

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042523\
 Data File : BF133046.D
 Acq On : 26 Apr 2023 01:03
 Operator : CG\JU
 Sample : 02270-25
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-16-0-2-20230413

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: BF133046.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.292	371	375	382	rVB	65097	73428	1.84%	0.203%
2	4.934	478	484	495	rVB	1249953	1460936	36.70%	4.039%
3	5.357	551	556	559	rBV	3639549	3335511	83.80%	9.221%
4	5.751	619	623	629	rBV	62693	60612	1.52%	0.168%
5	6.381	725	730	733	rBV	3550402	3359952	84.41%	9.288%
6	6.739	787	791	794	rBV	1644187	1234976	31.03%	3.414%
7	7.304	882	887	890	rBV	2695882	2231061	56.05%	6.168%
8	8.022	1006	1009	1012	rBV	1988467	1604925	40.32%	4.437%
9	9.098	1188	1192	1195	rBV	4662364	3980508	100.00%	11.004%
10	9.774	1303	1307	1310	rBV	2237941	1796649	45.14%	4.967%
11	10.486	1424	1428	1431	rBV	445098	342518	8.60%	0.947%
12	10.563	1436	1441	1444	rBV	2420986	2170416	54.53%	6.000%
13	11.257	1555	1559	1561	rBV	2019205	1712491	43.02%	4.734%
14	11.280	1561	1563	1566	rVV	628252	461667	11.60%	1.276%
15	11.327	1566	1571	1574	rVB	114257	99056	2.49%	0.274%
16	11.486	1592	1598	1600	rBV	54589	56526	1.42%	0.156%
17	11.757	1641	1644	1646	rBV	82539	68192	1.71%	0.189%
18	11.792	1646	1650	1653	rVV2	351410	374117	9.40%	1.034%
19	11.827	1653	1656	1659	rVV2	82349	93051	2.34%	0.257%
20	11.868	1659	1663	1665	rVV2	109226	130648	3.28%	0.361%
21	11.886	1665	1666	1672	rVB	58003	49646	1.25%	0.137%
22	12.051	1691	1694	1696	rBV2	78502	76078	1.91%	0.210%
23	12.068	1696	1697	1702	rVB	73137	53691	1.35%	0.148%
24	12.304	1734	1737	1740	rBV	46284	46136	1.16%	0.128%
25	12.386	1749	1751	1756	rVB2	51958	60154	1.51%	0.166%
26	12.463	1761	1764	1768	rVV	818113	700627	17.60%	1.937%
27	12.580	1778	1784	1788	rBV3	178524	231415	5.81%	0.640%
28	12.692	1797	1803	1807	rBV	702205	679564	17.07%	1.879%
29	12.845	1825	1829	1832	rBV	3583296	3231712	81.19%	8.934%
30	12.910	1836	1840	1844	rBV4	52221	85228	2.14%	0.236%
31	12.998	1852	1855	1857	rBV3	42385	49234	1.24%	0.136%
32	13.021	1857	1859	1864	rVB2	77117	69764	1.75%	0.193%
33	13.086	1867	1870	1873	rVB2	93928	76419	1.92%	0.211%
34	13.121	1873	1876	1879	rBV2	82873	86002	2.16%	0.238%
35	13.321	1907	1910	1917	rVB3	53842	54922	1.38%	0.152%
36	13.521	1942	1944	1946	rBV	55916	50048	1.26%	0.138%

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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

37	13.633	1960	1963	1967	rBV2	58928	81500	2.05%	0.225%
38	13.733	1977	1980	1982	rBV2	50535	45951	1.15%	0.127%
39	13.757	1982	1984	1987	rVV	63328	47456	1.19%	0.131%
40	13.827	1990	1996	2002	rVV8	49425	161867	4.07%	0.447%
41	13.886	2002	2006	2009	rVV2	1573751	1761052	44.24%	4.868%
42	13.915	2009	2011	2013	rVB	302934	224976	5.65%	0.622%
43	14.104	2040	2043	2048	rVB2	67296	70675	1.78%	0.195%
44	14.380	2087	2090	2095	rVB2	104123	109187	2.74%	0.302%
45	14.815	2161	2164	2168	rVB	205442	193558	4.86%	0.535%
46	14.904	2175	2179	2182	rBV	286247	401744	10.09%	1.111%
47	15.004	2193	2196	2200	rVB2	253368	267995	6.73%	0.741%
48	15.192	2225	2228	2234	rVB	188507	221056	5.55%	0.611%
49	15.251	2234	2238	2242	rBV	226245	249874	6.28%	0.691%
50	15.315	2244	2249	2252	rBV	927609	1146413	28.80%	3.169%
51	15.556	2286	2290	2296	rVB	104806	149579	3.76%	0.413%
52	15.780	2324	2328	2334	rVB	145108	205189	5.15%	0.567%
53	16.533	2451	2456	2462	rVB5	74377	131322	3.30%	0.363%
54	16.686	2477	2482	2489	rVB2	86545	174345	4.38%	0.482%
55	16.821	2501	2505	2508	rBV2	45396	77528	1.95%	0.214%
56	17.098	2548	2552	2560	rVB	66187	119763	3.01%	0.331%
57	18.233	2739	2745	2750	rBV10	34459	85560	2.15%	0.237%

