

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050423\
 Data File : BF133227.D
 Acq On : 04 May 2023 13:12
 Operator : CG\JU
 Sample : 02588-03
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 ZONE-B-6-9-05012023

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: BF133227.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.716	266	277	285	rBV	116556	173993	3.91%	0.524%
2	4.928	476	483	492	rVB	75907	109027	2.45%	0.328%
3	5.340	548	553	556	rBV	4506030	4363171	97.97%	13.145%
4	6.369	722	728	731	rBV	4275668	4453789	100.00%	13.418%
5	6.728	785	789	792	rBV	1401765	1216134	27.31%	3.664%
6	7.139	851	859	866	rBV	50847	63588	1.43%	0.192%
7	7.292	880	885	888	rBV	3165091	2812950	63.16%	8.474%
8	8.010	1003	1007	1010	rBV	2141853	1633457	36.68%	4.921%
9	9.086	1186	1190	1193	rBV	5197256	4213573	94.61%	12.694%
10	9.763	1301	1305	1308	rVB	2210758	1779789	39.96%	5.362%
11	10.474	1422	1426	1429	rVB	336248	290004	6.51%	0.874%
12	10.545	1434	1438	1442	rBV	2279790	2170973	48.74%	6.540%
13	10.592	1443	1446	1452	rVB	137933	125728	2.82%	0.379%
14	10.686	1458	1462	1467	rVB2	41018	53925	1.21%	0.162%
15	11.239	1553	1556	1559	rBV	1910955	1766518	39.66%	5.322%
16	11.263	1559	1560	1563	rVB	198787	123382	2.77%	0.372%
17	11.774	1643	1647	1652	rBV2	140871	186771	4.19%	0.563%
18	11.851	1657	1660	1663	rBV	44942	49660	1.12%	0.150%
19	12.451	1759	1762	1765	rBV	329416	248575	5.58%	0.749%
20	12.563	1776	1781	1793	rVB	318553	506910	11.38%	1.527%
21	12.680	1796	1801	1803	rVB	204764	208173	4.67%	0.627%
22	12.827	1822	1826	1830	rVB	3629605	3341729	75.03%	10.067%
23	13.074	1865	1868	1871	rBV2	62975	65327	1.47%	0.197%
24	13.310	1906	1908	1915	rVB	92233	105878	2.38%	0.319%
25	13.786	1983	1989	1994	rBV5	68695	140353	3.15%	0.423%
