

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120123\
 Data File : BF136363.D
 Acq On : 02 Dec 2023 06:15
 Operator : CG\JU
 Sample : 05521-01
 Misc :
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-1-COMP

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-BF112723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136363.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.045	497	503	510	rBV	49486	60446	2.93%	0.385%
2	5.445	566	571	574	rBV	2231275	2059714	100.00%	13.119%
3	6.439	735	740	743	rBV	2118661	1911203	92.79%	12.173%
4	6.804	799	802	806	rVB	942902	724821	35.19%	4.617%
5	7.363	892	897	900	rBV	1392849	1224209	59.44%	7.797%
6	8.080	1015	1019	1023	rBV	1031304	833391	40.46%	5.308%
7	9.157	1198	1202	1206	rBV	2213859	1954125	94.87%	12.446%
8	9.280	1220	1223	1227	rBV2	24937	23474	1.14%	0.150%
9	9.839	1311	1318	1321	rBV	884532	738659	35.86%	4.705%
10	10.098	1358	1362	1367	rBV2	29609	27646	1.34%	0.176%
11	10.627	1448	1452	1463	rBV	1034152	886835	43.06%	5.649%
12	11.327	1567	1571	1574	rBV	752915	637121	30.93%	4.058%
13	11.798	1646	1651	1654	rBV4	24364	33338	1.62%	0.212%
14	11.868	1659	1663	1667	rBV	267012	248165	12.05%	1.581%