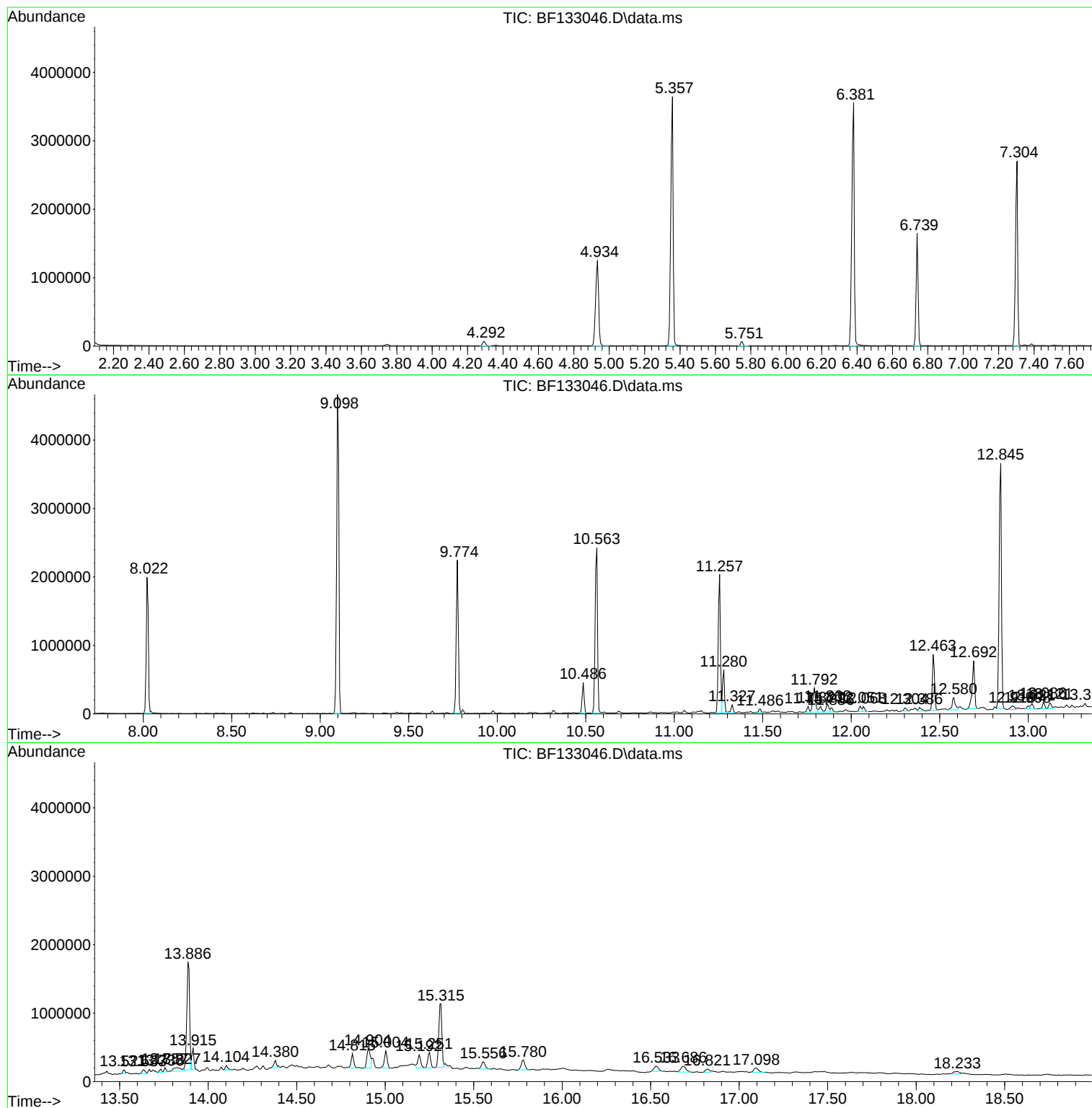
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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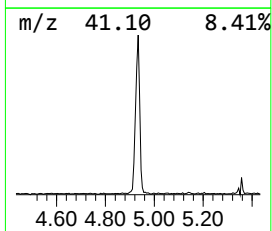
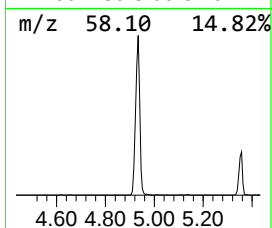
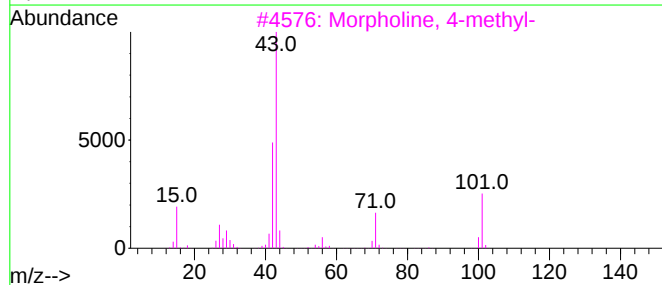
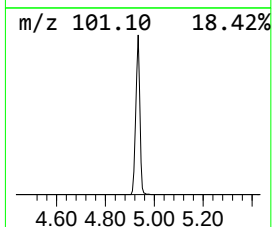
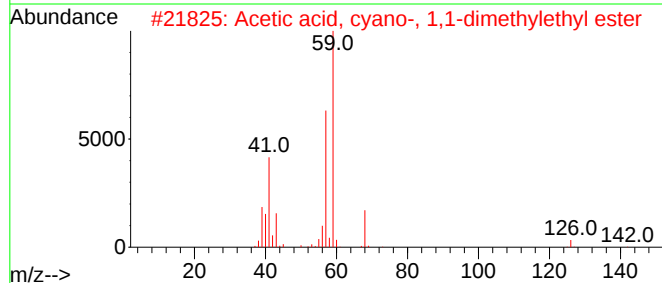
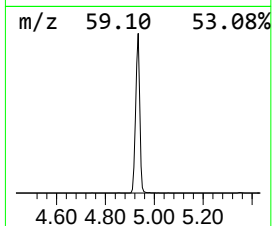
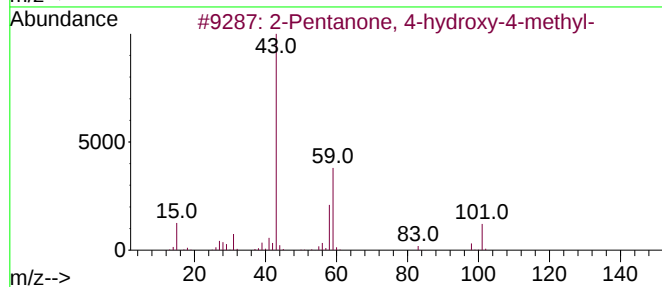
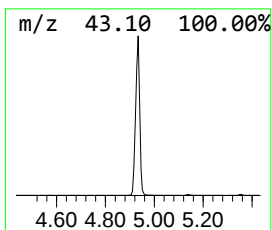
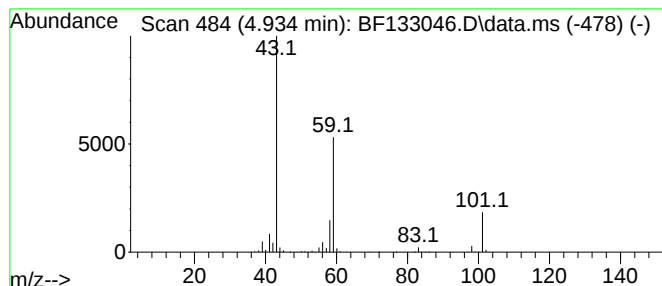
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.934	23.66 ng	1460940	1,4-Dichlorobenzene-d4	6.739

