

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082323\
 Data File : BF134899.D
 Acq On : 23 Aug 2023 12:24
 Operator : CG\JU
 Sample : 04091-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-A

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-BF082223.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134899.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.422	562	567	570	rBV	2669624	2445277	88.23%	11.184%
2	6.428	733	738	741	rBV	2568548	2451804	88.47%	11.214%
3	6.622	768	771	777	rBV	39996	39862	1.44%	0.182%
4	6.792	796	800	803	rBV	1032680	787733	28.42%	3.603%
5	7.351	890	895	898	rBV	1772607	1569538	56.63%	7.179%
6	8.069	1013	1017	1021	rBV	1260205	1043793	37.66%	4.774%
7	9.151	1196	1201	1204	rBV	3189241	2771410	100.00%	12.676%
8	9.269	1218	1221	1224	rVB	41576	33004	1.19%	0.151%
9	9.827	1312	1316	1320	rBV	1514333	1225006	44.20%	5.603%
10	10.621	1446	1451	1454	rBV	2332499	2034009	73.39%	9.303%
11	11.321	1566	1570	1573	rBV	1515219	1269984	45.82%	5.809%
12	11.392	1577	1582	1586	rVB3	28342	30738	1.11%	0.141%
13	11.857	1657	1661	1666	rBV	355936	355934	12.84%	1.628%