15	12.545	1772	1778	1781	rBV	64320	78959	3.83%	0.503%
16	12.657	1793	1797	1802	rBV	60389	67954	3.30%	0.433%
17	12.774	1811	1817	1821	rBV	48640	50537	2.45%	0.322%
18	12.927	1839	1843	1846	rBV	2153362	1798360	87.31%	11.454%
19	13.163	1878	1883	1887	rBV2	36198	41547	2.02%	0.265%
20	13.415	1922	1926	1931	rVB2	38543	56158	2.73%	0.358%
21	13.839	1996	1998	2002	rVB	31870	28077	1.36%	0.179%
22	13.915	2005	2011	2014	rBV8	41109	97151	4.72%	0.619%
23	13.980	2017	2022	2025	rBV2	836965	887205	43.07%	5.651%
24	14.080	2036	2039	2043	rVB5	18213	24257	1.18%	0.154%
25	14.462	2100	2104	2109	rBV3	52551	73189	3.55%	0.466%
26	14.857	2168	2171	2175	rVB2	30931	35415	1.72%	0.226%
27	14.927	2180	2183	2188	rVB2	74097	78884	3.83%	0.502%
28	15.027	2197	2200	2203	rBV3	23726	29985	1.46%	0.191%
29	15.080	2206	2209	2212	rVV	64845	70337	3.41%	0.448%
30	15.127	2213	2217	2222	rVB	74648	96529	4.69%	0.615%
31	15.462	2269	2274	2280	rBV	414919	551872	26.79%	3.515%
32	15.727	2317	2319	2325	rVB6	23452	34052	1.65%	0.217%
33	15.974	2356	2361	2371	rVB	99568	165300	8.03%	1.053%
34	17.339	2590	2593	2602	rVB9	37315	71425	3.47%	0.455%

Sum of corrected areas: 15700340

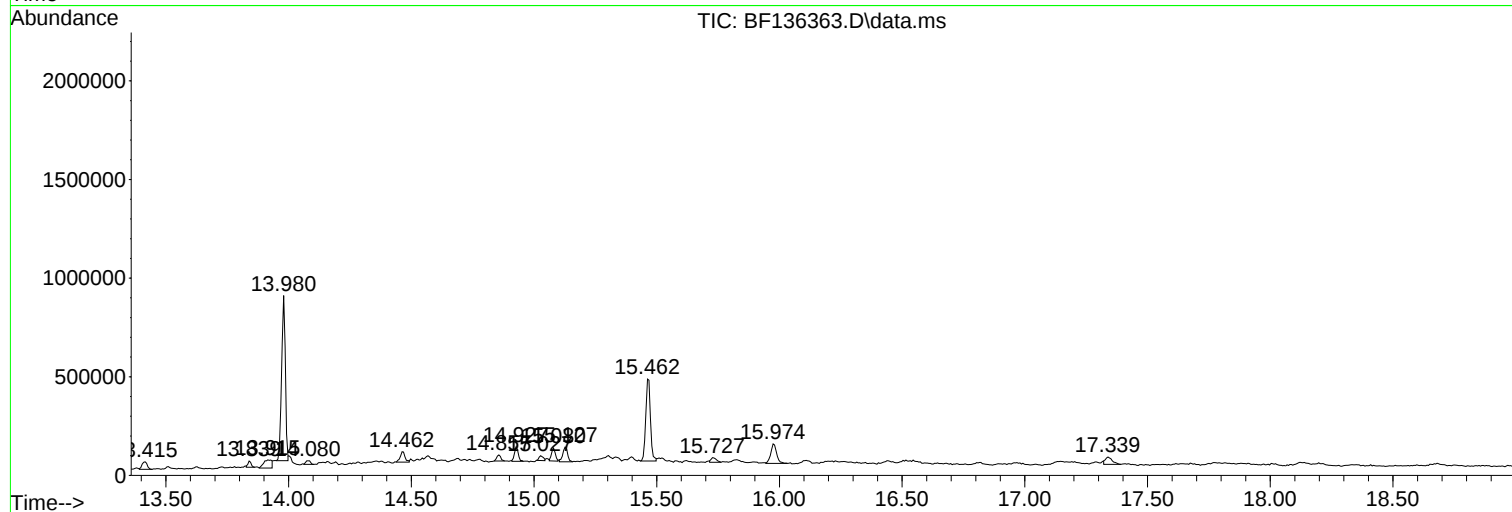