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9		



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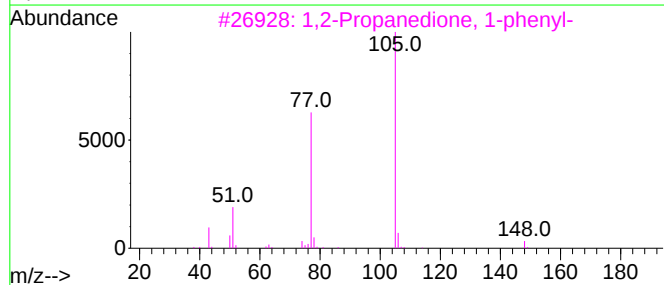
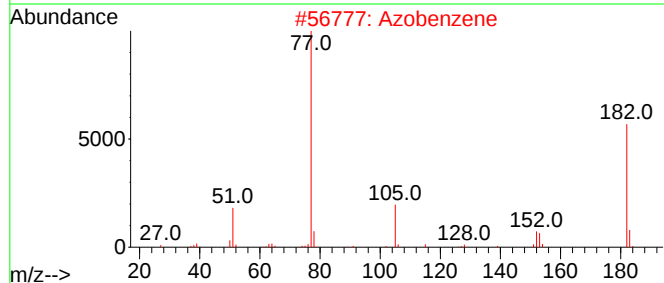
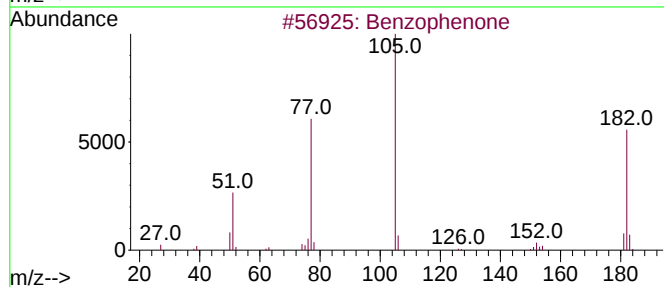
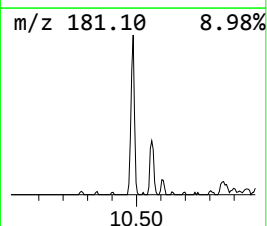
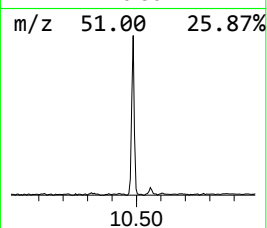
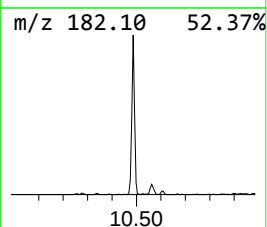
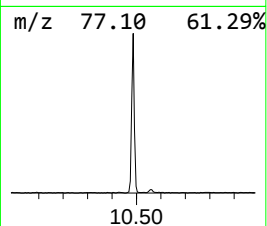
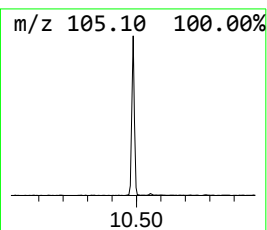
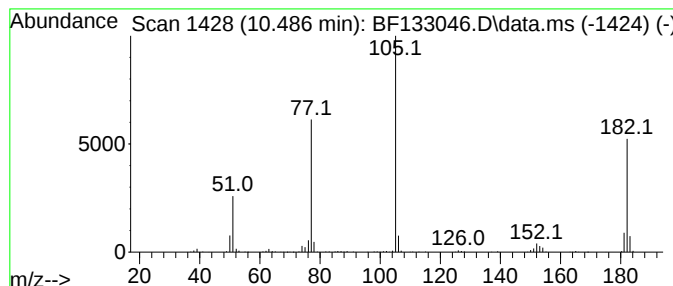
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.486	3.81 ng	342518	Acenaphthene-d10	9.774

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	64
3			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47
4			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
5			Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	47



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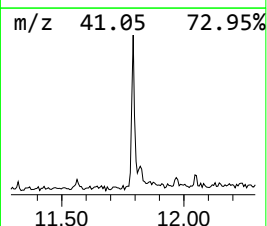
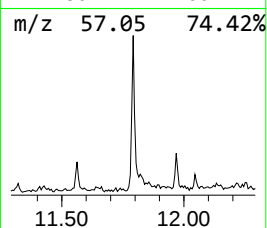
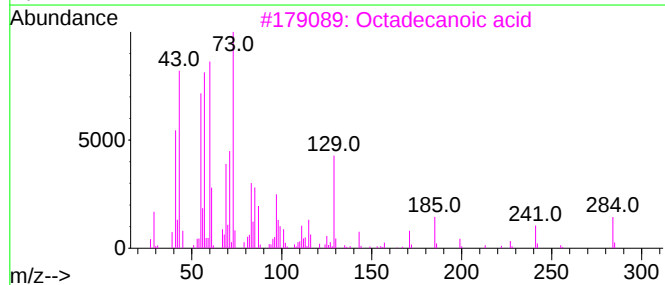
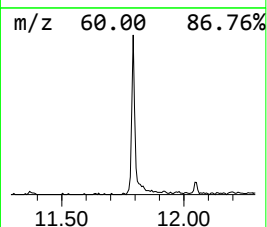
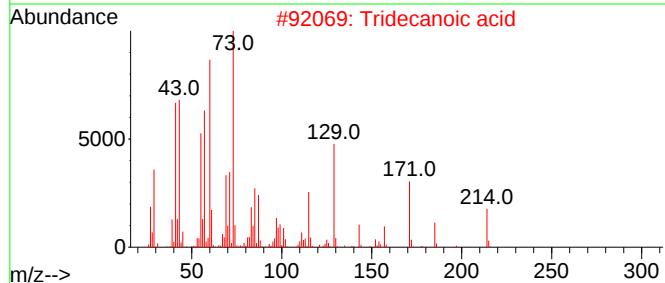
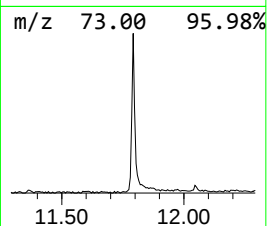
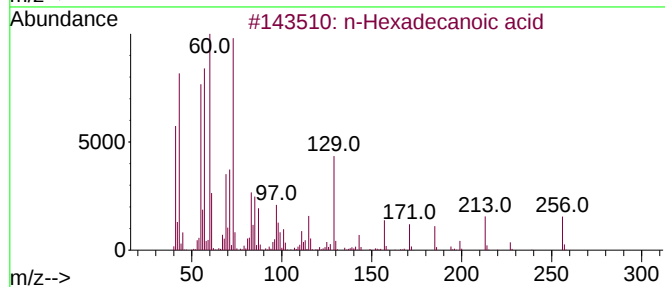
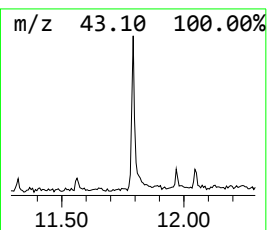
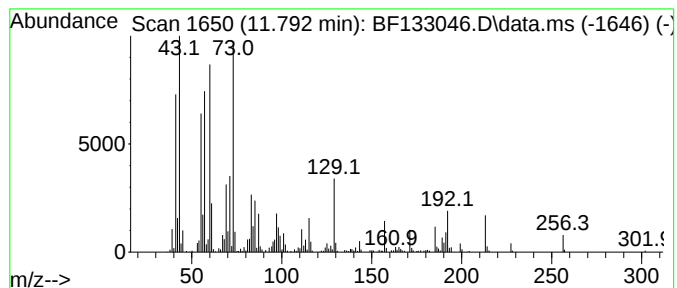
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.792	4.37 ng	374117	Phenanthrene-d10	11.257

