

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
 Data File : BF136433.D
 Acq On : 06 Dec 2023 17:45
 Operator : CG\JU
 Sample : 05602-11
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 ROUTE-4-TP-6

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-BF120523.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136433.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	10	13	23	rVB3	19719	28856	1.99%	0.278%
2	3.875	300	304	310	rVB2	18342	23957	1.65%	0.231%
3	5.022	496	499	503	rVB	38512	41534	2.87%	0.400%
4	5.428	564	568	571	rBV	1491470	1240831	85.71%	11.948%
5	6.428	734	738	741	rBV	1251061	1094050	75.58%	10.535%
6	6.798	797	801	804	rBV	535957	434075	29.99%	4.180%
7	7.351	891	895	899	rBV	788983	684385	47.28%	6.590%
8	8.075	1014	1018	1021	rBV	564405	462300	31.93%	4.452%
9	9.151	1197	1201	1204	rBV	1390539	1094499	75.61%	10.539%
10	9.269	1218	1221	1231	rVB	120266	136355	9.42%	1.313%
11	9.827	1313	1316	1320	rVB	551698	430766	29.76%	4.148%
12	10.616	1447	1450	1455	rBV	750328	681752	47.09%	6.565%
13	10.745	1469	1472	1478	rVB4	17232	26304	1.82%	0.253%