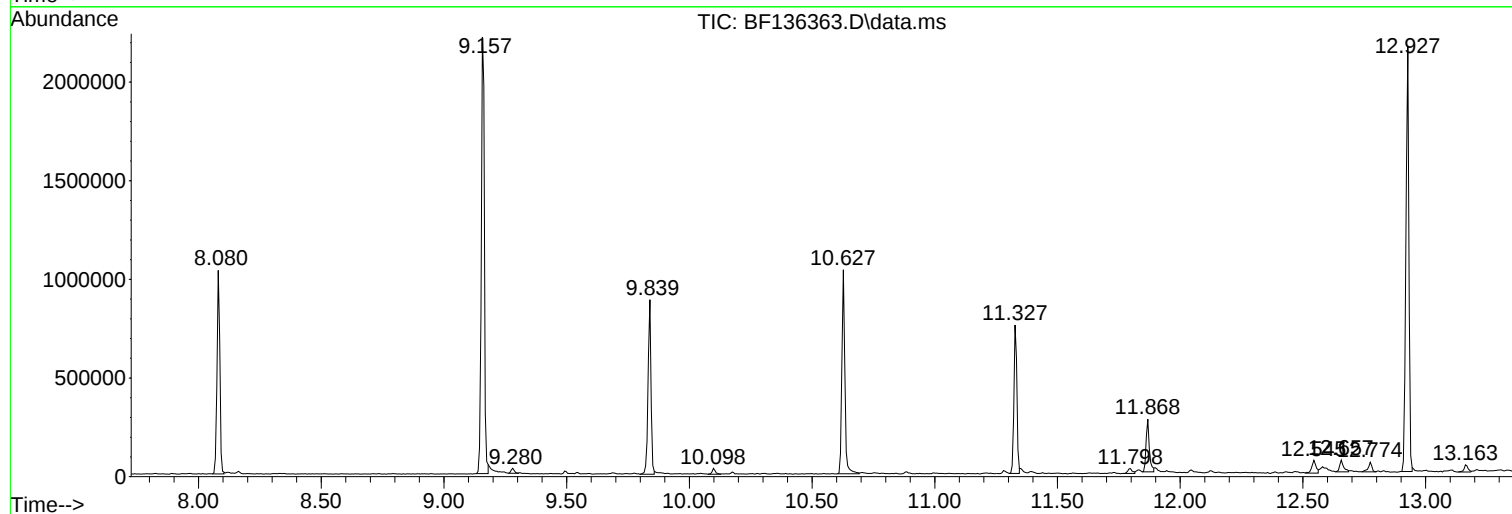
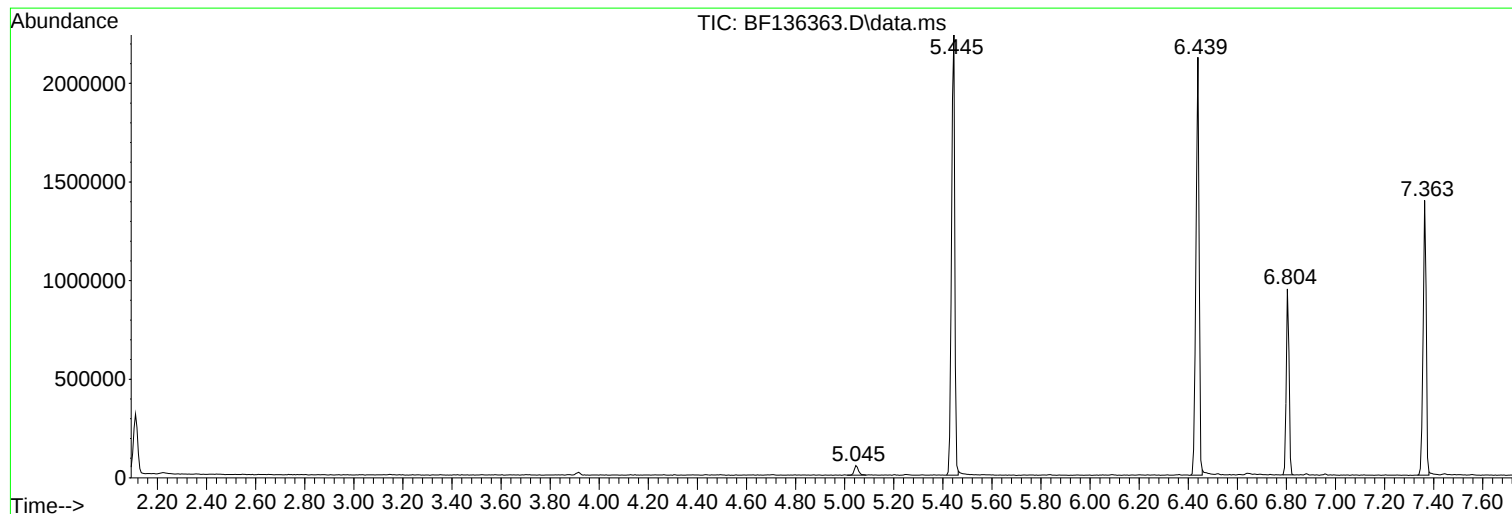
Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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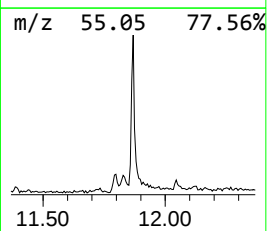
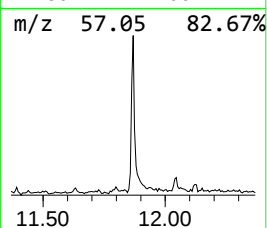
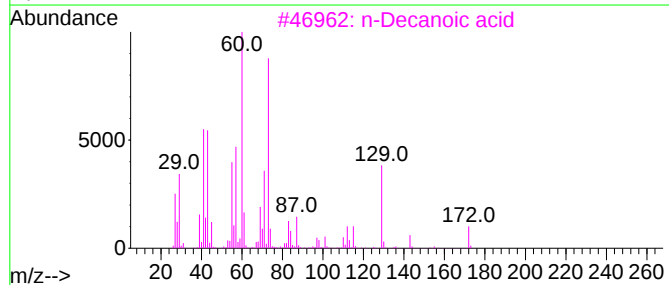
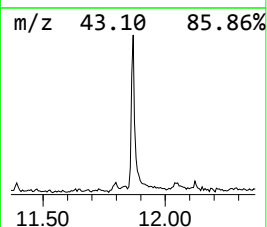
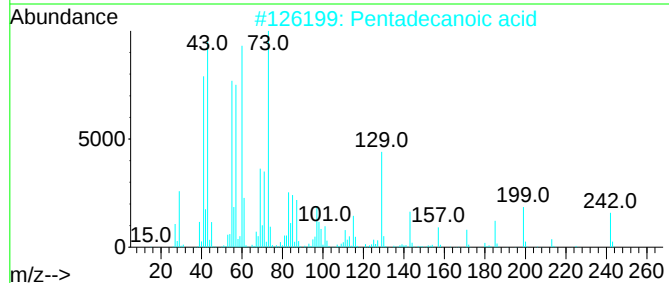
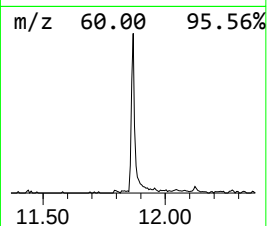
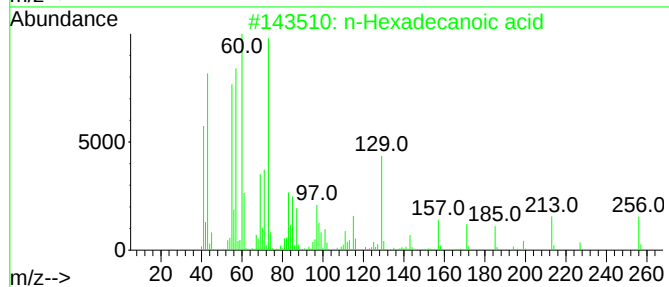
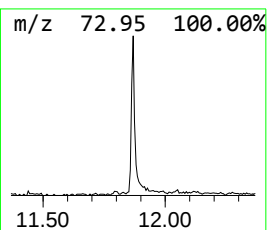
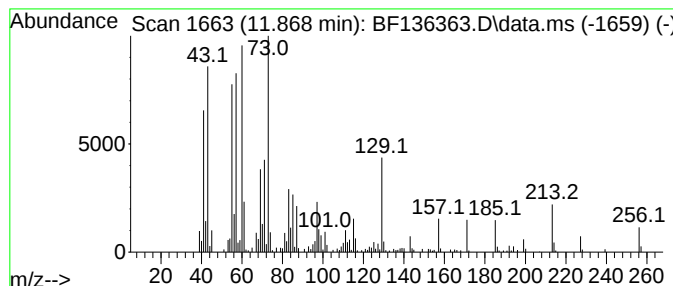
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.868	7.79 ng	248165	Phenanthrene-d10	11.327

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			n-Decanoic acid	172	C10H20O2	000334-48-5	76
4			Undecanoic acid	186	C11H22O2	000112-37-8	68
5			Tridecanoic acid	214	C13H26O2	000638-53-9	58



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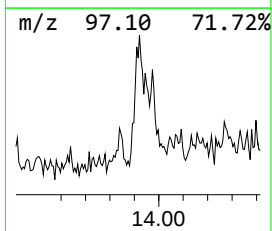
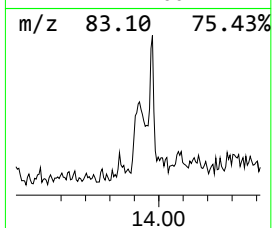
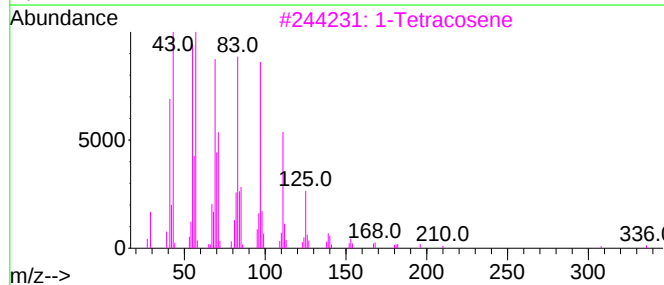
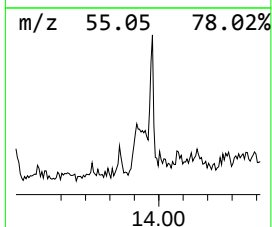
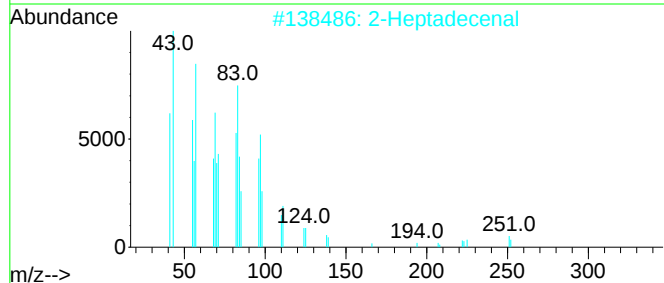
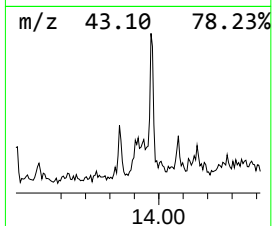