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	97
3			Octadecanoic acid	284	C18H36O2	000057-11-4	76
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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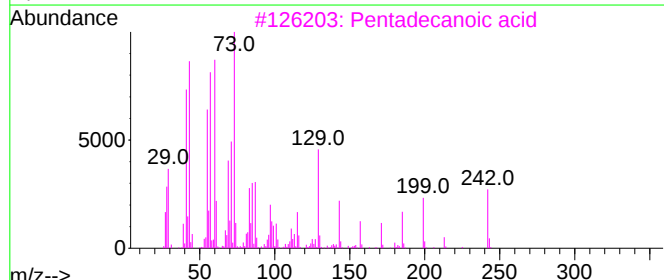
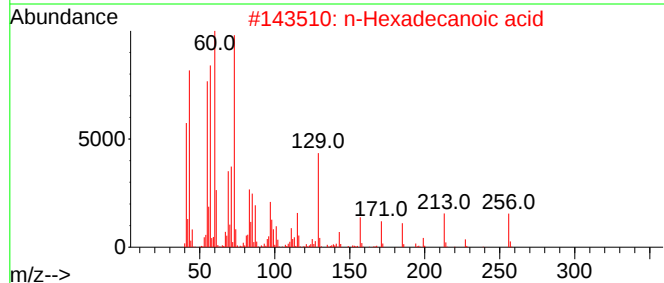
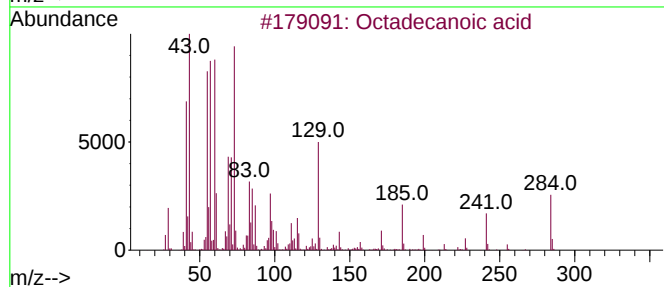
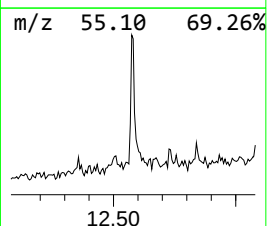
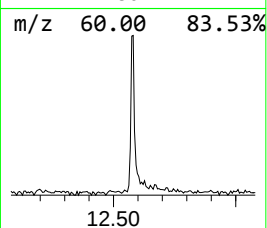
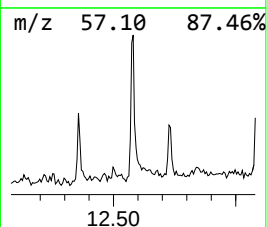
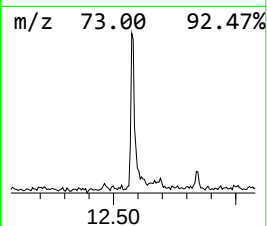
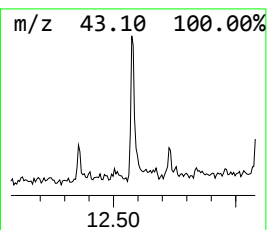
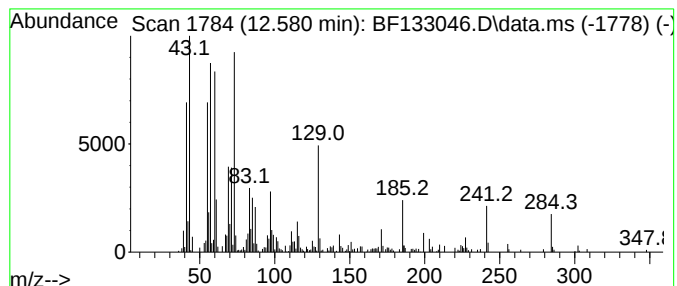
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.580	2.63 ng	231415	Chrysene-d12	13.892

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			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			n-Decanoic acid	172	C10H20O2	000334-48-5	60



