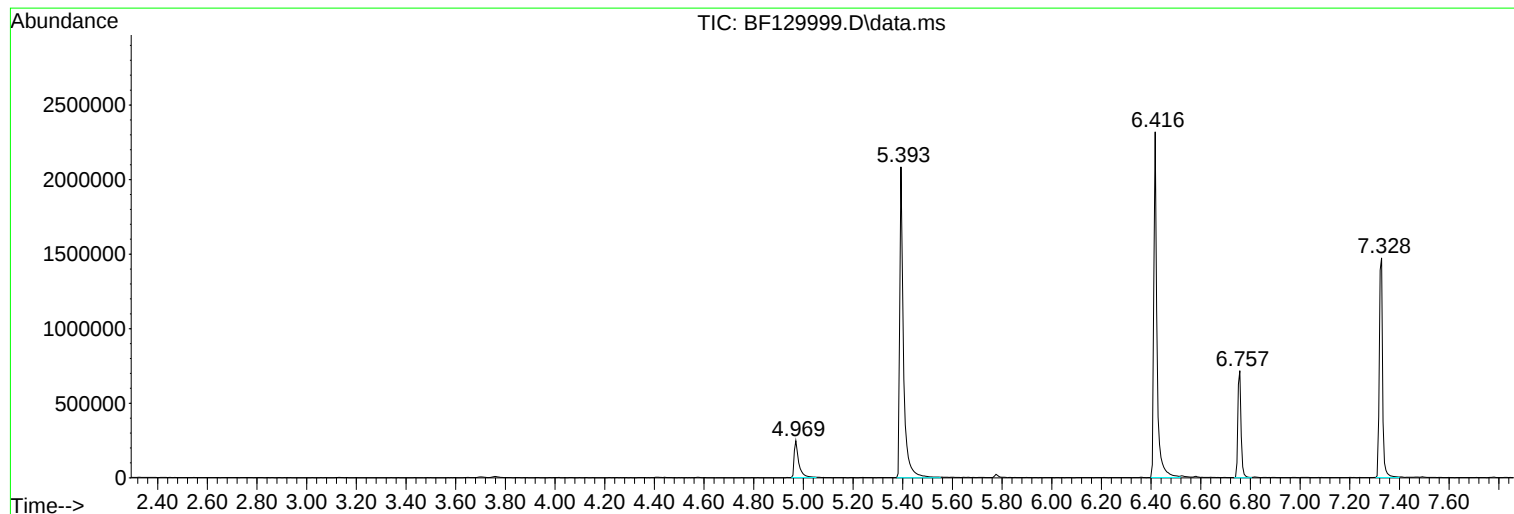
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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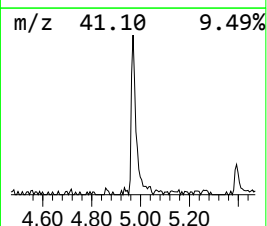
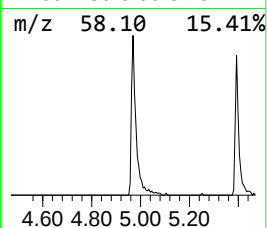
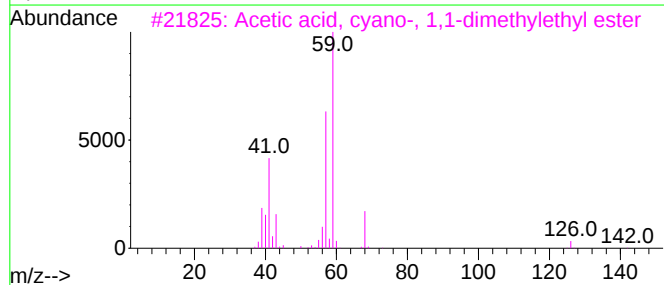
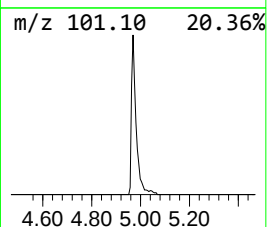
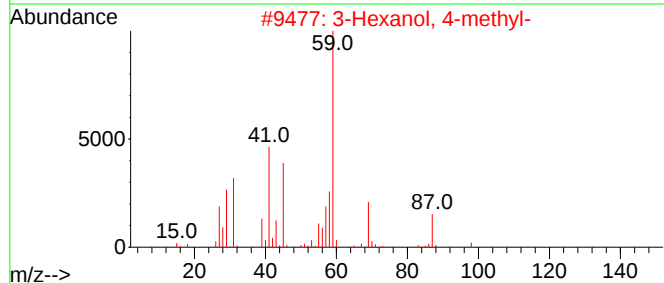
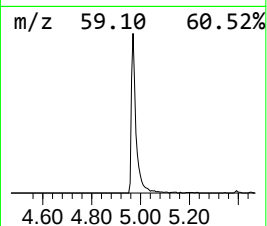
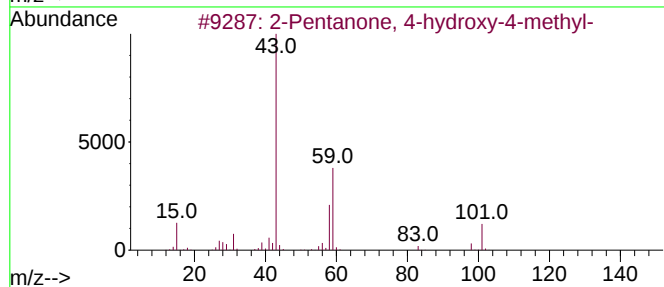
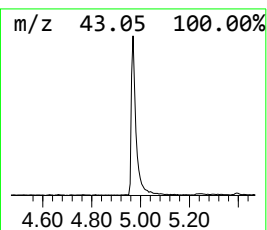
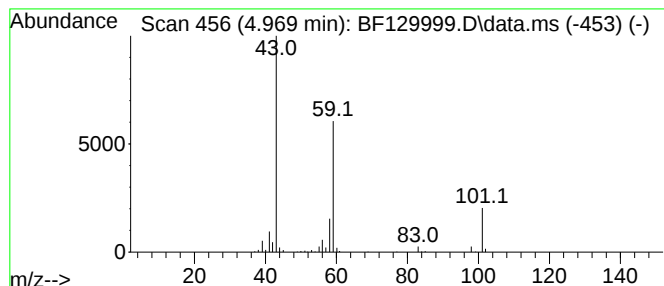
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.969	9.89 ng	321433	1,4-Dichlorobenzene-d4	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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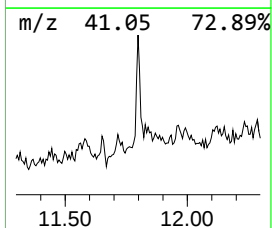
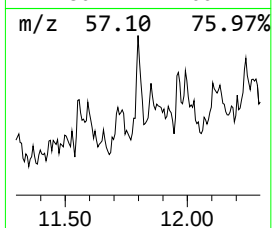
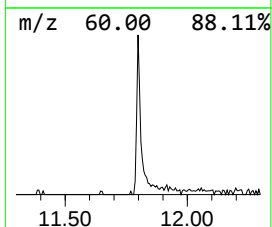
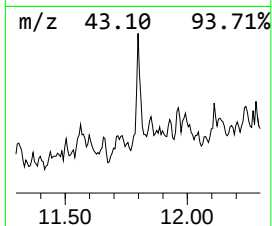
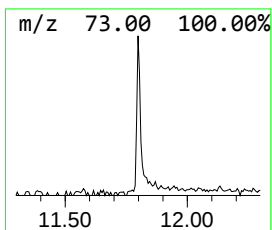
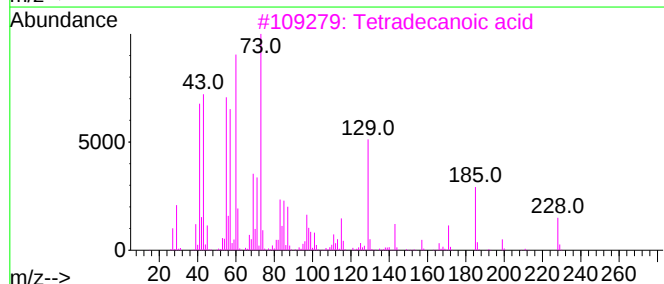
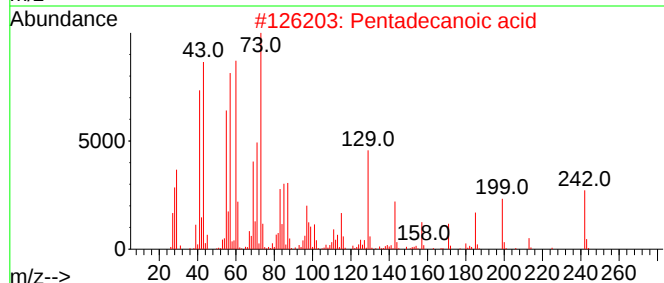
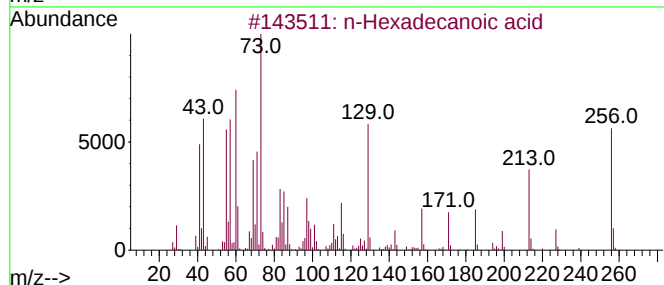
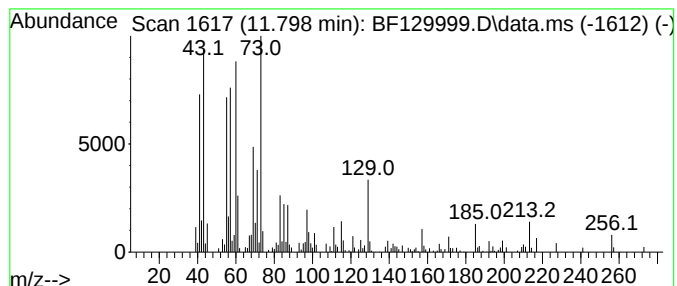