26	13.874	2000	2004	2007	rBV	1176205	1068831	24.00%	3.220%
27	14.057	2032	2035	2039	rVB2	61336	58154	1.31%	0.175%
28	14.362	2084	2087	2090	rVB2	88397	81965	1.84%	0.247%
29	14.657	2135	2137	2144	rVB	84753	82177	1.85%	0.248%
30	14.886	2173	2176	2179	rBV	90423	121519	2.73%	0.366%
31	14.980	2189	2192	2197	rVB2	131640	157293	3.53%	0.474%
32	15.174	2222	2225	2230	rVB	56321	74719	1.68%	0.225%
33	15.233	2232	2235	2240	rVB	72252	78933	1.77%	0.238%
34	15.292	2241	2245	2249	rBV	985552	1151981	25.87%	3.471%
35	15.751	2319	2323	2328	rVB	90476	114335	2.57%	0.344%

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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

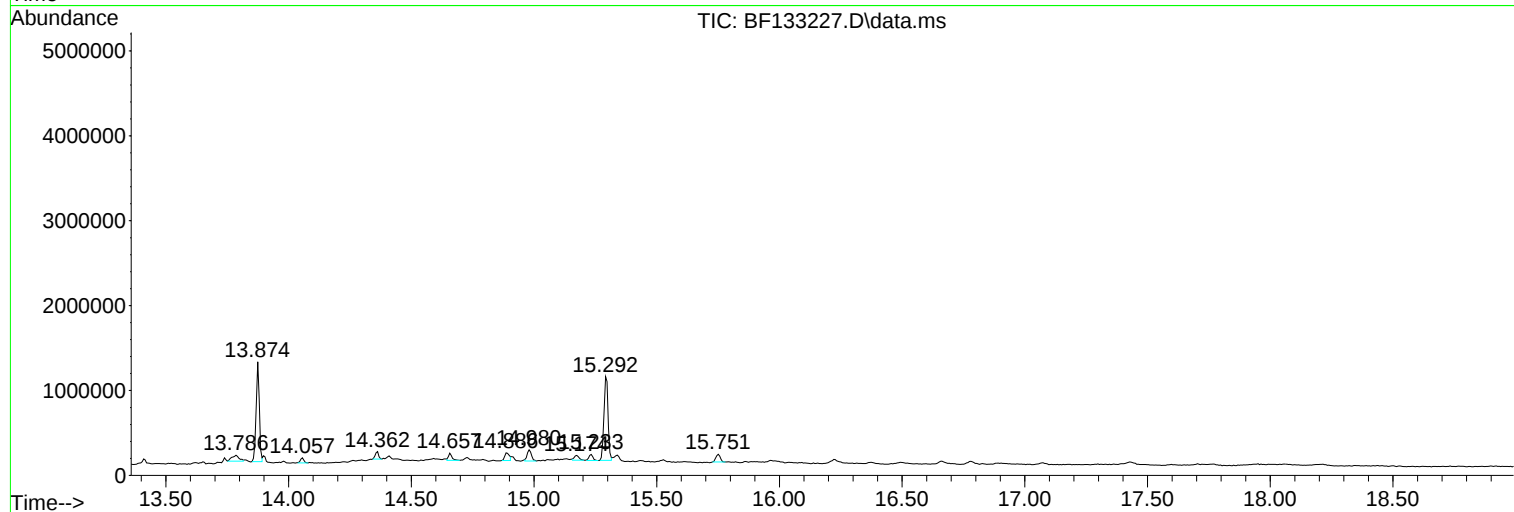
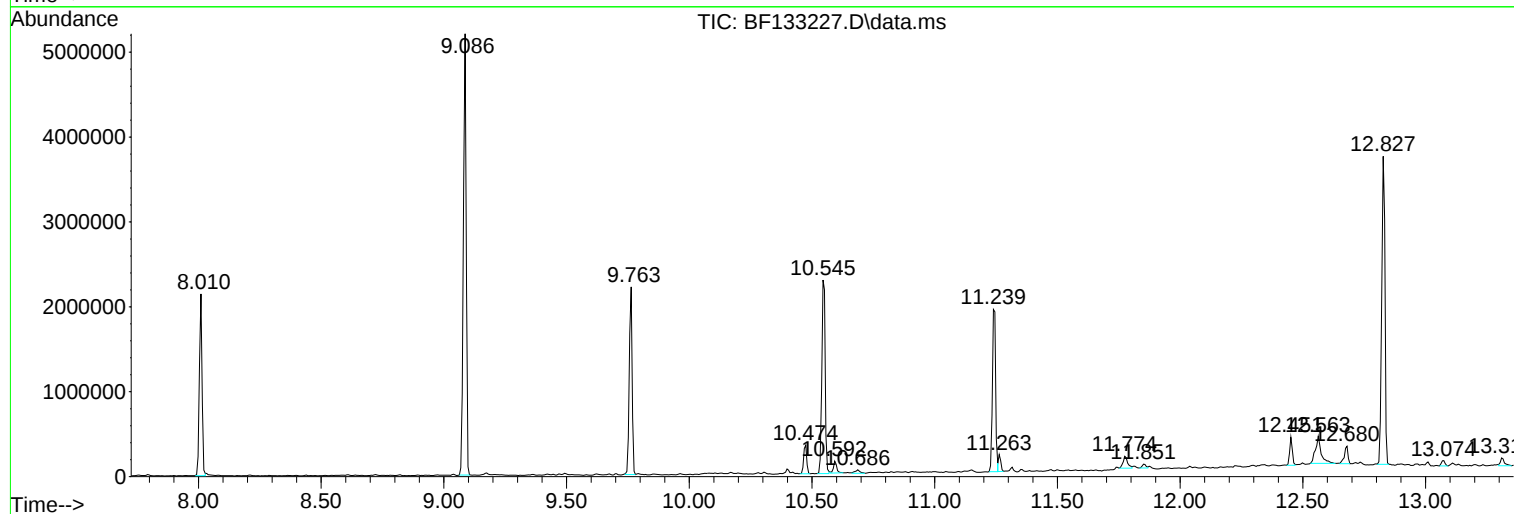
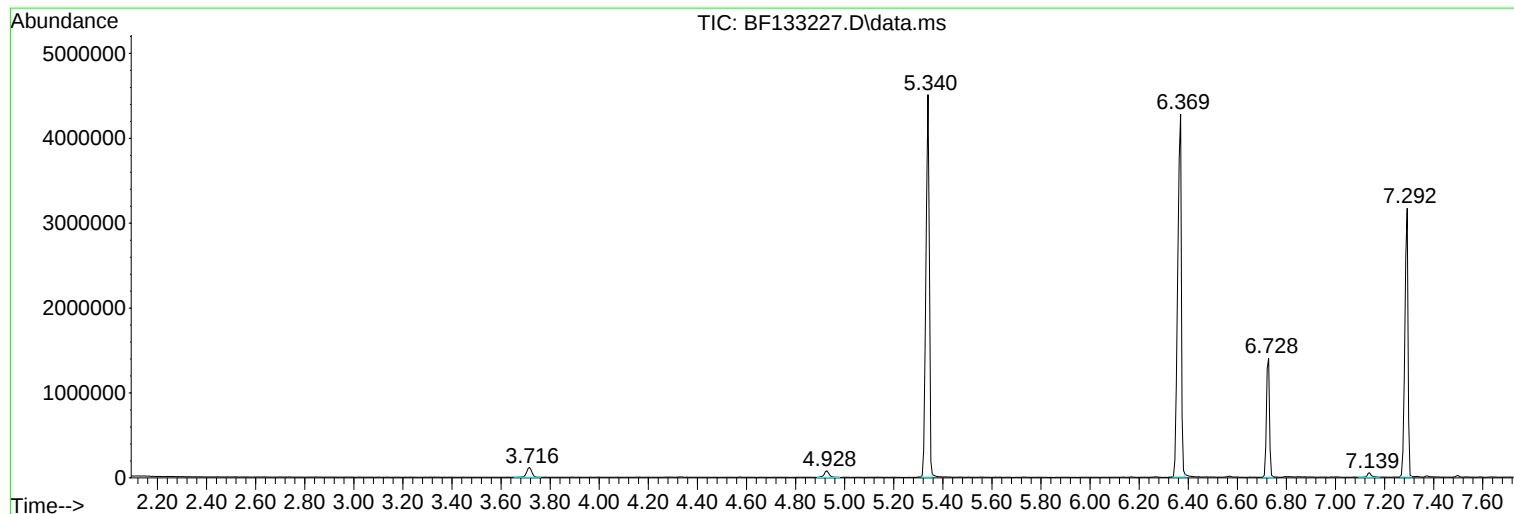
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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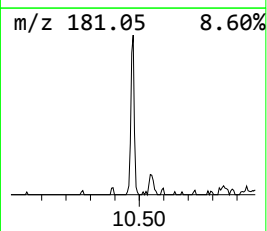
