

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120823\
 Data File : BF136475.D
 Acq On : 08 Dec 2023 19:12
 Operator : CG\JU
 Sample : 05629-04
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 72-11985

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: BF136475.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.028	496	500	511	rVB	234876	258487	11.40%	1.576%
2	5.440	565	570	573	rBV	1996417	1937438	85.45%	11.816%
3	6.440	735	740	743	rBV	2071209	1918090	84.60%	11.698%
4	6.793	797	800	804	rVB	774832	663447	29.26%	4.046%
5	7.357	890	896	899	rBV	1421907	1220415	53.83%	7.443%
6	8.075	1013	1018	1021	rBV	1003808	873104	38.51%	5.325%
7	9.151	1195	1201	1204	rBV	2858908	2267327	100.00%	13.828%
8	9.828	1312	1316	1319	rBV	1198099	910988	40.18%	5.556%
9	10.622	1446	1451	1454	rBV	1235973	1114980	49.18%	6.800%
10	10.728	1465	1469	1475	rBV	31912	32178	1.42%	0.196%
11	11.322	1566	1570	1572	rBV	831728	763480	33.67%	4.656%
12	11.339	1572	1573	1577	rVB	37525	28585	1.26%	0.174%
13	11.857	1657	1661	1666	rBV	193802	184903	8.16%	1.128%
14	12.533	1773	1776	1781	rBV	91545	84509	3.73%	0.515%
15	12.645	1791	1795	1800	rBV4	37966	45815	2.02%	0.279%
16	12.763	1809	1815	1818	rBV	70711	84904	3.74%	0.518%
17	12.916	1837	1841	1844	rBV	1917290	1574609	69.45%	9.603%
18	13.898	2003	2008	2012	rBV4	34200	74907	3.30%	0.457%
19	13.969	2016	2020	2024	rBV	649982	697725	30.77%	4.255%
20	14.069	2035	2037	2041	rVB4	29065	31607	1.39%	0.193%
21	14.457	2099	2103	2106	rBV5	43442	50272	2.22%	0.307%
22	14.616	2126	2130	2135	rBV	644798	615852	27.16%	3.756%
23	14.839	2165	2168	2174	rVB5	40772	64790	2.86%	0.395%
24	14.910	2178	2180	2185	rVB6	33308	40367	1.78%	0.246%
25	15.016	2195	2198	2202	rBV2	34967	56629	2.50%	0.345%
26	15.110	2211	2214	2220	rVB3	40610	49993	2.20%	0.305%
27	15.280	2240	2243	2247	rVB5	29977	34883	1.54%	0.213%
28	15.380	2258	2260	2264	rVB	24727	28862	1.27%	0.176%
29	15.451	2267	2272	2278	rBV	457777	585574	25.83%	3.571%
