

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071923\
 Data File : BF134359.D
 Acq On : 19 Jul 2023 15:17
 Operator : CG\JU
 Sample : 03597-10
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RB-46-(2-5)

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-BF062623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134359.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	4	10	19	rVB	362086	467903	28.39%	3.738%
2	5.093	507	511	520	rVB	17668	23824	1.45%	0.190%
3	5.481	572	577	593	rBV	1382244	1375617	83.47%	10.991%
4	6.481	742	747	761	rBV	1509608	1395411	84.67%	11.149%
5	6.669	775	779	796	rVB	23295	40548	2.46%	0.324%
6	6.840	804	808	815	rBV	496921	437754	26.56%	3.498%
7	7.398	899	903	914	rBV	916560	906698	55.02%	7.244%
8	8.116	1021	1025	1028	rBV	693180	544187	33.02%	4.348%
9	9.192	1204	1208	1211	rBV	2133882	1647979	100.00%	13.167%
10	9.304	1224	1227	1230	rBV	23160	20992	1.27%	0.168%
11	9.875	1320	1324	1327	rBV	717911	561847	34.09%	4.489%
12	10.669	1455	1459	1474	rBV	1159508	996301	60.46%	7.960%
13	11.369	1574	1578	1581	rBV	632009	537098	32.59%	4.291%
14	11.392	1581	1582	1586	rVV	144705	91633	5.56%	0.732%
15	11.433	1586	1589	1594	rVB2	19891	28129	1.71%	0.225%
16	11.610	1613	1619	1624	rBV2	15451	20531	1.25%	0.164%
17	11.898	1665	1668	1675	rVB2	177152	168115	10.20%	1.343%
18	11.986	1679	1683	1686	rBV2	22587	25766	1.56%	0.206%
19	12.204	1717	1720	1725	rVB	26377	22661	1.38%	0.181%
20	12.592	1782	1786	1789	rBV	209242	178964	10.86%	1.430%
21	12.686	1799	1802	1807	rBV2	36763	44475	2.70%	0.355%
22	12.822	1820	1825	1829	rBV	177889	171135	10.38%	1.367%
23	12.969	1841	1850	1853	rBV	1259278	1221328	74.11%	9.758%
24	13.039	1858	1862	1867	rVV3	13016	23112	1.40%	0.185%
25	13.151	1879	1881	1884	rVB2	21657	20648	1.25%	0.165%
