

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030724\
 Data File : BF137531.D
 Acq On : 07 Mar 2024 15:47
 Operator : CG\JU
 Sample : P1688-02
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-2

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-BF022924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137531.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	12	17	29	rVB	1142712	1579234	41.63%	5.151%
2	5.140	516	519	523	rBV	44733	52556	1.39%	0.171%
3	5.528	581	585	606	rBV	3548459	3333776	87.88%	10.873%
4	6.510	748	752	779	rBV	3465389	3515088	92.66%	11.464%
5	6.869	810	813	822	rBV	1367059	1232263	32.48%	4.019%
6	7.428	904	908	920	rBV	2300320	2134827	56.27%	6.963%
7	8.145	1026	1030	1045	rBV	1777130	1665294	43.90%	5.431%
8	8.469	1080	1085	1097	rBV	20188	51169	1.35%	0.167%
9	9.222	1209	1213	1225	rBV	4402876	3793564	100.00%	12.373%
10	9.339	1230	1233	1238	rVB	78596	80186	2.11%	0.262%
11	9.898	1325	1328	1341	rBV	1933867	1857537	48.97%	6.058%
12	10.004	1341	1346	1354	rVB3	51608	79350	2.09%	0.259%
13	10.692	1459	1463	1482	rBV	2176292	2098668	55.32%	6.845%
14	11.398	1579	1583	1592	rBV	1864709	1745972	46.02%	5.694%
15	11.939	1670	1675	1696	rBV	358904	670767	17.68%	2.188%
16	12.733	1806	1810	1822	rBV3	68651	133320	3.51%	0.435%
17	12.998	1851	1855	1868	rVB	3596383	3270689	86.22%	10.667%
18	13.239	1893	1896	1899	rBV2	56134	45741	1.21%	0.149%
19	13.586	1950	1955	1958	rBV2	114682	129065	3.40%	0.421%
20	13.921	2008	2012	2021	rBV	207479	287723	7.58%	0.938%
21	14.057	2032	2035	2041	rBV	1146263	1073343	28.29%	3.501%
22	14.110	2041	2044	2049	rVB3	40374	60152	1.59%	0.196%
23	14.239	2063	2066	2069	rVB	104460	84676	2.23%	0.276%
24	14.551	2115	2119	2128	rBV	105001	150516	3.97%	0.491%
25	14.857	2168	2171	2173	rBV2	64931	77272	2.04%	0.252%
