

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010824\
 Data File : BF137002.D
 Acq On : 08 Jan 2024 19:03
 Operator : CG\JU
 Sample : P1056-03
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MR-311P-30-32

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-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137002.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	12	16	26	rVB2	18587	25490	1.62%	0.244%
2	5.022	496	499	506	rBV	56629	68922	4.38%	0.659%
3	5.428	565	568	584	rBV	1228907	1229244	78.07%	11.745%
4	6.434	735	739	755	rBV	1410798	1251590	79.49%	11.958%
5	6.781	795	798	802	rBV	490766	380127	24.14%	3.632%
6	7.346	890	894	897	rBV	944912	809384	51.41%	7.733%
7	8.057	1011	1015	1020	rBV	624949	512129	32.53%	4.893%
8	9.134	1194	1198	1202	rBV	1652943	1574478	100.00%	15.043%
9	9.210	1209	1211	1216	rVB	25561	23815	1.51%	0.228%
10	9.746	1294	1302	1306	rBV	38344	38463	2.44%	0.367%
11	9.816	1310	1314	1321	rVB	687047	567752	36.06%	5.425%
12	10.245	1385	1387	1390	rVB	24757	18067	1.15%	0.173%
13	10.610	1445	1449	1460	rBV	964509	914180	58.06%	8.735%
14	10.722	1465	1468	1475	rVB2	11784	15855	1.01%	0.151%
15	11.310	1564	1568	1571	rBV	681560	573352	36.42%	5.478%
16	11.839	1655	1658	1671	rBV2	169022	211318	13.42%	2.019%
17	12.634	1789	1793	1801	rBV	42655	60533	3.84%	0.578%
18	12.716	1804	1807	1812	rVB2	19690	19549	1.24%	0.187%
19	12.904	1835	1839	1842	rBV	1534818	1286563	81.71%	12.292%
20	13.445	1927	1931	1933	rBV	60067	52141	3.31%	0.498%
21	13.810	1989	1993	1999	rVB2	15380	18353	1.17%	0.175%