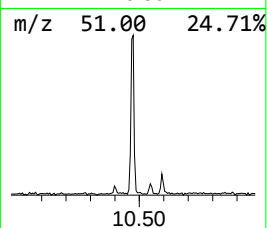
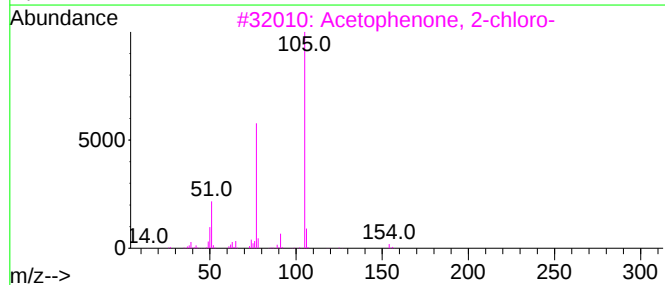
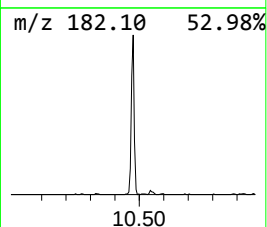
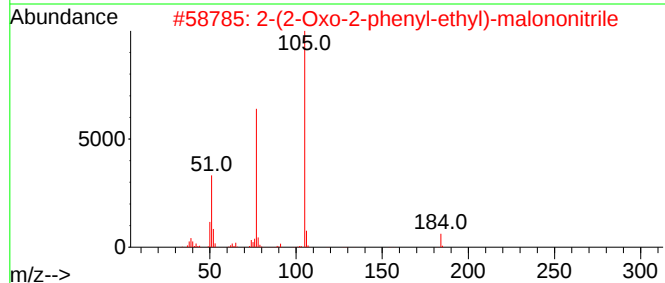
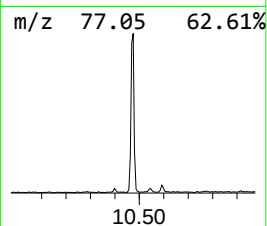
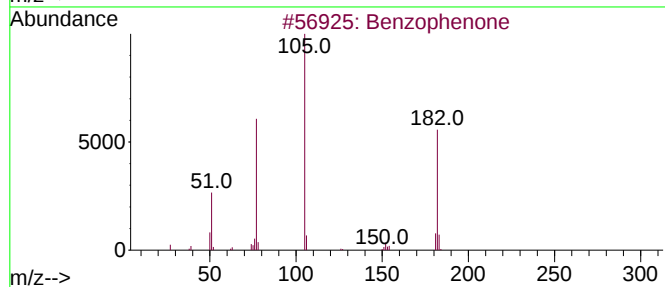
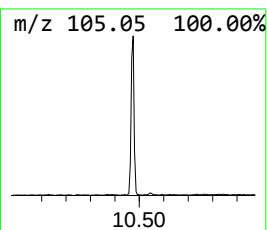
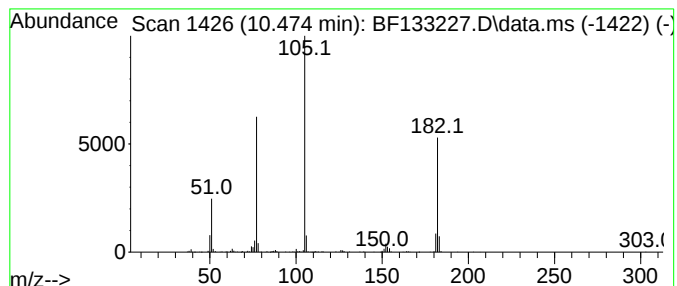
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.475	3.26 ng	290004	Acenaphthene-d10	9.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			2-(2-Oxo-2-phenyl-ethyl)-malononitrile	184	C11H8N2O	1000296-76-9	47
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	47
4			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47
5			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47



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Instrument :
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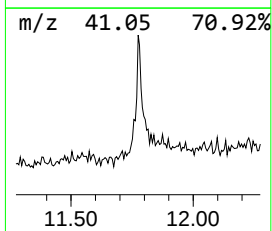