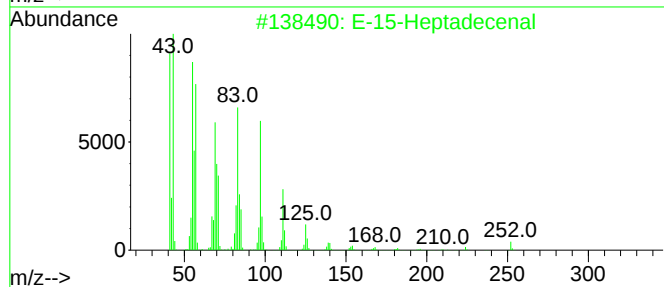
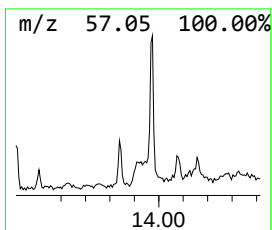
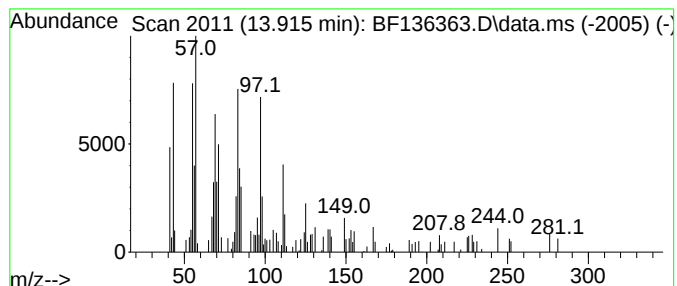
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Peak Number 3 E-15-Heptadecenal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.915	2.19 ng	97151	Chrysene-d12	13.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal			252	C17H32O	1000130-97-9	94
2	2-Heptadecenal			252	C17H32O	1000143-48-6	90
3	1-Tetracosene			336	C24H48	010192-32-2	87
4	Heptafluorobutyric acid, hexadec...			438	C20H33F7O2	006385-15-5	87
5	Pentafluoropropionic acid, hexad...			388	C19H33F5O2	006222-07-7	87



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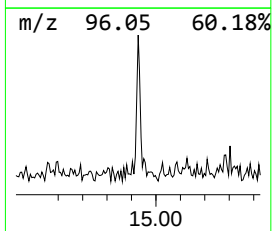
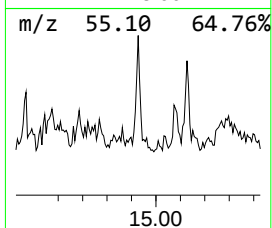
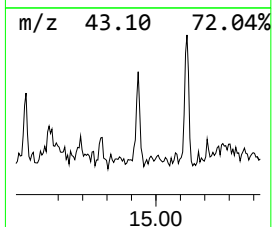
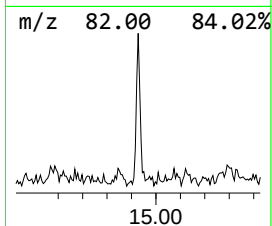
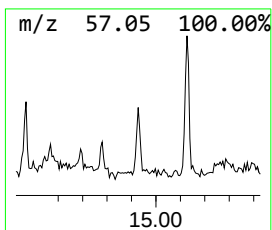
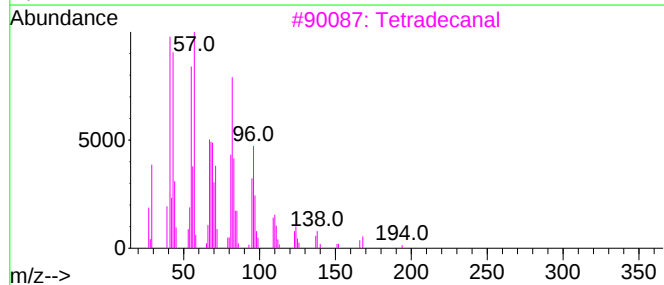
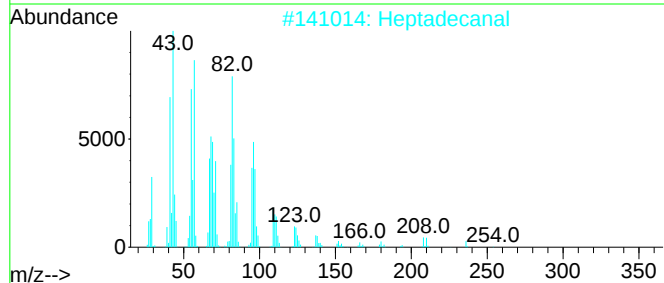
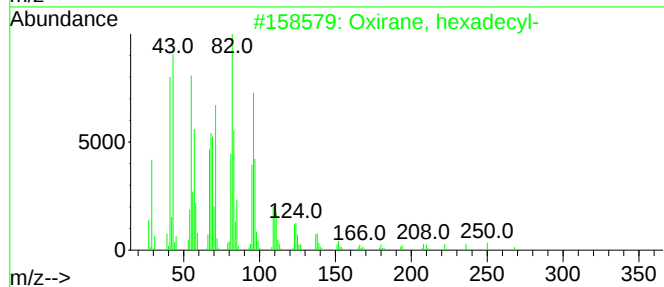
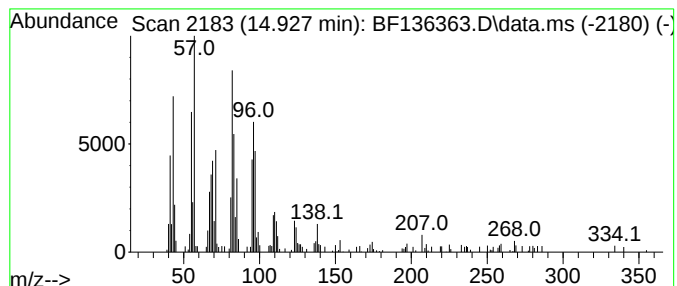
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Peak Number 4 Oxirane, hexadecyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.927	2.86 ng	78884	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	90