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.798	5.36 ng	171687	Phenanthrene-d10	11.281

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		Tridecanoic acid	214	C13H26O2	000638-53-9	72
5		Nonanoic acid	158	C9H18O2	000112-05-0	53



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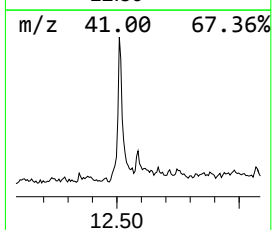
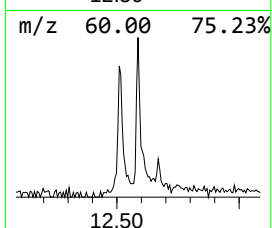
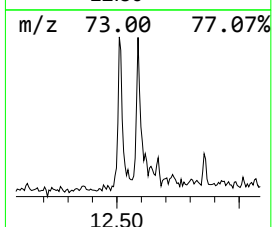
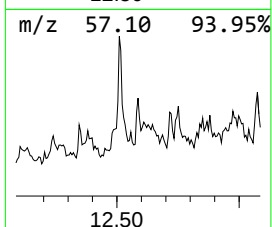
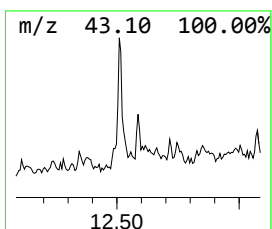
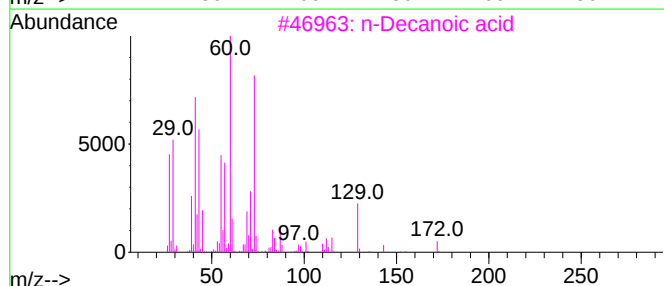
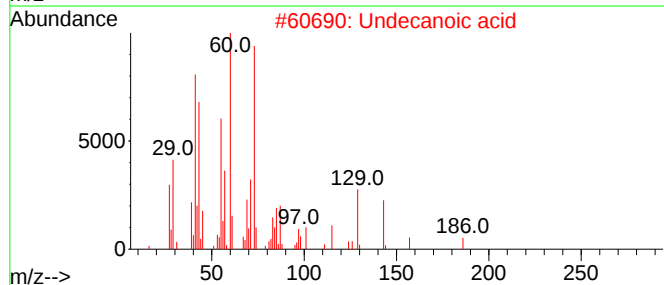
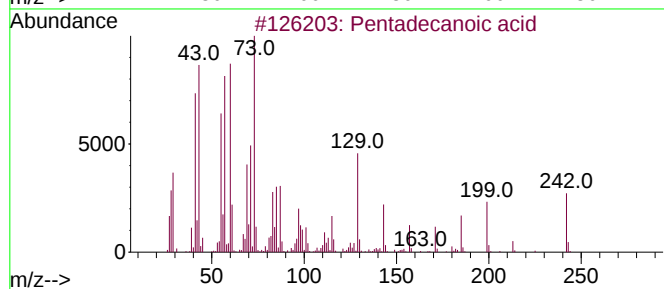
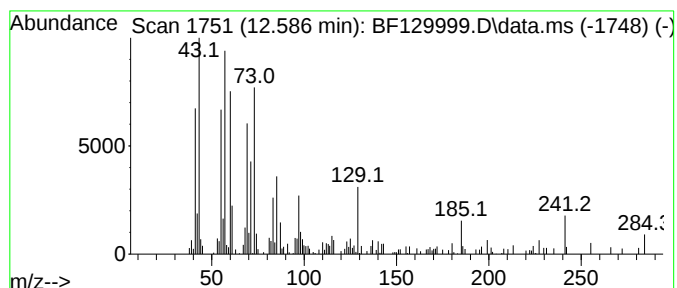
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Pentadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.586	2.71 ng	86748	Phenanthrene-d10	11.281

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	80
2			Undecanoic acid	186	C11H22O2	000112-37-8	53
3			n-Decanoic acid	172	C10H20O2	000334-48-5	46
4			Heptanoic acid	130	C7H14O2	000111-14-8	38
5			N-Acetylisoaxazolidine	115	C5H9NO2	115615-36-6	30



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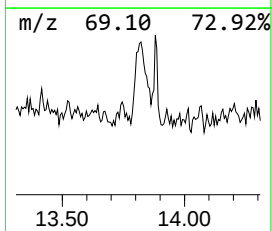