22	13.916	2003	2011	2013	rVV6	17239	43548	2.77%	0.416%
23	13.969	2016	2020	2028	rVB	341608	341435	21.69%	3.262%
24	14.128	2043	2047	2050	rBV2	17833	18799	1.19%	0.180%
25	14.433	2096	2099	2104	rVB2	17270	16669	1.06%	0.159%
26	14.816	2161	2164	2168	rVB3	14747	18567	1.18%	0.177%
27	15.451	2267	2272	2279	rBV	267617	359486	22.83%	3.435%
28	15.916	2347	2351	2357	rBV6	9755	16474	1.05%	0.157%

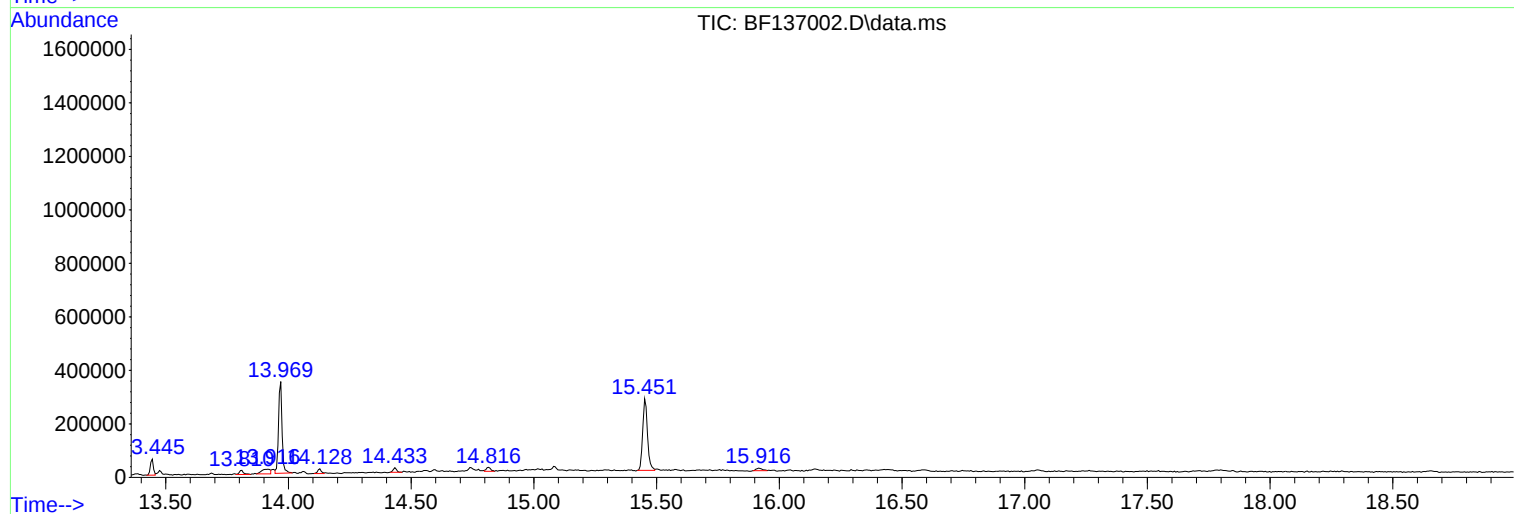
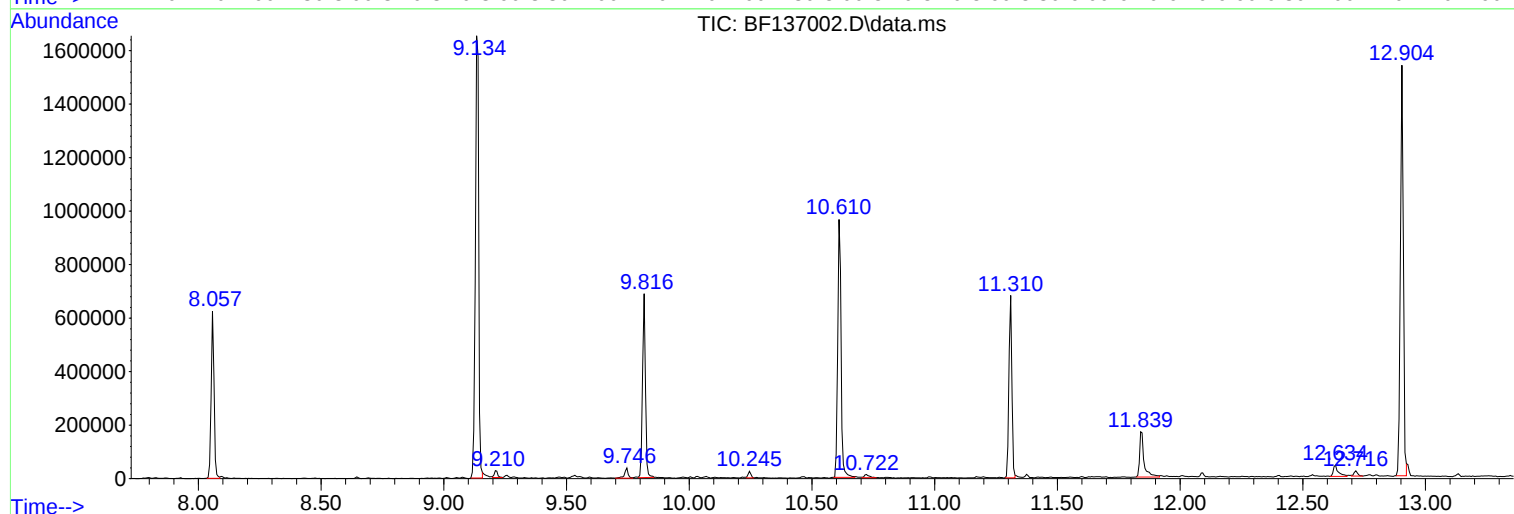
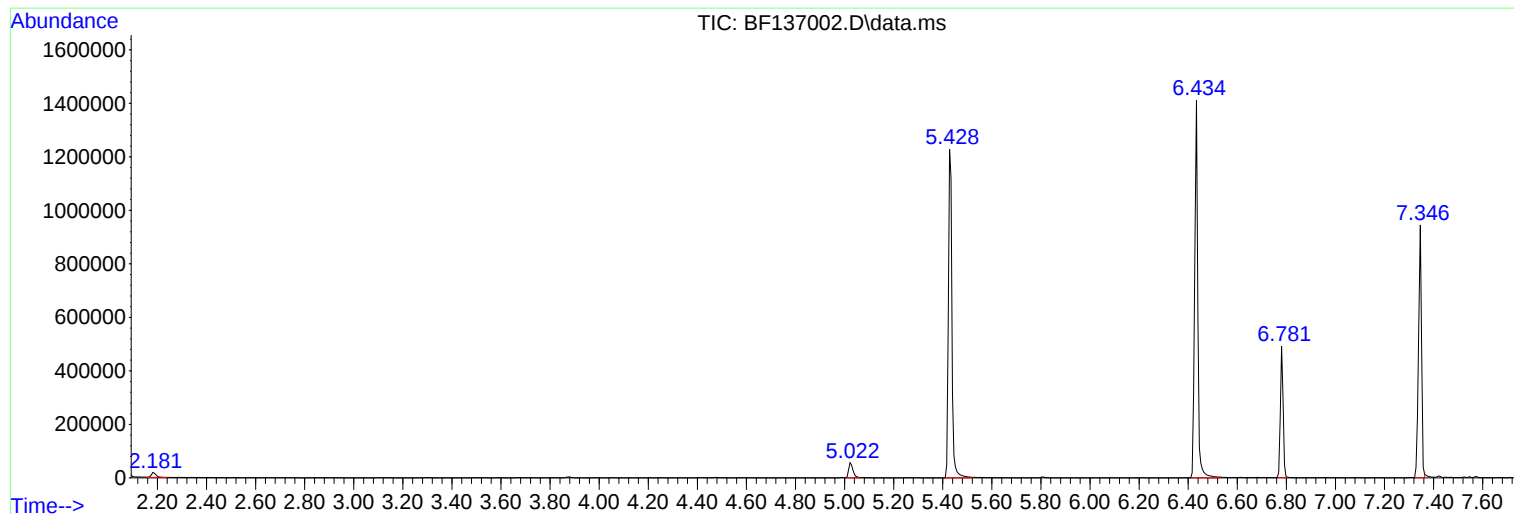
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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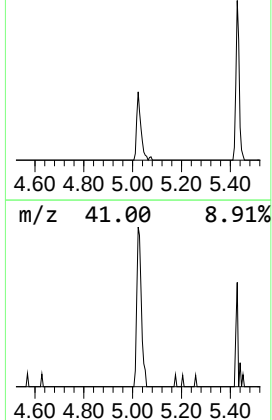
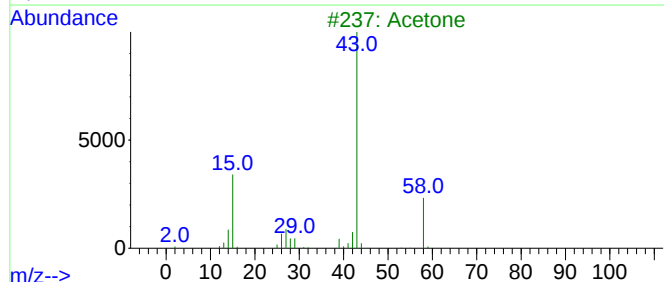
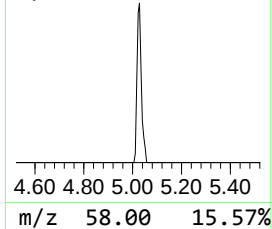
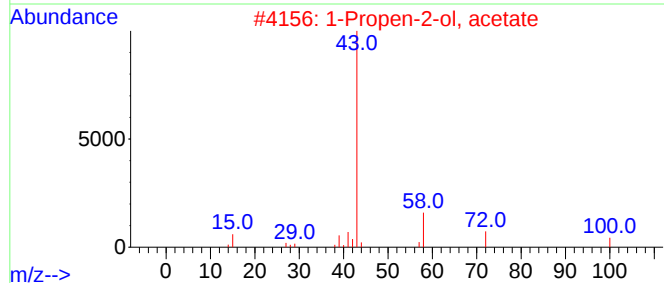