14	11.321	1566	1570	1573	rBV	592615	520523	35.96%	5.012%
15	11.721	1633	1638	1641	rVB6	10353	18022	1.24%	0.174%
16	11.857	1657	1661	1670	rBV2	168910	188907	13.05%	1.819%
17	12.110	1698	1704	1716	rBV2	20813	52777	3.65%	0.508%
18	12.374	1744	1749	1752	rBV5	26505	31230	2.16%	0.301%
19	12.533	1773	1776	1779	rBV	65245	61168	4.23%	0.589%
20	12.580	1781	1784	1788	rVB3	31819	37164	2.57%	0.358%
21	12.645	1792	1795	1801	rVV2	48179	52446	3.62%	0.505%
22	12.763	1812	1815	1818	rVB	61604	57817	3.99%	0.557%
23	12.915	1837	1841	1844	rBV	1714529	1447629	100.00%	13.940%
24	13.104	1869	1873	1877	rVB	381876	325455	22.48%	3.134%
25	13.151	1879	1881	1886	rVB4	20253	24825	1.71%	0.239%
26	13.327	1908	1911	1914	rBV4	17534	21417	1.48%	0.206%
27	13.968	2017	2020	2024	rVB	524468	512262	35.39%	4.933%
28	14.145	2048	2050	2054	rBV5	25239	28123	1.94%	0.271%
29	14.457	2100	2103	2105	rVB	47986	45782	3.16%	0.441%
30	15.109	2211	2214	2219	rVB	94461	117251	8.10%	1.129%
31	15.451	2268	2272	2277	rBV	300697	347592	24.01%	3.347%
32	15.956	2354	2358	2362	rBV2	75975	114833	7.93%	1.106%

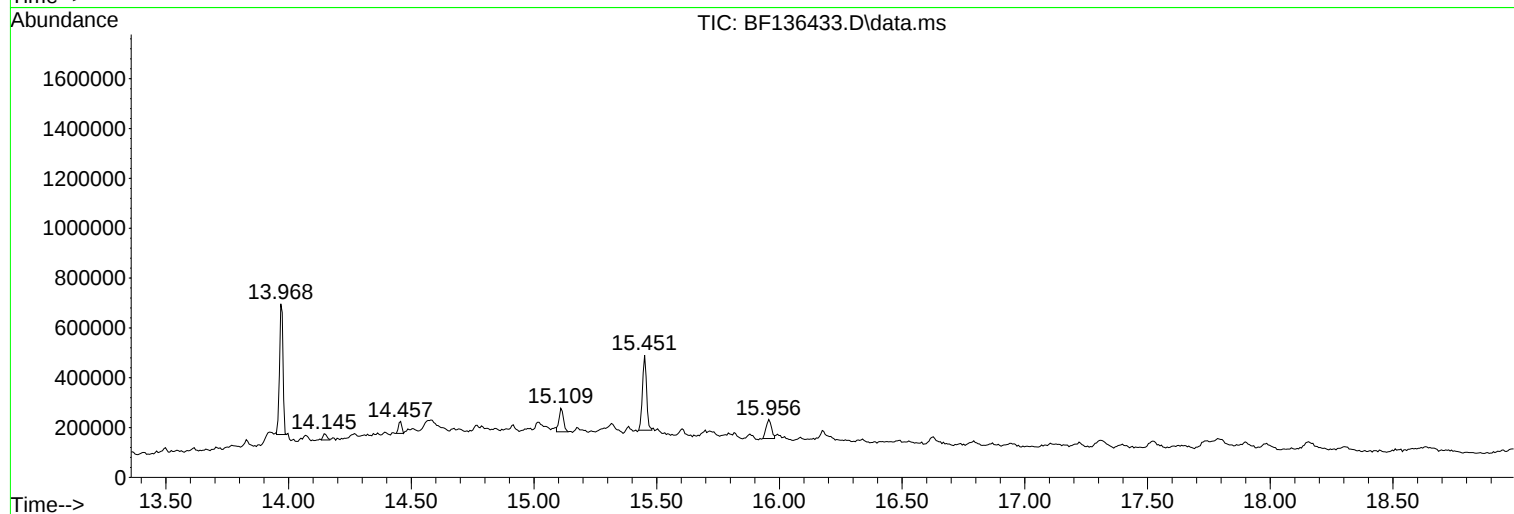