14	12.539	1772	1777	1781	rBV	98123	97513	3.52%	0.446%
15	12.645	1792	1795	1802	rBV	86704	108640	3.92%	0.497%
16	12.768	1809	1816	1819	rBV	120685	133896	4.83%	0.612%
17	12.921	1837	1842	1845	rBV	2731789	2531807	91.35%	11.580%
18	13.504	1935	1941	1943	rBV2	37582	35565	1.28%	0.163%
19	13.833	1991	1997	1999	rBV2	124735	177478	6.40%	0.812%
20	13.974	2014	2021	2024	rBV	972646	894594	32.28%	4.092%
21	13.998	2024	2025	2033	rVB	59213	45338	1.64%	0.207%
22	14.074	2033	2038	2042	rBV2	94385	104574	3.77%	0.478%
23	14.151	2048	2051	2056	rVB	34736	32994	1.19%	0.151%
24	14.462	2100	2104	2111	rBV	86459	102716	3.71%	0.470%
25	14.768	2153	2156	2162	rVB	28385	31593	1.14%	0.145%
26	14.845	2165	2169	2177	rBV	76259	108906	3.93%	0.498%
27	15.015	2194	2198	2201	rBV	44615	62970	2.27%	0.288%
28	15.045	2201	2203	2209	rVB2	29054	33331	1.20%	0.152%
29	15.115	2211	2215	2221	rBV2	24618	37147	1.34%	0.170%
30	15.286	2239	2244	2247	rBV2	70891	104628	3.78%	0.479%
31	15.380	2257	2260	2264	rVB	34717	35982	1.30%	0.165%
32	15.445	2266	2271	2278	rBV	660670	843993	30.45%	3.860%
33	15.792	2325	2330	2340	rVB	50880	103558	3.74%	0.474%