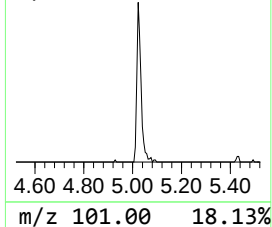
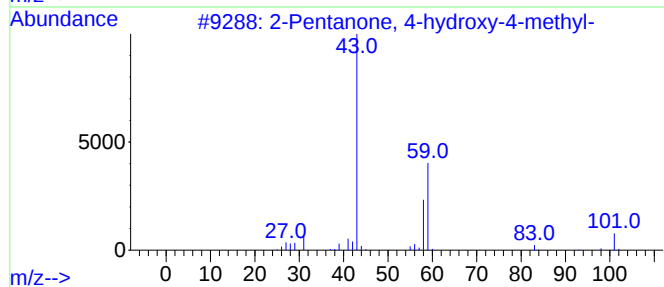
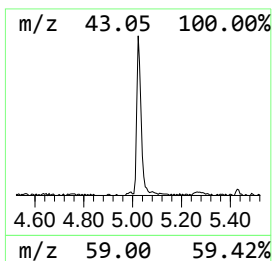
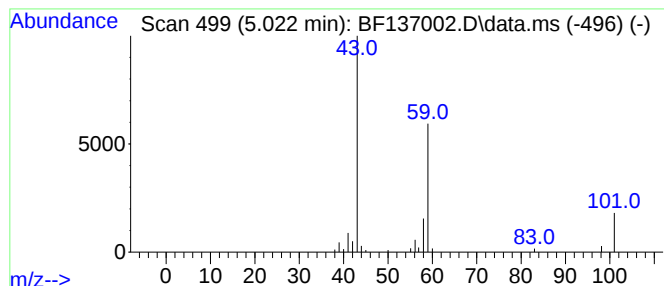
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	3.63 ng	68922	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
3			Acetone	58	C3H6O	000067-64-1	9
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Acetamide, N-(cyanomethyl)-	98	C4H6N2O	004814-80-6	9



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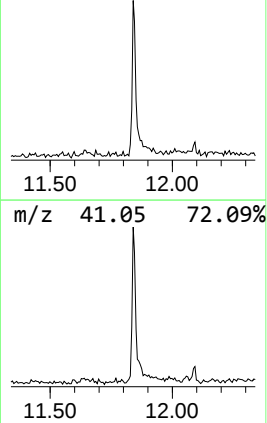
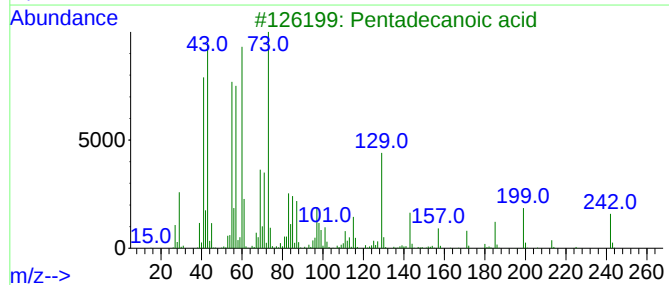
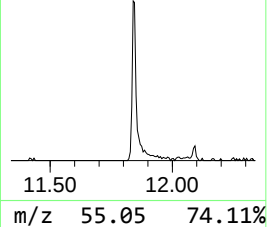
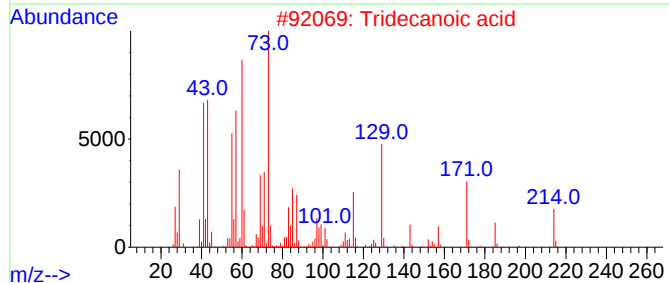
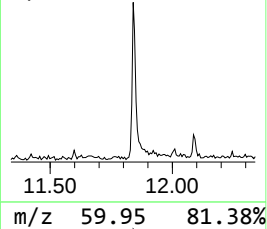
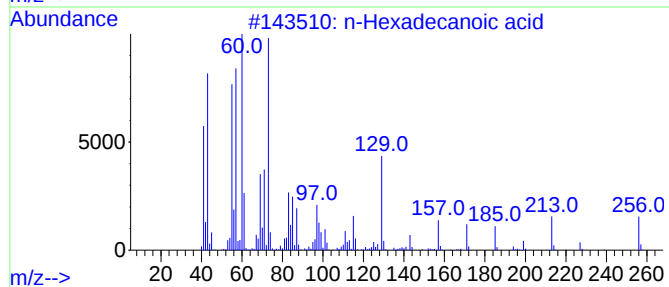
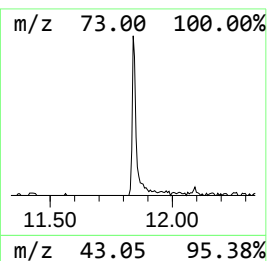