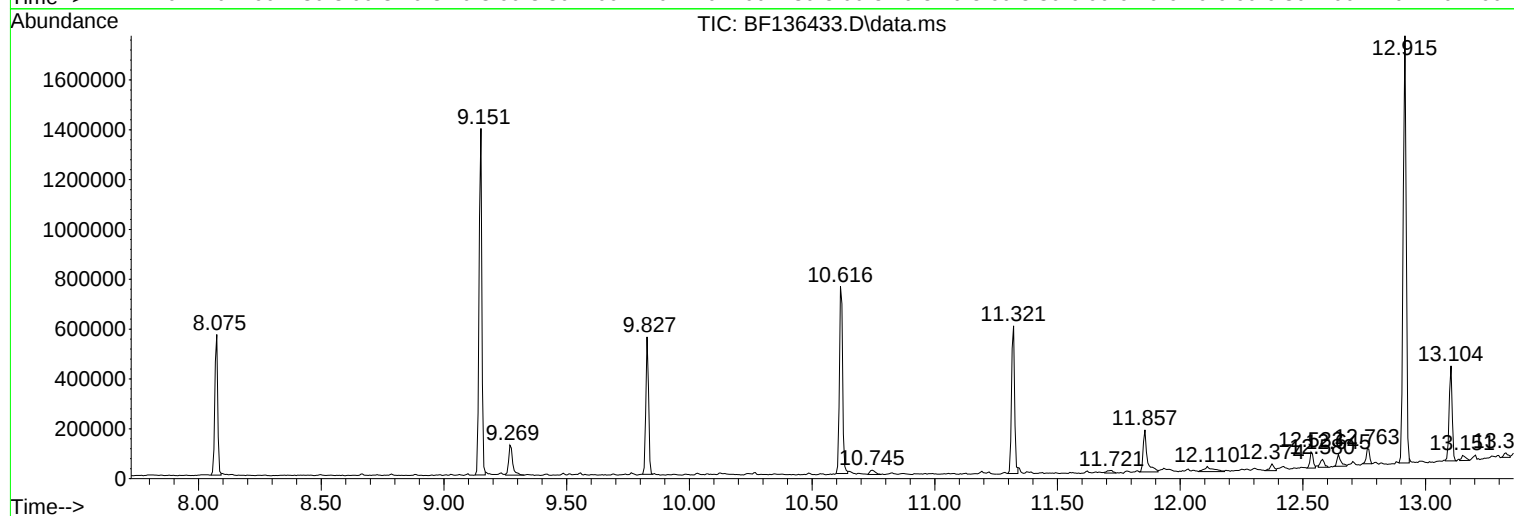
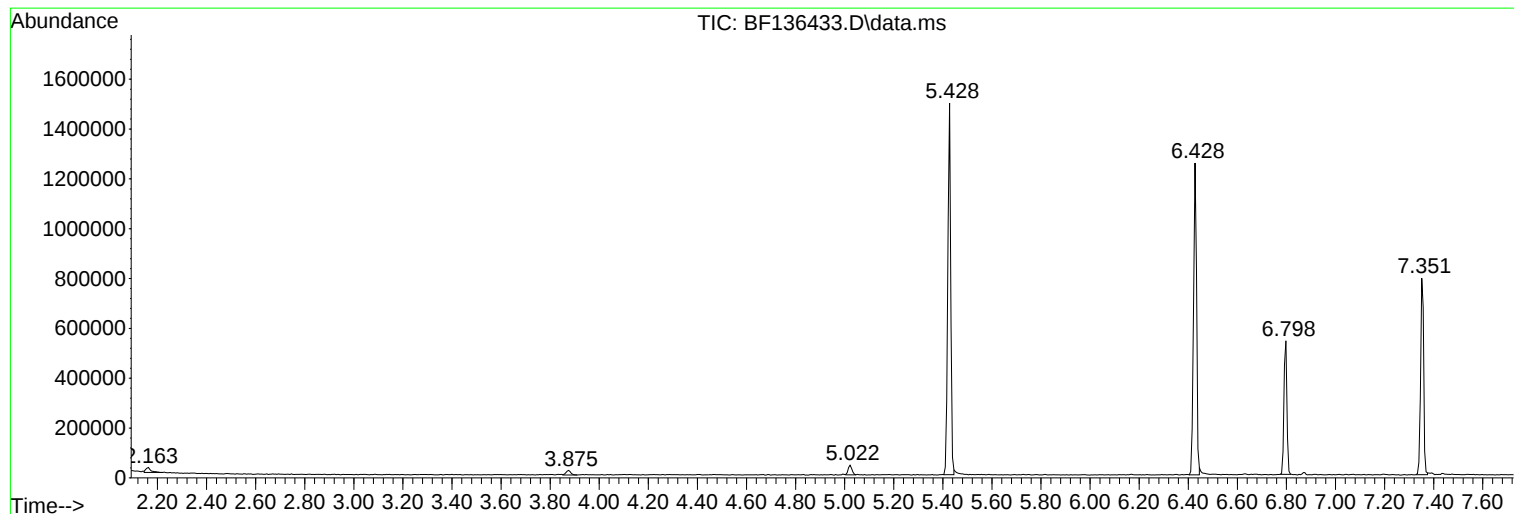
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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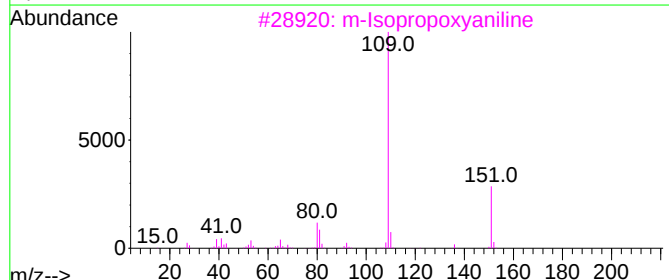
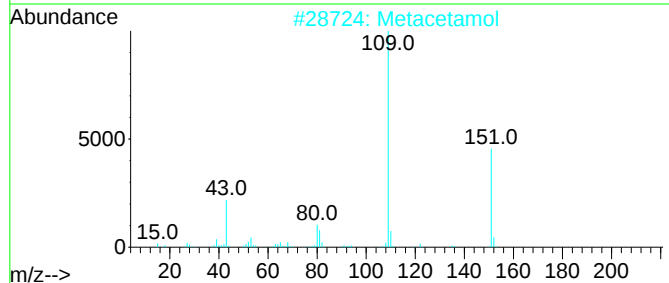
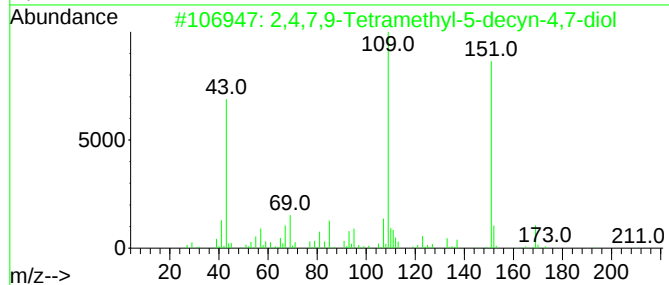
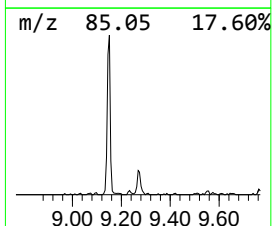
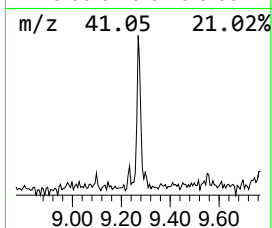
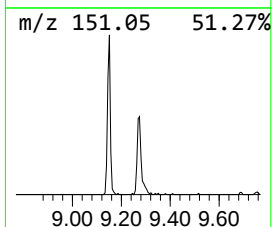
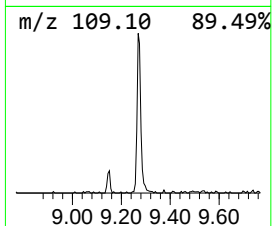
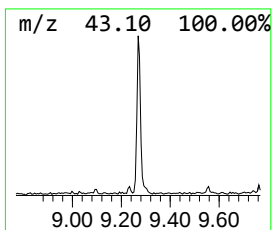
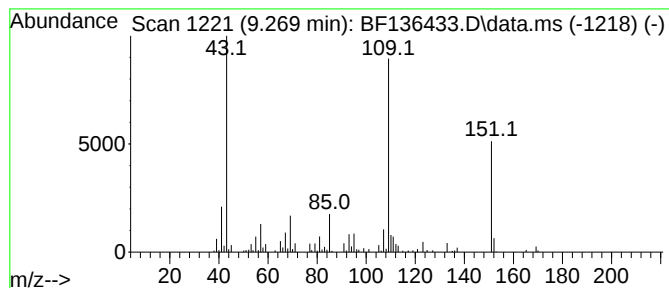
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.269	6.33 ng	136355	Acenaphthene-d10	9.827

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	90	
2	Metacetamol	151	C8H9NO2	000621-42-1	59	
3	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	59	
4	Acetaminophen	151	C8H9NO2	000103-90-2	45	
5	2,4-Heptadienal, 2,4-dimethyl-	138	C9H14O	042452-48-2	43	



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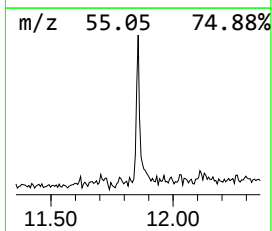
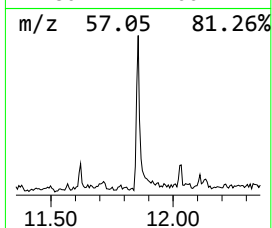
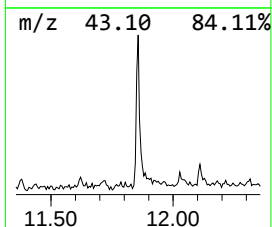