34	15.951	2352	2357	2362	rBV6	20024	35036	1.26%	0.160%
35	16.403	2428	2434	2441	rBV3	35844	76913	2.78%	0.352%
36	17.150	2555	2561	2570	rVB7	22108	65959	2.38%	0.302%

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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-BF082223.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

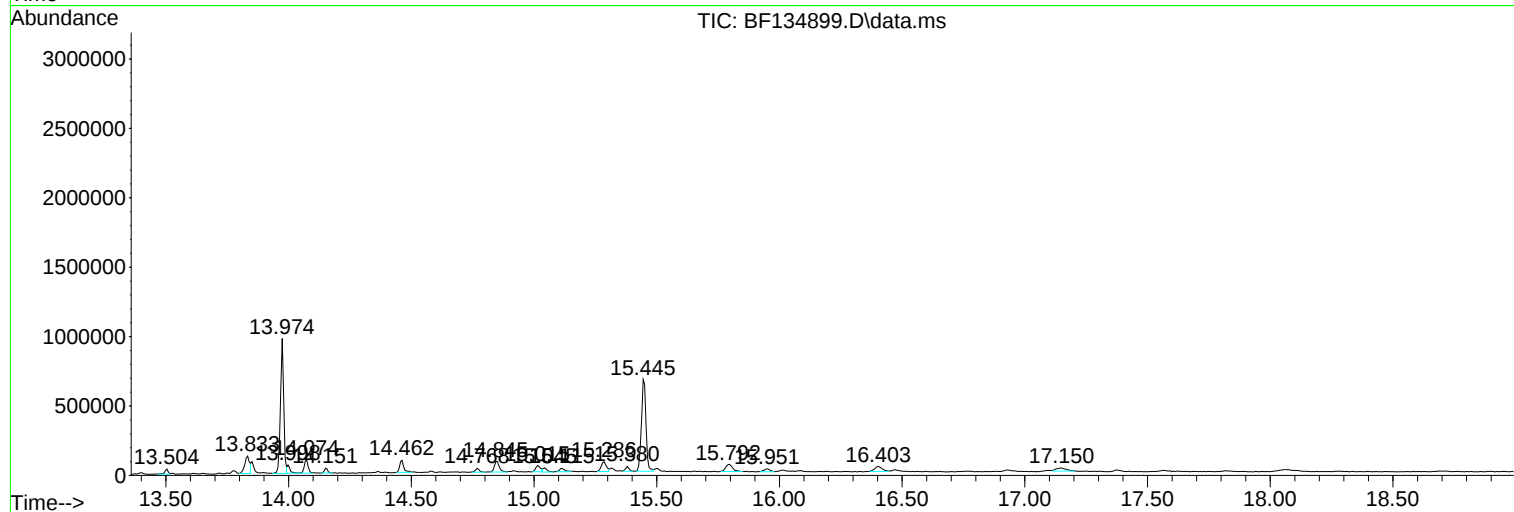
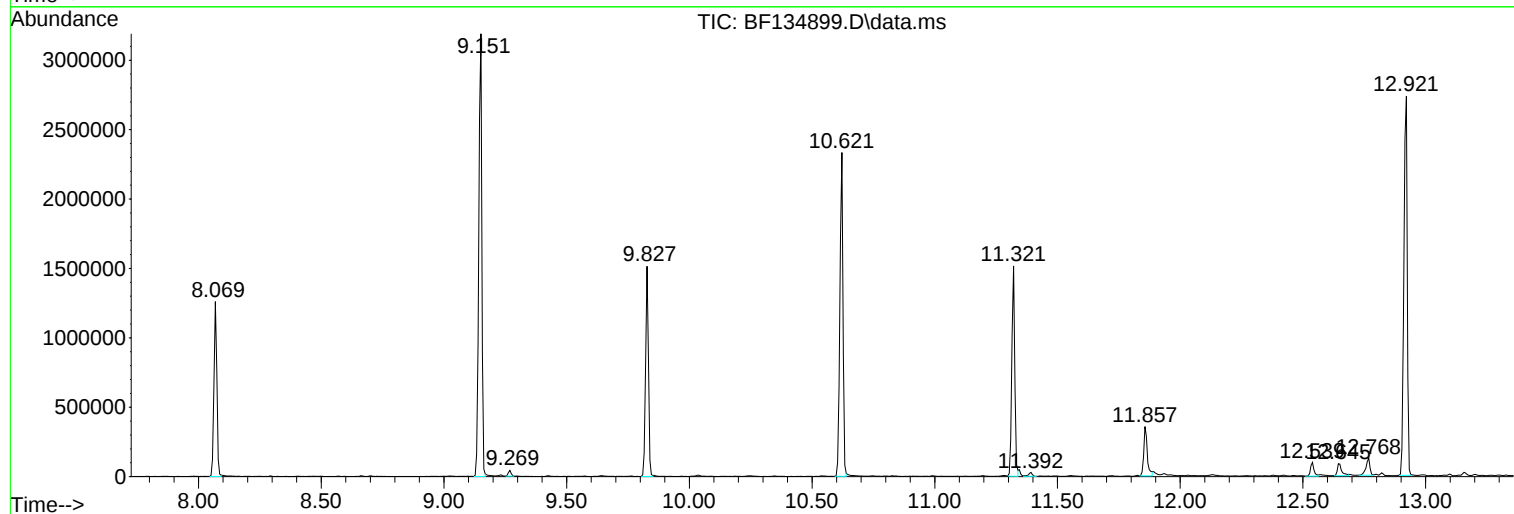
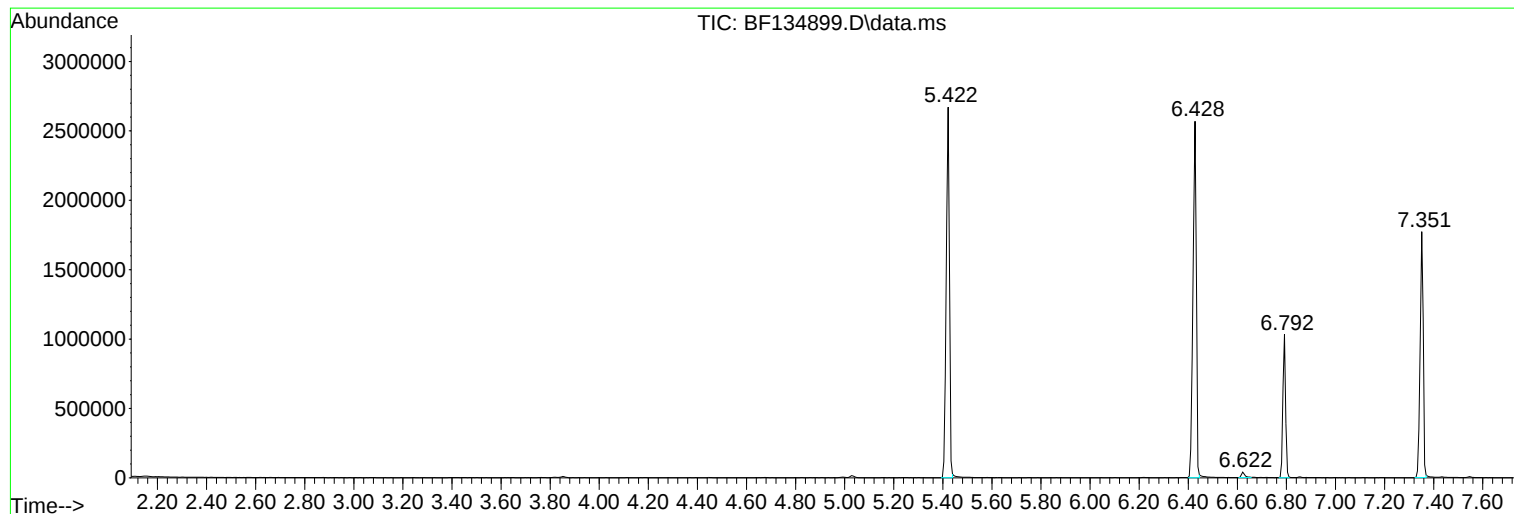
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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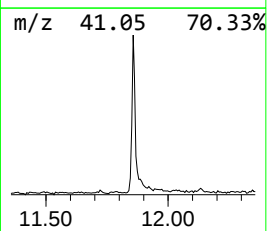
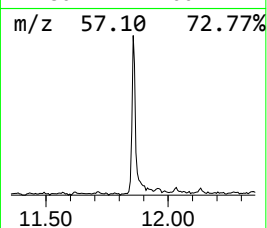
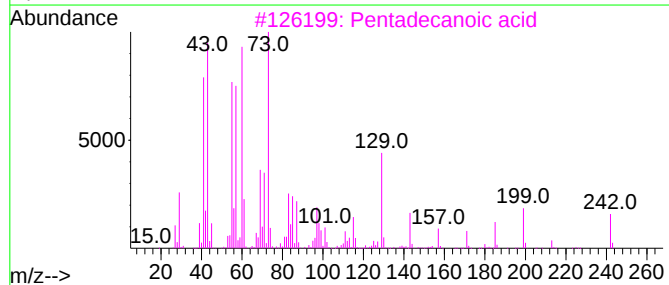
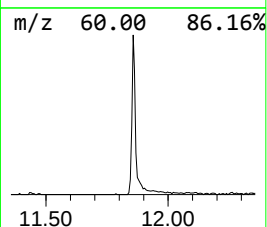
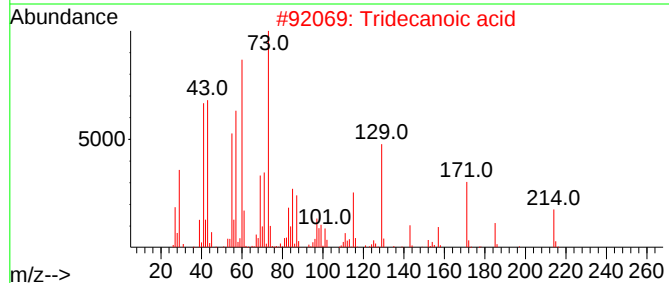
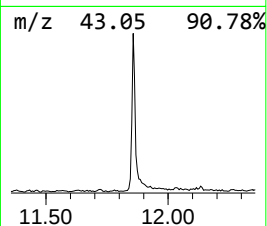
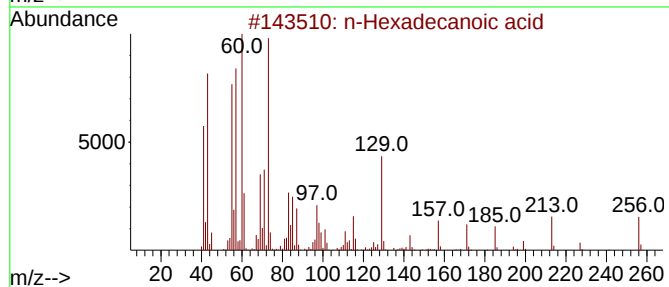
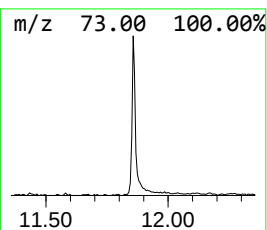
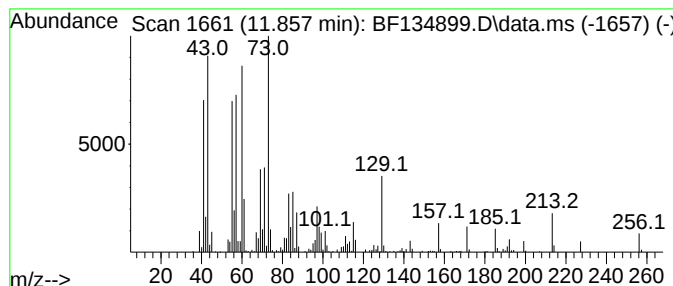
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	5.61 ng	355934	Phenanthrene-d10	11.321

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	92
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60