26	14.957	2184	2188	2195	rVB	58714	77364	2.04%	0.252%
27	15.245	2233	2237	2244	rVB	53487	68656	1.81%	0.224%
28	15.462	2270	2274	2284	rVB10	20555	44239	1.17%	0.144%
29	15.598	2291	2297	2305	rBV	844760	1154999	30.45%	3.767%
30	15.668	2306	2309	2315	rVB2	40140	57355	1.51%	0.187%
31	16.162	2388	2393	2394	rBV2	35608	55400	1.46%	0.181%

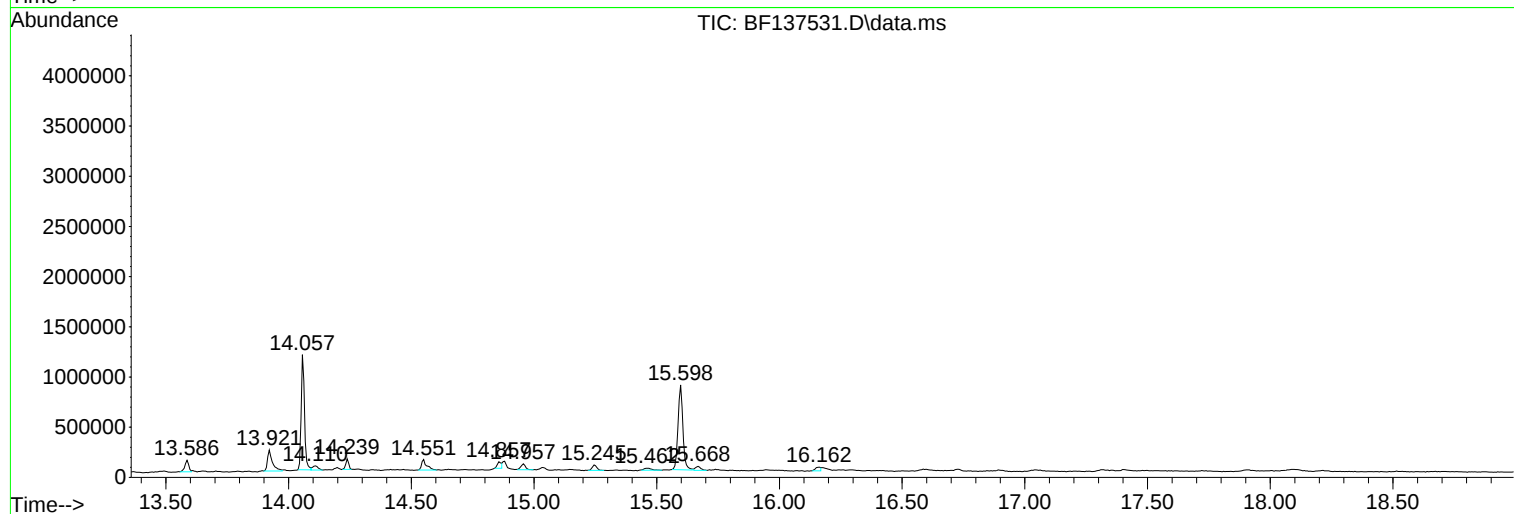
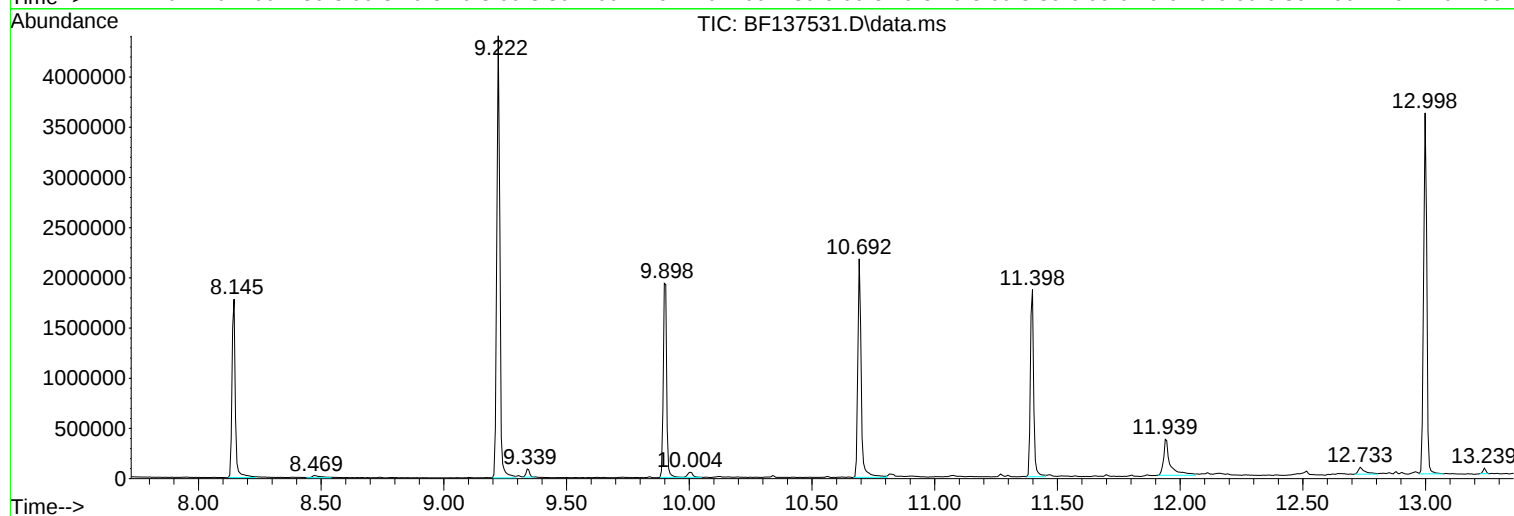
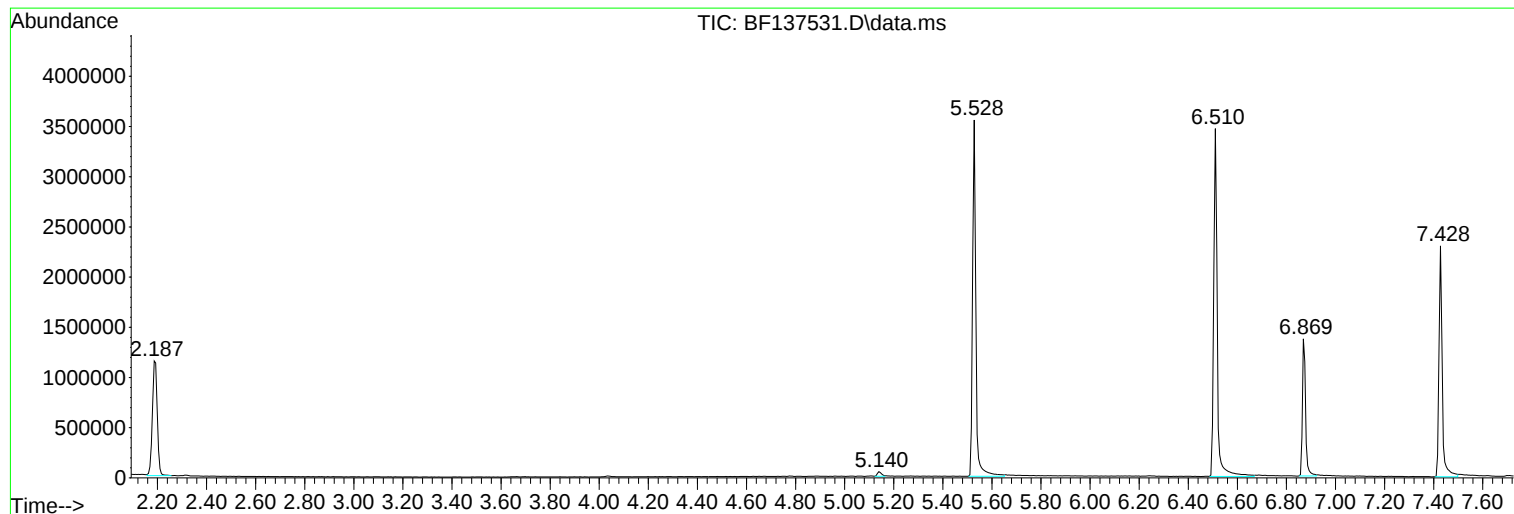
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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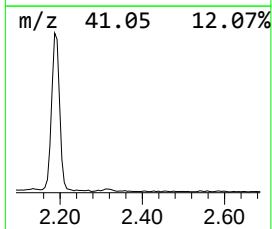
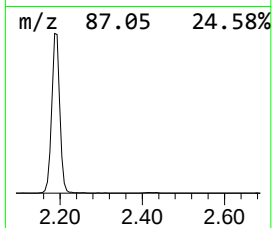
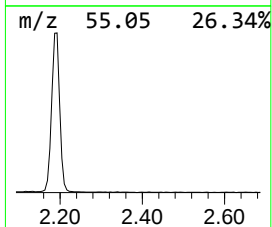
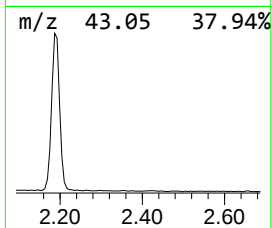
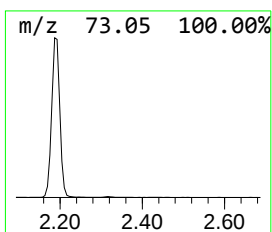
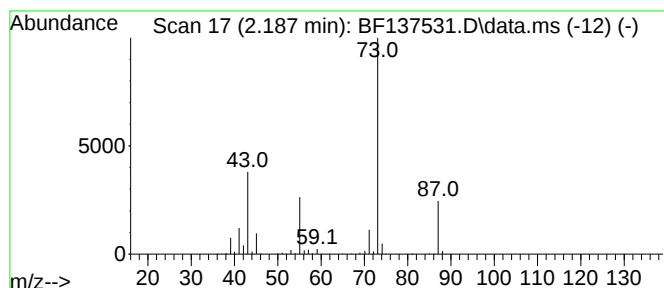
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.187	25.63 ng	1579230	1,4-Dichlorobenzene-d4	6.869

