

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082322\
 Data File : BF129965.D
 Acq On : 23 Aug 2022 22:04
 Operator : CG\JU
 Sample : N4292-01
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TR-04-082222

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-BF081422.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129965.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.998	458	461	479	rBV	374032	467443	13.42%	1.819%
2	5.416	529	532	556	rBV	2964060	3108931	89.25%	12.098%
3	6.440	702	706	719	rBV	3224662	3028053	86.93%	11.783%
4	6.775	759	763	769	rBV	1150374	914909	26.26%	3.560%
5	7.345	856	860	863	rBV	2249295	1964357	56.39%	7.644%
6	8.057	977	981	984	rBV	1440606	1158596	33.26%	4.509%
7	8.081	984	985	988	rVB	73048	39899	1.15%	0.155%
8	8.769	1098	1102	1105	rBV	63697	53278	1.53%	0.207%
9	8.869	1116	1119	1124	rVB	46405	39432	1.13%	0.153%
10	9.134	1158	1164	1167	rBV	3829228	3483392	100.00%	13.555%
11	9.810	1273	1279	1282	rBV	1433360	1124083	32.27%	4.374%
12	9.839	1282	1284	1291	rVB	81582	79159	2.27%	0.308%
13	10.016	1311	1314	1317	rBV	54650	46452	1.33%	0.181%
14	10.357	1369	1372	1378	rVB	52270	51197	1.47%	0.199%
15	10.604	1410	1414	1424	rBV	1978123	1676927	48.14%	6.526%
16	10.710	1428	1432	1439	rVV3	34655	62970	1.81%	0.245%
17	11.298	1529	1532	1535	rBV	1101759	896635	25.74%	3.489%
18	11.322	1535	1536	1541	rVB	188862	140924	4.05%	0.548%
19	11.822	1618	1621	1627	rVB3	136637	154288	4.43%	0.600%
20	11.916	1634	1637	1639	rBV2	40474	44725	1.28%	0.174%
21	11.986	1646	1649	1651	rBV	37741	42936	1.23%	0.167%
22	12.516	1735	1739	1740	rBV	321416	293089	8.41%	1.141%
23	12.533	1740	1742	1752	rVB	644402	826649	23.73%	3.217%
24	12.610	1752	1755	1759	rBV2	77840	96263	2.76%	0.375%
25	12.745	1775	1778	1781	rVB	214544	172132	4.94%	0.670%