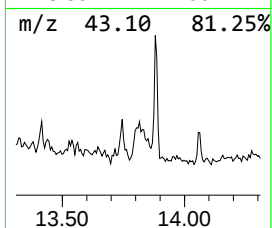
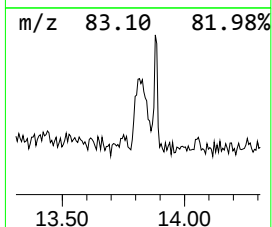
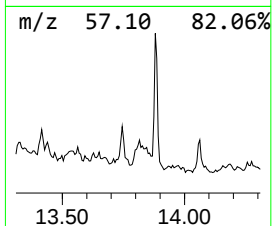
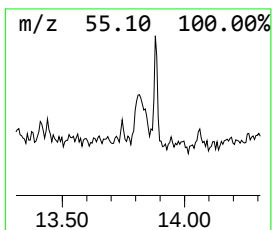
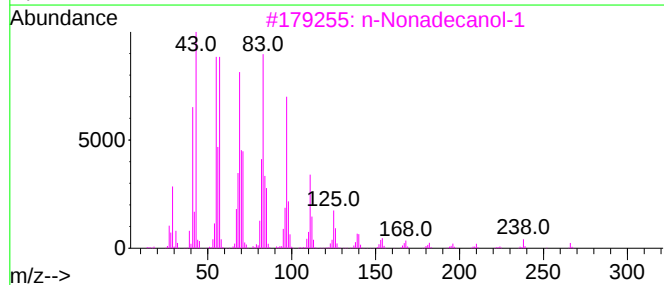
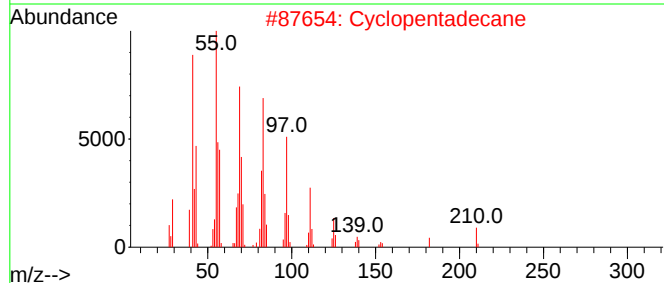
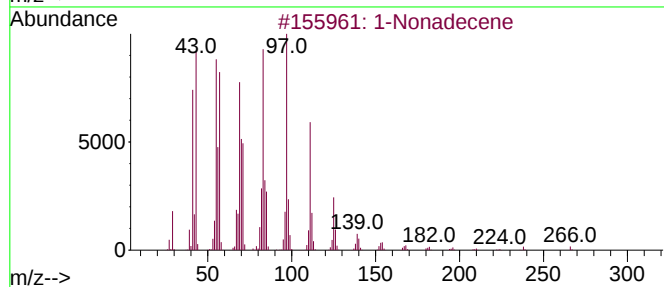
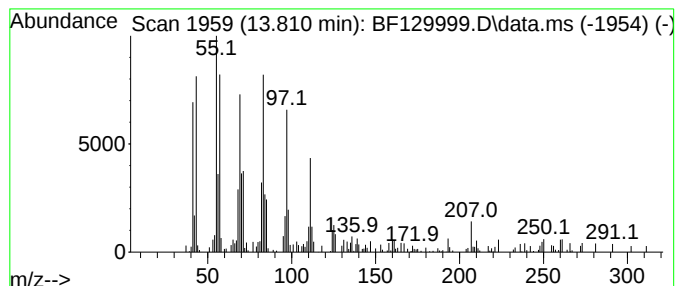
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1-Nonadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.810	4.74 ng	199672	Chrysene-d12	13.927

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Nonadecene	266	C19H38	018435-45-5	96
2			Cyclopentadecane	210	C15H30	000295-48-7	96
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	93
4			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	93
5			4-Methyl-E-9-octadecene	266	C19H38	1000130-87-1	93



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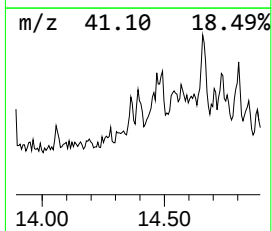
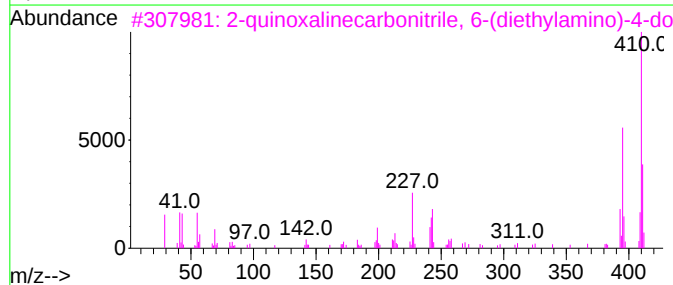
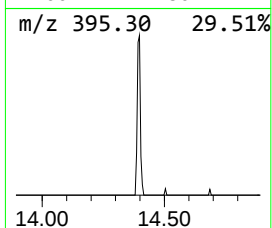
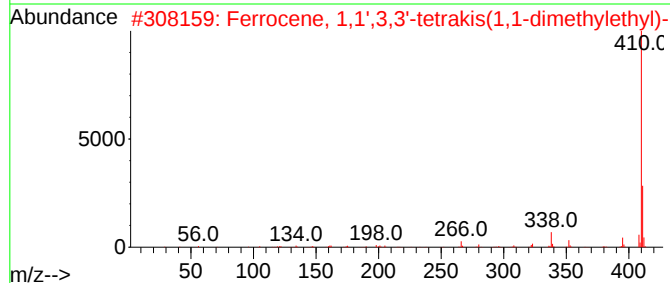
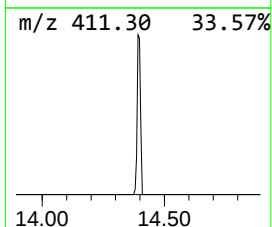