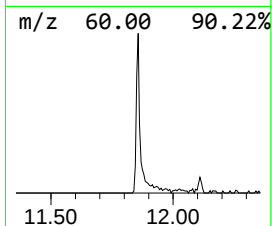
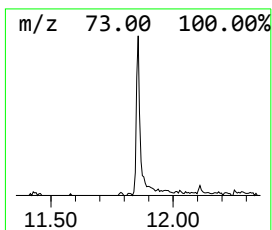
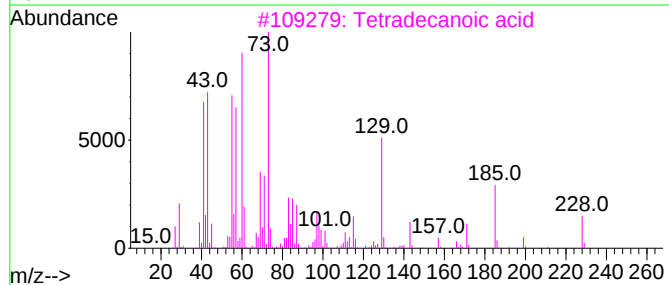
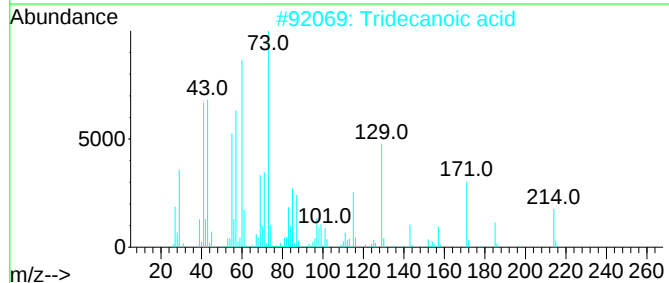
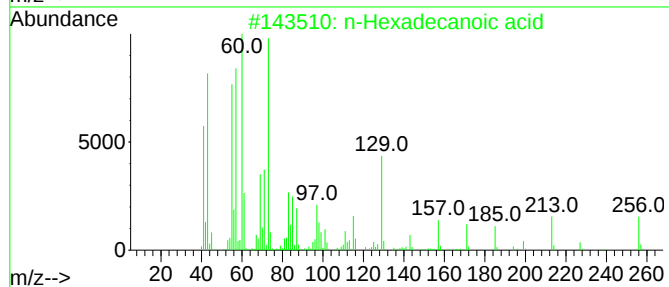
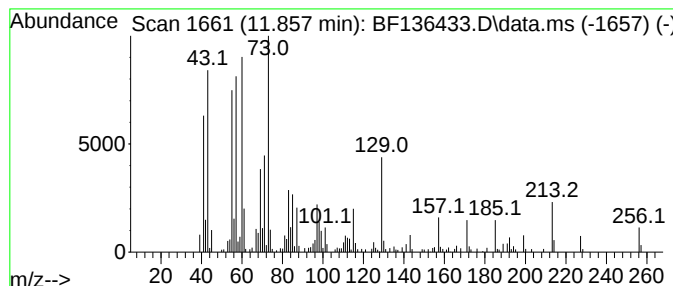
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	7.26 ng	188907	Phenanthrene-d10	11.322

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			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5			Undecanoic acid	186	C11H22O2	000112-37-8	68



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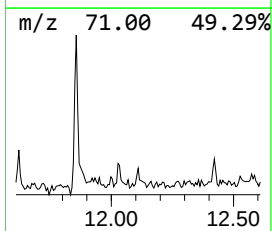
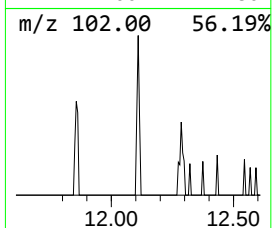
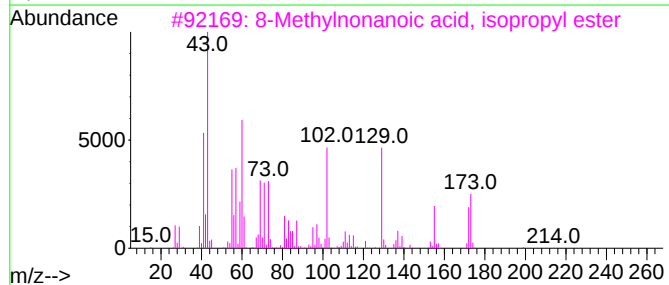
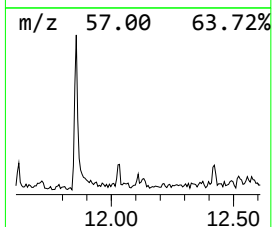
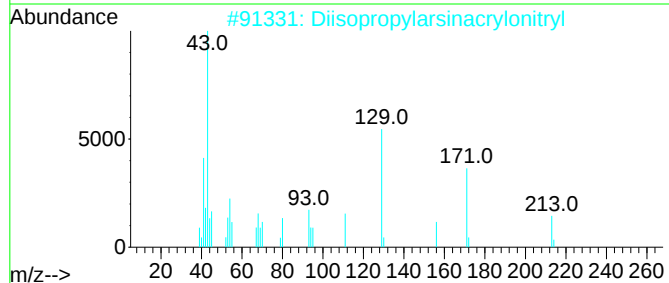
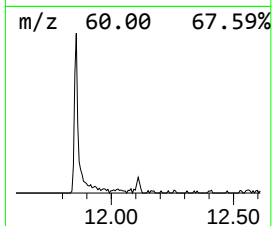
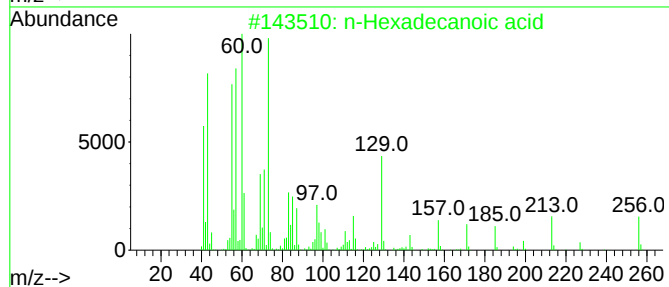
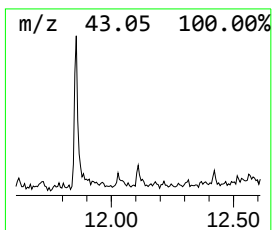
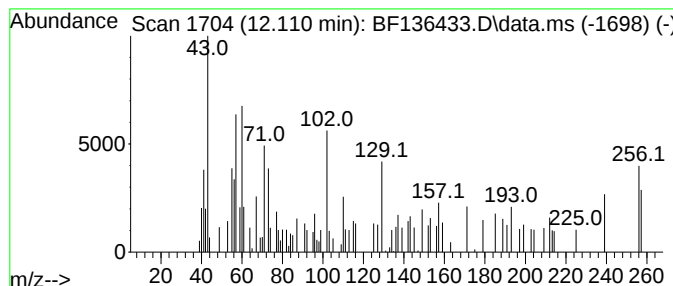
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 unknown12.110 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.110	2.03 ng	52777	Phenanthrene-d10	11.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	43