2			Heptadecanal	254	C17H34O	1000376-70-0	86
3			Tetradecanal	212	C14H28O	000124-25-4	83
4			Octadecanal	268	C18H36O	000638-66-4	68
5			Tetracosanal	352	C24H48O	057866-08-7	68



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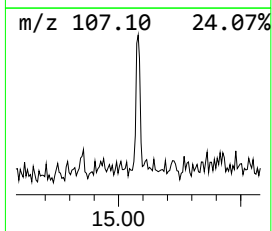
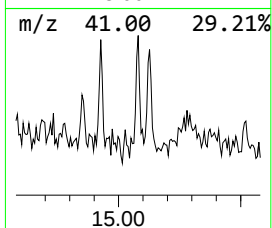
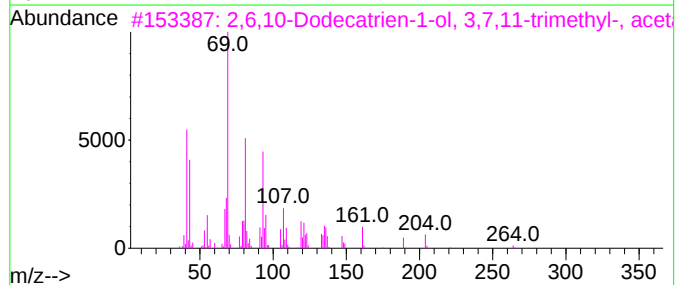
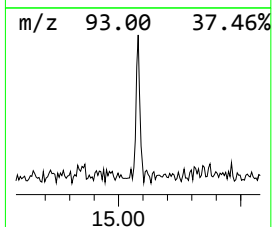
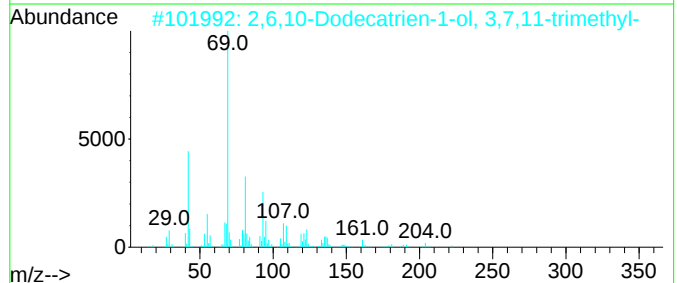
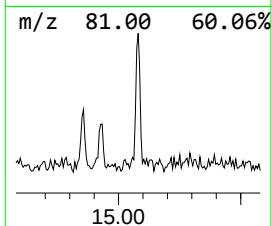
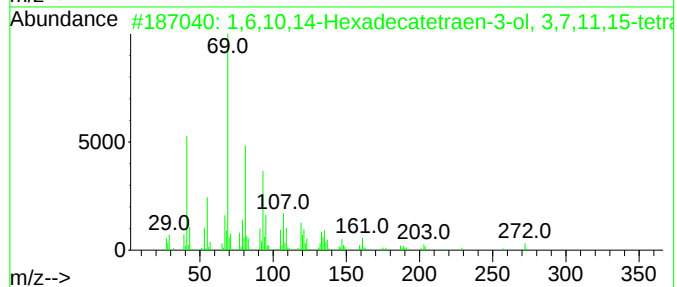
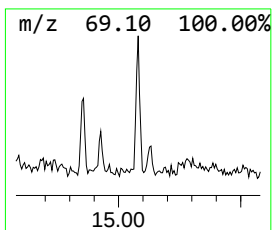
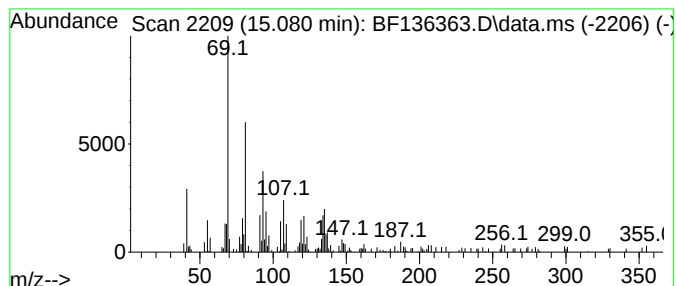
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Peak Number 5 1,6,10,14-Hexadecatetraen-3... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.080	2.55 ng	70337	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6,10,14-Hexadecatetraen-3-ol, ...	290	C20H34O	001113-21-9	86		
2	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	81		
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	80		
4	(E,E,E)-3,7,11,15-Tetramethylhex...	272	C20H32	077898-97-6	72		