30	15.710	2314	2316	2320	rVB4	25444	27786	1.23%	0.169%
31	15.951	2353	2357	2364	rBV3	39261	73819	3.26%	0.450%

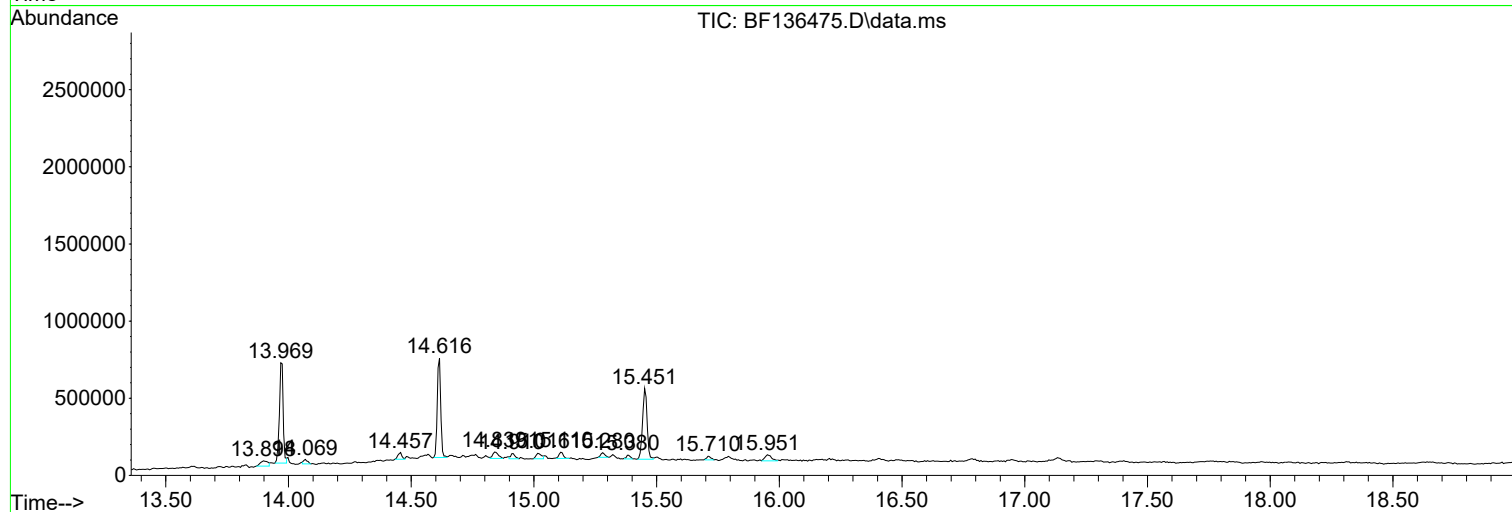
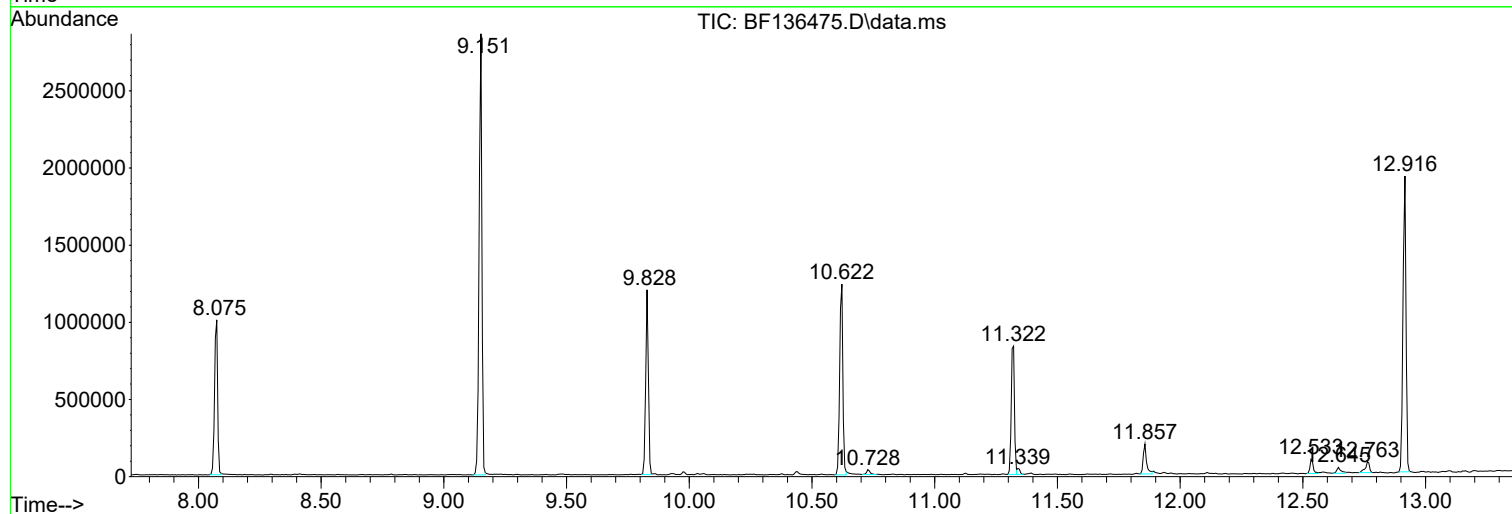
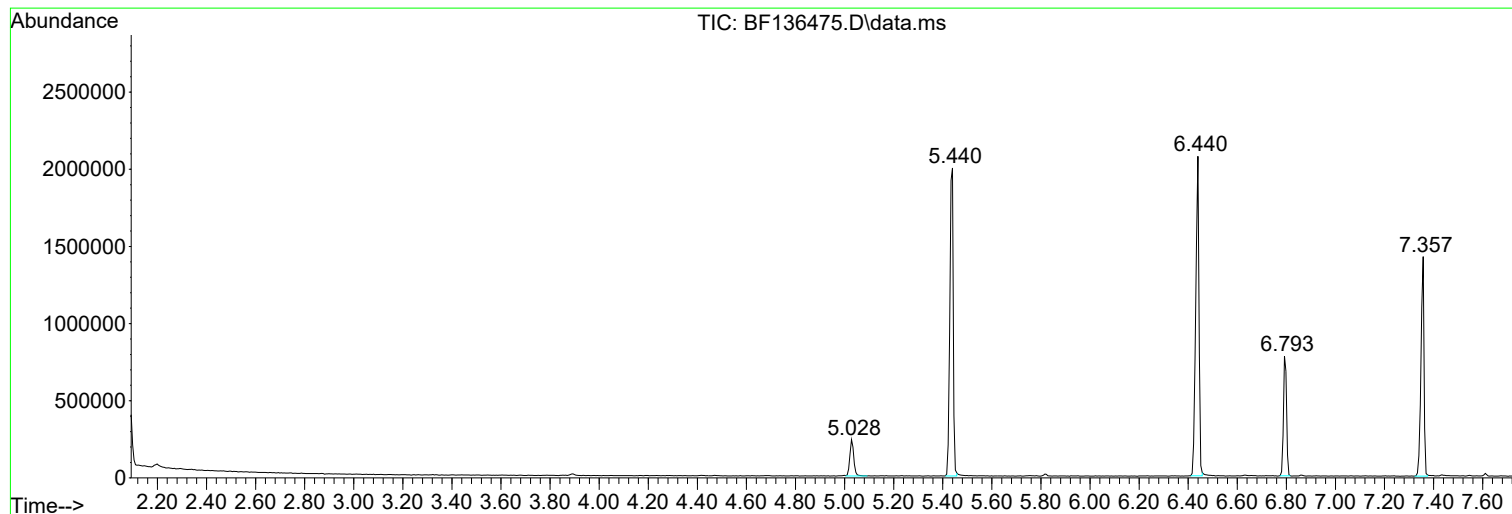
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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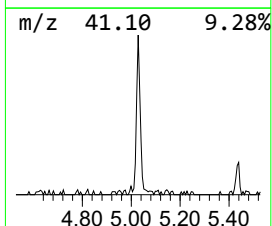
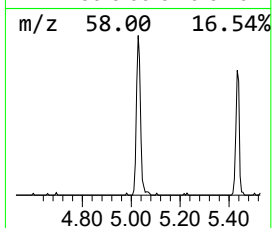
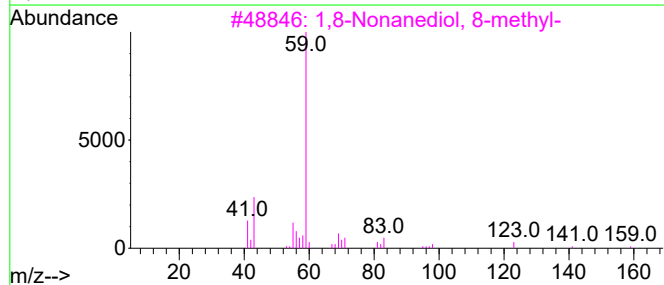
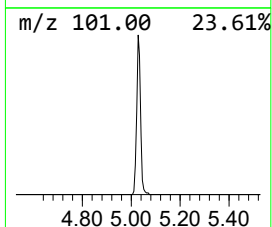
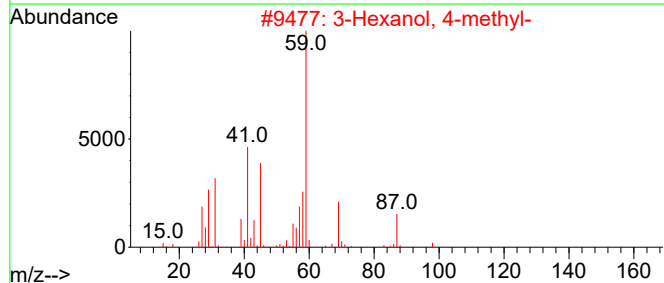
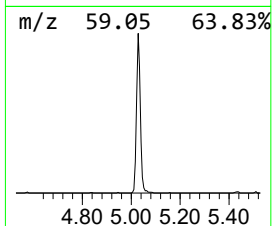
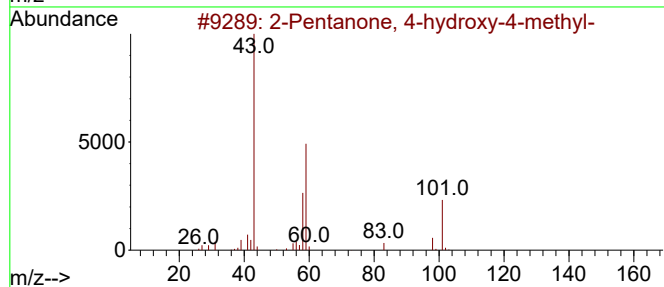
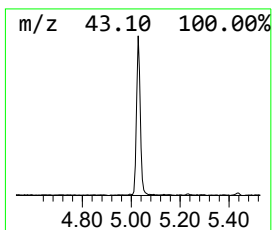
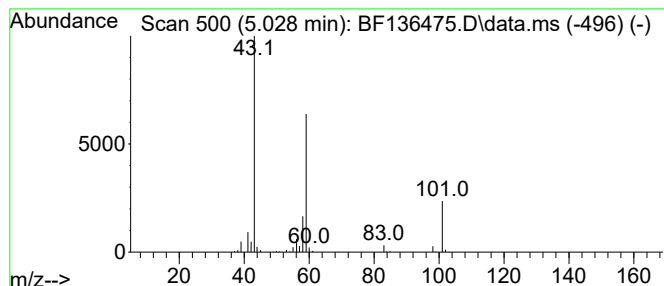
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TIC Library : C:\Database\NIST20.L
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.028	7.79 ng	258487	1,4-Dichlorobenzene-d4	6.793

