

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050223\
 Data File : BF133183.D
 Acq On : 02 May 2023 12:11
 Operator : CG\JU
 Sample : 02521-05
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GMW-10

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-BF042123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133183.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	9	13	20	rVB	60020	73273	1.20%	0.179%
2	4.916	478	481	490	rVB	75089	94076	1.54%	0.229%
3	5.340	549	553	557	rBV	3060365	2654240	43.33%	6.472%
4	6.363	723	727	730	rBV	2132890	1702790	27.80%	4.152%
5	6.728	786	789	797	rVB	1678454	1347812	22.01%	3.286%
6	7.298	880	886	889	rBV	3755923	3631685	59.29%	8.855%
7	8.016	1004	1008	1011	rBV	2193963	1789368	29.21%	4.363%
8	8.081	1015	1019	1025	rVB2	87949	120332	1.96%	0.293%
9	8.404	1070	1074	1079	rBV	124895	113420	1.85%	0.277%
10	9.092	1185	1191	1194	rBV	6666818	6111173	99.77%	14.901%
11	9.581	1271	1274	1285	rVB5	52041	73251	1.20%	0.179%
12	9.769	1302	1306	1309	rBV	2147587	1975652	32.26%	4.817%
13	10.480	1423	1427	1430	rBV	1280586	986876	16.11%	2.406%
14	10.557	1435	1440	1443	rBV	4029270	3842660	62.74%	9.370%
15	10.675	1458	1460	1468	rVB	113744	142028	2.32%	0.346%
16	11.127	1534	1537	1539	rBV	176570	141484	2.31%	0.345%
17	11.198	1546	1549	1554	rBV4	86998	135859	2.22%	0.331%
18	11.251	1554	1558	1561	rVV	2171994	1968780	32.14%	4.801%
19	11.551	1606	1609	1612	rBV	190625	147725	2.41%	0.360%
20	11.651	1623	1626	1631	rVB	97432	86996	1.42%	0.212%
21	11.716	1633	1637	1640	rBV3	63912	95538	1.56%	0.233%
22	11.792	1645	1650	1658	rBV	1997142	2098587	34.26%	5.117%
23	11.957	1675	1678	1682	rVB	152606	135298	2.21%	0.330%
24	12.345	1742	1744	1748	rVB	123607	123138	2.01%	0.300%
25	12.574	1779	1783	1794	rBV	1210897	1296814	21.17%	3.162%
26	12.721	1805	1808	1811	rVB	90576	67929	1.11%	0.166%
27	12.839	1823	1828	1831	rBV	5942115	6125022	100.00%	14.935%
28	13.074	1866	1868	1872	rBV	62151	65322	1.07%	0.159%
29	13.757	1980	1984	1999	rBV2	352041	817009	13.34%	1.992%