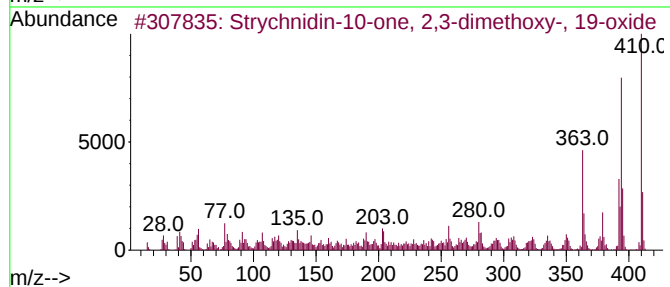
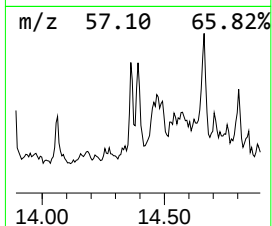
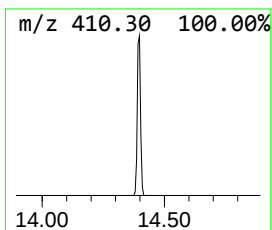
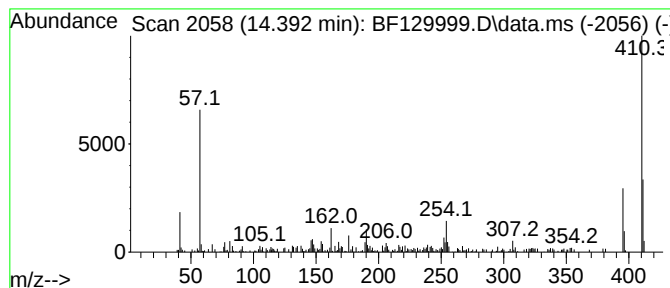
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Strychnidin-10-one, 2,3-dim... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.392	2.03 ng	85536	Chrysene-d12	13.927

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Strychnidin-10-one, 2,3-dimethox...	410	C23H26N2O5	017301-81-4	72
2			Ferrocene, 1,1',3,3'-tetrakis(1,...	410	C26H42Fe	001317-17-5	58
3			2-quinolinecarbonitrile, 6-(di...	410	C25H38N4O	1000399-06-1	50
4			Silane, diphenyl(4-biphenyloxy)p...	410	C27H26O2Si	1000367-49-5	38
5			2'-Hydroxy-3,3',4'-trimethoxycha...	410	C20H17F3O6	1010453-84-8	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082522\
Data File : BF129999.D
Acq On : 25 Aug 2022 14:58
Operator : CG\JU
Sample : N4292-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TR-04-082222

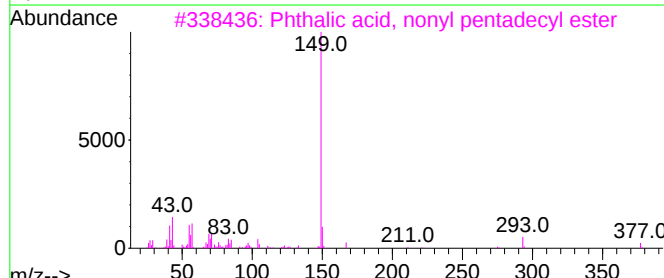
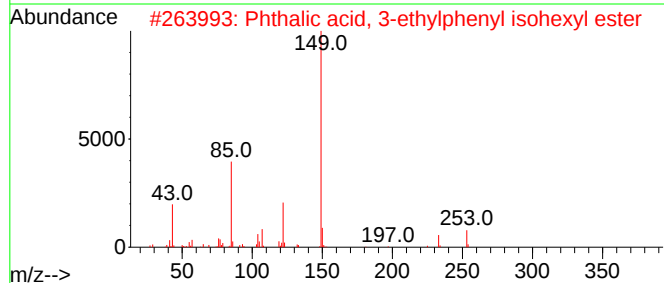
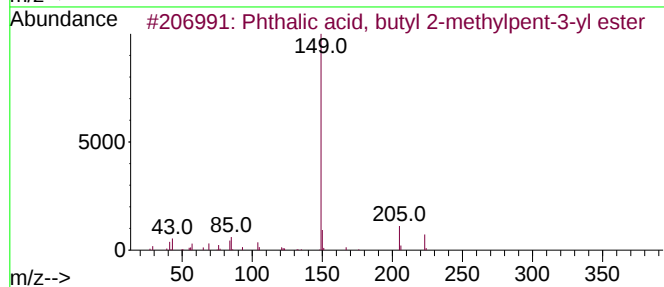
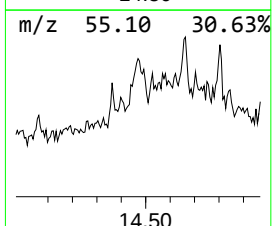