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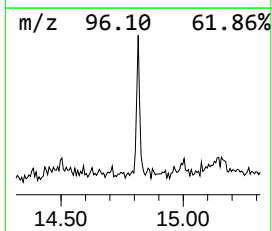
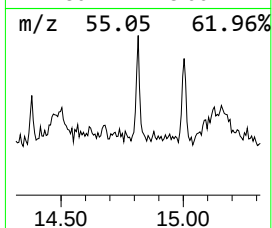
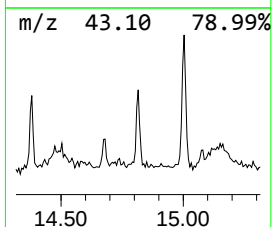
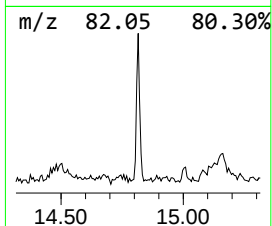
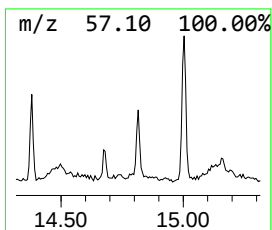
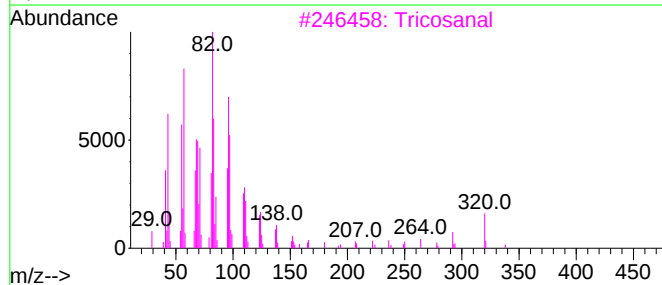
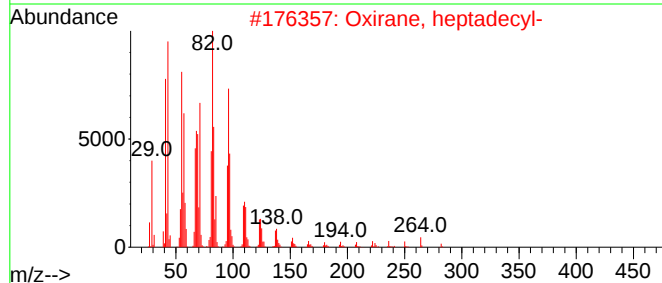
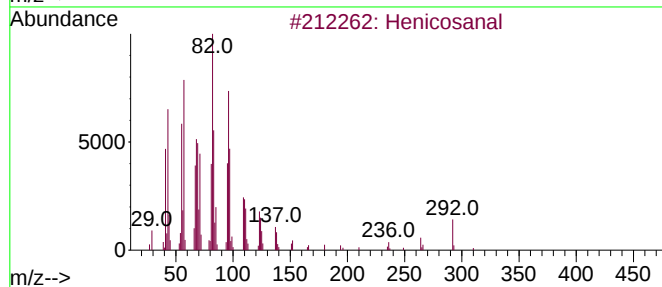
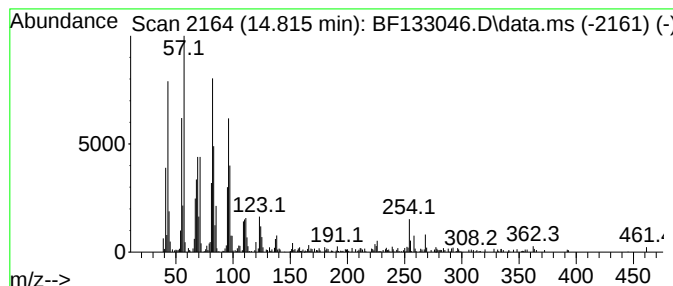
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Henicosanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.815	3.38 ng	193558	Perylene-d12	15.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Henicosanal	310	C21H42O	051227-32-8	94
2			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	93
3			Tricosanal	338	C23H46O	072934-02-2	87
4			16-Octadecenal	266	C18H34O	056554-87-1	86
5			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042523\
Data File : BF133046.D
Acq On : 26 Apr 2023 01:03
Operator : CG\JU
Sample : 02270-25
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-16-0-2-20230413

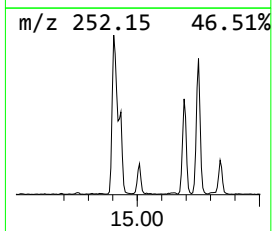
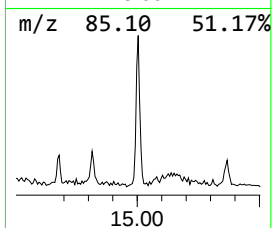
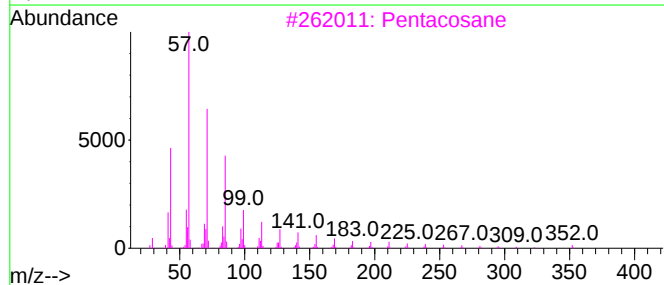
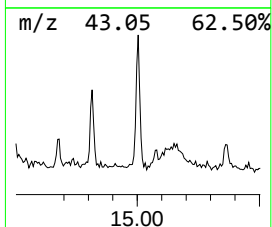
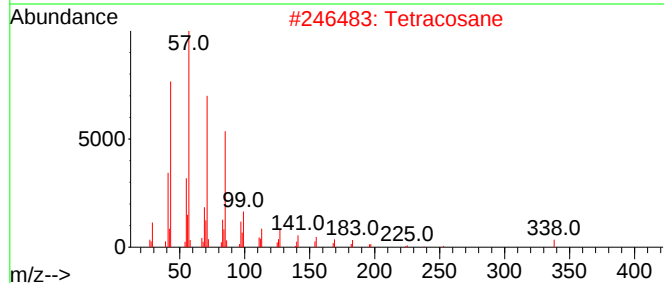
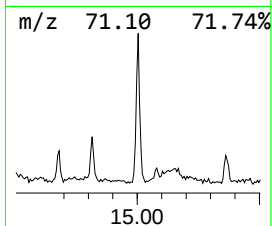
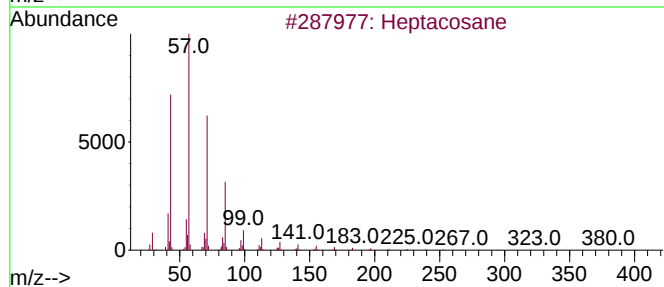
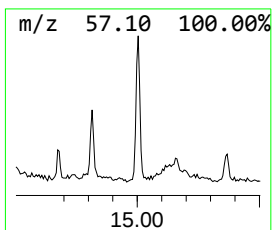
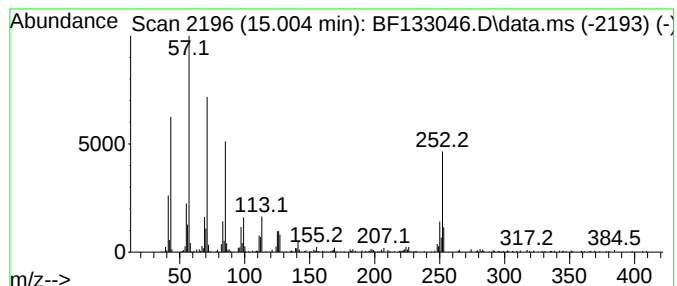
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown15.004 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.004	4.68 ng	267995	Perylene-d12	15.315