30	13.880	2001	2005	2009	rBV	1634140	1525575	24.91%	3.720%
31	14.733	2147	2150	2154	rVB	141082	133321	2.18%	0.325%
32	14.986	2190	2193	2197	rVB	69288	78455	1.28%	0.191%
33	15.304	2242	2247	2251	rBV	980135	1107870	18.09%	2.701%
34	15.345	2252	2254	2259	rVB	72217	85290	1.39%	0.208%
35	15.757	2321	2324	2330	rVB	79859	116058	1.89%	0.283%

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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-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

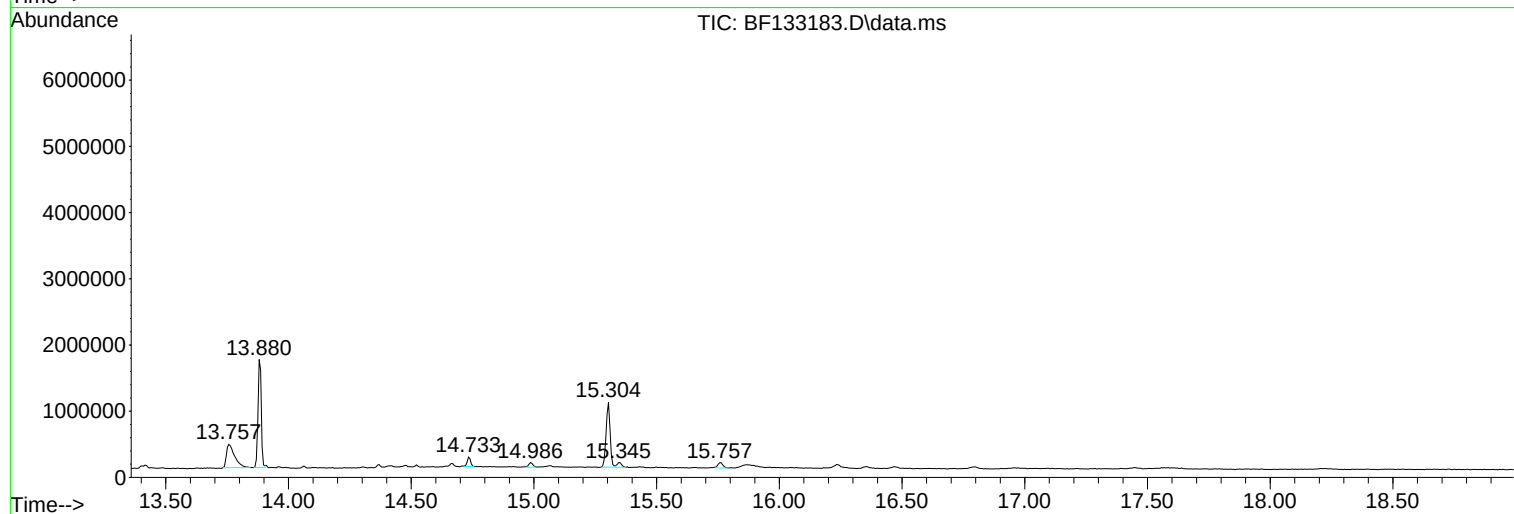
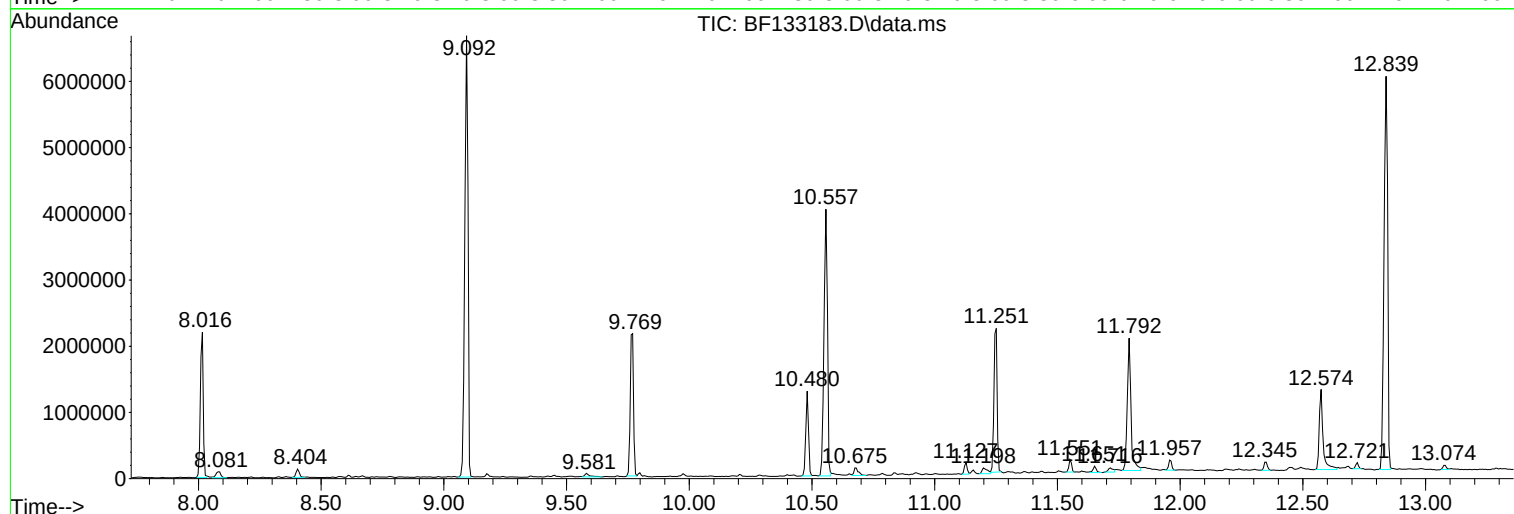
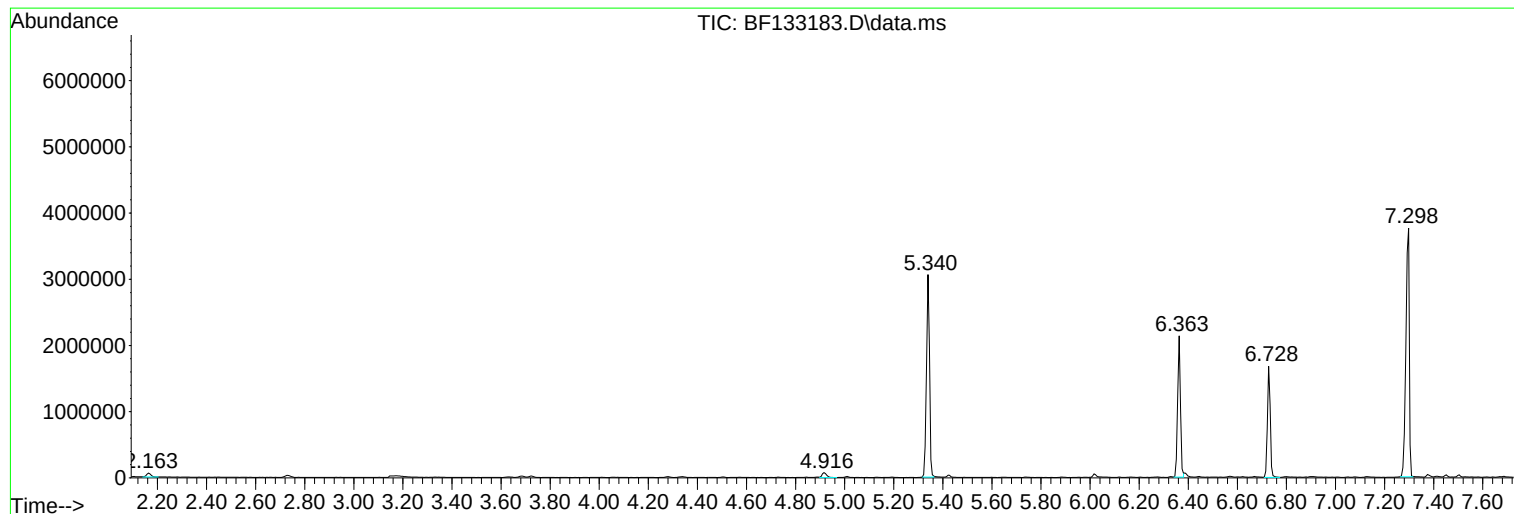
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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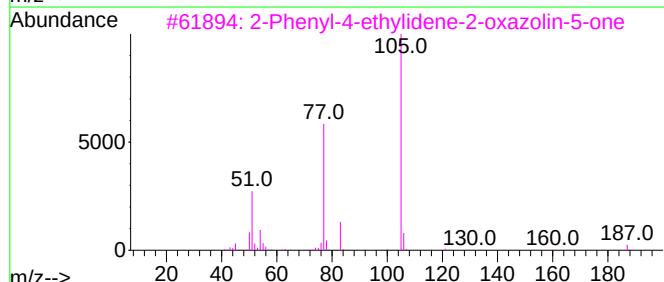
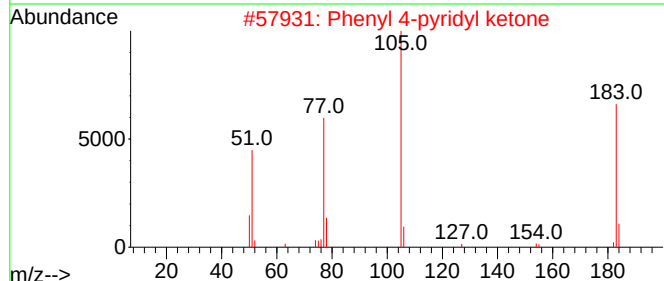
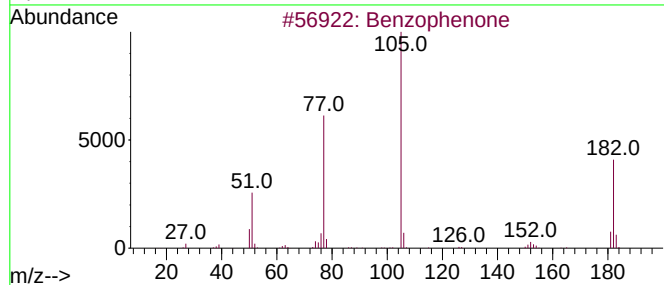
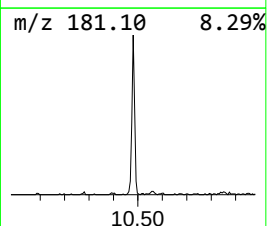
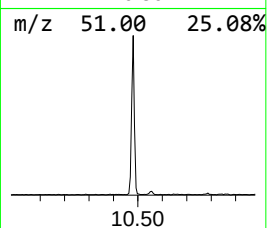
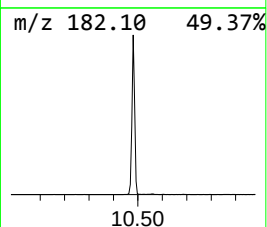