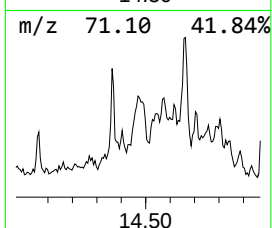
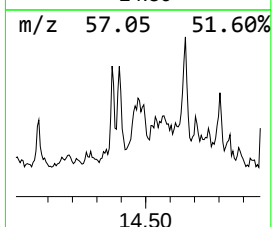
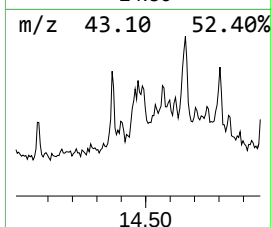
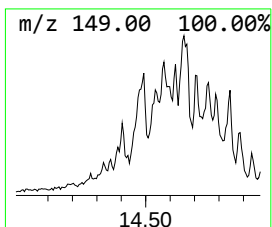
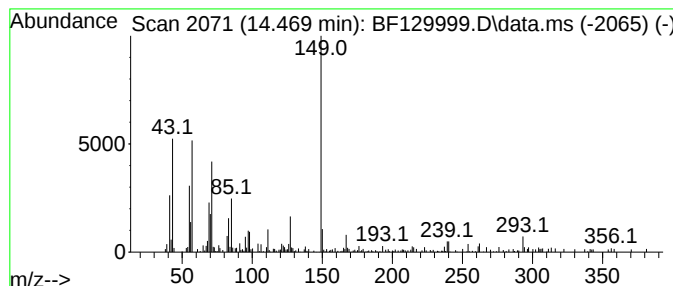
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown14.469 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.469	4.31 ng	181496	Chrysene-d12	13.927

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic acid, butyl 2-methylpen...	306	C18H26O4	1000356-90-8	43
2			Phthalic acid, 3-ethylphenyl iso...	354	C22H26O4	1000357-08-0	43
3			Phthalic acid, nonyl pentadecyl ...	502	C32H54O4	1000308-92-7	43
4			Phthalic acid, monoamide, N-meth...	339	C21H25NO3	1000322-84-3	43
5			Phthalic acid, 3,3-dimethylbut-2...	306	C18H26O4	1000357-00-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082522\
Data File : BF129999.D
Acq On : 25 Aug 2022 14:58
Operator : CG\JU
Sample : N4292-01
Misc :
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BNA_F
ClientSampleId :
TR-04-082222

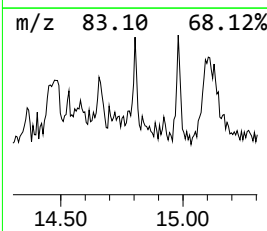
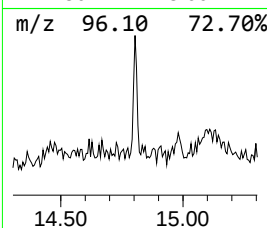
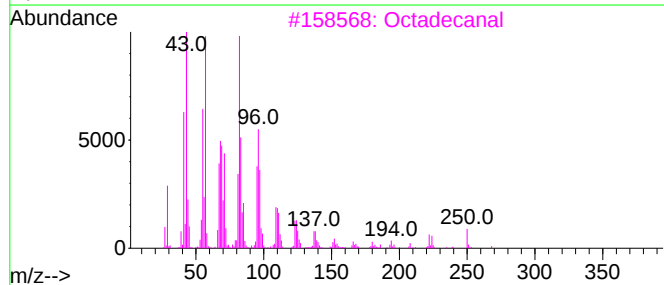