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	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	23		



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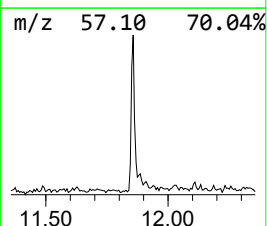
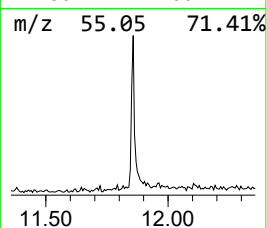
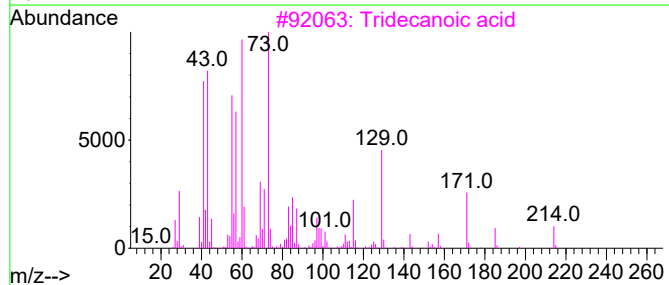
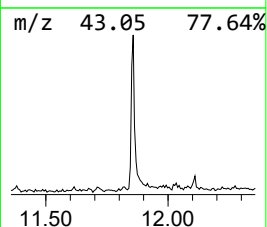
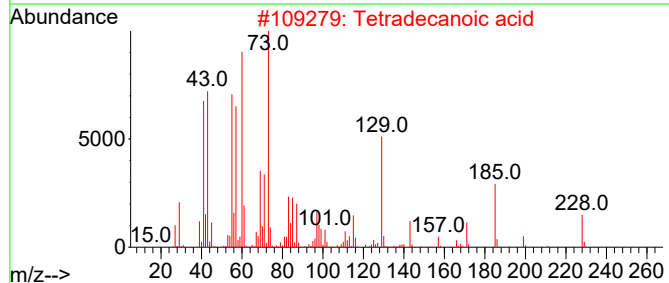
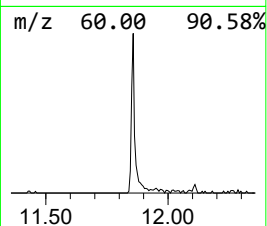
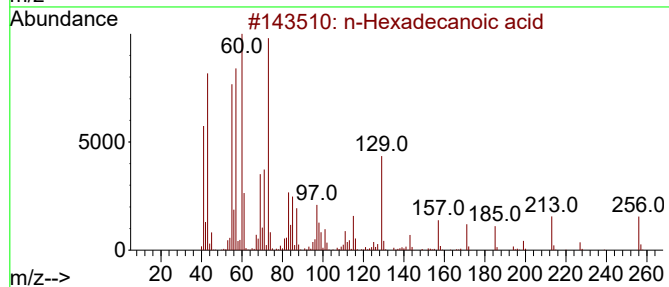
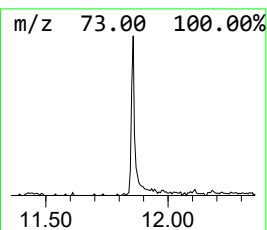
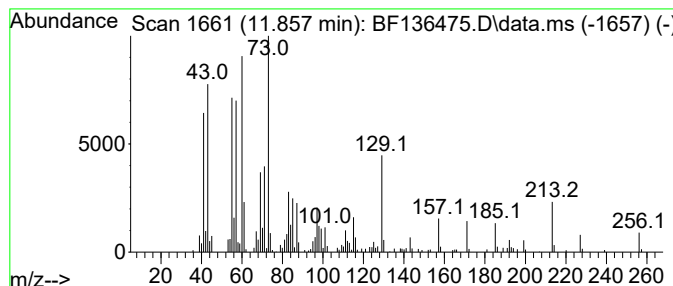
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	4.84 ng	184903	Phenanthrene-d10	11.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5			n-Decanoic acid	172	C10H20O2	000334-48-5	68



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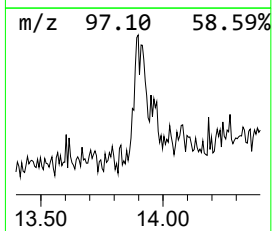
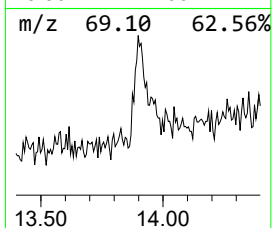
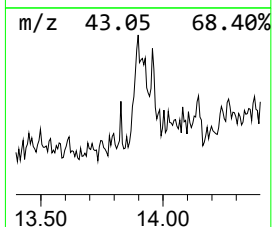
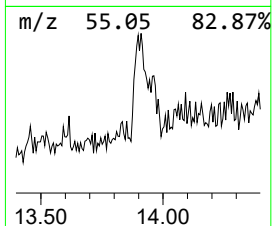
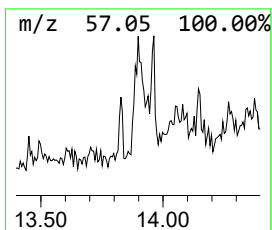
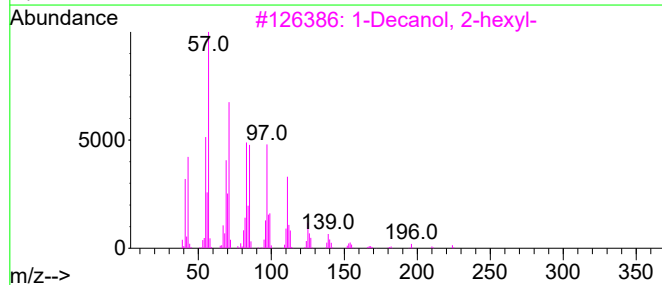