26	13.257	1896	1899	1903	rVB	23810	21641	1.31%	0.173%
27	13.669	1966	1969	1973	rVB	23692	21848	1.33%	0.175%
28	13.780	1982	1988	1990	rBV3	20963	26390	1.60%	0.211%
29	13.892	2001	2007	2016	rBV5	58460	126962	7.70%	1.014%
30	14.033	2024	2031	2034	rBV2	471187	525679	31.90%	4.200%
31	14.057	2034	2035	2040	rVV	102520	89186	5.41%	0.713%
32	14.121	2043	2046	2051	rVB2	62321	77858	4.72%	0.622%
33	14.421	2095	2097	2100	rVB	24435	20789	1.26%	0.166%
34	14.498	2107	2110	2113	rBV3	17758	23917	1.45%	0.191%
35	15.092	2207	2211	2215	rBV	71525	123692	7.51%	0.988%
36	15.410	2262	2265	2271	rVB	41669	59104	3.59%	0.472%

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RB-46-(2-5)

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-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.474	2271	2276	2281	rBV	57104	78174	4.74%	0.625%
38	15.539	2282	2287	2300	rVB	247656	348067	21.12%	2.781%

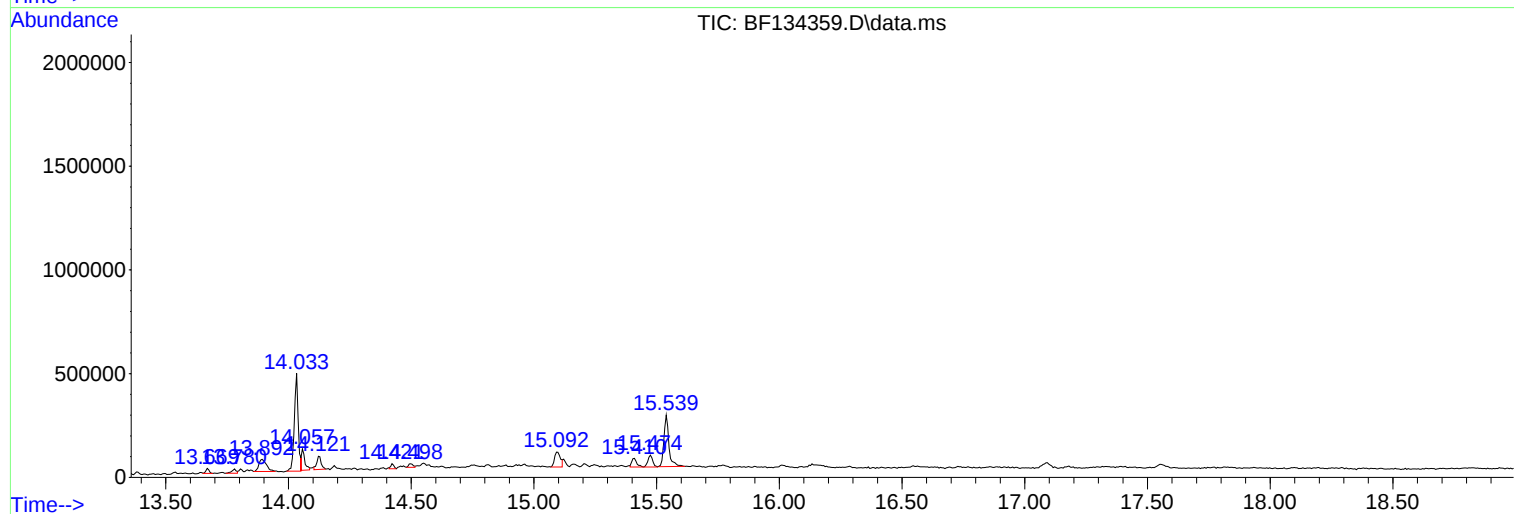
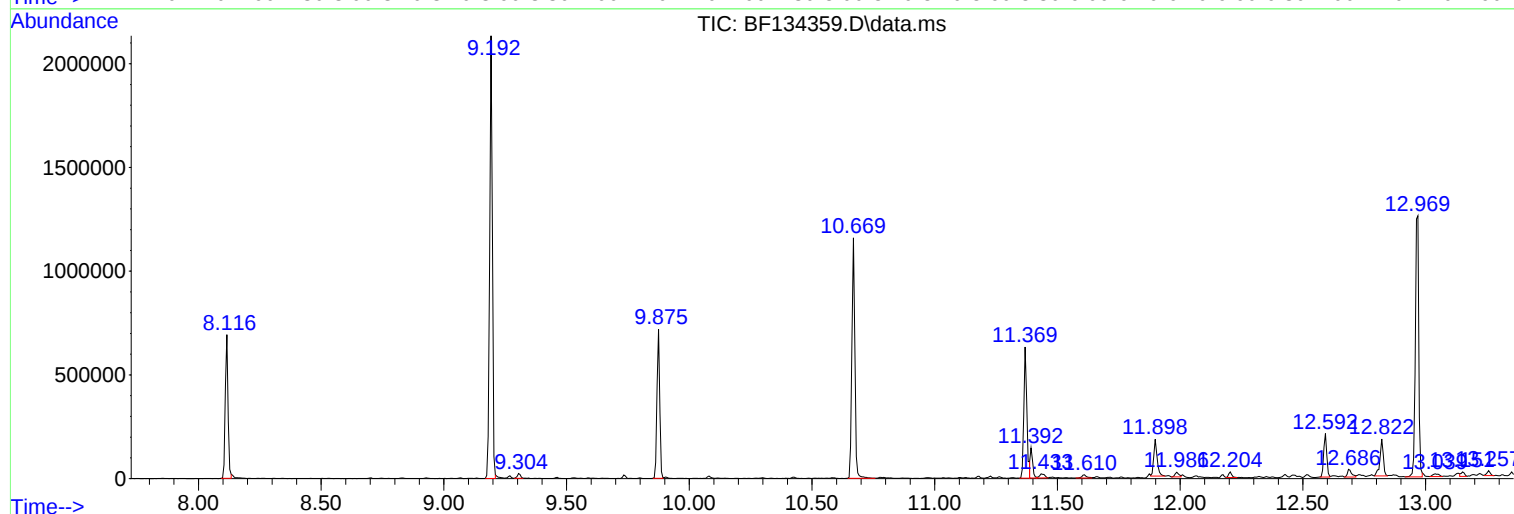
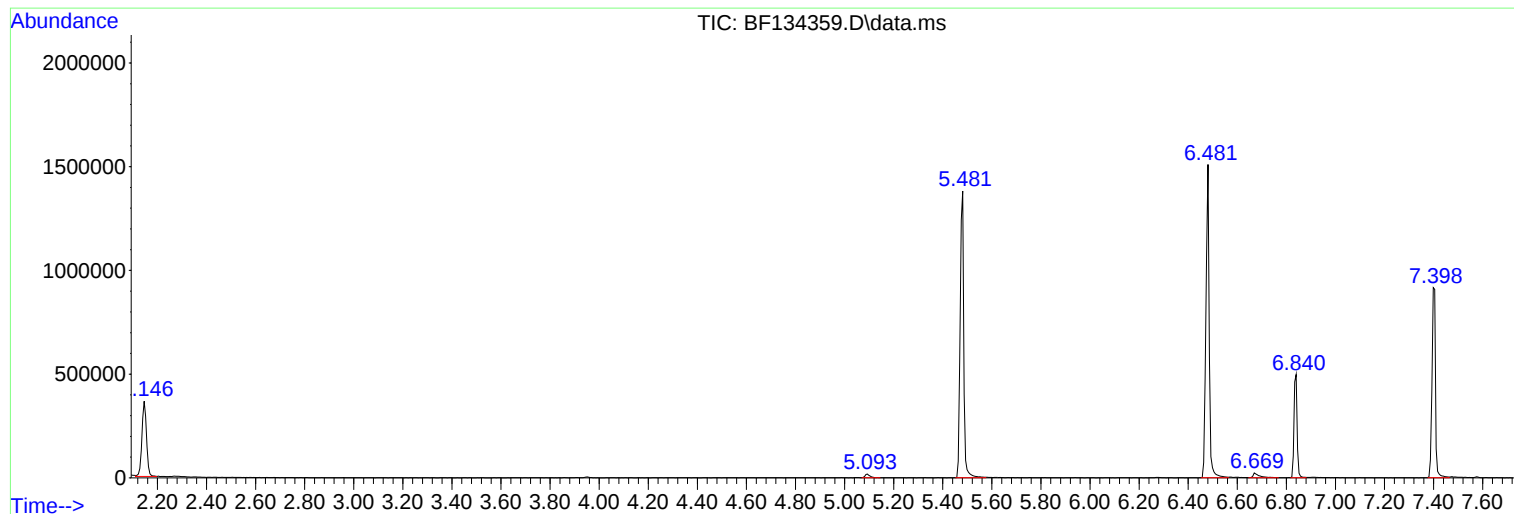
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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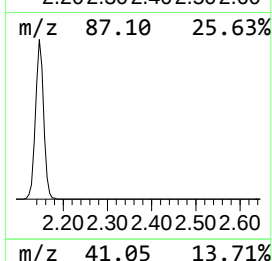
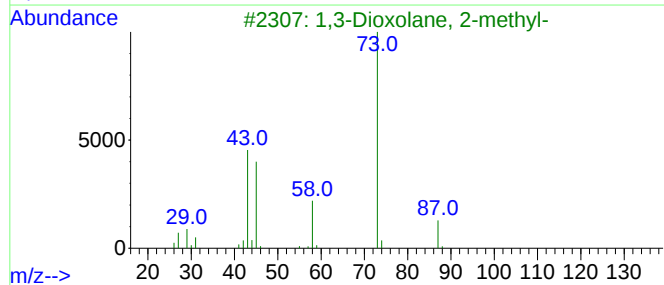
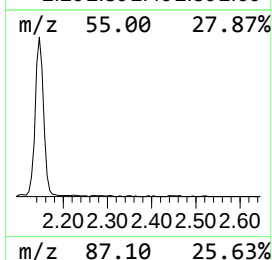
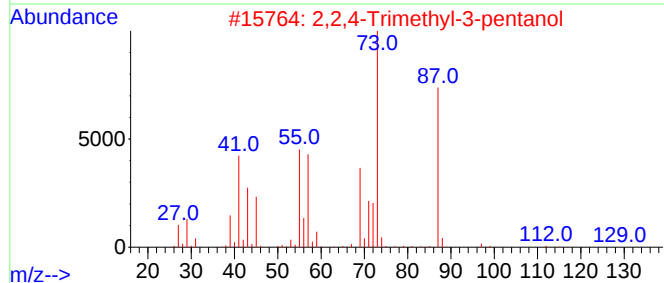
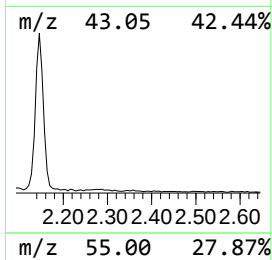
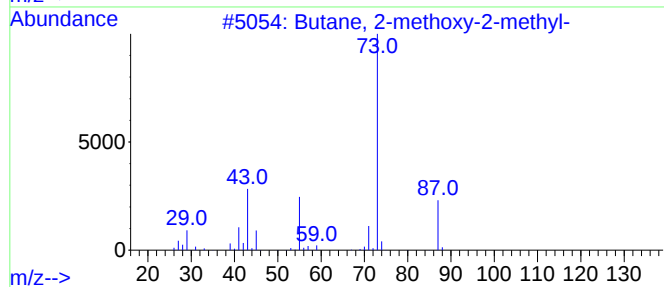
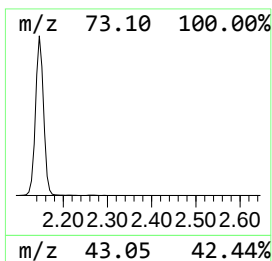
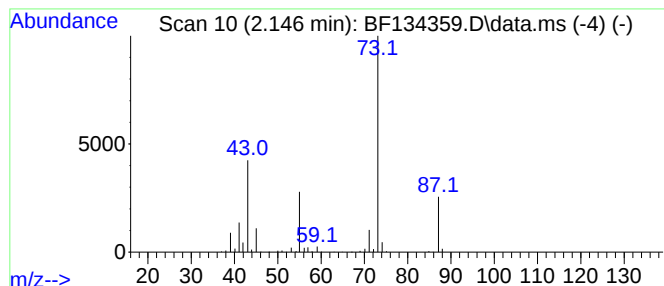
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	21.38 ng	467903	1,4-Dichlorobenzene-d4	6.840

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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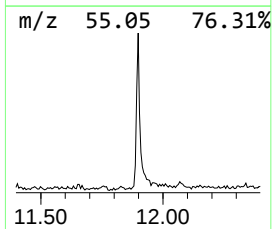