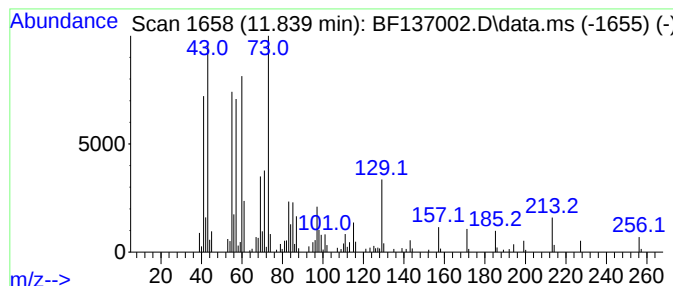
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	7.37 ng	211318	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	47



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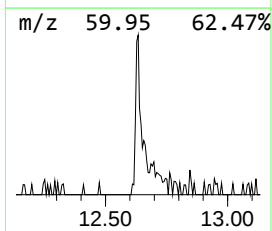
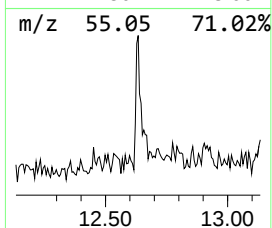
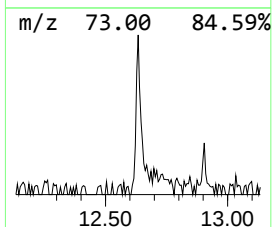
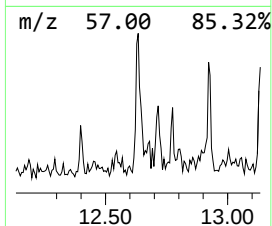
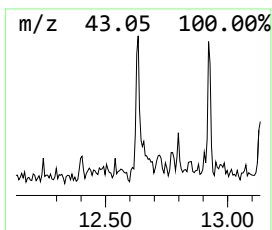
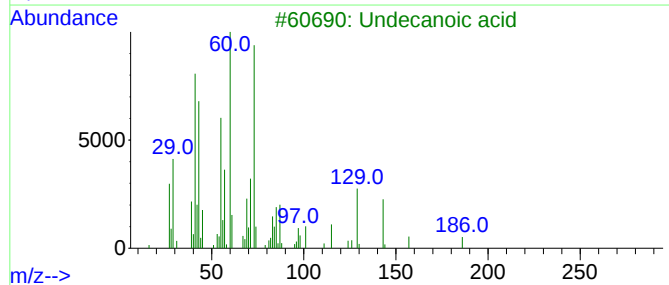
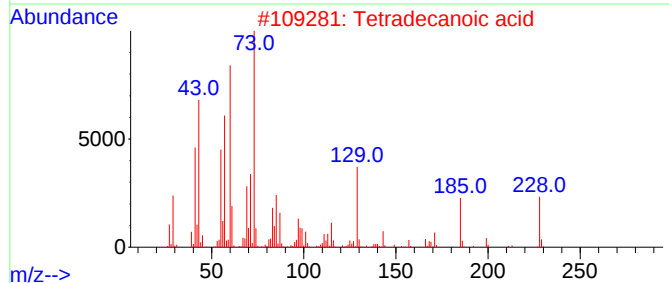
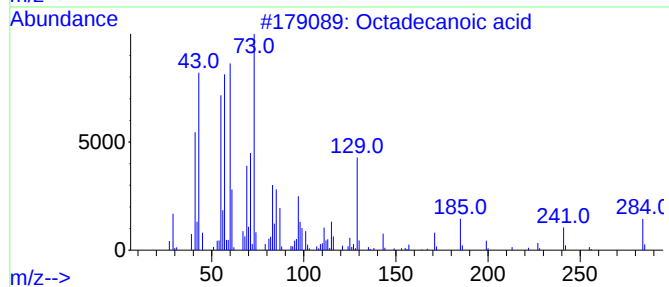
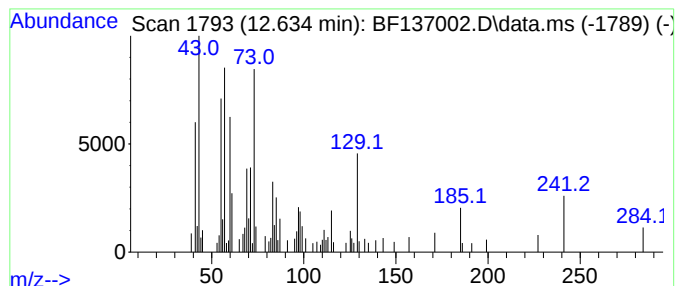
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.634	2.11 ng	60533	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	49
3			Undecanoic acid	186	C11H22O2	000112-37-8	30