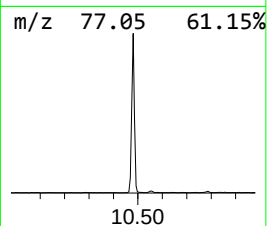
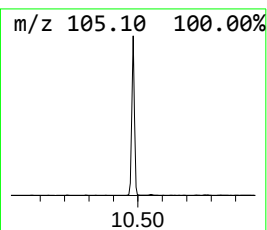
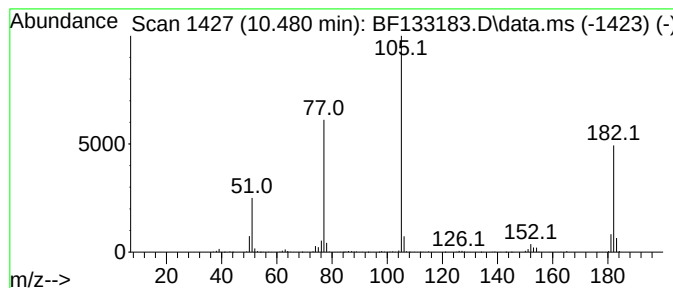
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.480	9.99 ng	986876	Acenaphthene-d10	9.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	50
3			2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	47
4			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47
5			5-[N-Benzoylaminoethyl]tetrazole	203	C9H9N5O	1000227-36-3	47



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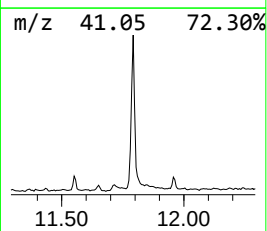
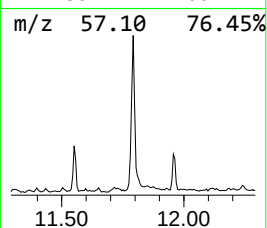
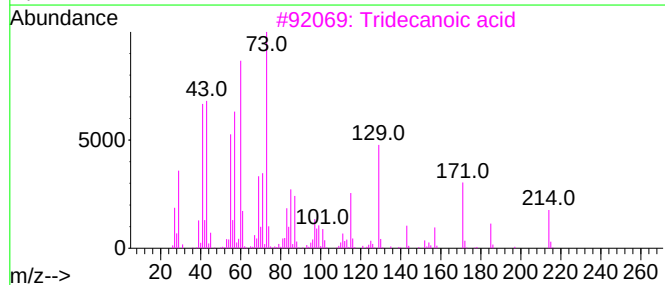
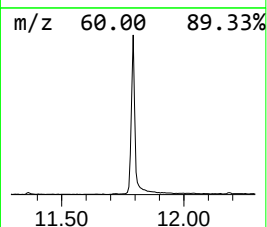
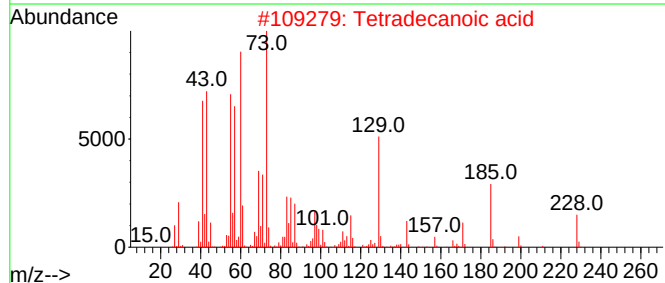
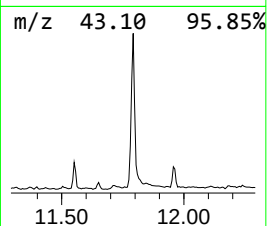
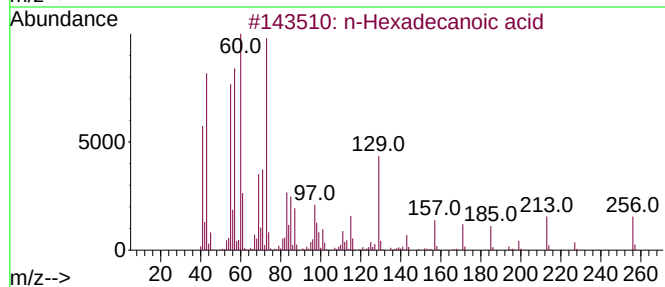
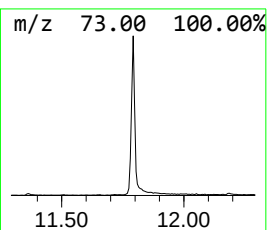
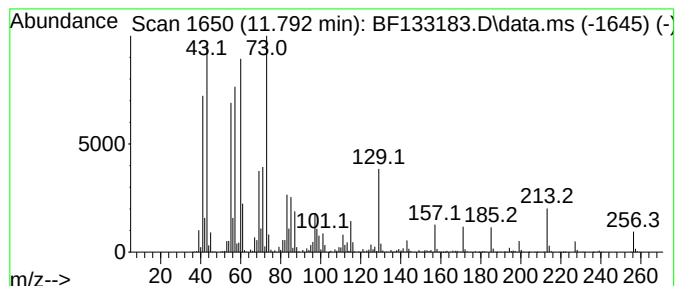
Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.792	21.32 ng	2098590	Phenanthrene-d10		11.251	