2			Diisopropylarsinacrylonitryl	213	C9H16AsN	077376-96-6	25
3			8-Methylnonanoic acid, isopropyl...	214	C13H26O2	1000452-00-6	25
4			n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	22
5			Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	14



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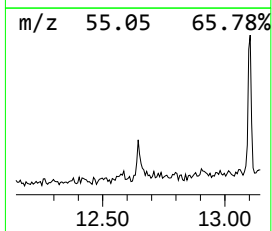
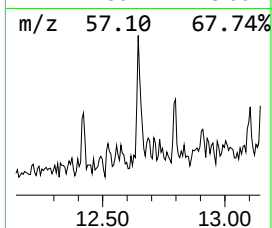
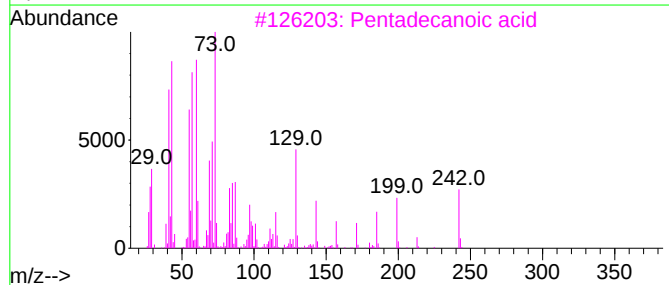
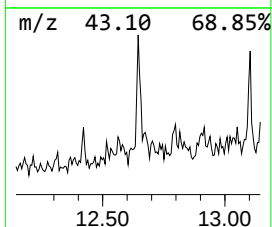
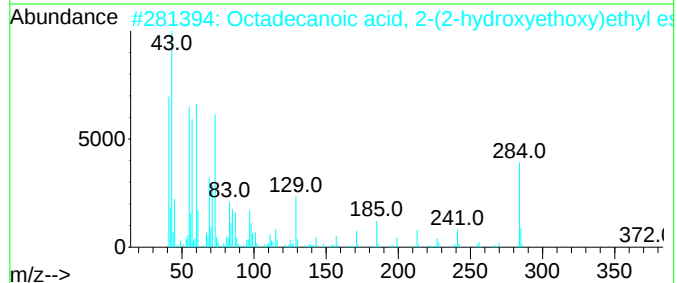
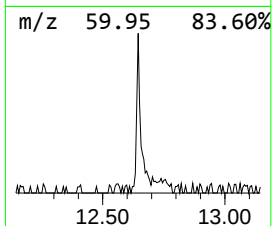
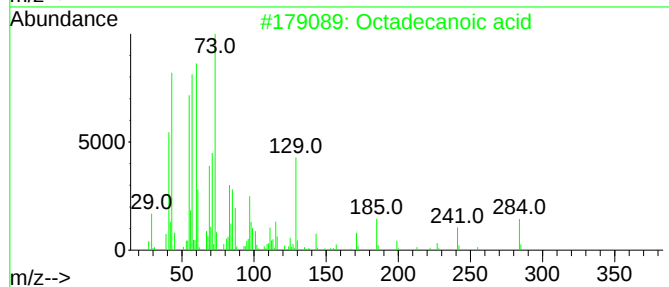
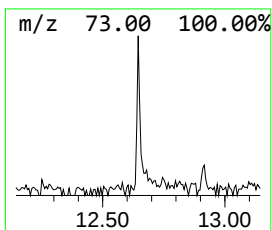
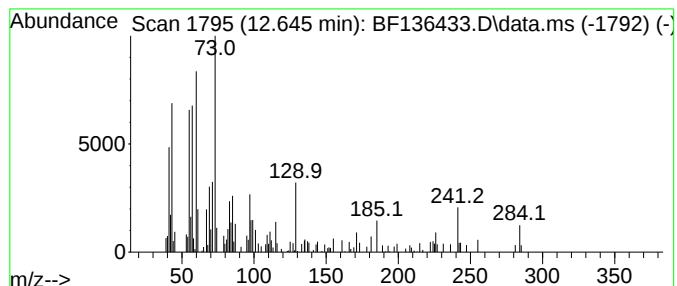
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.645	2.02 ng	52446	Phenanthrene-d10	11.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4			Tridecanoic acid	214	C13H26O2	000638-53-9	64
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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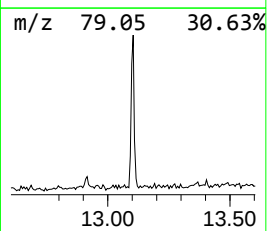