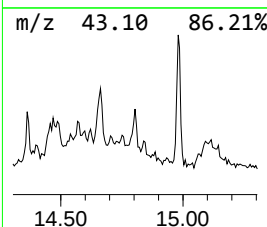
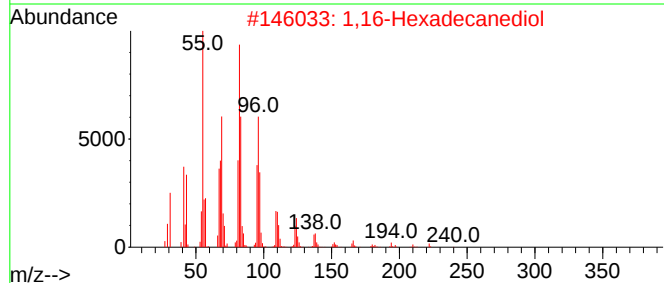
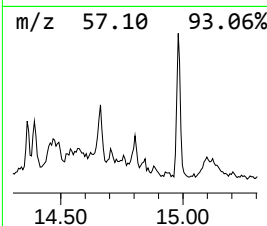
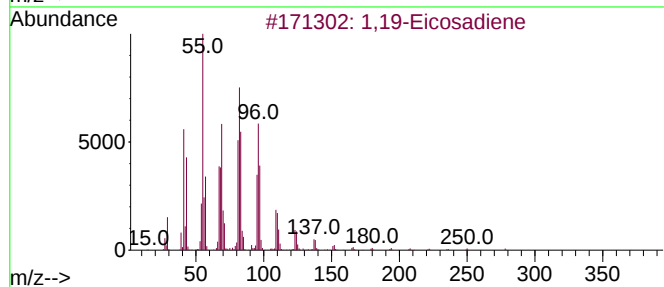
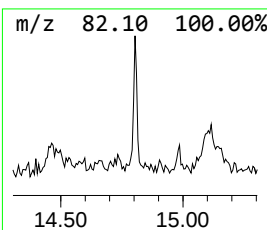
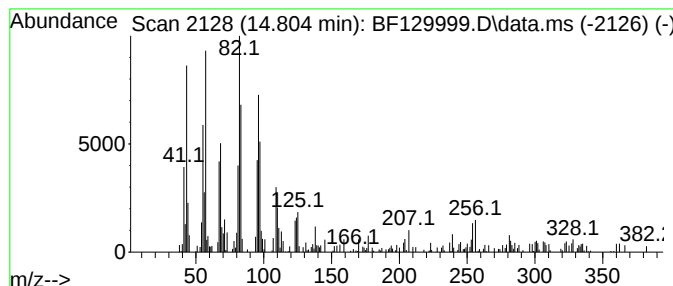
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1,19-Eicosadiene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.804	2.25 ng	80315	Perylene-d12	15.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,19-Eicosadiene	278	C20H38	014811-95-1	91
2			1,16-Hexadecanediol	258	C16H34O2	007735-42-4	90
3			Octadecanal	268	C18H36O	000638-66-4	90
4			Bicyclo[10.8.0]eicosane, cis-	278	C20H38	1000155-82-2	89
5			Pentadecanal-	226	C15H30O	002765-11-9	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082522\
Data File : BF129999.D
Acq On : 25 Aug 2022 14:58
Operator : CG\JU
Sample : N4292-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-04-082222

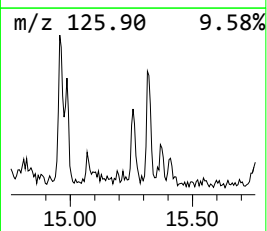
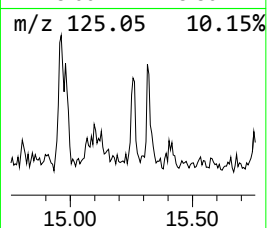
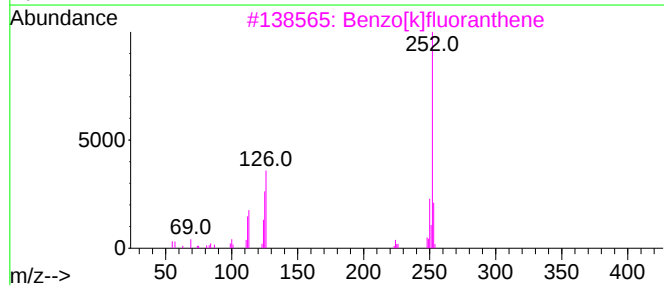
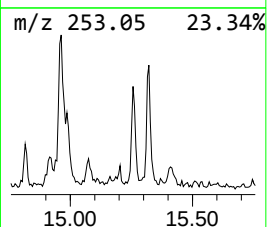
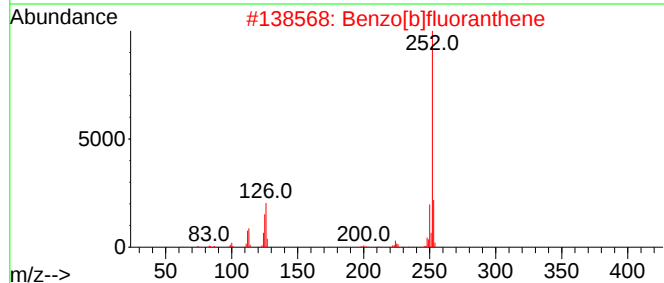