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptacosane	380	C27H56	000593-49-7	48
2		Tetracosane	338	C24H50	000646-31-1	46
3		Pentacosane	352	C25H52	000629-99-2	45
4		Hexacosane	366	C26H54	000630-01-3	45
5		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042523\
Data File : BF133046.D
Acq On : 26 Apr 2023 01:03
Operator : CG\JU
Sample : 02270-25
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-16-0-2-20230413

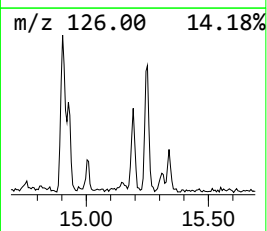
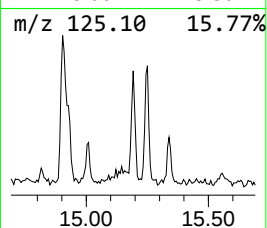
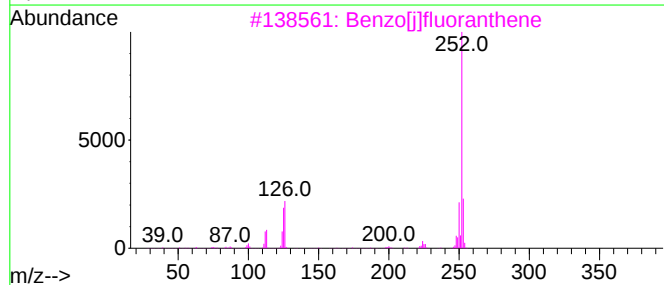
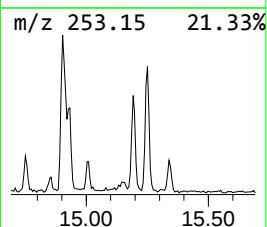
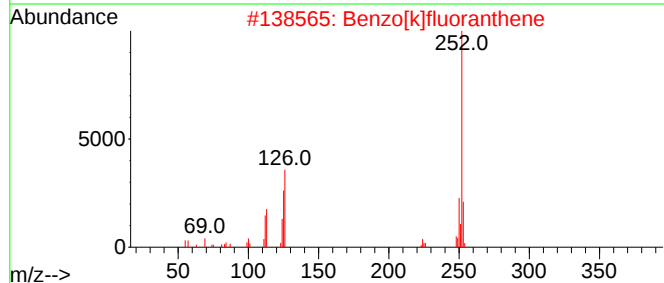
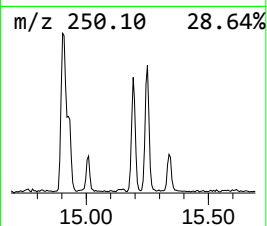
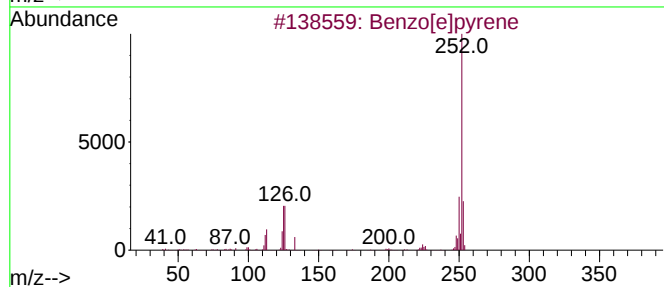
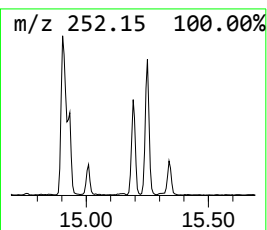
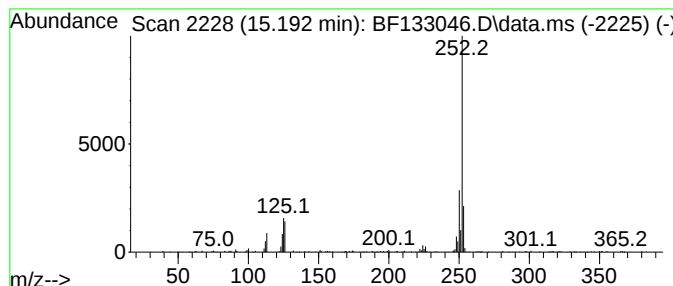
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.192	3.86 ng	221056	Perylene-d12	15.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	98
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
3			Benzo[j]fluoranthene	252	C20H12	000205-82-3	95
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
5			Benzo[a]pyrene	252	C20H12	000050-32-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042523\
Data File : BF133046.D
Acq On : 26 Apr 2023 01:03
Operator : CG\JU
Sample : 02270-25
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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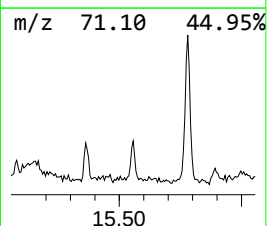
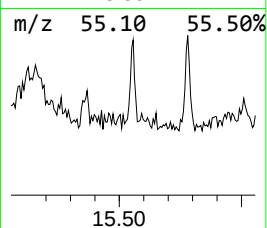
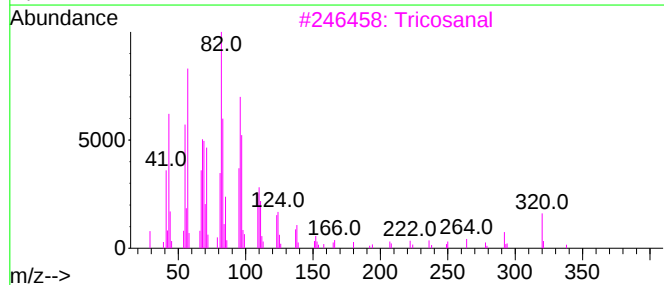
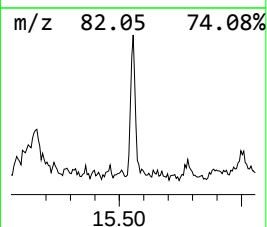
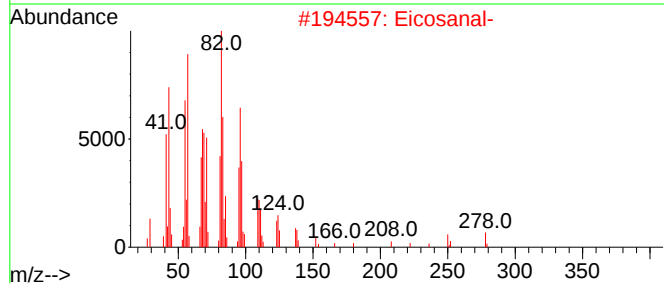
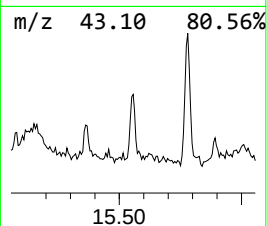
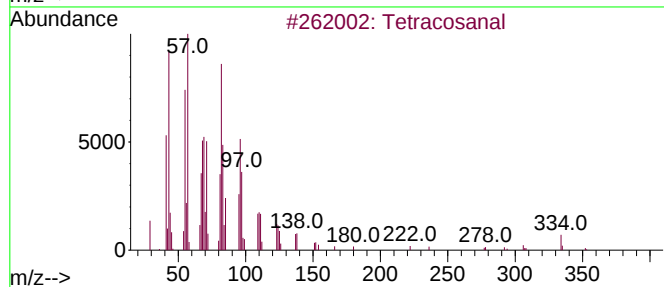
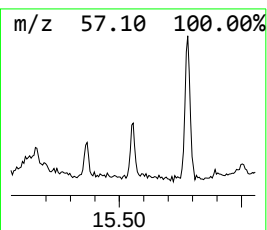
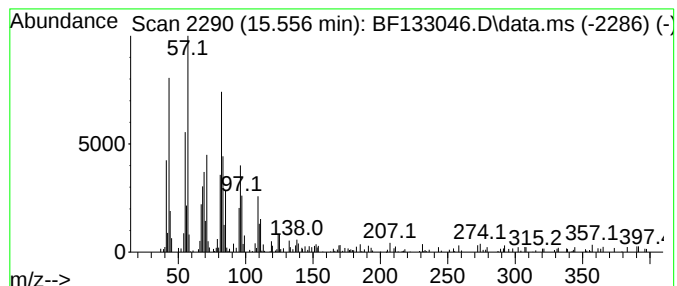
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetracosanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.557	2.61 ng	149579	Perylene-d12	15.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosanal	352	C24H48O	057866-08-7	93
2			Eicosanal-	296	C20H40O	002400-66-0	74
3			Tricosanal	338	C23H46O	072934-02-2	72
4			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	68
5			Hexacosanal	380	C26H52O	026627-85-0	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042523\
Data File : BF133046.D
Acq On : 26 Apr 2023 01:03
Operator : CG\JU
Sample : 02270-25
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-16-0-2-20230413