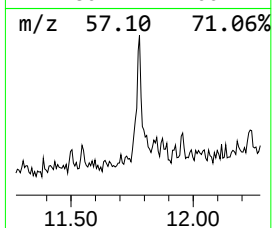
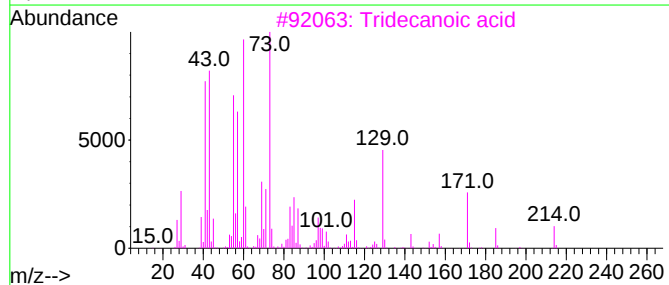
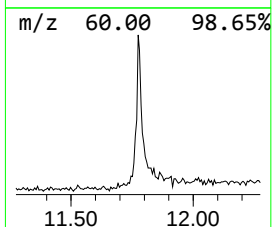
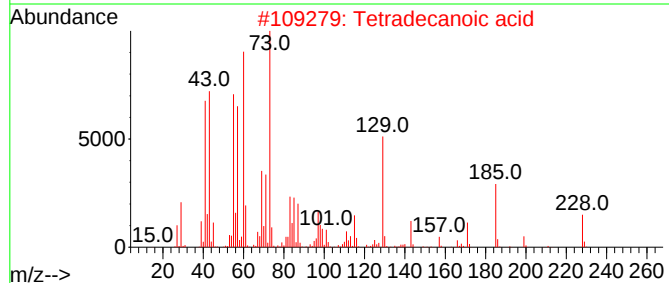
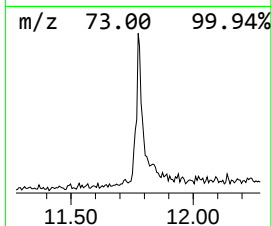
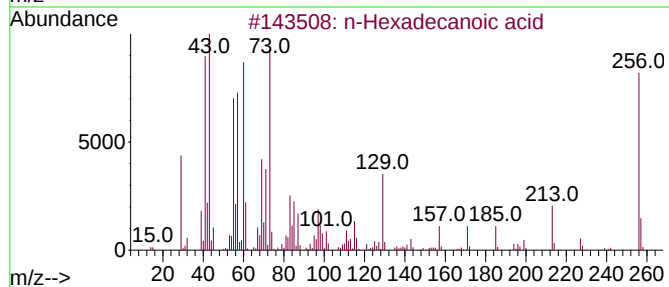
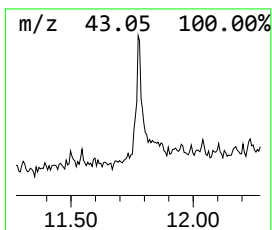
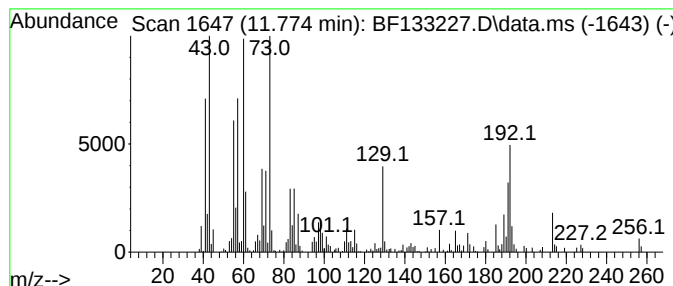
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.774	2.11 ng	186771	Phenanthrene-d10	11.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93		
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	91		
3	Tridecanoic acid	214	C13H26O2	000638-53-9	86		
4	n-Decanoic acid	172	C10H20O2	000334-48-5	55		
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	53		



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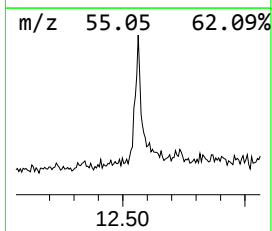
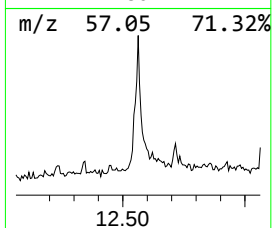