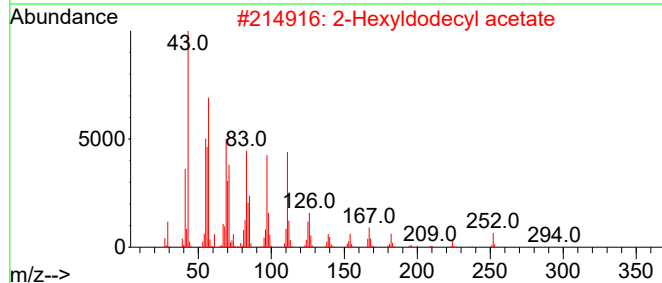
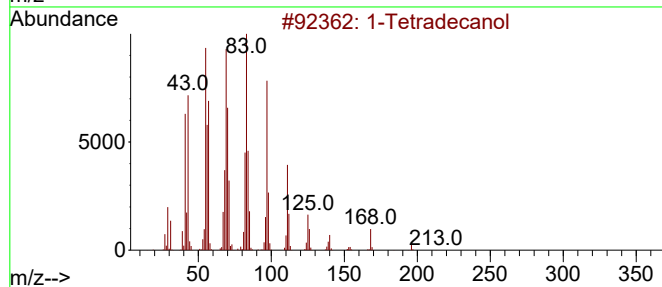
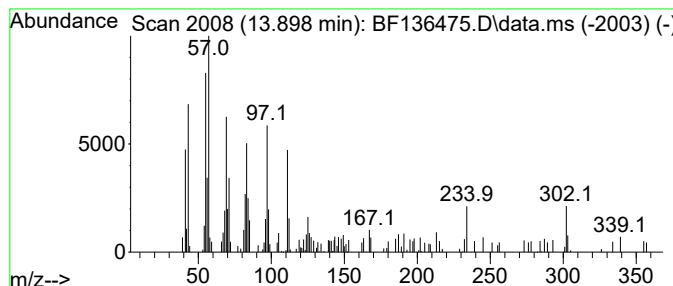
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Peak Number 5 1-Tetradecanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	2.15 ng	74907	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetradecanol			214	C14H30O	000112-72-1	64
2	2-Hexyldodecyl acetate			312	C20H40O2	1000368-55-9	64
3	1-Decanol, 2-hexyl-			242	C16H34O	002425-77-6	64
4	Heptafluorobutyric acid, pentade...			424	C19H31F7O2	959261-23-5	58
5	Trifluoroacetic acid,n-tridecyl ...			296	C15H27F3O2	053800-02-5	58



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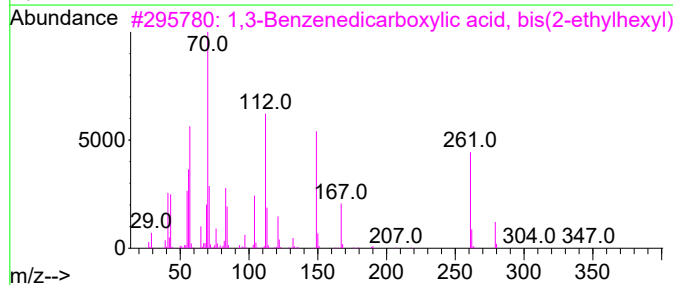
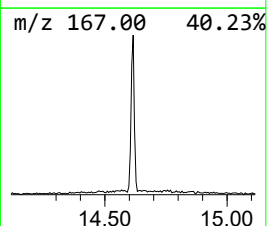
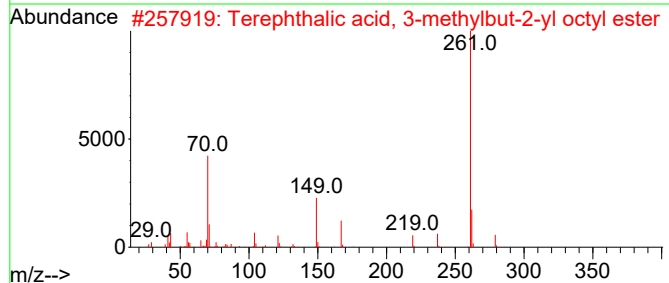
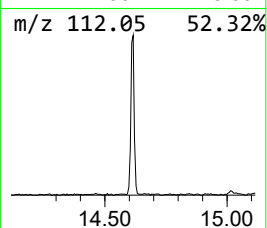
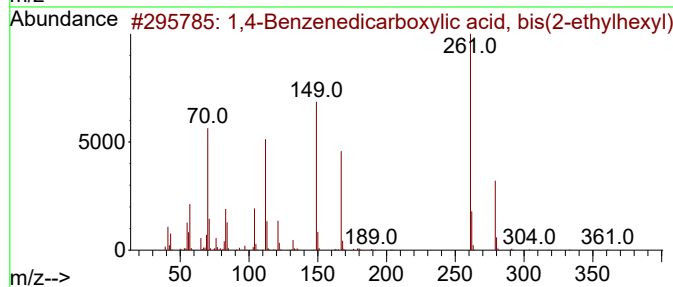
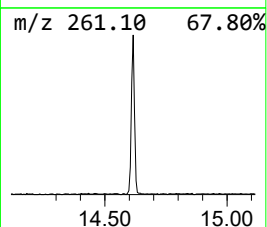
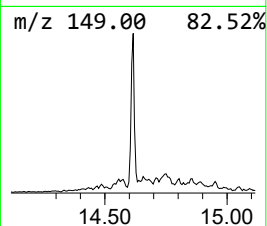