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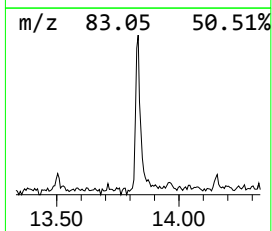
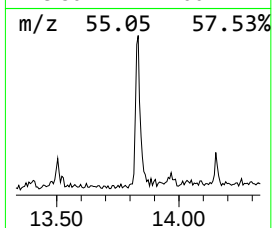
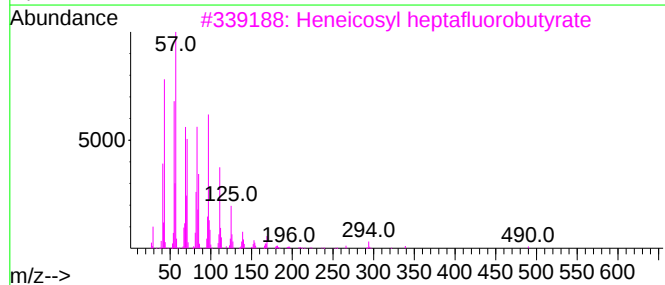
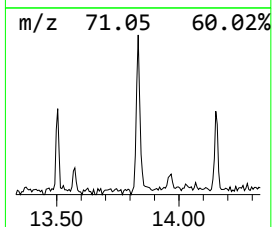
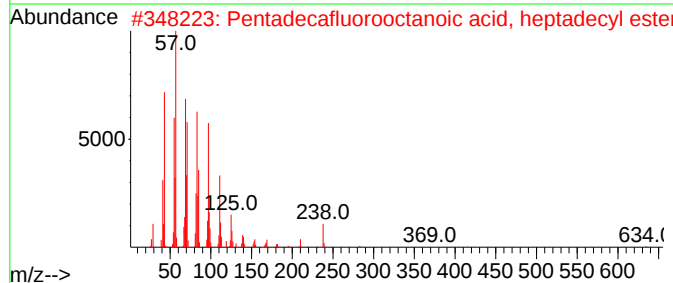
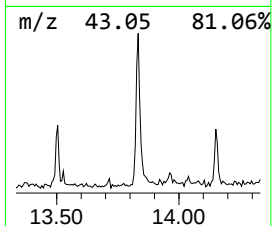
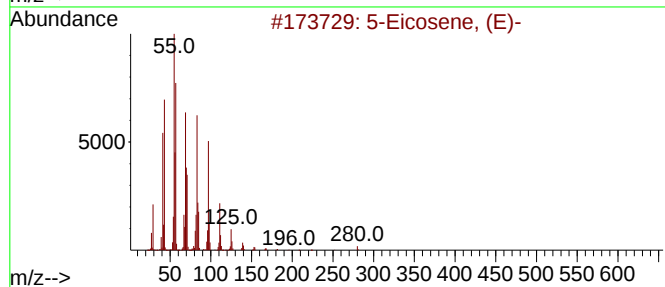
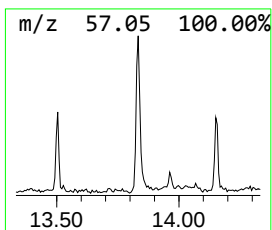
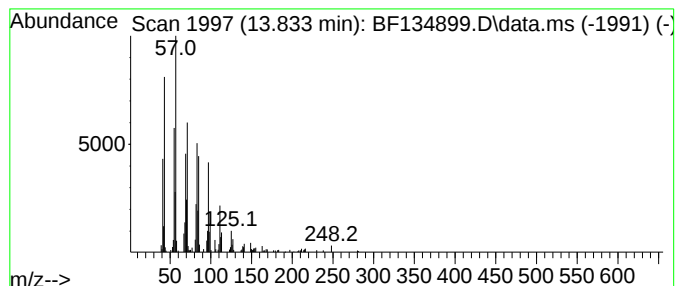
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Peak Number 3 5-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.833	3.97 ng	177478	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Eicosene, (E)-	280	C20H40	074685-30-6	95
2			Pentadecafluorooctanoic acid, he...	652	C25H35F15O2	1000406-04-7	87
3			Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	87
4			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
5			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	87



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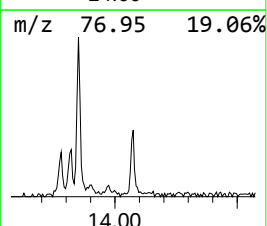
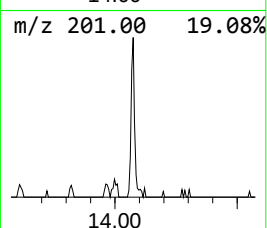
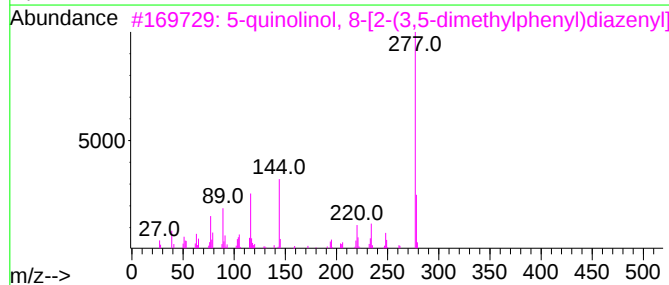