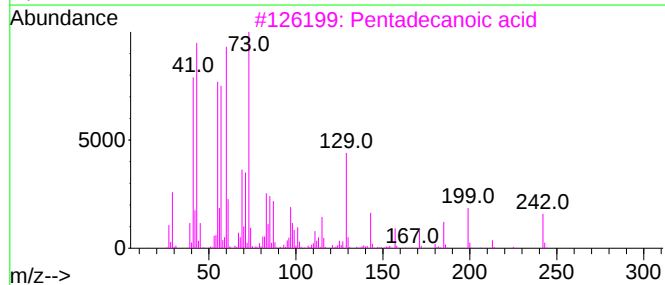
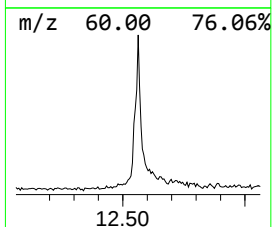
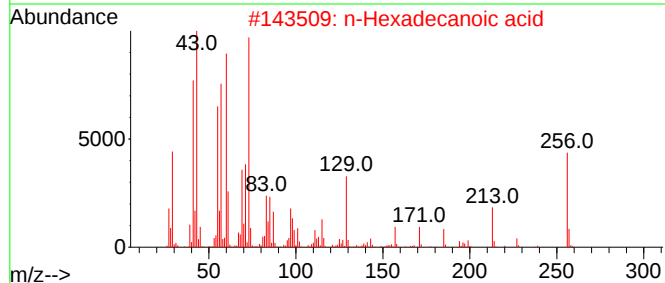
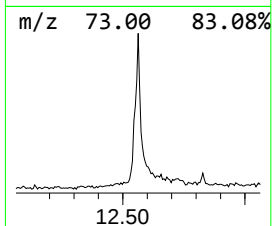
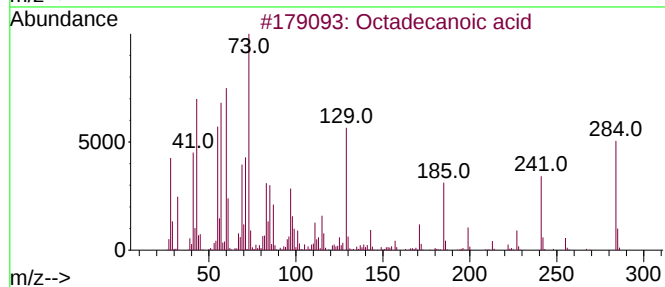
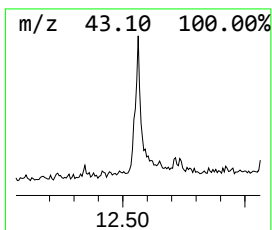
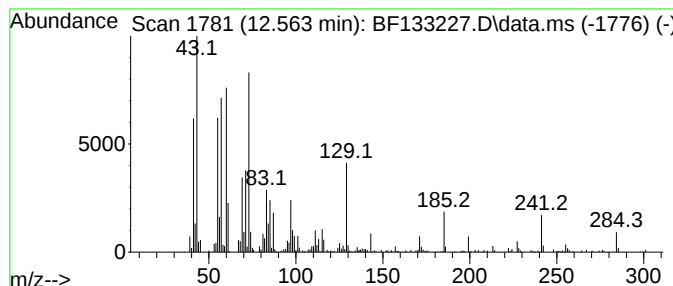
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.563	9.49 ng	506910	Chrysene-d12	13.874

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	86
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72



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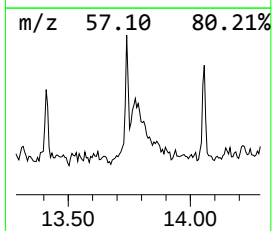
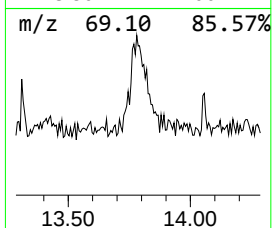
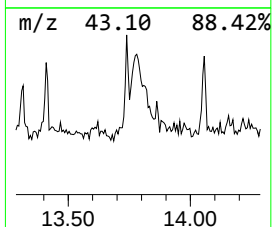
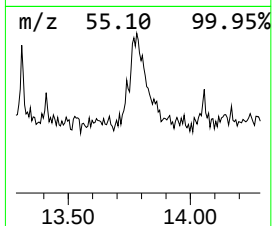
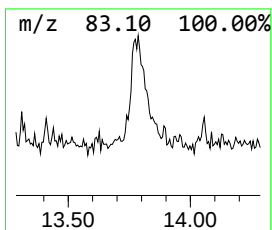
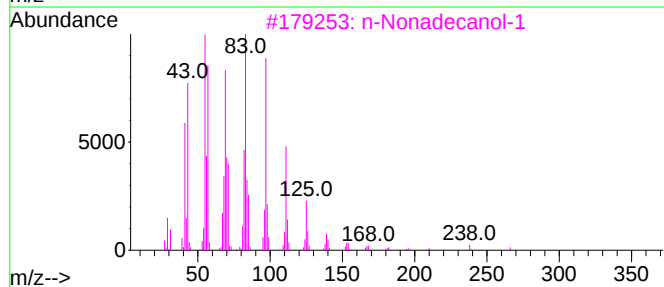
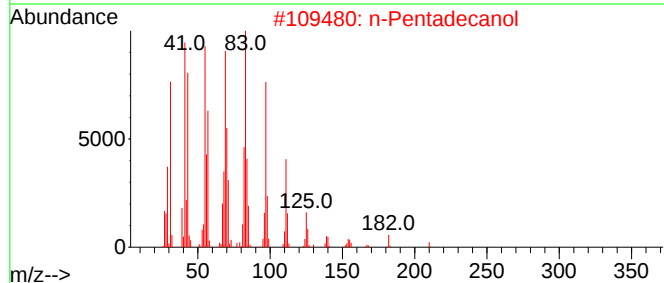
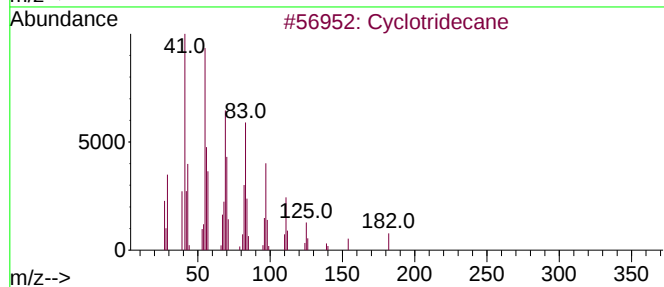