5	(E,E)-7,11,15-Trimethyl-3-methyl...	272	C20H32	070901-63-2	59		



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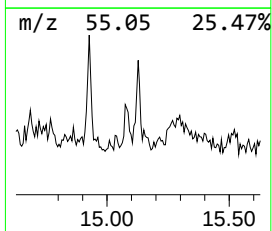
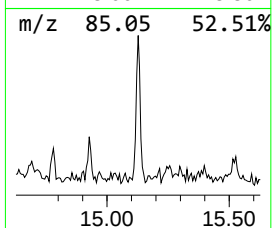
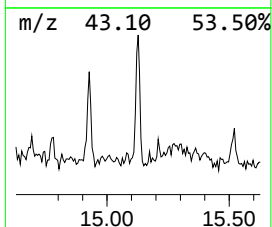
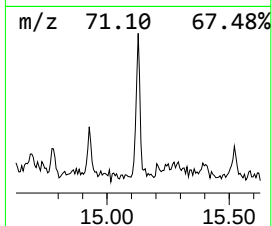
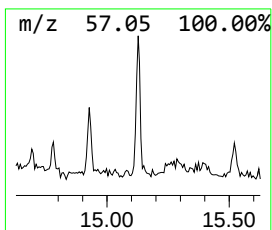
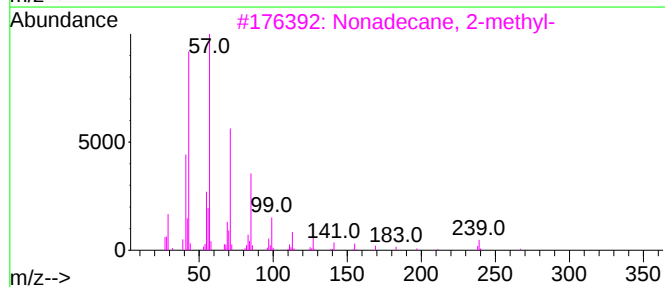
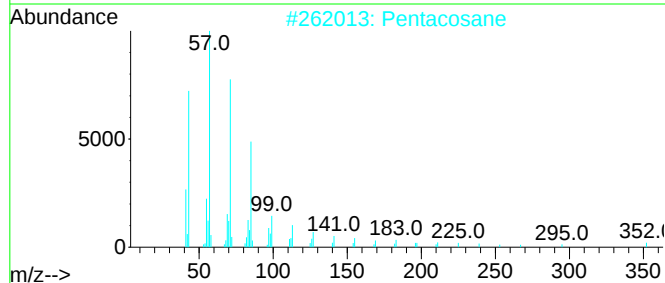
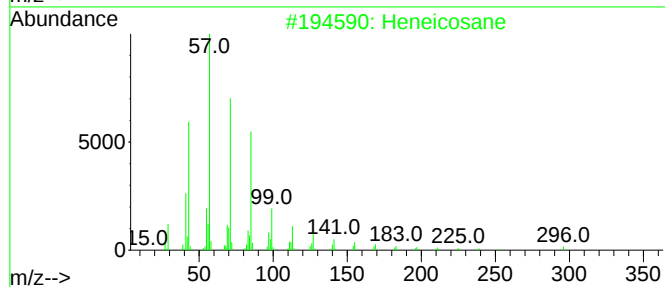
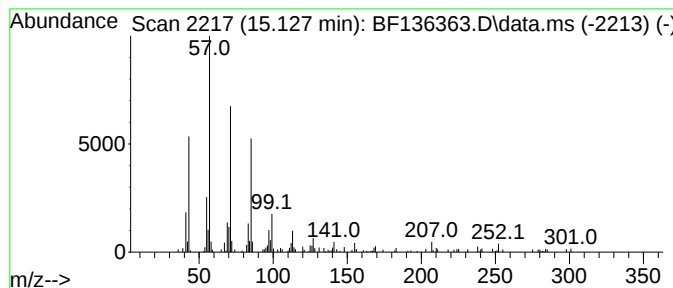
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Peak Number 6 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.127	3.50 ng	96529	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	87
2			Pentacosane	352	C25H52	000629-99-2	87
3			Nonadecane, 2-methyl-	282	C20H42	001560-86-7	87
4			Eicosane	282	C20H42	000112-95-8	87
5			Octacosane	394	C28H58	000630-02-4	87



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ClientSampleId :
SP-1-COMP

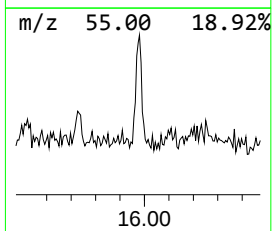
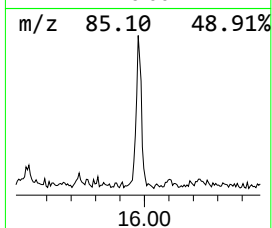
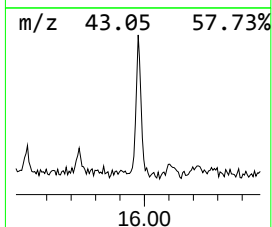
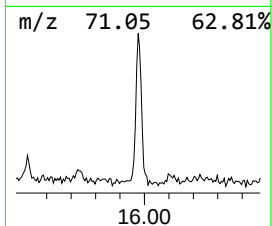
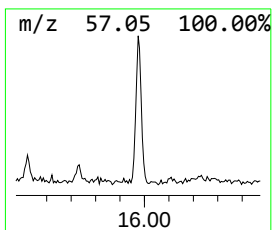