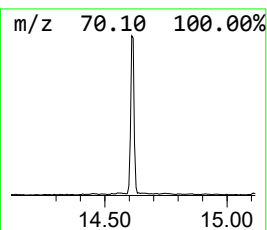
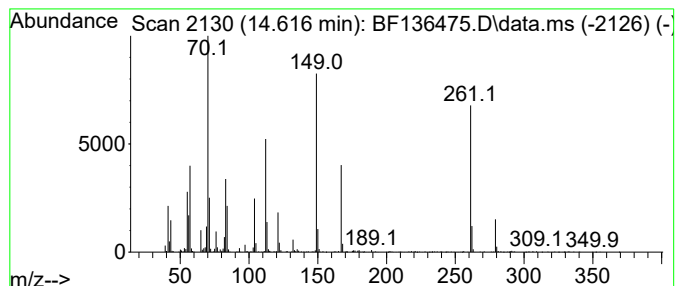
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Peak Number 6 1,4-Benzenedicarboxylic aci... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.616	17.65 ng	615852	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	87
2			Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	72
3			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	62
4			Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	43
5			Terephthalic acid, 4-fluoro-2-me...	402	C23H27F O5	1000415-83-4	35



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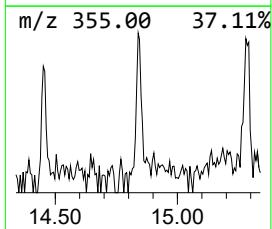
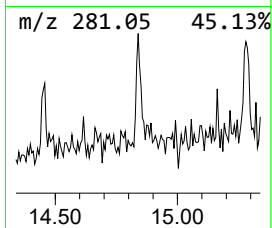
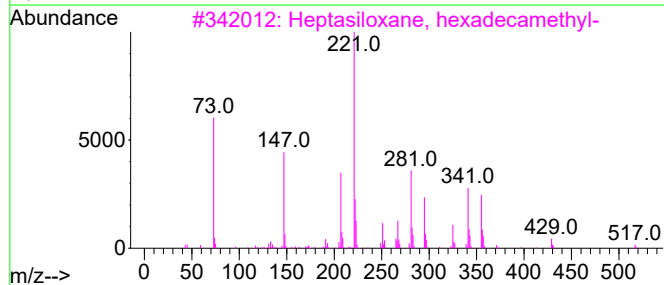
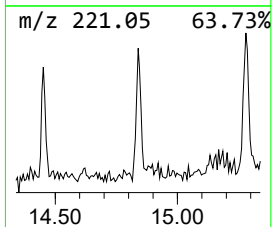
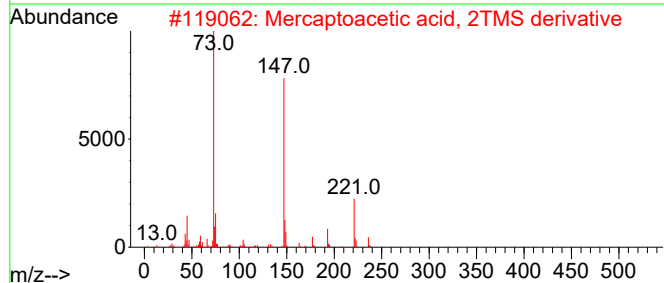
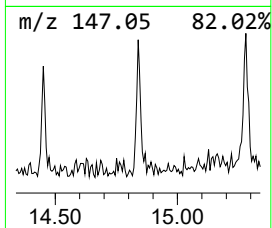
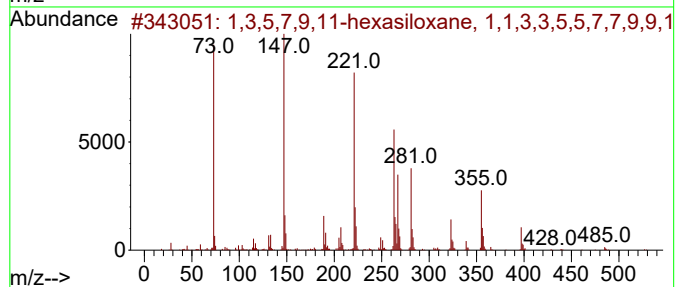
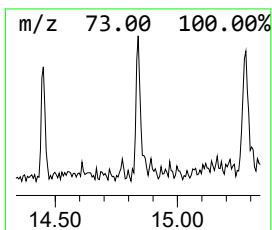