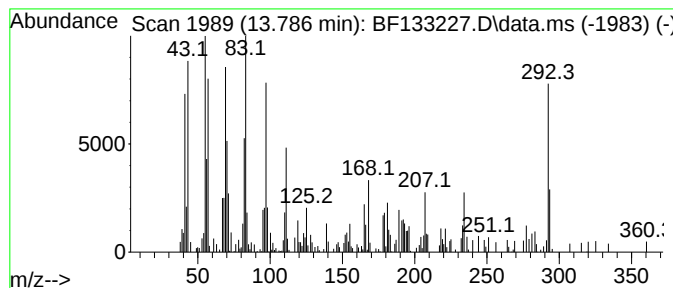
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Cyclotridecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.786	2.63 ng	140353	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotridecane	182	C13H26	000295-02-3	83
2			n-Pentadecanol	228	C15H32O	000629-76-5	60
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	60
4			Cetene	224	C16H32	000629-73-2	56
5			1-Hexadecanol	242	C16H34O	036653-82-4	53



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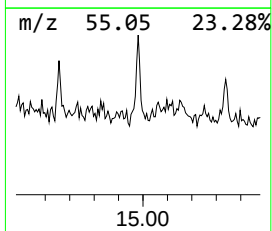
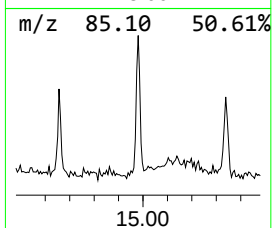
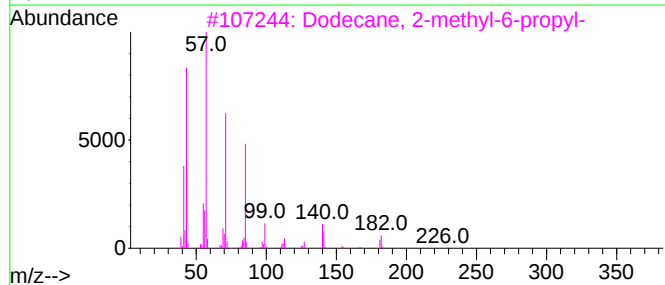
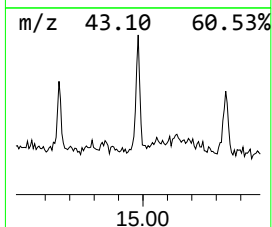
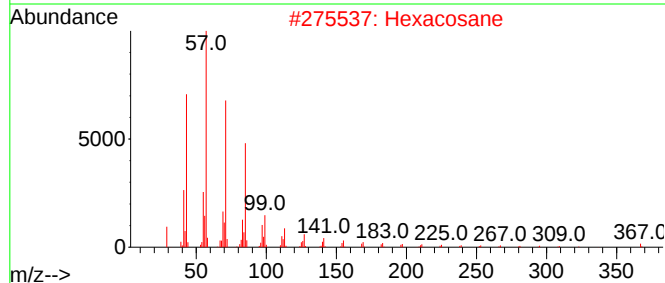
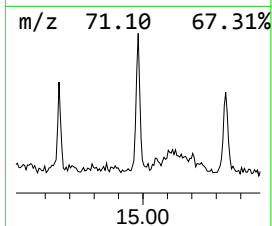
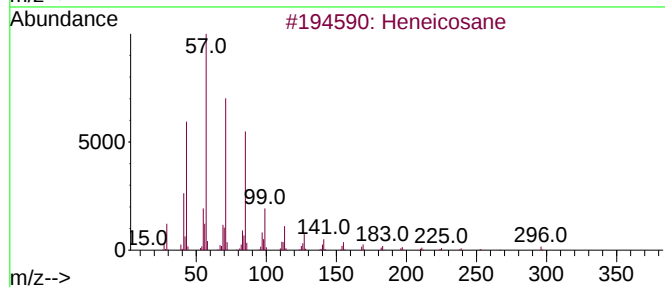
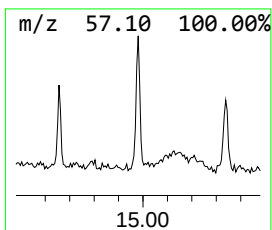
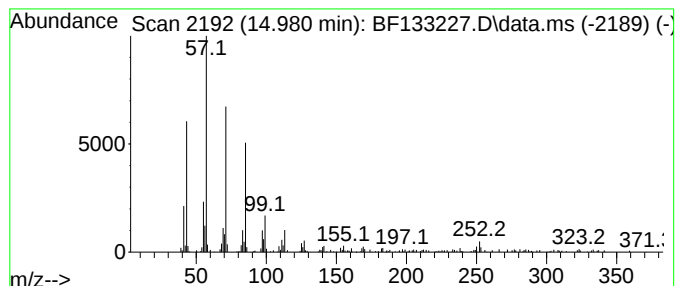
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.980	2.73 ng	157293	Perylene-d12	15.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	87
2			Hexacosane	366	C26H54	000630-01-3	76
3			Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	74
4			Hexatriacontane	507	C36H74	000630-06-8	64
5			Tetradecane, 4-methyl-	212	C15H32	025117-24-2	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050423\
Data File : BF133227.D
Acq On : 04 May 2023 13:12
Operator : CG\JU
Sample : 02588-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ZONE-B-6-9-05012023

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzophenone	10.475	3.3	ng	290004	3	9.763	1779790	20.0
n-Hexadecanoic ...	11.774	2.1	ng	186771	4	11.245	1766520	20.0
Octadecanoic acid	12.563	9.5	ng	506910	5	13.874	1068830	20.0
Cyclotridecane	13.786	2.6	ng	140353	5	13.874	1068830	20.0
Heneicosane	14.980	2.7	ng	157293	6	15.292	1151980	20.0