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	92
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	91
5	n-Decanoic acid		172	C10H20O2	000334-48-5	62



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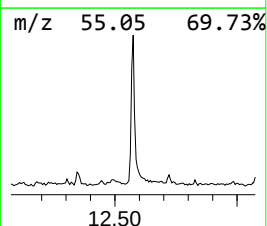
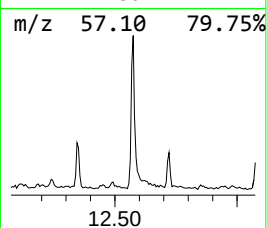
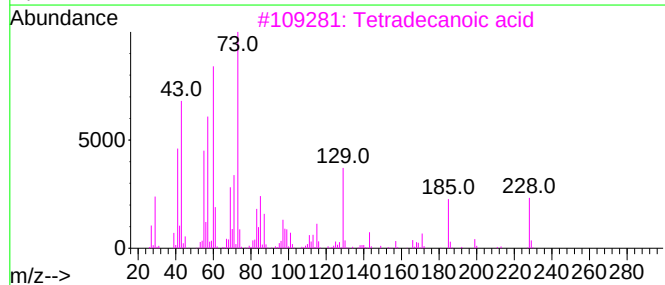
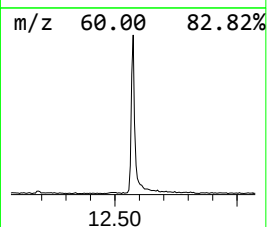
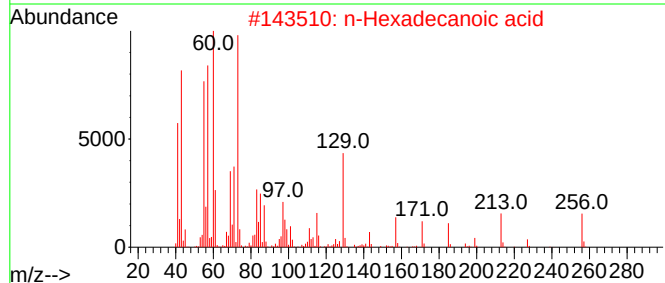
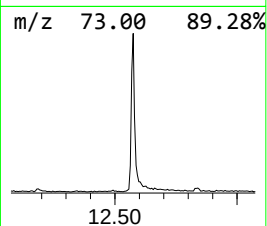
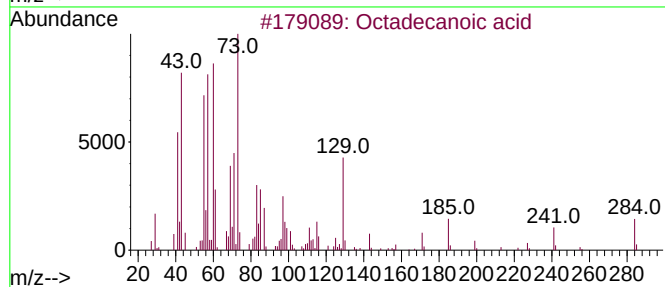
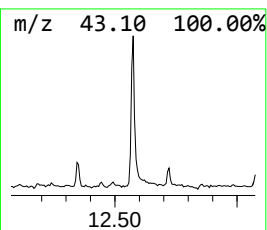
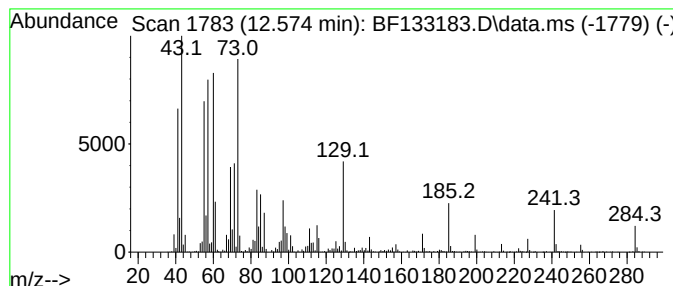
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.574	17.00 ng	1296810	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			Tridecanoic acid	214	C13H26O2	000638-53-9	76
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	76



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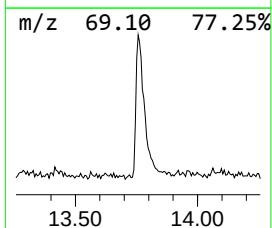
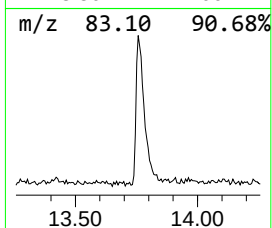