4			Oxalic acid, propyl tetradecyl e...	328	C19H36O4	1000309-26-7	30
5			Oxalic acid, cyclobutyl heptadec...	382	C23H42O4	1000309-70-7	18



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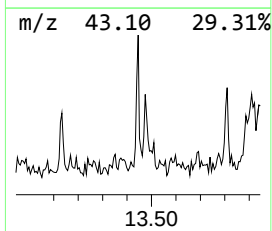
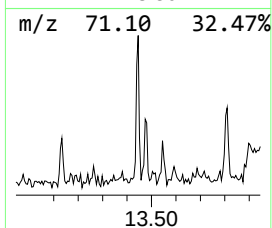
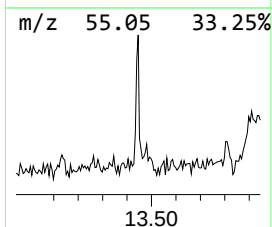
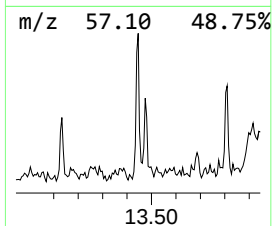
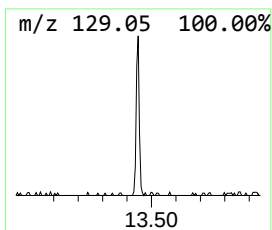
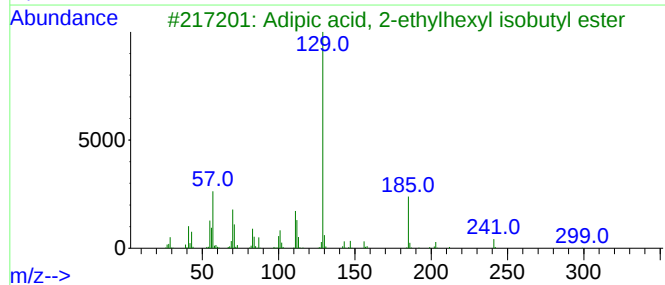
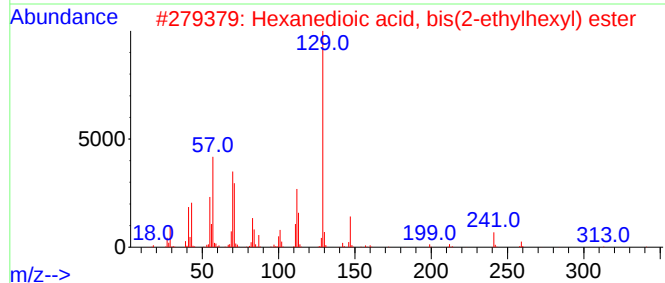
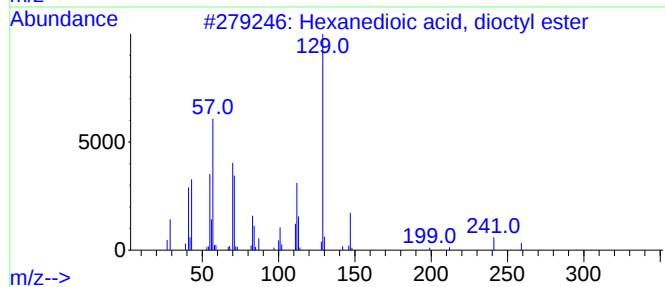
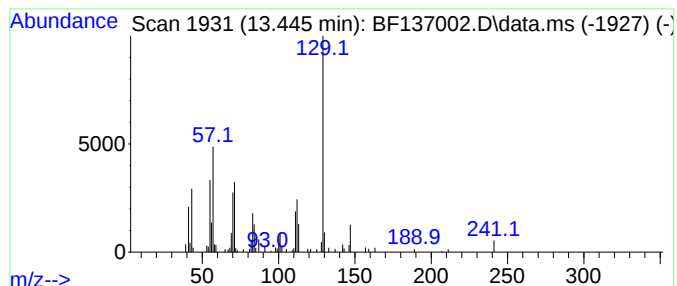
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexanedioic acid, dioctyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.445	3.05 ng	52141	Chrysene-d12	13.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	91