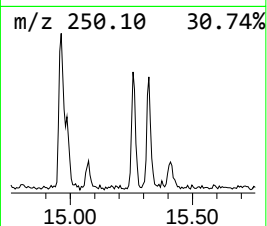
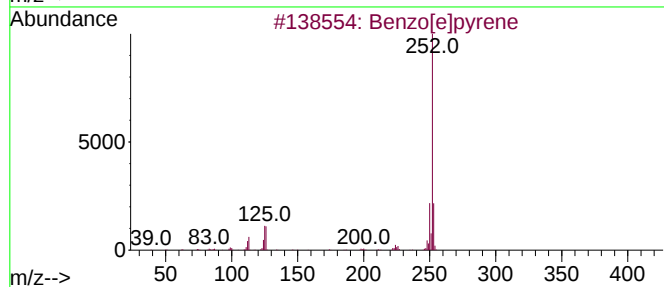
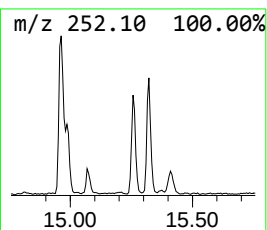
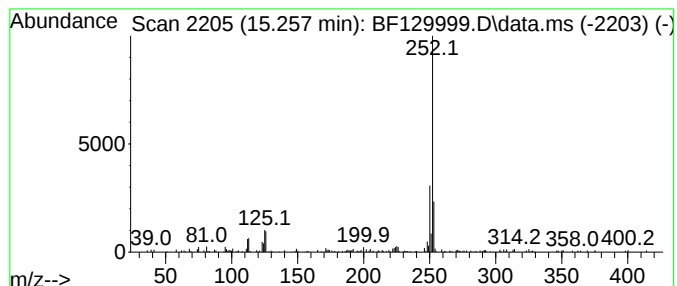
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzo[e]pyrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.257	2.03 ng	72258	Perylene-d12	15.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	93
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	90
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	76
4			Perylene	252	C20H12	000198-55-0	74
5			Benzo[a]pyrene	252	C20H12	000050-32-8	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082522\
Data File : BF129999.D
Acq On : 25 Aug 2022 14:58
Operator : CG\JU
Sample : N4292-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

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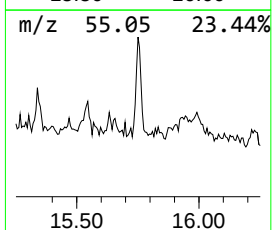
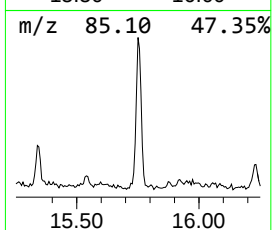
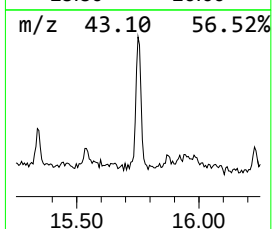
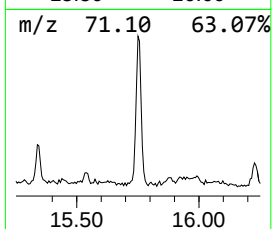
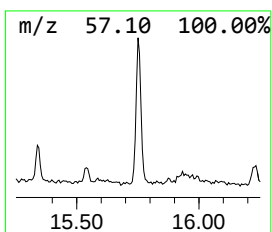
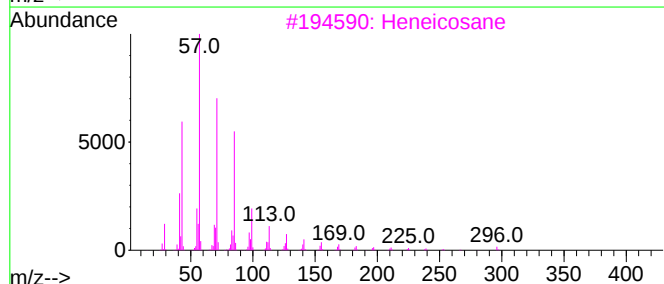
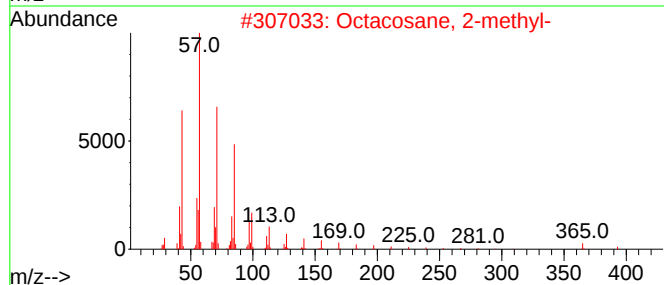