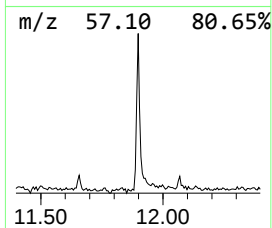
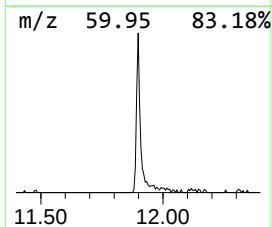
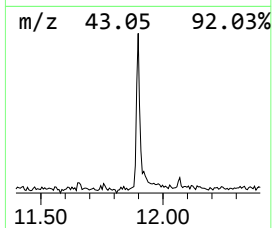
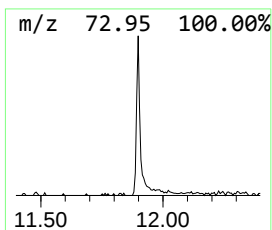
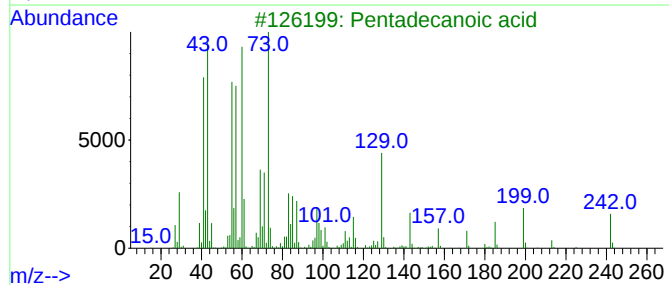
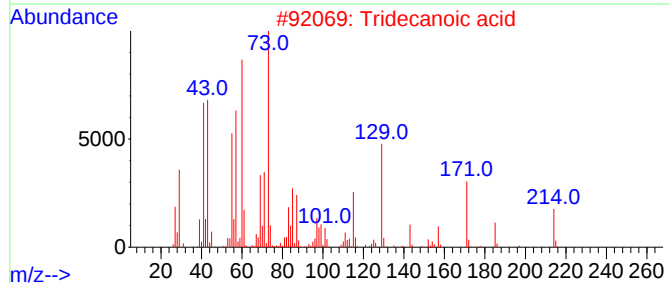
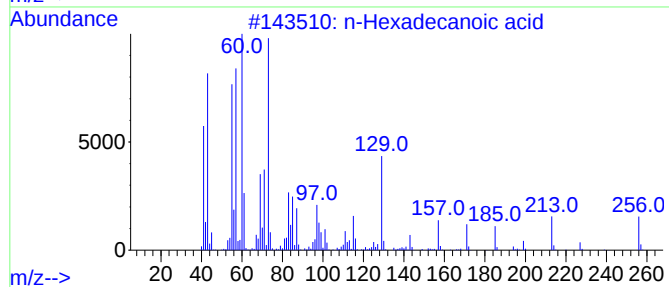
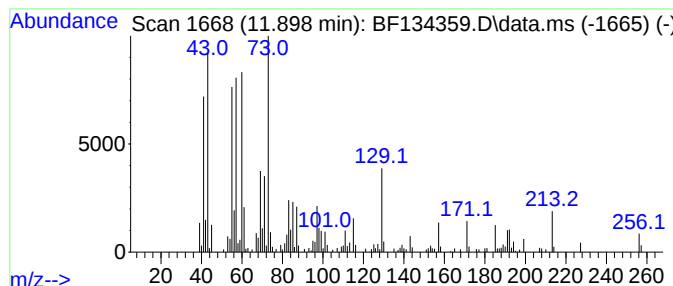
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	6.26 ng	168115	Phenanthrene-d10	11.369

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	76



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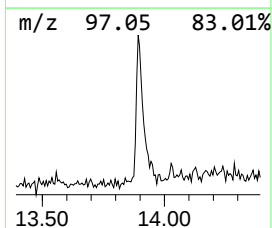
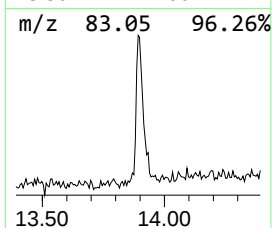
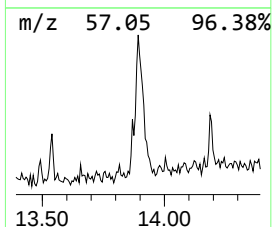
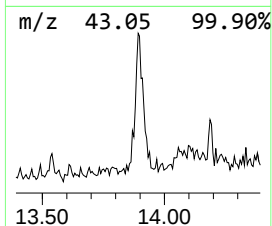
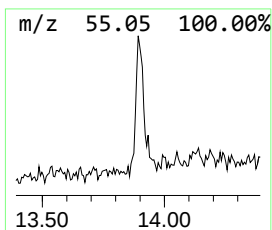
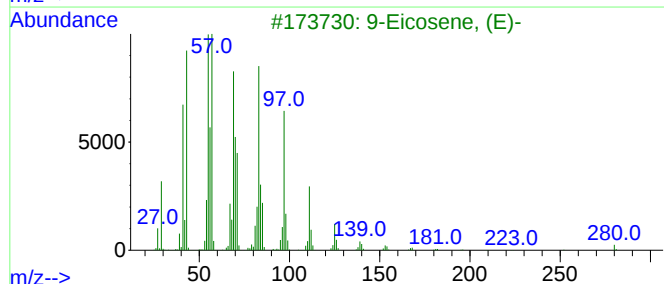
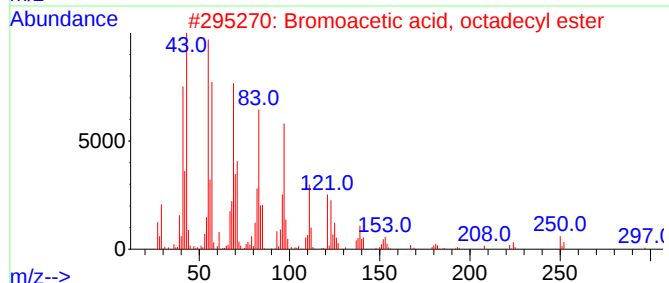
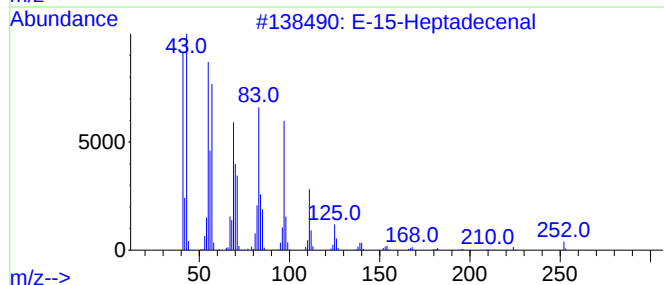
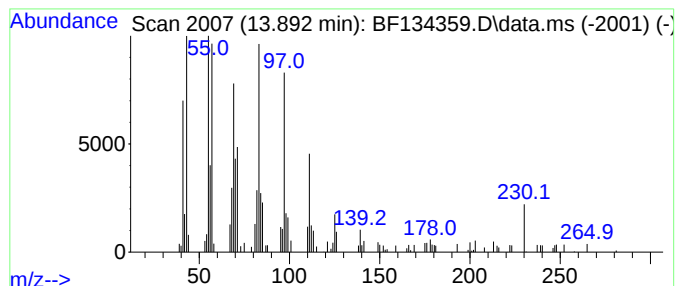