2			Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	91
3			Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1010324-48-0	59
4			Adipic acid, 2-ethylhexyl isohex...	342	C20H38O4	1000324-48-3	53
5			Adipic acid, cycloheptyl isohexy...	326	C19H34O4	1000324-71-8	50



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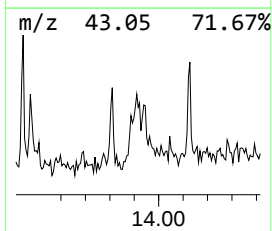
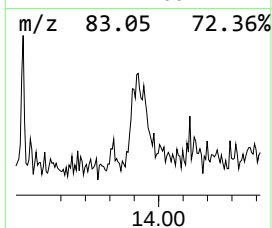
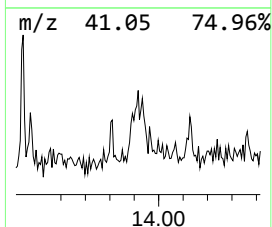
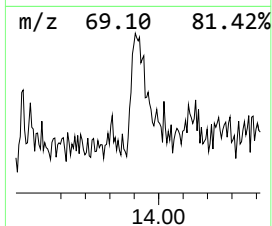
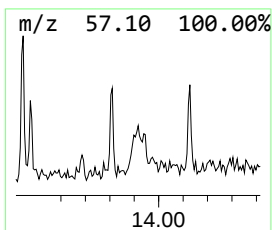
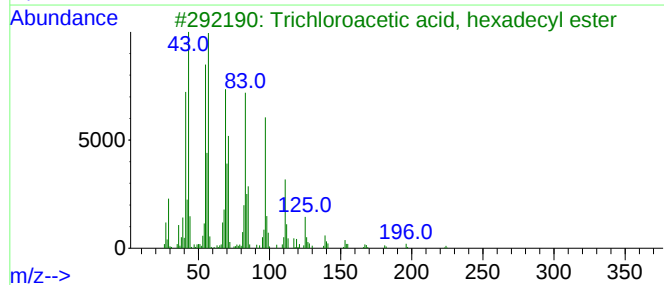
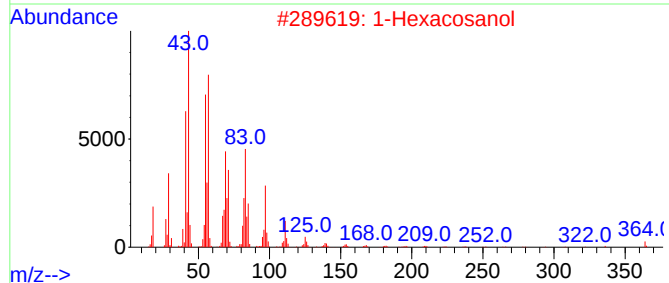
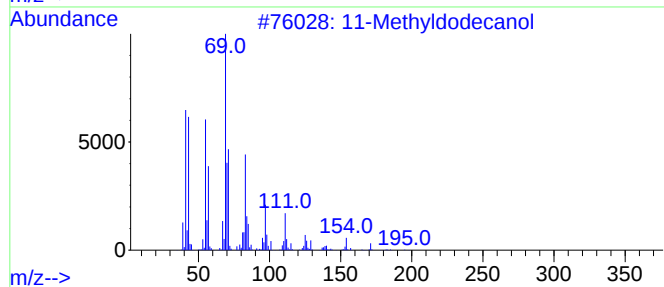
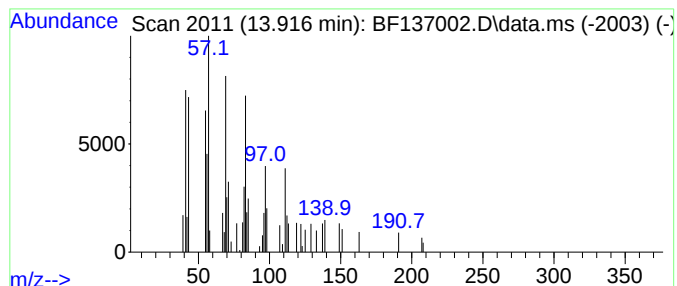
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 11-Methyldodecanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.916	2.55 ng	43548	Chrysene-d12	13.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11-Methyldodecanol	200	C13H28O	085763-57-1	58
2			1-Hexacosanol	382	C26H54O	000506-52-5	46
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	43
4			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	43
5			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	43



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.022	3.6	ng	68922	1	6.781	380127	20.0
n-Hexadecanoic ...	11.839	7.4	ng	211318	4	11.310	573352	20.0
Octadecanoic acid	12.634	2.1	ng	60533	4	11.310	573352	20.0
Hexanedioic aci...	13.445	3.0	ng	52141	5	13.969	341435	20.0
11-Methyldodecanol	13.916	2.5	ng	43548	5	13.969	341435	20.0