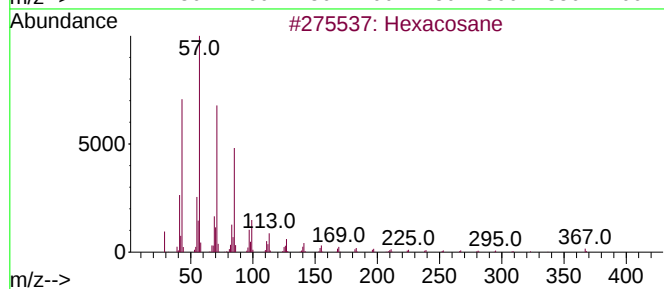
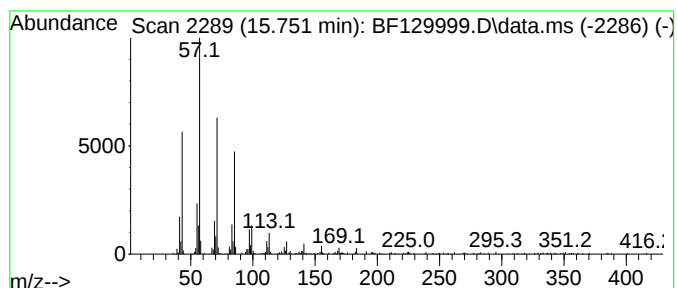
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.751	7.06 ng	251877	Perylene-d12	15.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	90
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
3			Heneicosane	296	C21H44	000629-94-7	90
4			Docosane	310	C22H46	000629-97-0	87
5			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082522\
Data File : BF129999.D
Acq On : 25 Aug 2022 14:58
Operator : CG\JU
Sample : N4292-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.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-...	4.969	9.9	ng	321433	1	6.757	650031	20.0
n-Hexadecanoic ...	11.798	5.4	ng	171687	4	11.281	640759	20.0
Pentadecanoic acid	12.586	2.7	ng	86748	4	11.281	640759	20.0
1-Nonadecene	13.810	4.7	ng	199672	5	13.927	842439	20.0
Strychnidin-10-...	14.392	2.0	ng	85536	5	13.927	842439	20.0
unknown14.469	14.469	4.3	ng	181496	5	13.927	842439	20.0
1,19-Eicosadiene	14.804	2.3	ng	80315	6	15.374	713130	20.0
Benzo[e]pyrene	15.257	2.0	ng	72258	6	15.374	713130	20.0
Hexacosane	15.751	7.1	ng	251877	6	15.374	713130	20.0