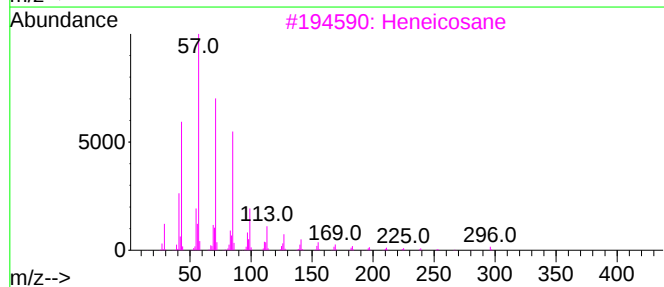
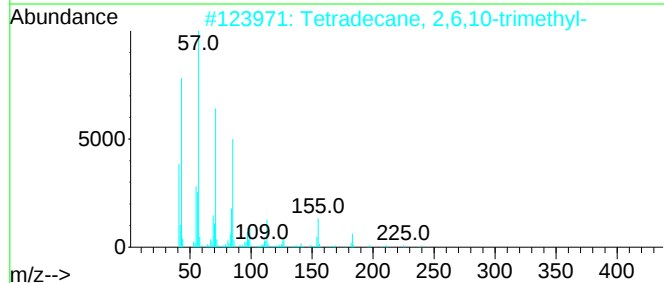
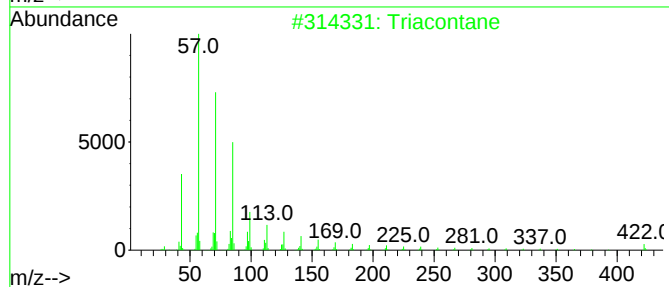
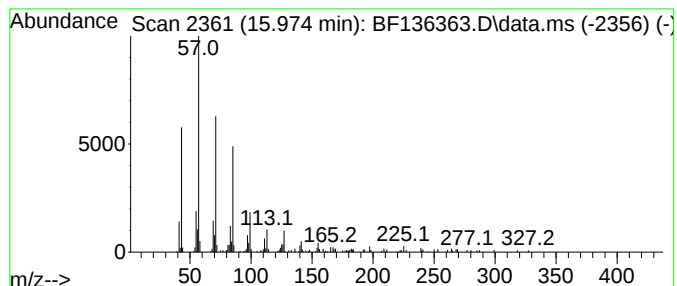
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Triacontane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.974	5.99 ng	165300	Perylene-d12	15.468

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Triacontane	422	C30H62	000638-68-6	90
2		Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	90
3		Heneicosane	296	C21H44	000629-94-7	90
4		Hexacosane	366	C26H54	000630-01-3	87
5		Hentriacontane	437	C31H64	000630-04-6	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120123\
Data File : BF136363.D
Acq On : 02 Dec 2023 06:15
Operator : CG\JU
Sample : 05521-01
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1-COMP

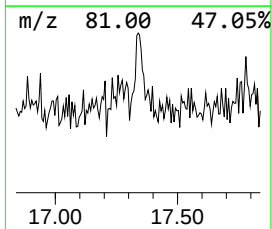
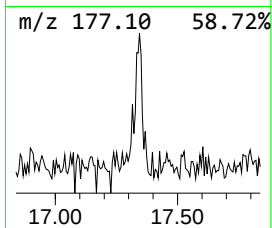
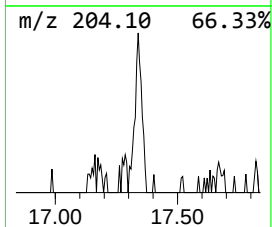
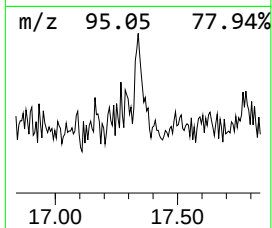
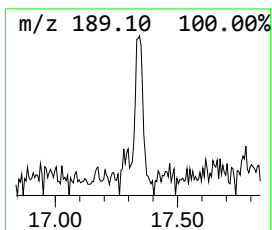
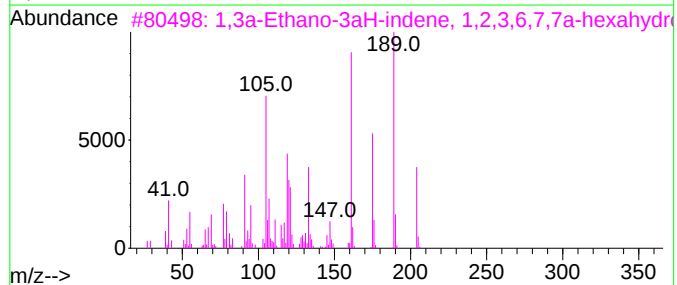
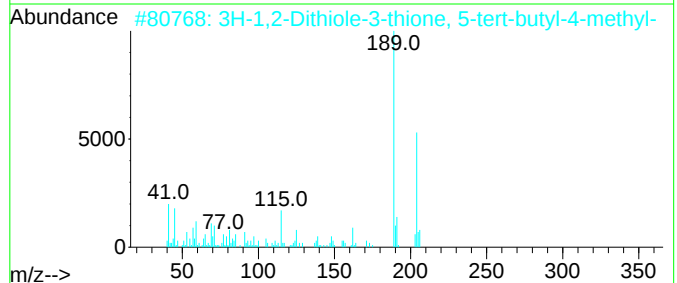
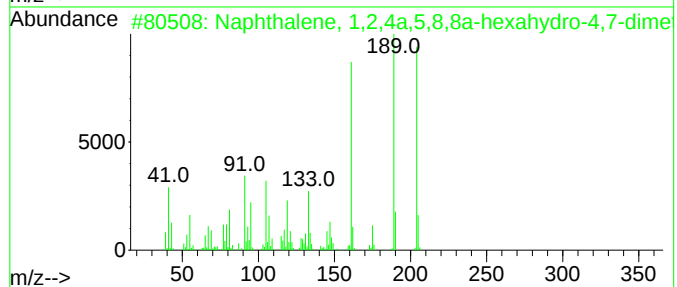
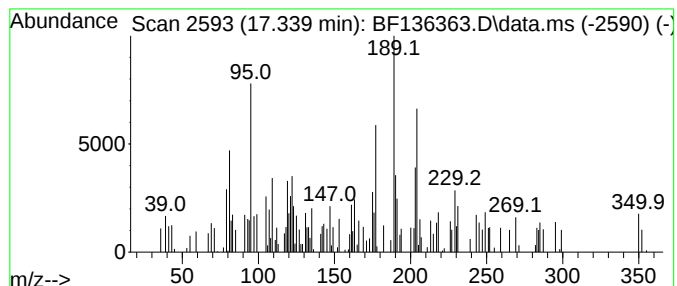