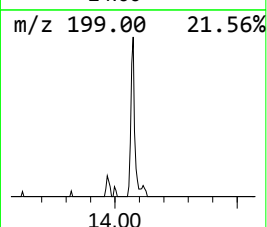
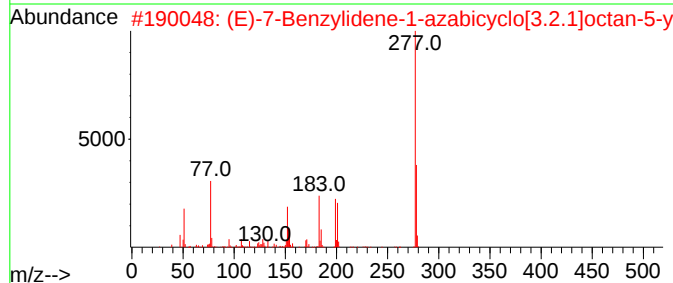
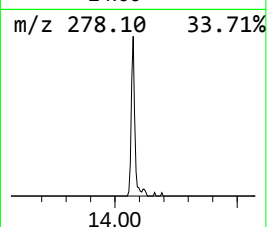
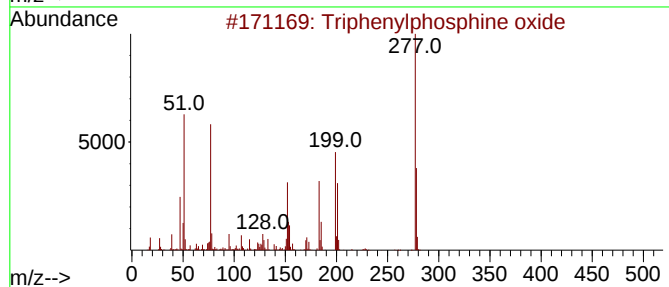
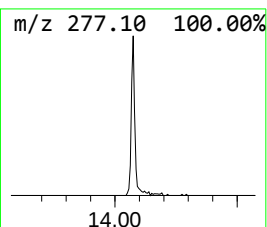
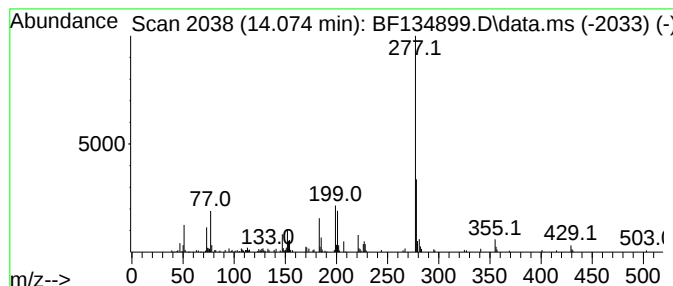
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Triphenylphosphine oxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.074	2.34 ng	104574	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	64
3			5-quinolinol, 8-[2-(3,5-dimethyl...]	277	C17H15N3O	1000397-10-2	50
4			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	40
5			Benzoic acid, 2-(diphenylphosphi...]	306	C19H15O2P	017261-28-8	36



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ALS Vial : 8 Sample Multiplier: 1

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ClientSampleId :
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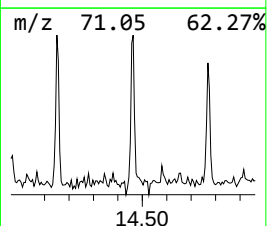
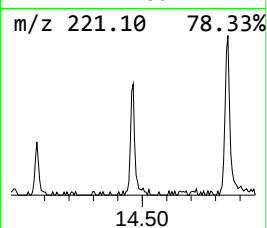
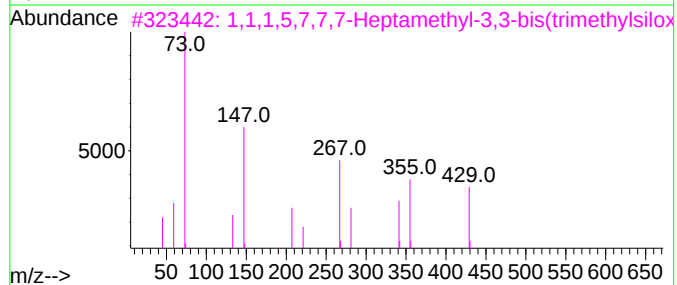
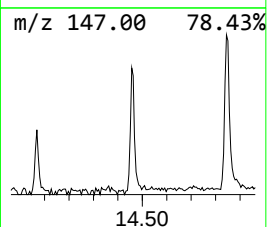
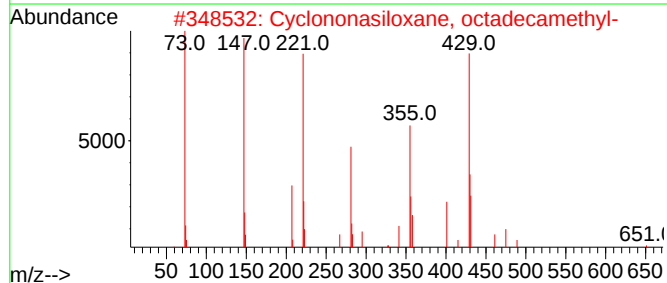
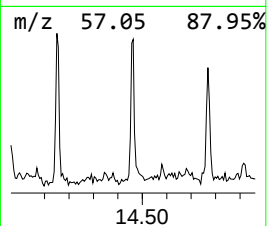