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	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	17



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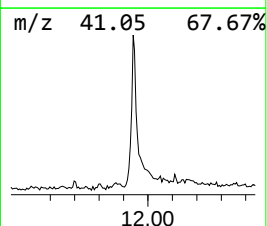
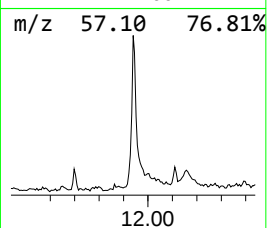
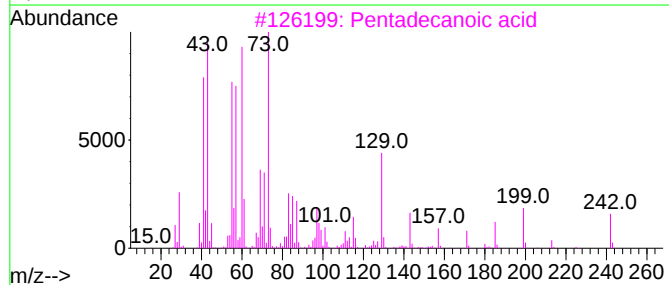
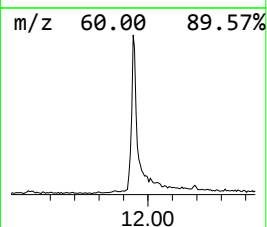
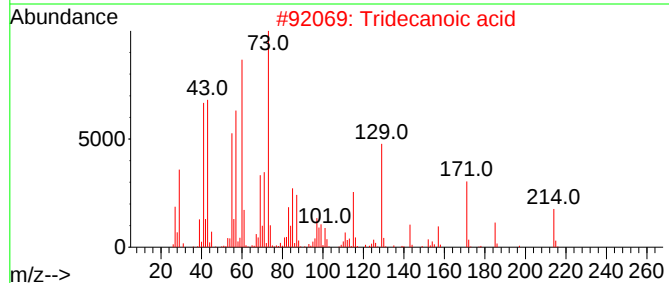
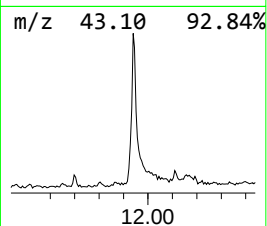
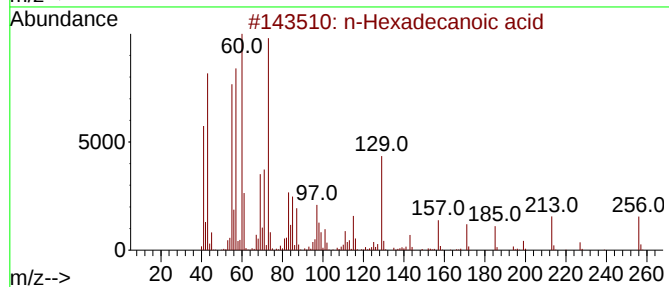
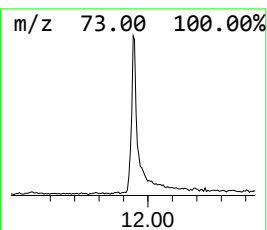
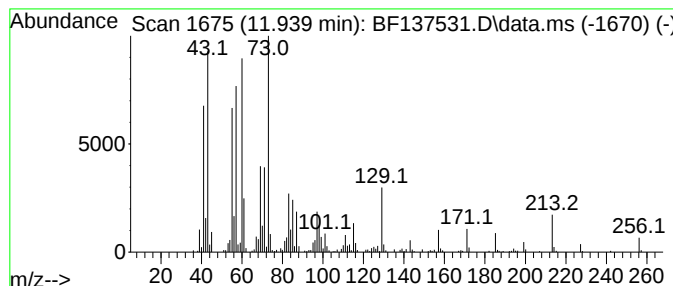
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.939	7.68 ng	670767	Phenanthrene-d10	11.398

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	89
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



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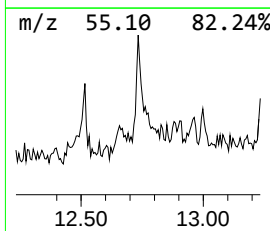
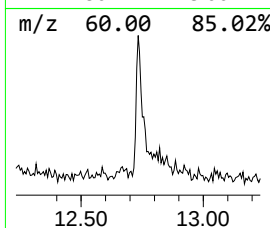