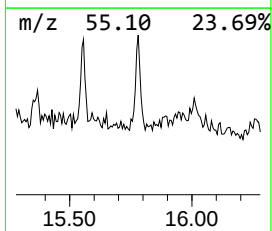
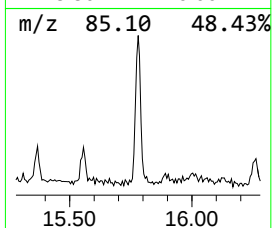
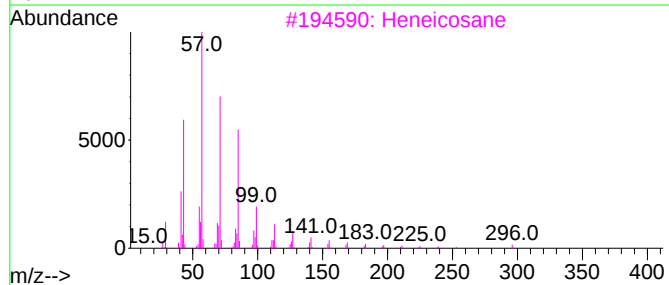
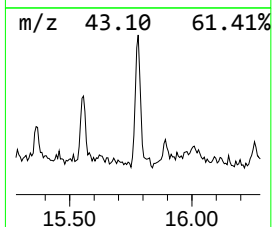
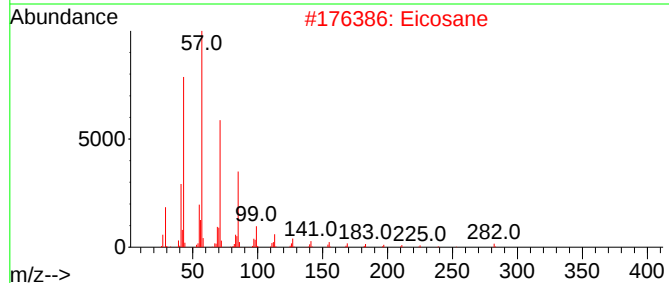
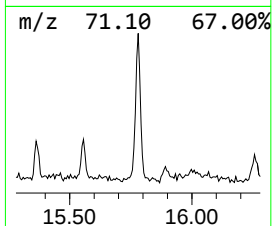
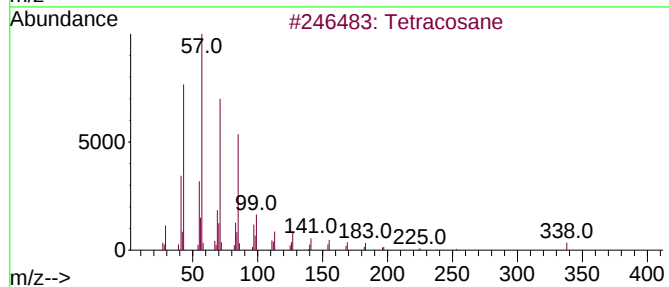
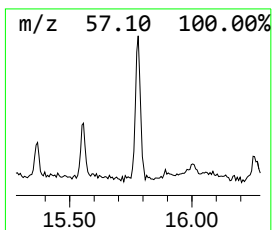
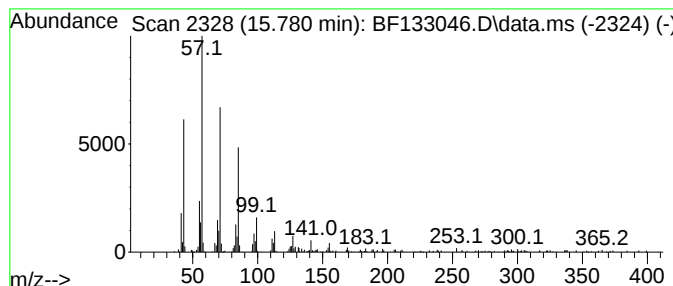
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.780	3.58 ng	205189	Perylene-d12	15.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	99
2			Eicosane	282	C20H42	000112-95-8	93
3			Heneicosane	296	C21H44	000629-94-7	90
4			Pentacosane	352	C25H52	000629-99-2	90
5			Tridecane, 6-propyl-	226	C16H34	055045-10-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042523\
Data File : BF133046.D
Acq On : 26 Apr 2023 01:03
Operator : CG\JU
Sample : 02270-25
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-16-0-2-20230413