26	12.880	1797	1801	1805	rBV	2550418	2338056	67.12%	9.098%
27	13.786	1950	1955	1964	rVB5	128338	303366	8.71%	1.181%
28	13.904	1972	1975	1978	rBV	324605	302895	8.70%	1.179%
29	13.945	1978	1982	1985	rVV2	748652	785057	22.54%	3.055%
30	13.974	1985	1987	1992	rVB	104564	98392	2.82%	0.383%
31	14.033	1995	1997	2002	rVB2	52231	54064	1.55%	0.210%
32	14.421	2059	2063	2070	rBV2	128021	200674	5.76%	0.781%
33	14.833	2130	2133	2136	rVB2	123683	122757	3.52%	0.478%
34	14.986	2156	2159	2160	rBV	66826	74640	2.14%	0.290%
35	15.010	2160	2163	2168	rVB	262897	300826	8.64%	1.171%
36	15.068	2169	2173	2175	rBV3	86309	145544	4.18%	0.566%

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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-BF081422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.280	2207	2209	2213	rVB	52228	50254	1.44%	0.196%
38	15.345	2218	2220	2223	rVV	69480	80820	2.32%	0.315%
39	15.404	2226	2230	2240	rVB	510681	643360	18.47%	2.504%
40	15.792	2292	2296	2300	rVB	170610	230149	6.61%	0.896%

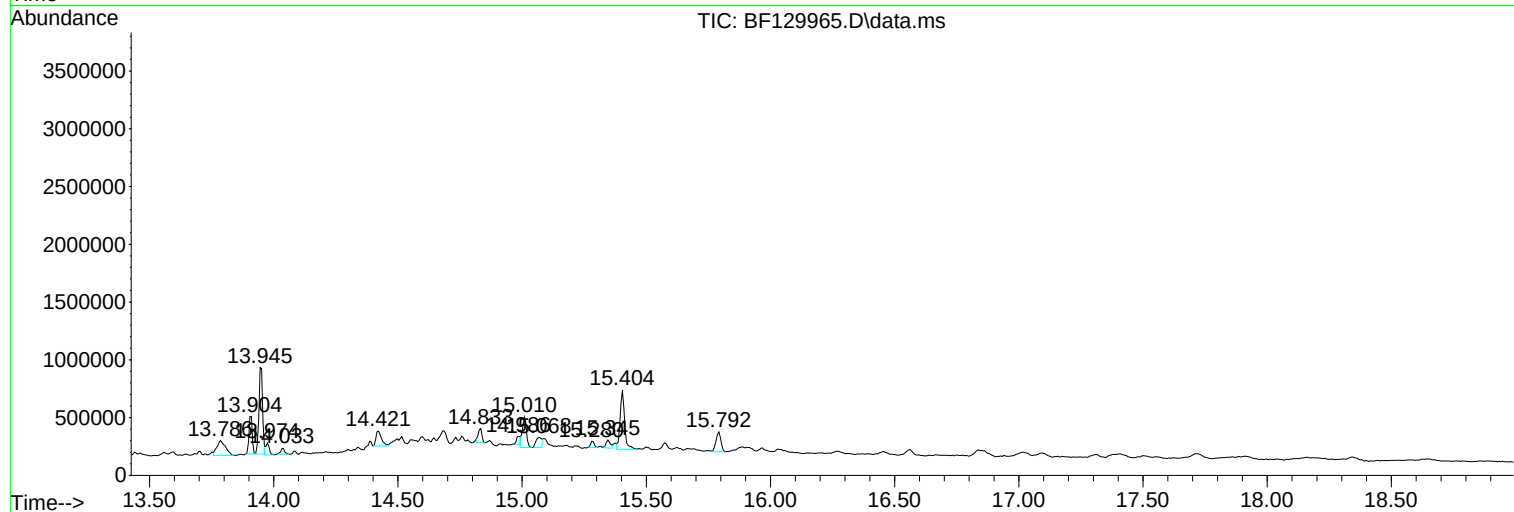
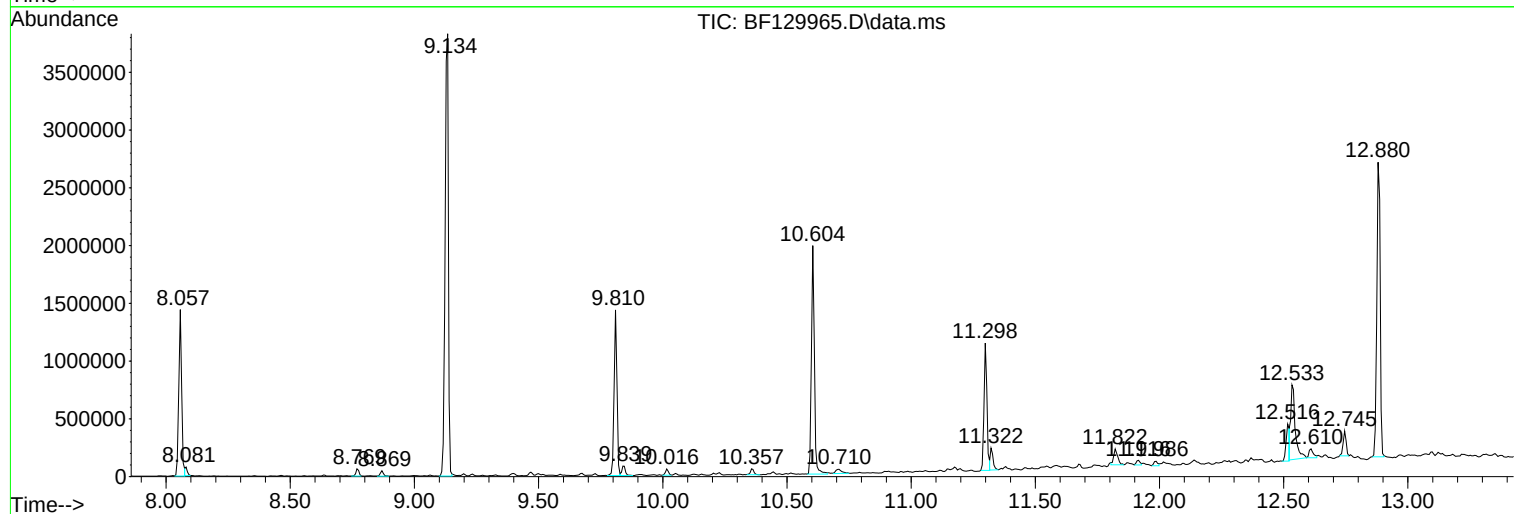
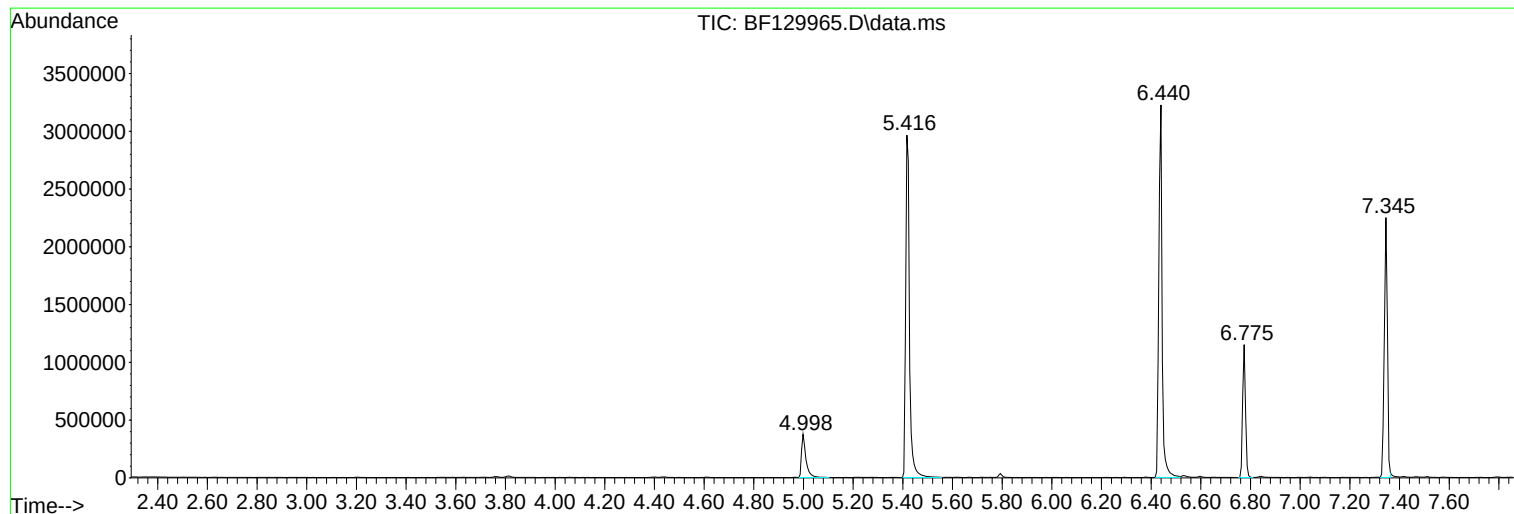
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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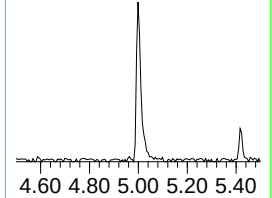
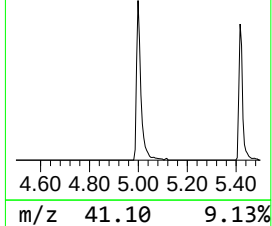
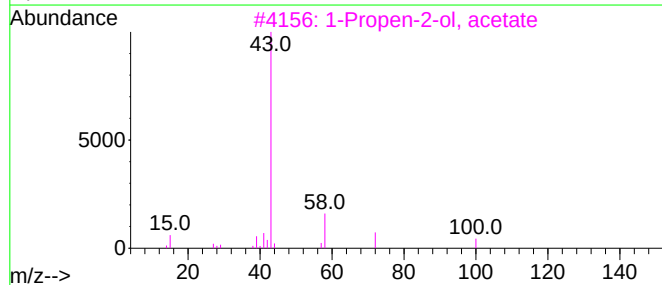
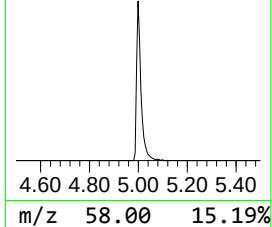
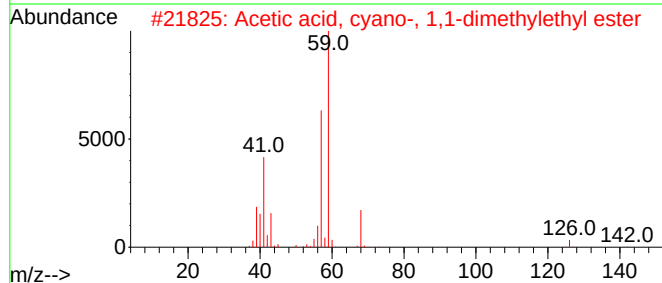
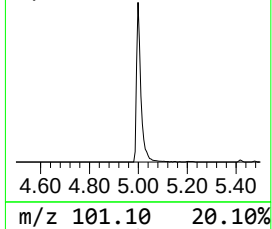
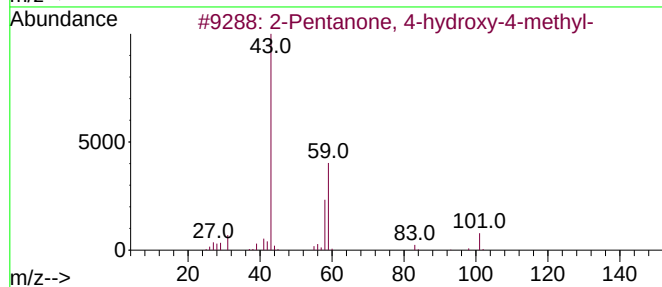
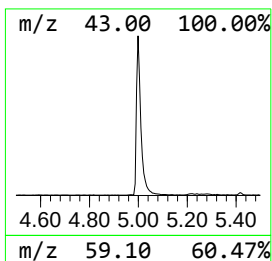
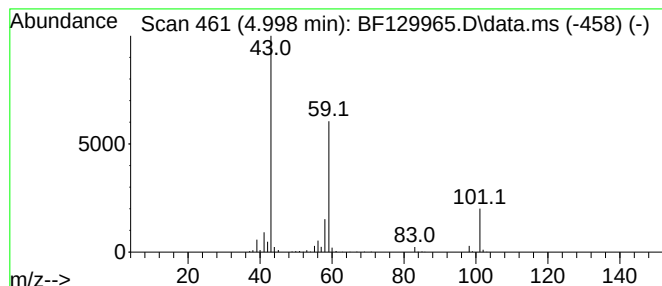
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.998	10.22 ng	467443	1,4-Dichlorobenzene-d4			6.775
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	10