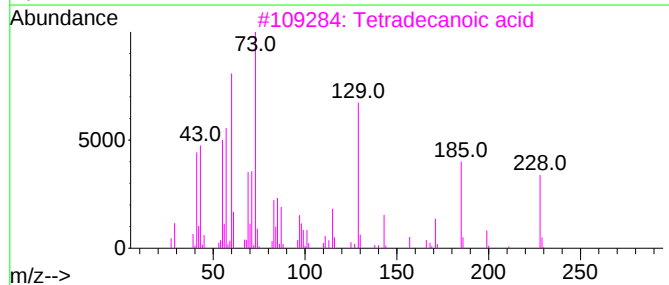
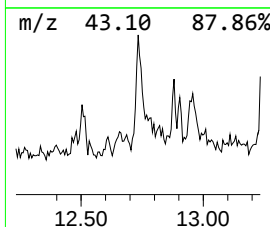
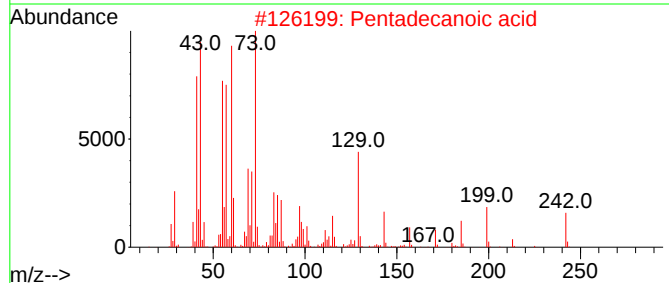
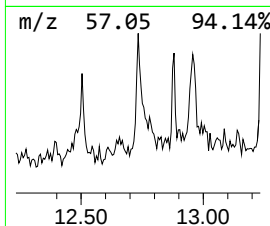
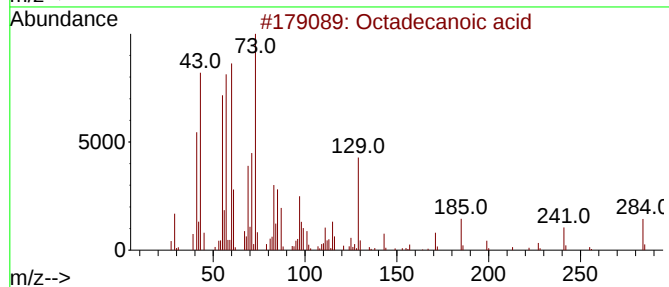
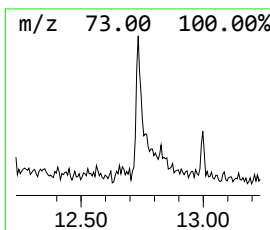
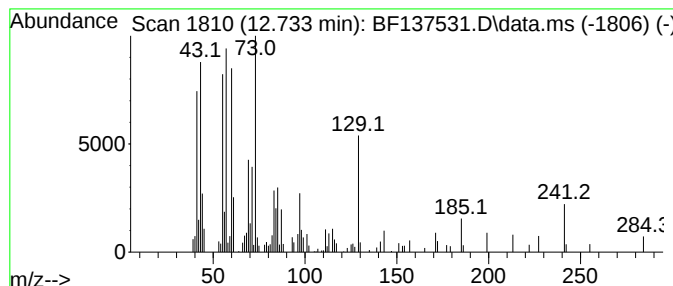
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.733	2.48 ng	133320	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	80
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			n-Decanoic acid	172	C10H20O2	000334-48-5	70
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64



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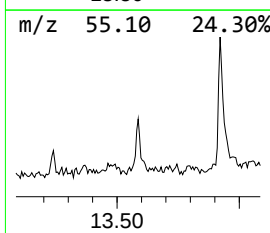
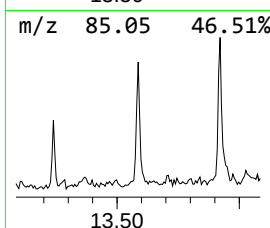
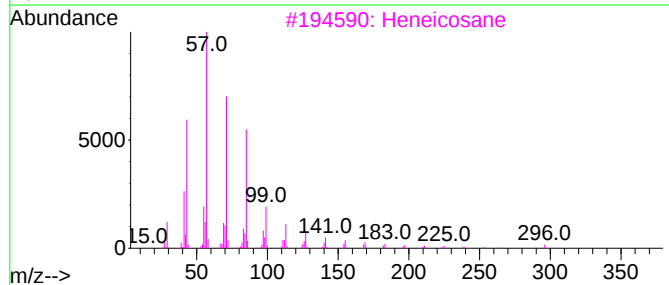
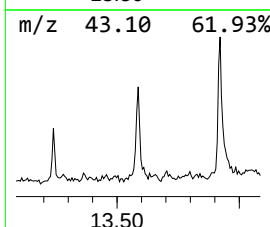
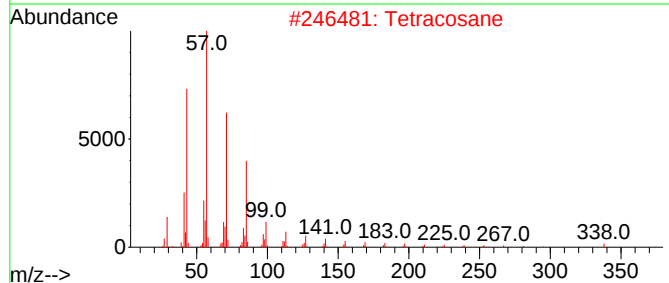
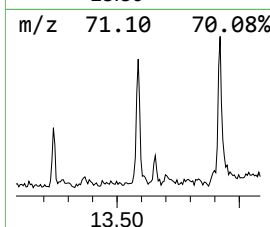