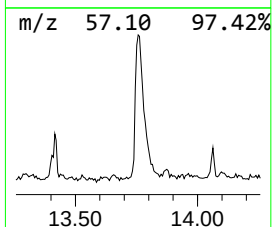
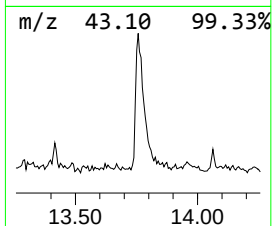
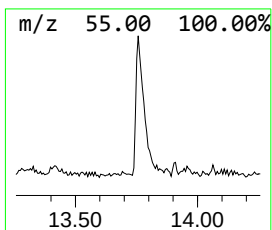
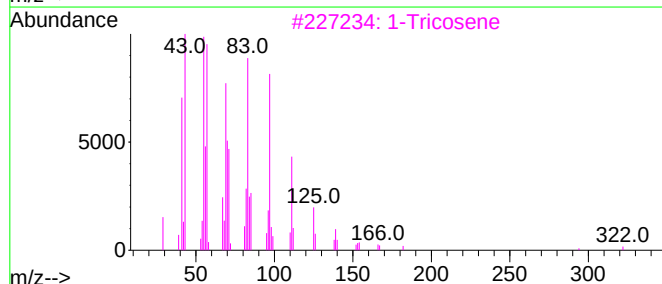
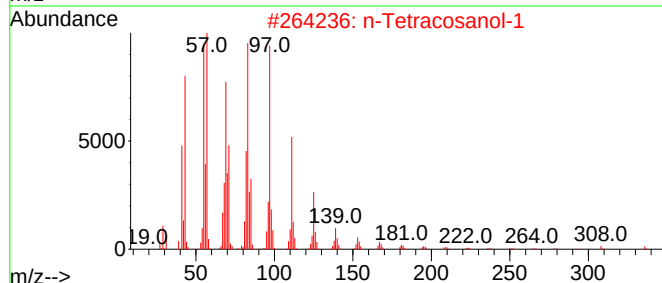
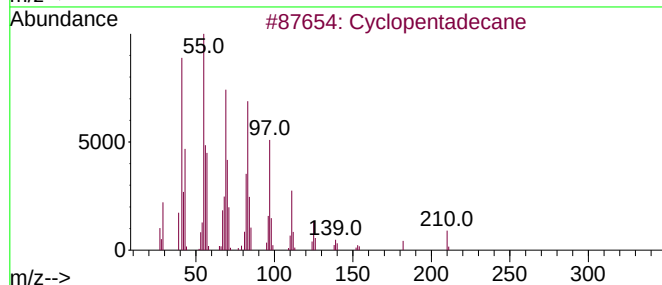
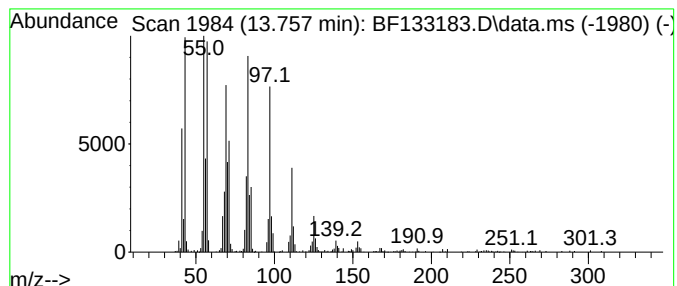
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 4 Cyclopentadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.757	10.71 ng	817009	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	96
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3			1-Tricosene	322	C23H46	018835-32-0	94
4			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94



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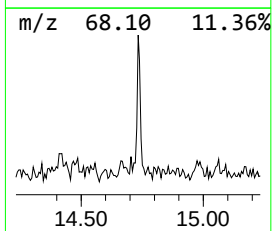
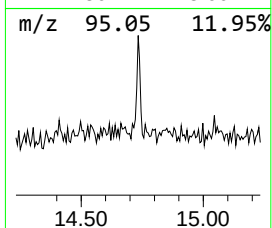
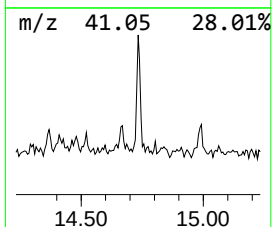
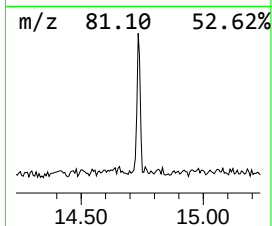
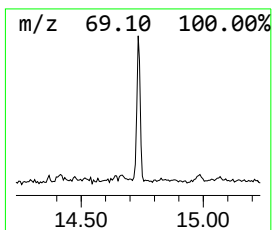
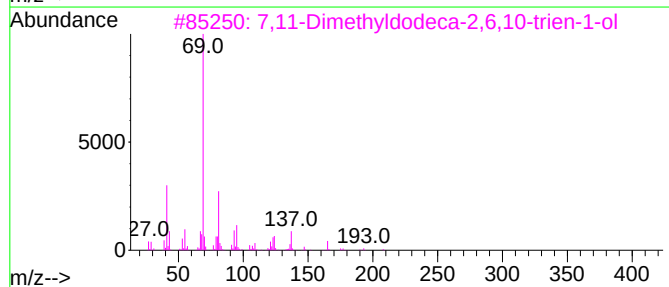
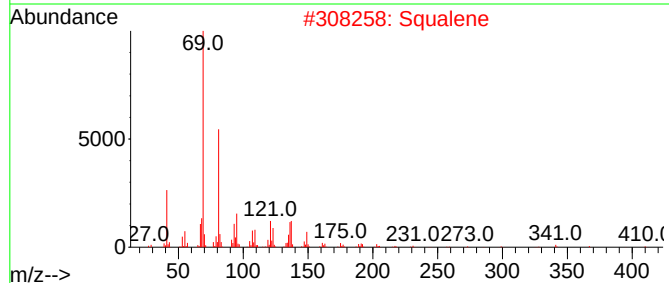