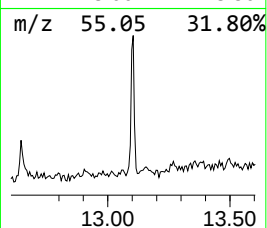
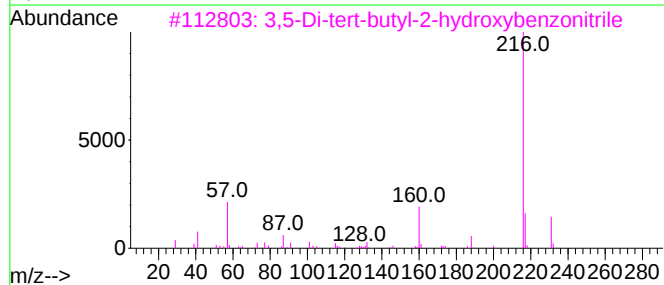
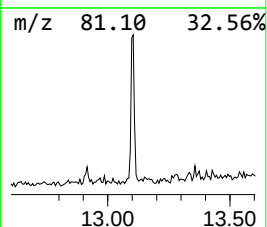
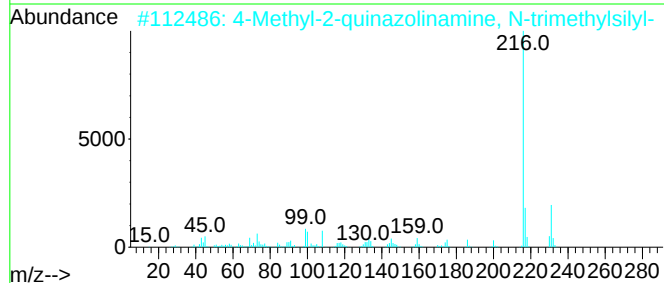
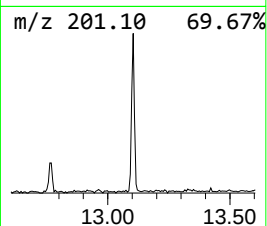
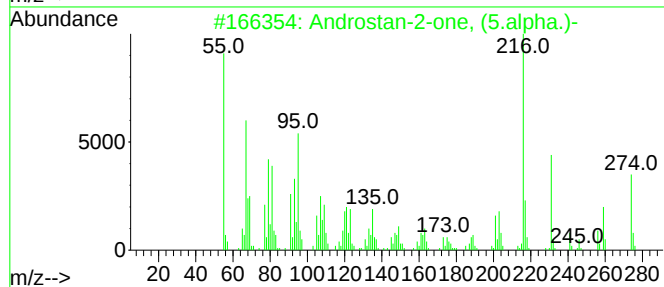
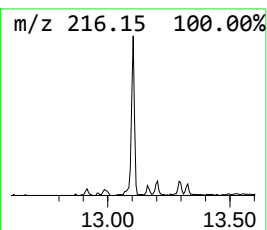
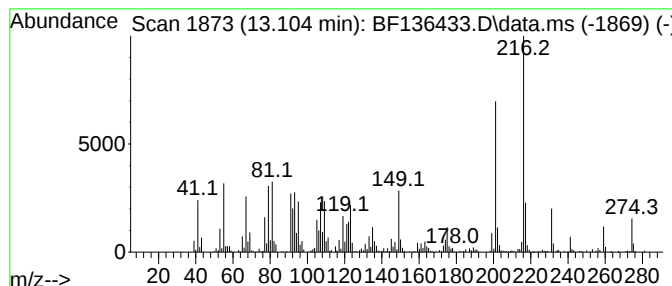
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Peak Number 7 unknown13.104 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.104	12.71 ng	325455	Chrysene-d12	13.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Androstan-2-one, (5.alpha.)-	274	C19H30O	001225-48-5	46
2			4-Methyl-2-quinazolinamine, N-tr...	231	C12H17N3Si	1010471-48-6	46
3			3,5-Di-tert-butyl-2-hydroxybenzo...	231	C15H21NO	095091-86-4	38
4			1,4-benzenediacetonitrile, 2,5-d...	216	C12H12N2O2	1000400-71-7	38
5			2-Pyrazolin-5-one, 4-acetyl-3-me...	216	C12H12N2O2	004173-74-4	38



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ClientSampleId :
ROUTE-4-TP-6

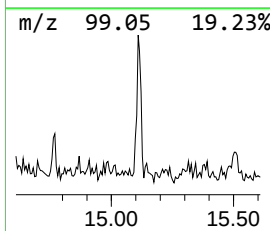
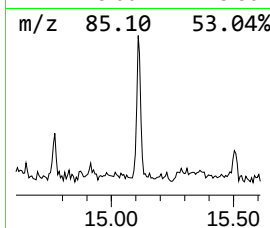
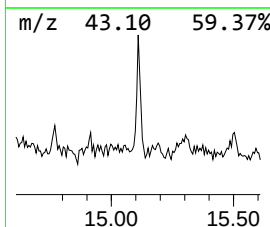