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown17.339 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.339	2.59 ng	71425	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,4a,5,8,8a-hexah...	204	C15H24	005951-61-1	30
2			3H-1,2-Dithiole-3-thione, 5-tert...	204	C8H12S3	013120-76-8	30
3			1,3a-Ethano-3aH-indene, 1,2,3,6,...	204	C15H24	004545-68-0	30
4			2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	207297-57-2	27
5			4a,8-Dimethyl-2-(prop-1-en-2-yl)...	204	C15H24	103827-22-1	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120123\
Data File : BF136363.D
Acq On : 02 Dec 2023 06:15
Operator : CG\JU
Sample : 05521-01
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.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
n-Hexadecanoic ...	11.868	7.8	ng	248165	4	11.327	637121	20.0
E-15-Heptadecenal	13.915	2.2	ng	97151	5	13.980	887205	20.0
Oxirane, hexade...	14.927	2.9	ng	78884	6	15.468	551872	20.0
1,6,10,14-Hexad...	15.080	2.5	ng	70337	6	15.468	551872	20.0
Heneicosane	15.127	3.5	ng	96529	6	15.468	551872	20.0
Triacontane	15.974	6.0	ng	165300	6	15.468	551872	20.0
unknown17.339	17.339	2.6	ng	71425	6	15.468	551872	20.0