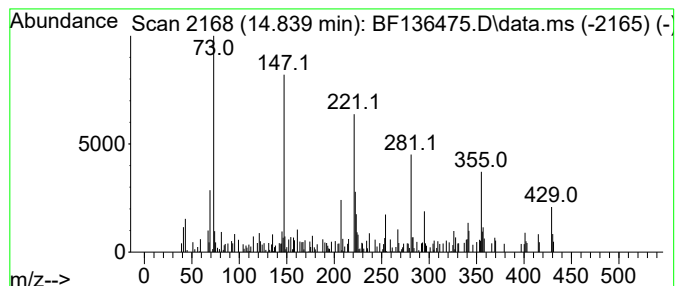
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Peak Number 7 unknown14.839 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.839	2.21 ng	64790	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5,7,9,11-hexasiloxane, 1,1,3...	542	C20H54O5Si6	1000458-50-7	42		
2	Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	37		
3	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	22		
4	Tetrazole, 1-(2-fluorophenyl)-5-...	342	C18H19FN4S	1000272-52-4	22		
5	1H-Purine-2,6-dione, 3,7-dihydro...	326	C18H22N4O2	333415-38-6	14		



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ClientSampleId :
72-11985

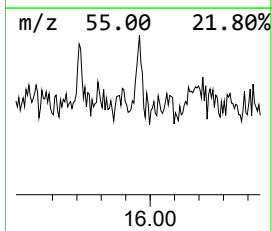
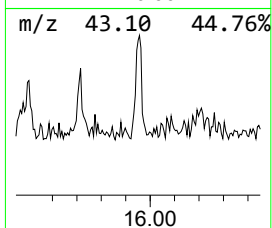
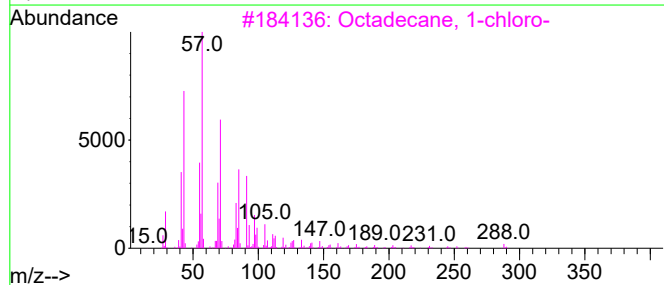
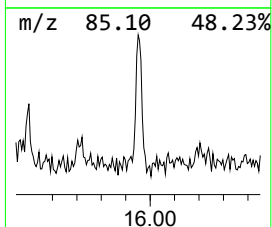
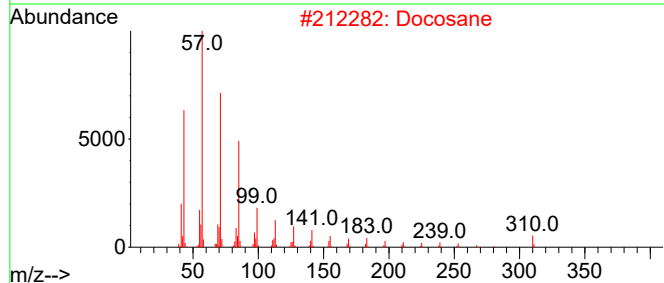
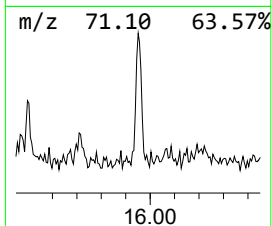
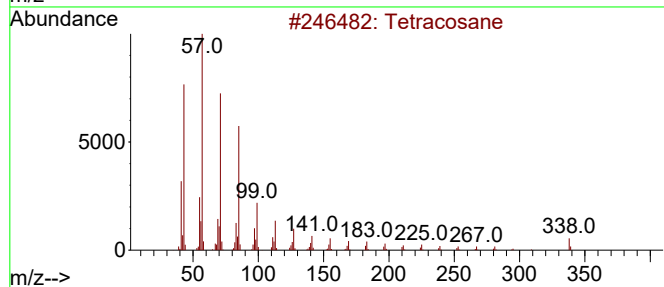
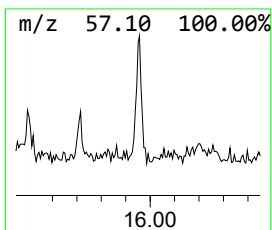