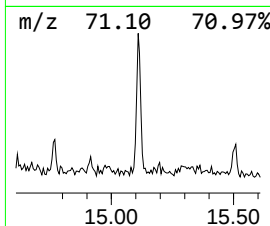
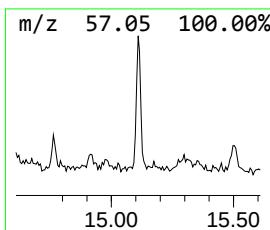
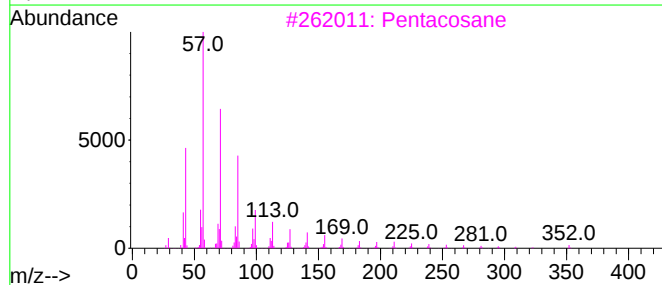
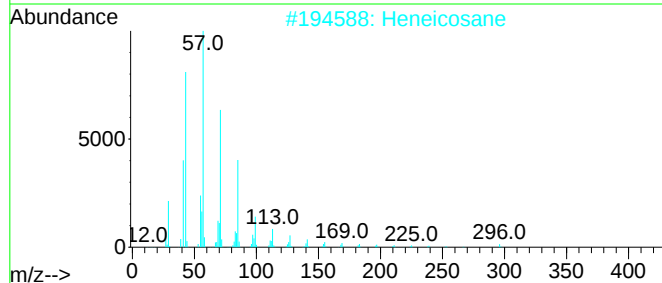
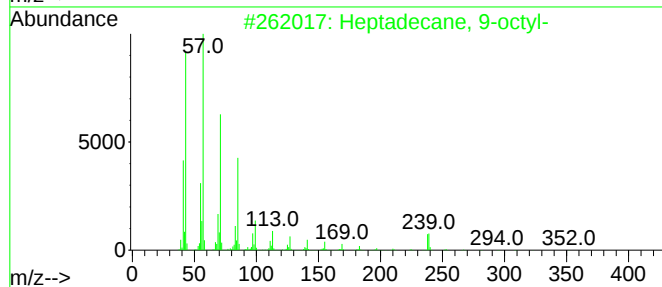
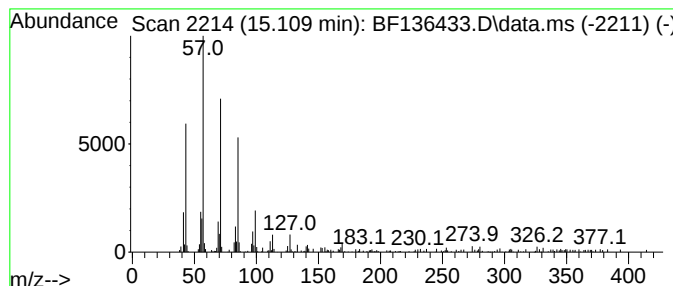
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecane, 9-octyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.109	6.75 ng	117251	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
2			Heneicosane	296	C21H44	000629-94-7	92
3			Pentacosane	352	C25H52	000629-99-2	86
4			Eicosane, 2-methyl-	296	C21H44	001560-84-5	70
5			Tetratetracontane	619	C44H90	007098-22-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
Data File : BF136433.D
Acq On : 06 Dec 2023 17:45
Operator : CG\JU
Sample : 05602-11
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ROUTE-4-TP-6

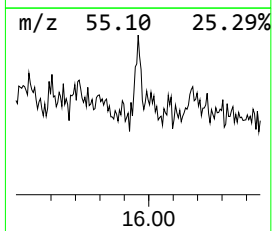
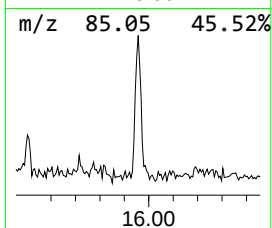
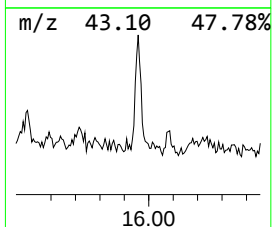
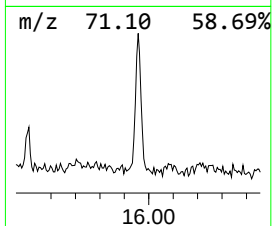
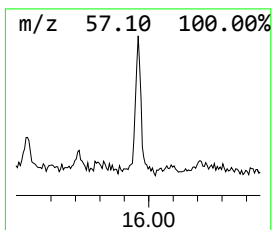
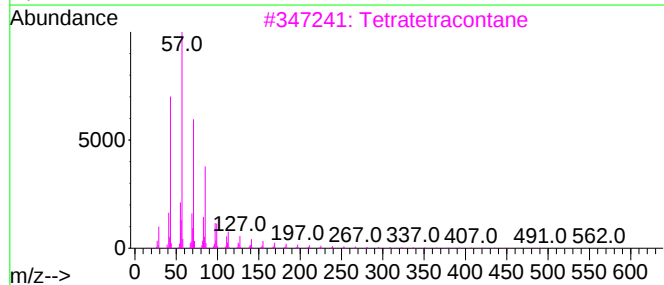