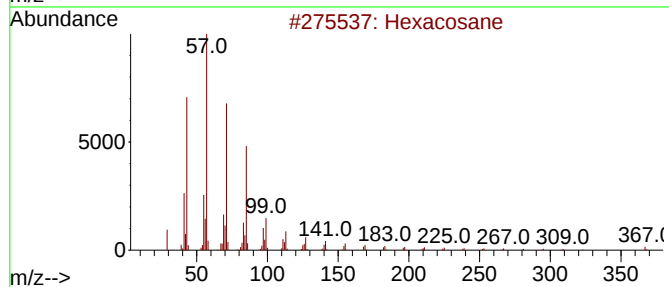
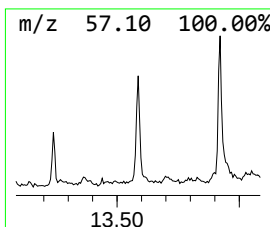
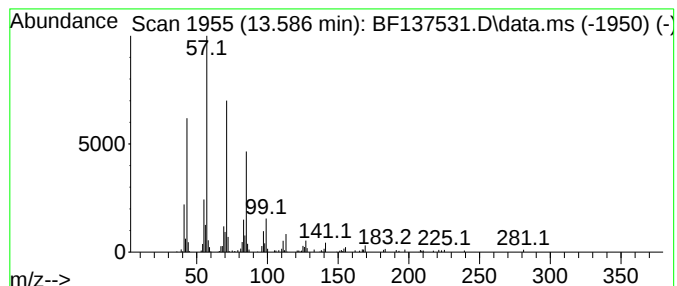
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.586	2.40 ng	129065	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			Tetracosane	338	C24H50	000646-31-1	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Pentacosane	352	C25H52	000629-99-2	91
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90



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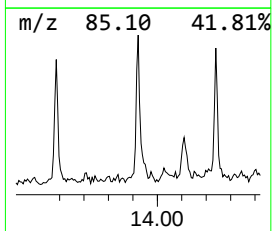
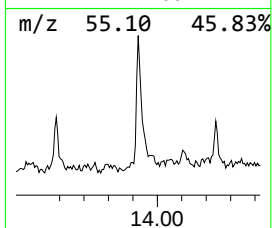
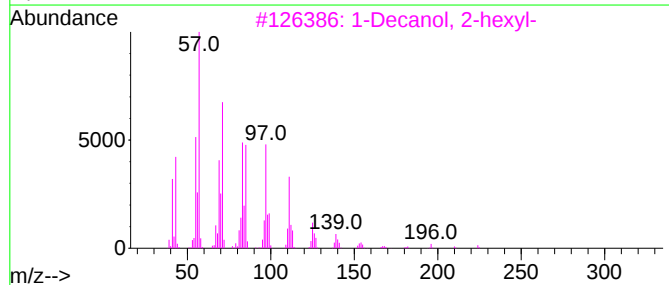
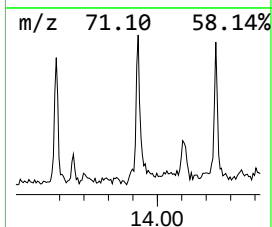
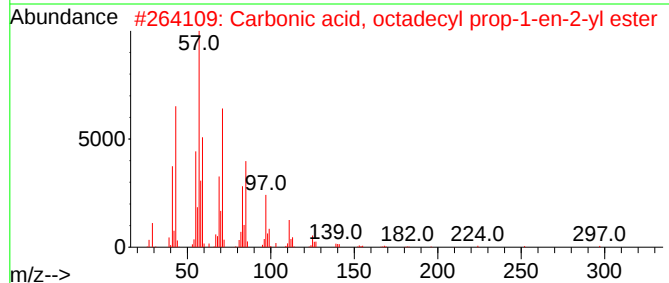
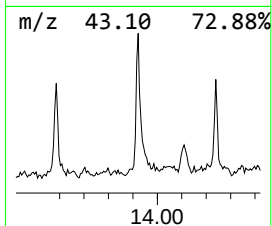
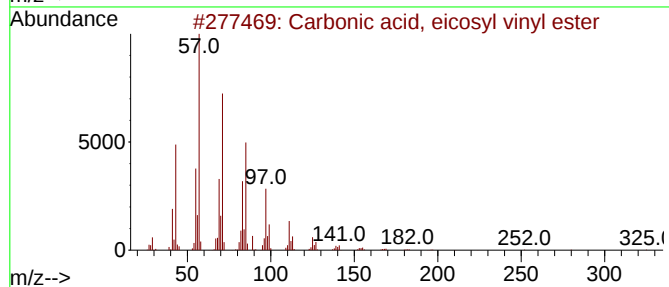
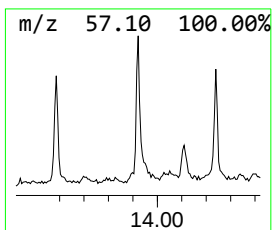
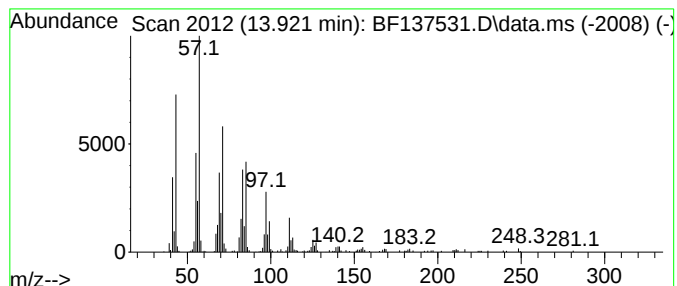