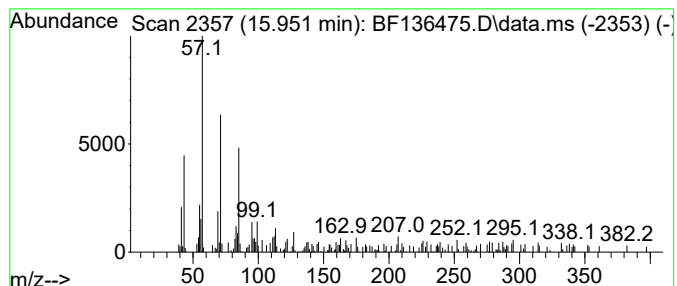
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.951	2.52 ng	73819	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	93
2			Docosane	310	C22H46	000629-97-0	83
3			Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	64
4			Hexadecane	226	C16H34	000544-76-3	58
5			Hexacosane	366	C26H54	000630-01-3	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120823\
Data File : BF136475.D
Acq On : 08 Dec 2023 19:12
Operator : CG\JU
Sample : 05629-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11985

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-Pentanone, 4-...	5.028	7.8	ng	258487	1	6.793	663447	20.0
n-Hexadecanoic ...	11.857	4.8	ng	184903	4	11.322	763480	20.0
1-Tetradecanol	13.898	2.1	ng	74907	5	13.974	697725	20.0
1,4-Benzenedica...	14.616	17.6	ng	615852	5	13.974	697725	20.0
unknown14.839	14.839	2.2	ng	64790	6	15.451	585574	20.0
Tetracosane	15.951	2.5	ng	73819	6	15.451	585574	20.0