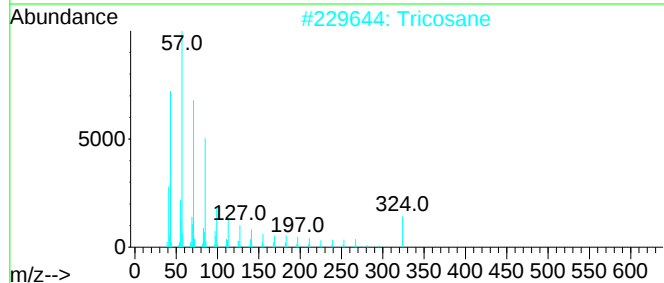
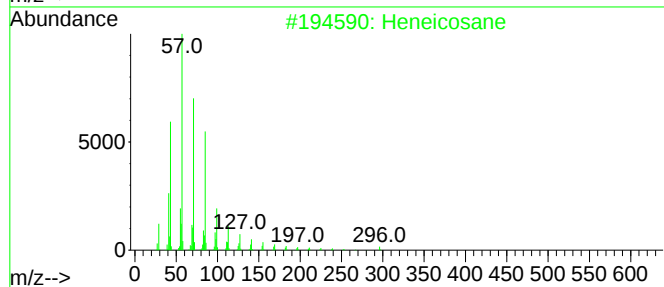
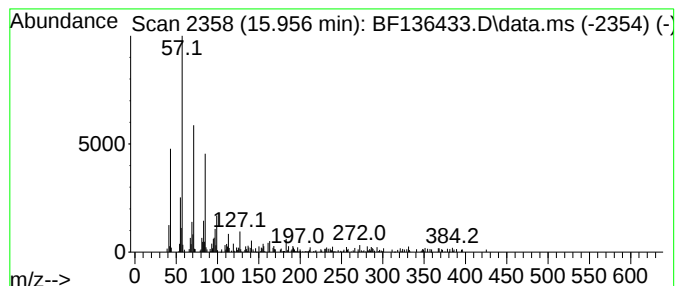
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.956	6.61 ng	114833	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	94
2			Tricosane	324	C23H48	000638-67-5	91
3			Tetratetracontane	619	C44H90	007098-22-8	90
4			Octacosane	394	C28H58	000630-02-4	87
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
Data File : BF136433.D
Acq On : 06 Dec 2023 17:45
Operator : CG\JU
Sample : 05602-11
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ROUTE-4-TP-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.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
2,4,7,9-Tetrame...	9.269	6.3	ng	136355	3	9.827	430766	20.0
n-Hexadecanoic ...	11.857	7.3	ng	188907	4	11.322	520523	20.0
unknown12.110	12.110	2.0	ng	52777	4	11.322	520523	20.0
Octadecanoic acid	12.645	2.0	ng	52446	4	11.322	520523	20.0
unknown13.104	13.104	12.7	ng	325455	5	13.968	512262	20.0
Heptadecane, 9-...	15.109	6.8	ng	117251	6	15.451	347592	20.0
Heneicosane	15.956	6.6	ng	114833	6	15.451	347592	20.0