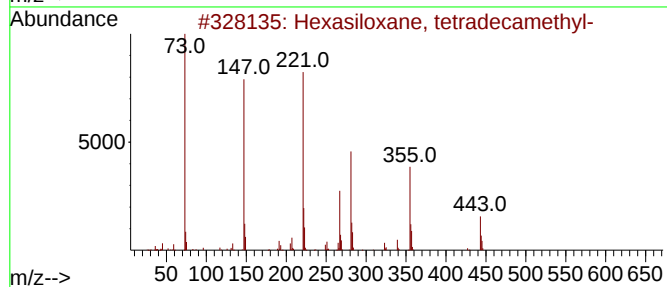
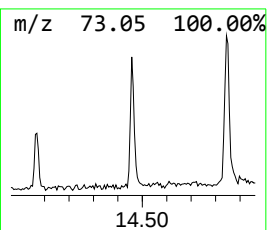
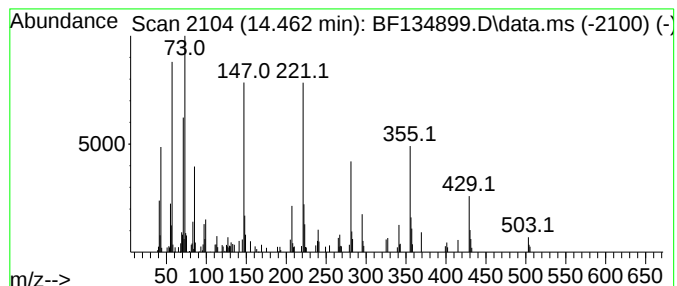
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Peak Number 5 Hexasiloxane, tetradecamethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.462	2.30 ng	102716	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	68
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	59
3			1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	38
4			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	32
5			Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	22



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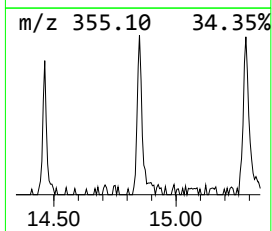
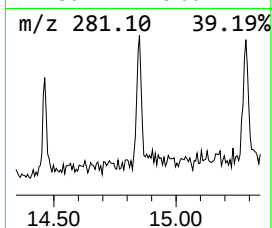
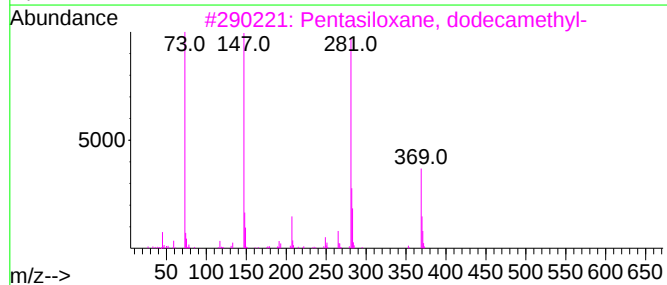
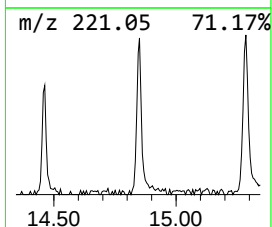
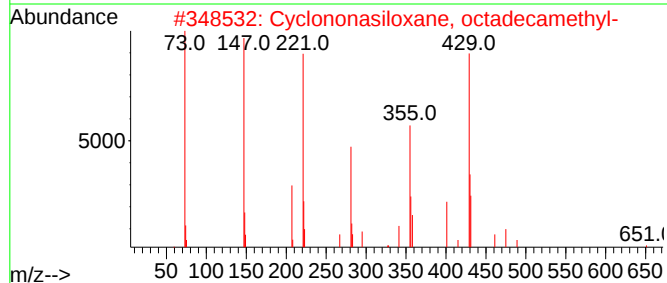
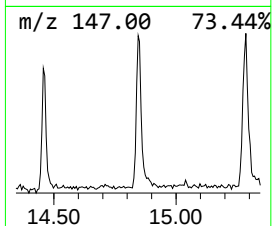
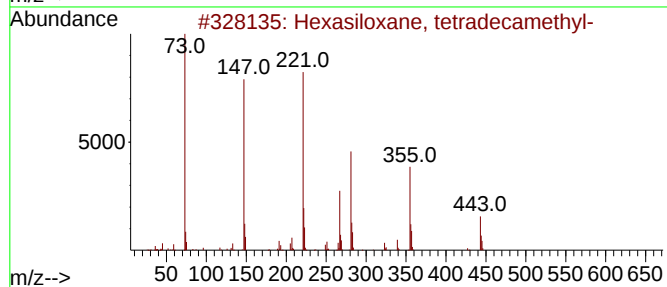
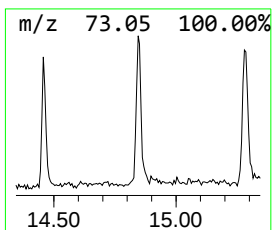
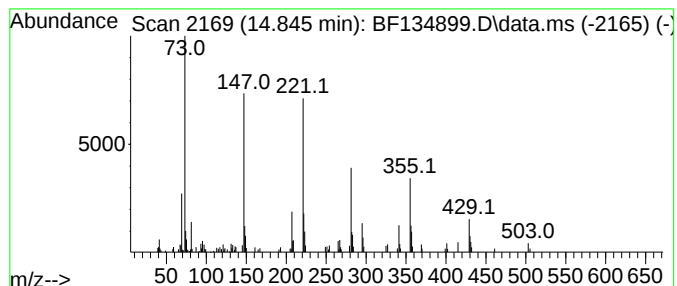
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cyclononasiloxane, octadeca... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.845	2.58 ng	108906	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	83