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 E-15-Heptadecenal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	4.83 ng	126962	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			E-15-Heptadecenal	252	C17H32O	1000130-97-9	95
2			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
3			9-Eicosene, (E)-	280	C20H40	074685-29-3	91
4			1-Octadecene	252	C18H36	000112-88-9	90
5			Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	87



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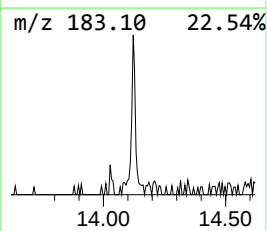
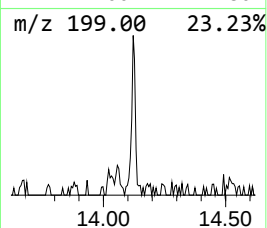
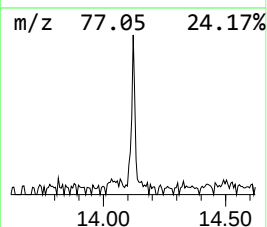
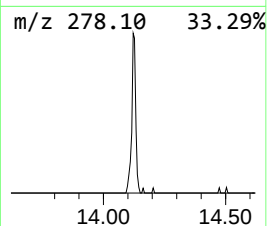
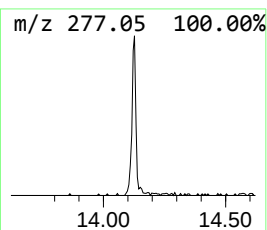
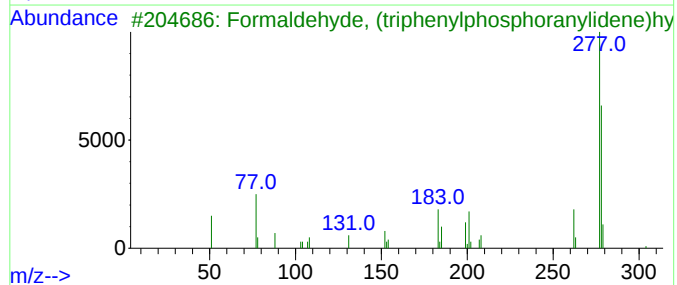
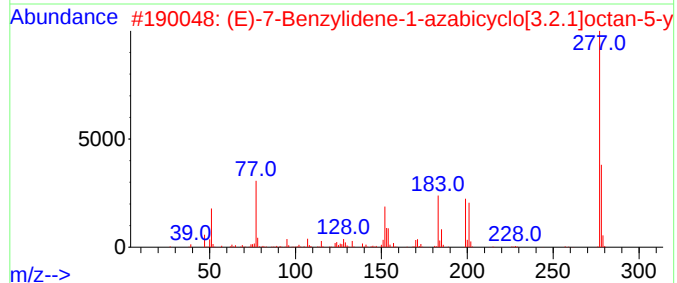
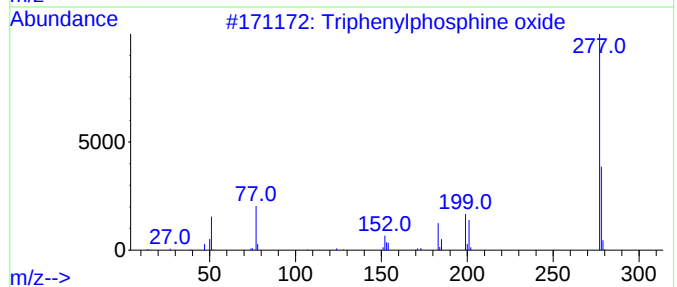