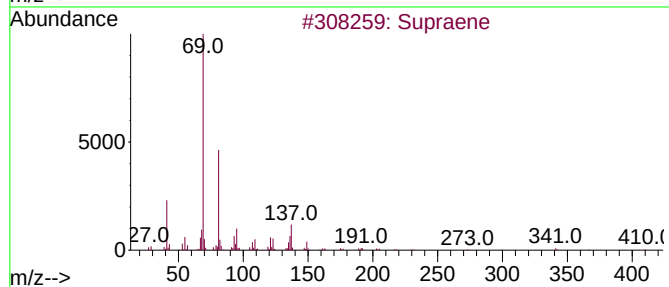
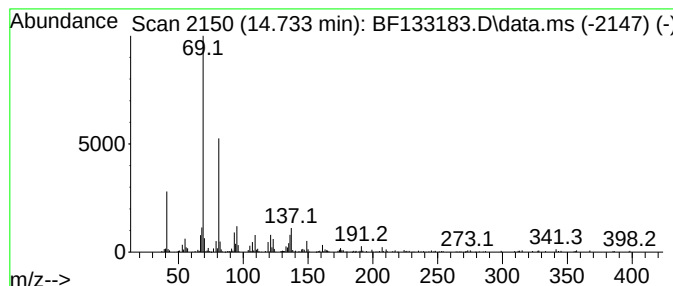
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.733	2.41 ng	133321	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			Squalene	410	C30H50	000111-02-4	90
3			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	80
4			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64
5			6,11-Dimethyl-2,6,10-dodecatrien...	208	C14H24O	1000196-53-3	64



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Data File : BF133183.D
Acq On : 02 May 2023 12:11
Operator : CG\JU
Sample : 02521-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GMW-10

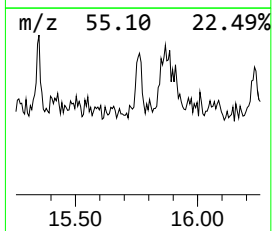
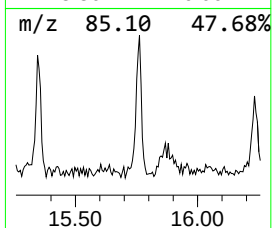
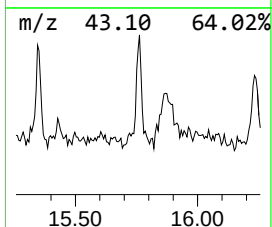
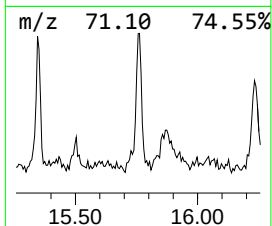
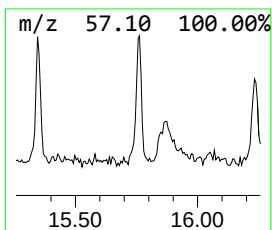
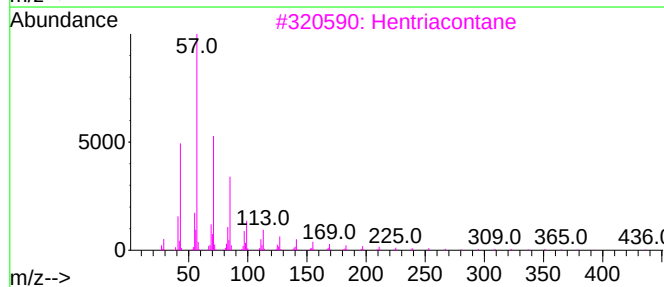
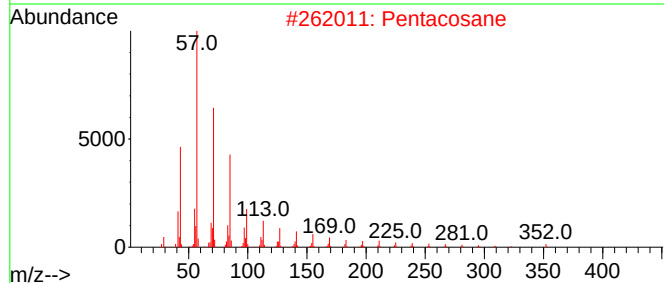
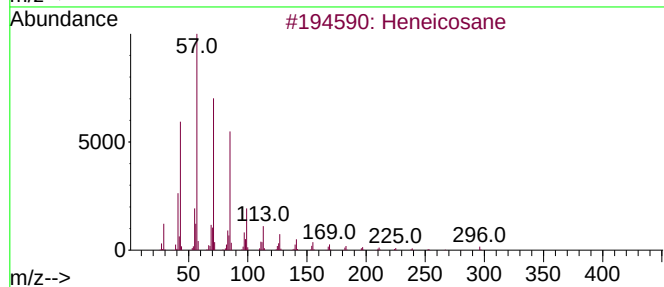
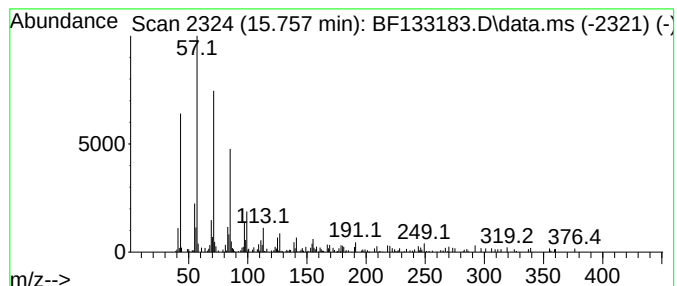
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.757	2.10 ng	116058	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	90
2			Pentacosane	352	C25H52	000629-99-2	90
3			Hentriacontane	437	C31H64	000630-04-6	87
4			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87
5			Octacosane	394	C28H58	000630-02-4	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050223\
Data File : BF133183.D
Acq On : 02 May 2023 12:11
Operator : CG\JU
Sample : 02521-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GMW-10

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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
Benzophenone	10.480	10.0	ng	986876	3	9.769	1975650	20.0
n-Hexadecanoic ...	11.792	21.3	ng	2098590	4	11.251	1968780	20.0
Octadecanoic acid	12.574	17.0	ng	1296810	5	13.880	1525580	20.0
Cyclopentadecane	13.757	10.7	ng	817009	5	13.880	1525580	20.0
Supraene	14.733	2.4	ng	133321	6	15.304	1107870	20.0
Heneicosane	15.757	2.1	ng	116058	6	15.304	1107870	20.0