4	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	9
5	Morpholine, 4-methyl-		101	C5H11NO	000109-02-4	9



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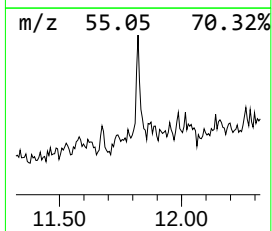
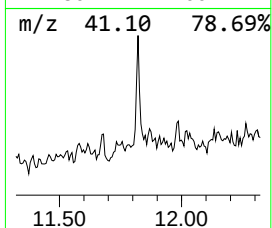
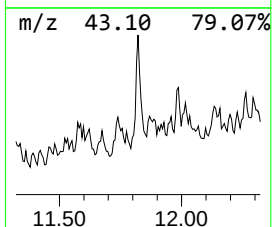
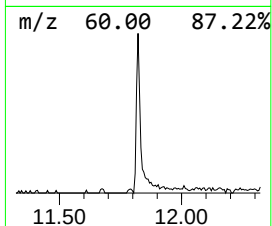
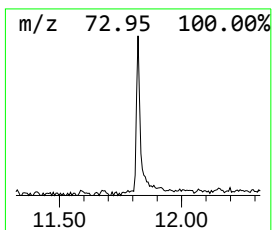
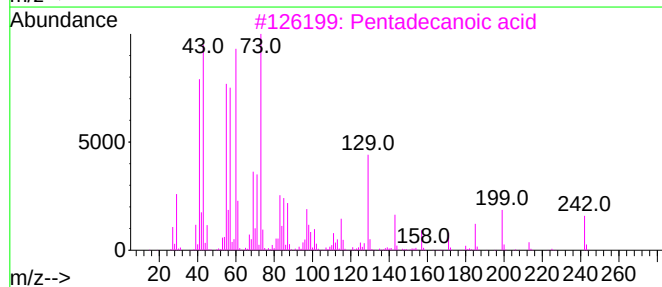
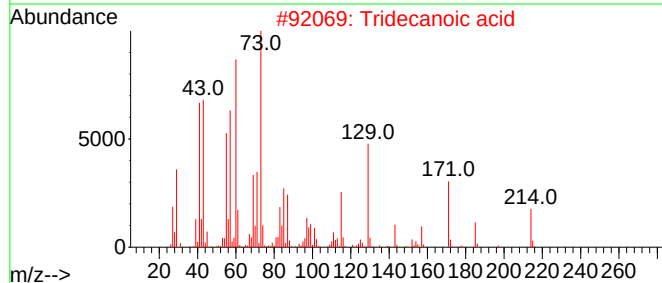
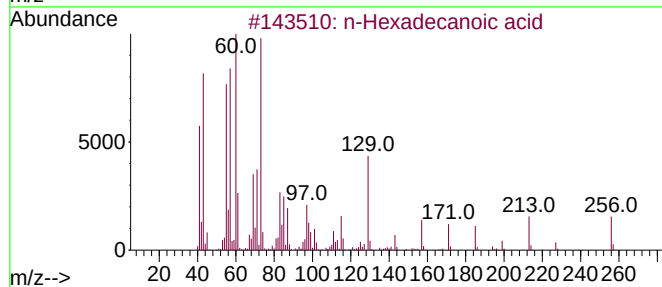
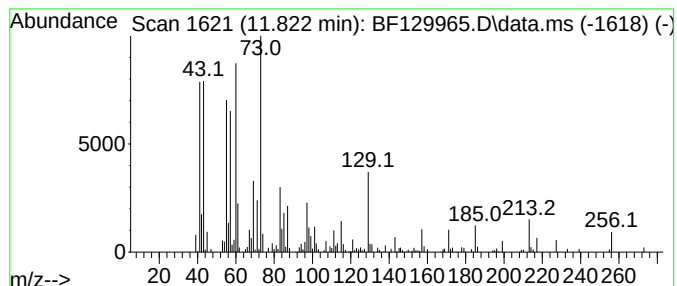
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.822	3.44 ng	154288	Phenanthrene-d10	11.298	
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	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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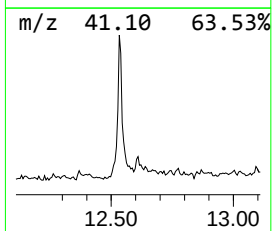
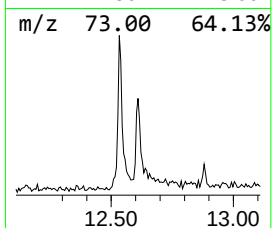
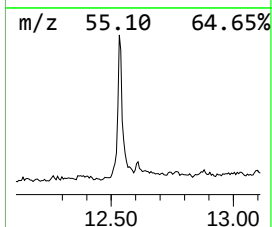