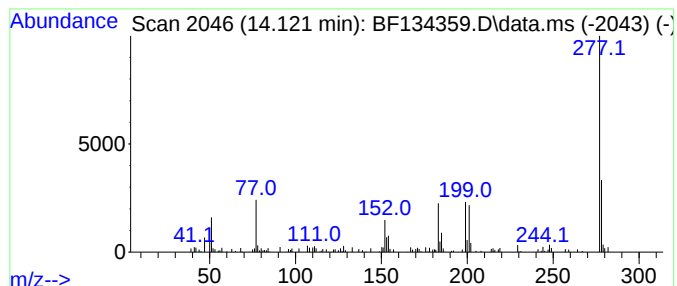
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.121	2.96 ng	77858	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	96
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	90
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4			Phenol, 2-(2,2-difluoro-1,3-benz...	277	C14H9F2NO3	1000274-10-8	43
5			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	37



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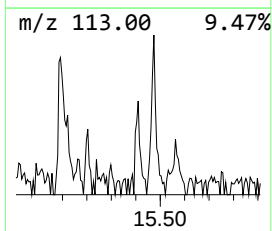
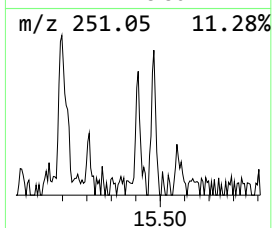
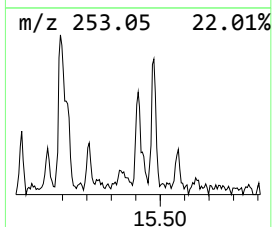
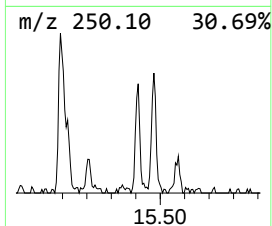
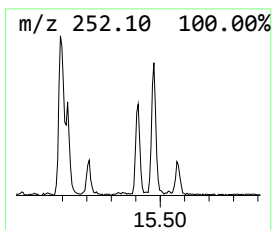
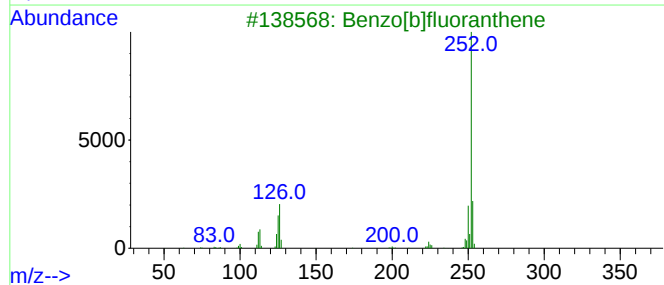
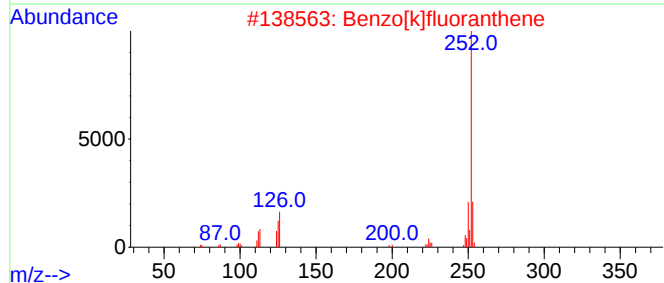
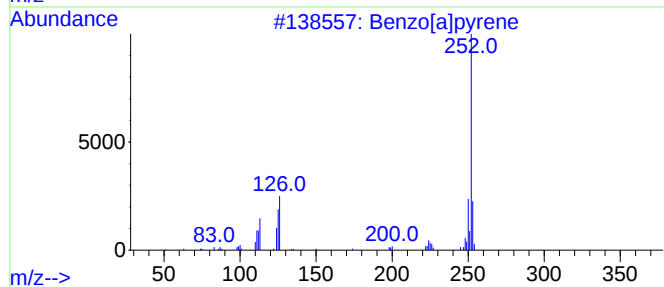
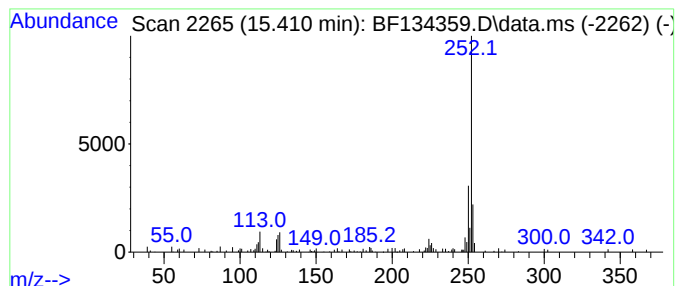
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.410	3.40 ng	59104	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[a]pyrene	252	C20H12	000050-32-8	94
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	87
4			Perylene	252	C20H12	000198-55-0	81
5			Benzo[e]pyrene	252	C20H12	000192-97-2	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071923\
Data File : BF134359.D
Acq On : 19 Jul 2023 15:17
Operator : CG\JU
Sample : 03597-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-46-(2-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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
Butane, 2-metho...	2.146	21.4	ng	467903	1	6.840	437754	20.0
n-Hexadecanoic ...	11.898	6.3	ng	168115	4	11.369	537098	20.0
E-15-Heptadecenal	13.892	4.8	ng	126962	5	14.033	525679	20.0
Triphenylphosph...	14.121	3.0	ng	77858	5	14.033	525679	20.0
Benzo[e]pyrene	15.410	3.4	ng	59104	6	15.539	348067	20.0