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	59
3			Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	46
4			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	46
5			Propanedioic acid, 2TMS derivative	248	C9H20O4Si2	018457-04-0	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082323\
Data File : BF134899.D
Acq On : 23 Aug 2023 12:24
Operator : CG\JU
Sample : 04091-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

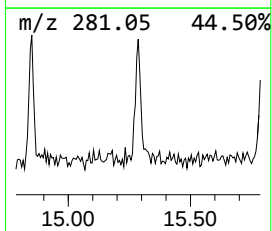
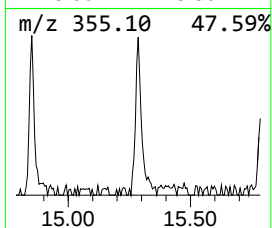
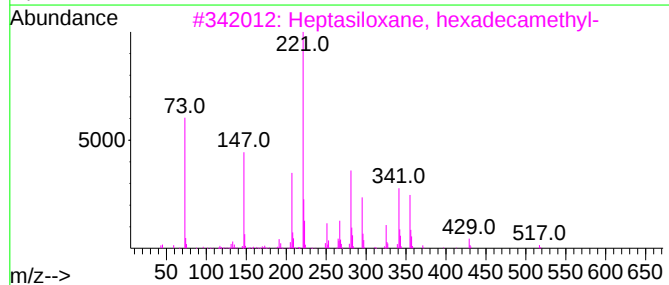
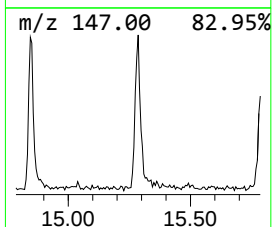
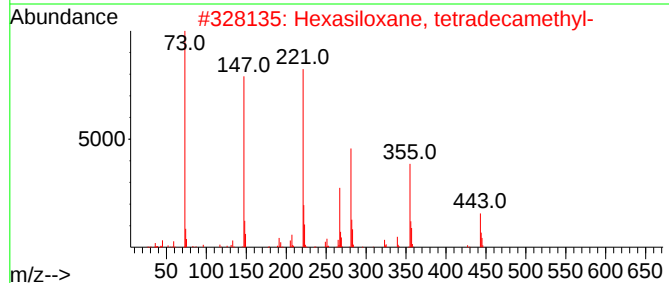
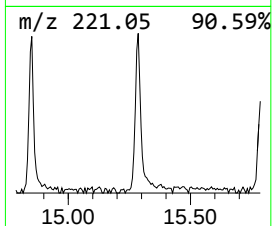
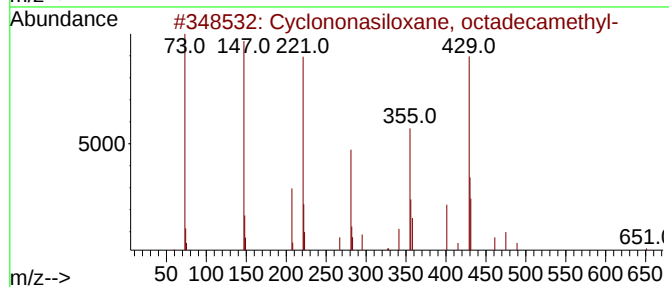
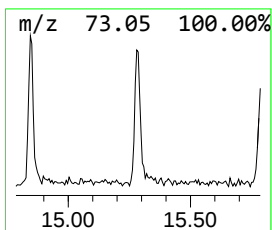
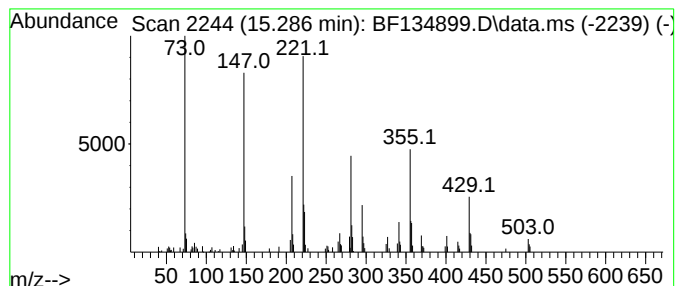
Instrument :
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ClientSampleId :
TP-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown15.286 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD			R.T.