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Carbonic acid, eicosyl vinyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.921	5.36 ng	287723	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	91
2			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	91
3			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	91
4			Hexadecyl nonyl ether	368	C25H52O	1000406-37-7	90
5			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	90



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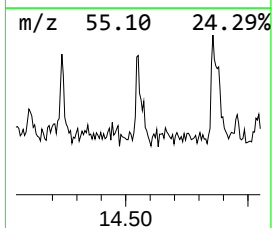
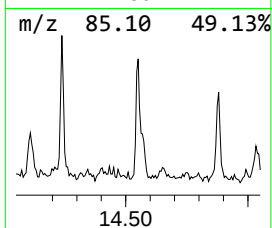
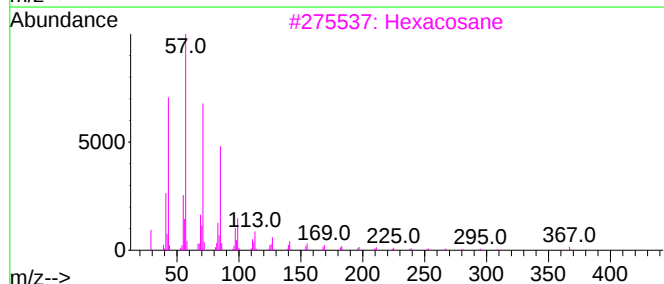
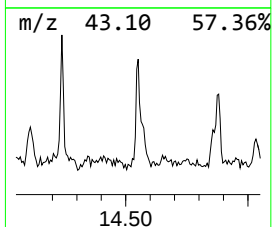
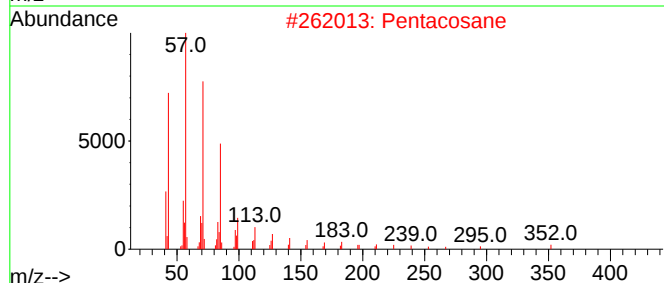
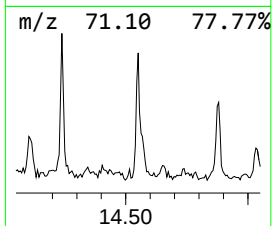
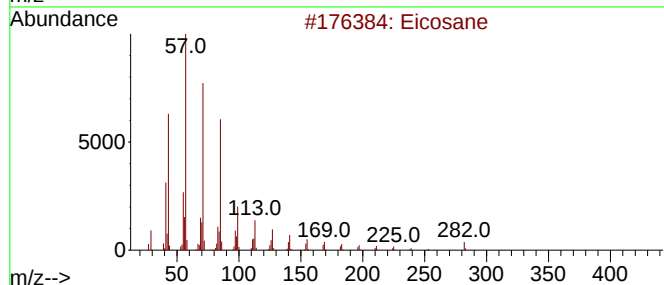
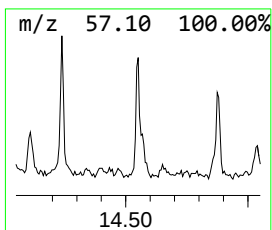
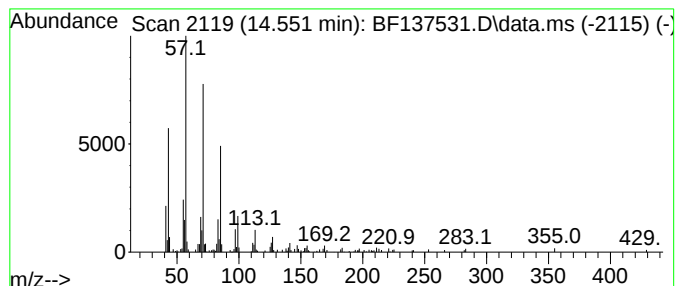
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.551	2.80 ng	150516	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane			282	C20H42	000112-95-8	94
2	Pentacosane			352	C25H52	000629-99-2	91
3	Hexacosane			366	C26H54	000630-01-3	91
4	Heneicosane			296	C21H44	000629-94-7	91
5	Octacosane			394	C28H58	000630-02-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030724\
Data File : BF137531.D
Acq On : 07 Mar 2024 15:47
Operator : CG\JU
Sample : P1688-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.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
Butane, 2-metho...	2.187	25.6	ng	1579230	1	6.869	1232260	20.0
n-Hexadecanoic ...	11.939	7.7	ng	670767	4	11.398	1745970	20.0
Octadecanoic acid	12.733	2.5	ng	133320	5	14.057	1073340	20.0
Hexacosane	13.586	2.4	ng	129065	5	14.057	1073340	20.0
Carbonic acid, ...	13.921	5.4	ng	287723	5	14.057	1073340	20.0
Eicosane	14.551	2.8	ng	150516	5	14.057	1073340	20.0