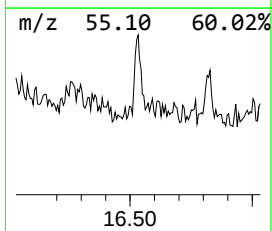
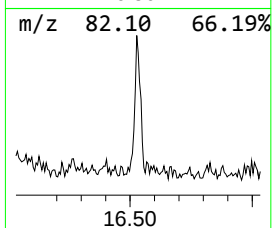
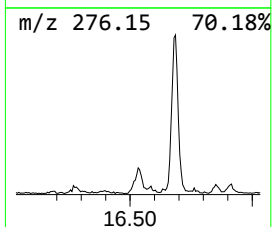
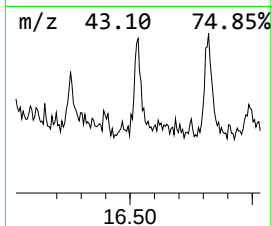
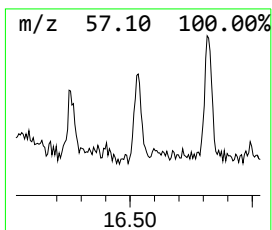
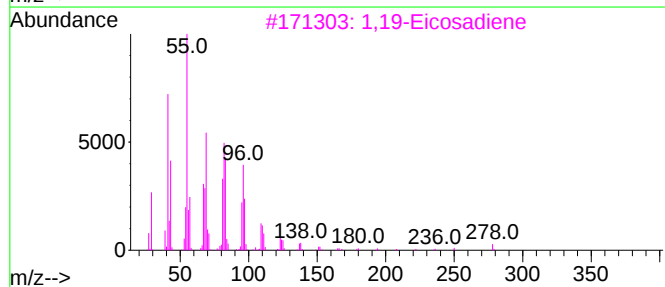
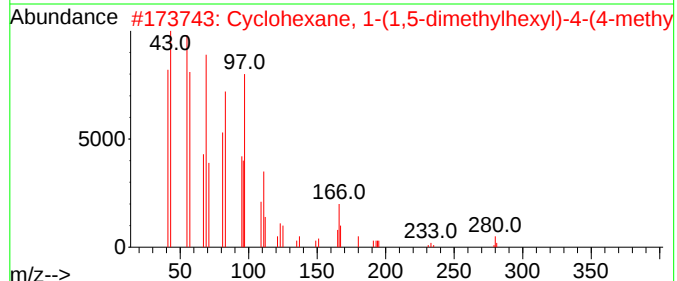
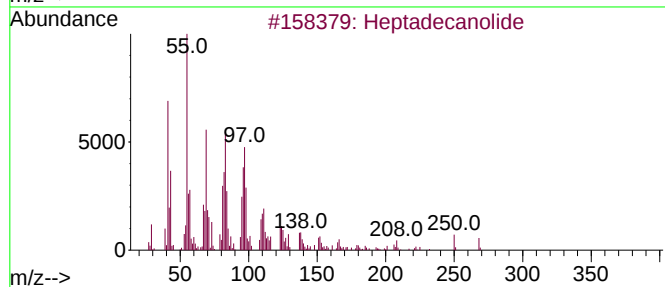
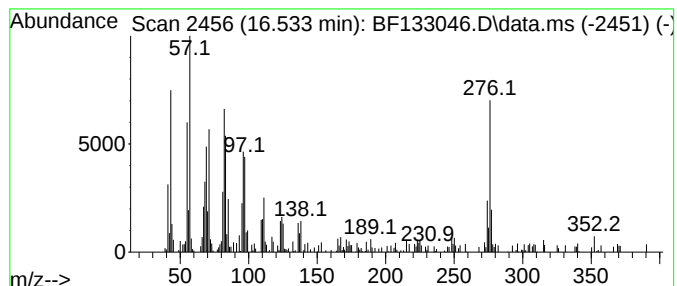
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptadecanolide Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.533	2.29 ng	131322	Perylene-d12	15.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecanolide	268	C17H32O2	005637-97-8	78
2			Cyclohexane, 1-(1,5-dimethylhexy...	280	C20H40	056009-20-2	64
3			1,19-Eicosadiene	278	C20H38	014811-95-1	52
4			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	46
5			trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042523\
Data File : BF133046.D
Acq On : 26 Apr 2023 01:03
Operator : CG\JU
Sample : 02270-25
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-16-0-2-20230413

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

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

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					#	RT	Resp	Conc
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Benzophenone	10.486	3.8	ng	342518	3	9.774	1796650	20.0
n-Hexadecanoic ...	11.792	4.4	ng	374117	4	11.257	1712490	20.0
Octadecanoic acid	12.580	2.6	ng	231415	5	13.892	1761050	20.0
Henicosanal	14.815	3.4	ng	193558	6	15.315	1146410	20.0
unknown15.004	15.004	4.7	ng	267995	6	15.315	1146410	20.0
Benzo[e]pyrene	15.192	3.9	ng	221056	6	15.315	1146410	20.0
Tetracosanal	15.557	2.6	ng	149579	6	15.315	1146410	20.0
Tetracosane	15.780	3.6	ng	205189	6	15.315	1146410	20.0
Heptadecanolide	16.533	2.3	ng	131322	6	15.315	1146410	20.0