15.286	2.48 ng	104628	Perylene-d12			15.445
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	78
2		Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	68
3		Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	42
4		Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	22
5		N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082323\
Data File : BF134899.D
Acq On : 23 Aug 2023 12:24
Operator : CG\JU
Sample : 04091-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-A

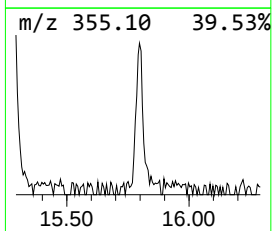
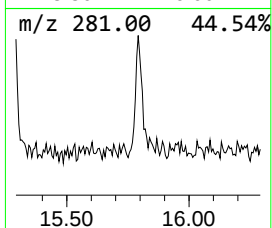
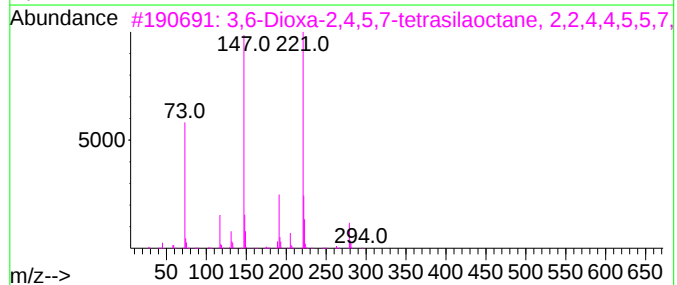
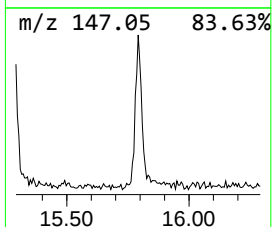
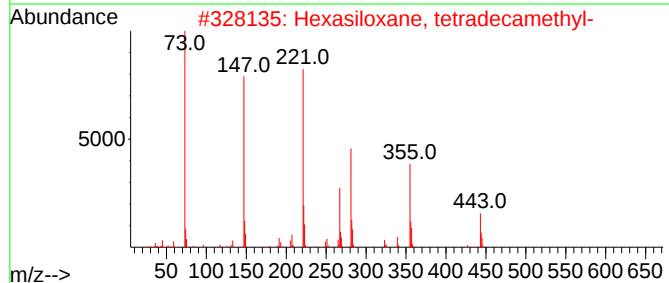
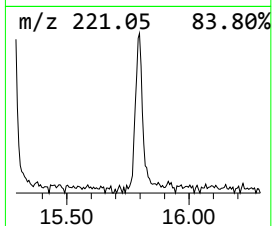
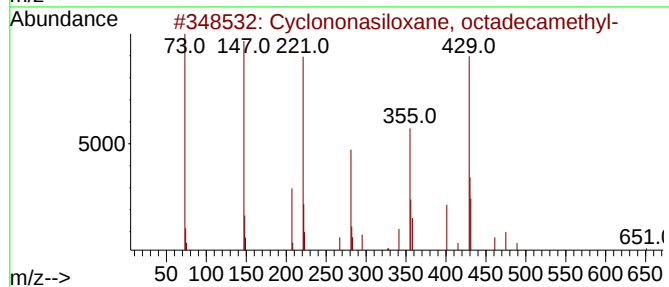
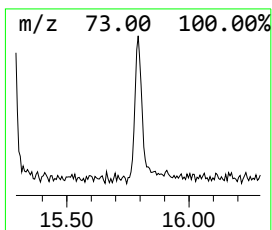
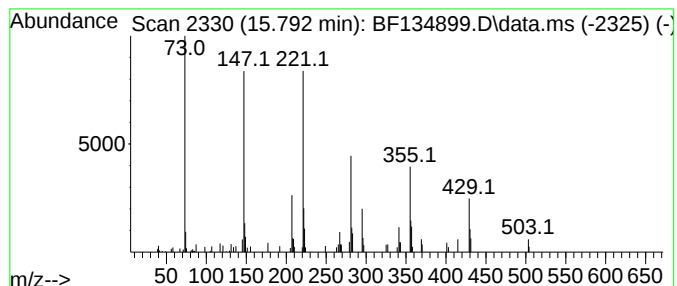
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown15.792 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.792	2.45 ng	103558	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	90
2			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	72
3			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	37
4			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	32
5			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082323\
Data File : BF134899.D
Acq On : 23 Aug 2023 12:24
Operator : CG\JU
Sample : 04091-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082223.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 ...	11.857	5.6	ng	355934	4	11.321	1269980	20.0
5-Eicosene, (E)-	13.833	4.0	ng	177478	5	13.974	894594	20.0
Triphenylphosph...	14.074	2.3	ng	104574	5	13.974	894594	20.0
Hexasiloxane, t...	14.462	2.3	ng	102716	5	13.974	894594	20.0
Cyclononasiloxa...	14.845	2.6	ng	108906	6	15.445	843993	20.0
unknown15.286	15.286	2.5	ng	104628	6	15.445	843993	20.0
unknown15.792	15.792	2.5	ng	103558	6	15.445	843993	20.0