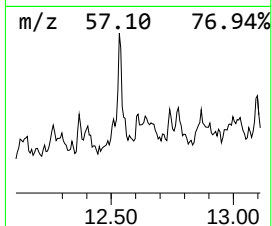
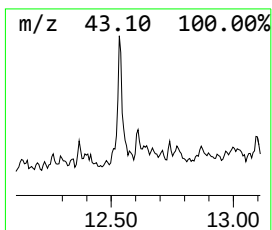
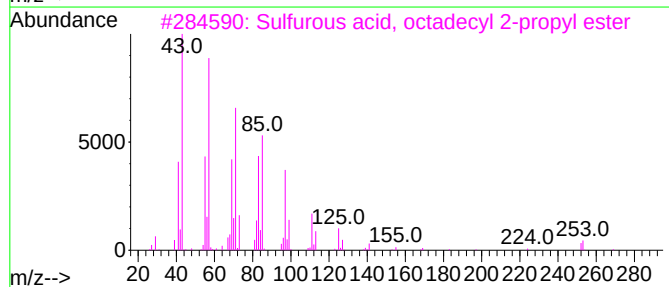
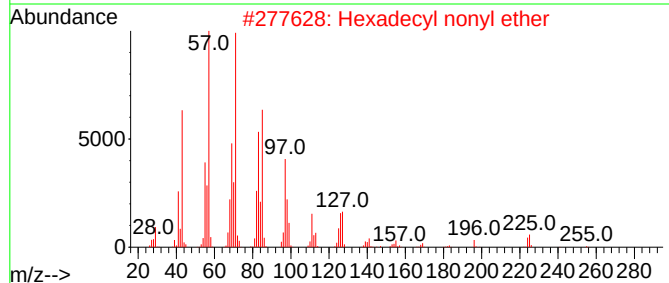
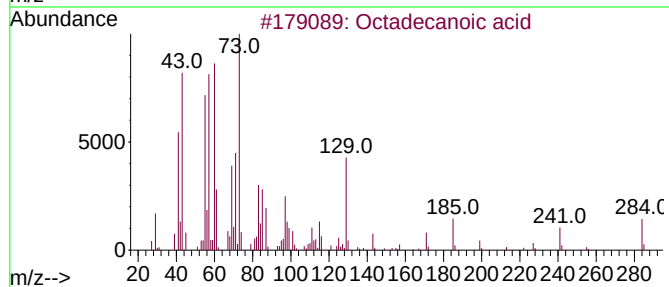
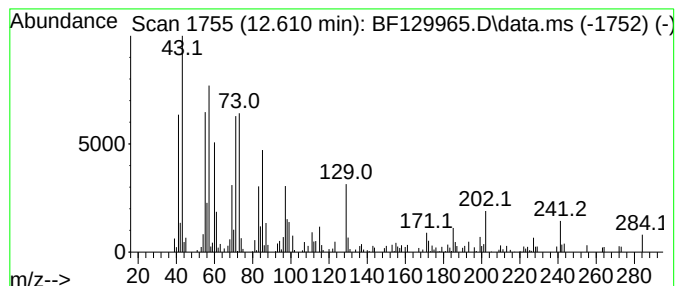
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.610	2.15 ng	96263	Phenanthrene-d10	11.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	90
2			Hexadecyl nonyl ether	368	C25H52O	1000406-37-7	45
3			Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	43
4			Eicosyl isobutyl ether	354	C24H50O	1000406-33-0	43
5			Nonyl tetradecyl ether	340	C23H48O	1000406-37-6	41



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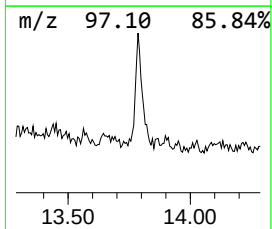
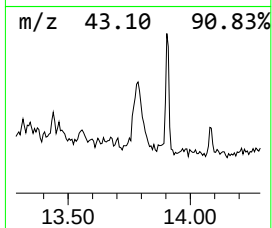
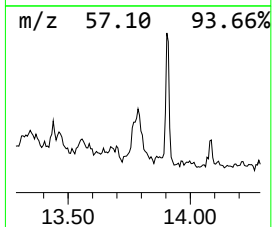
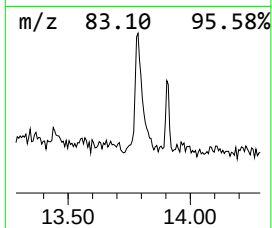
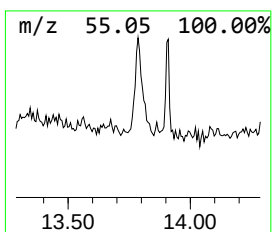
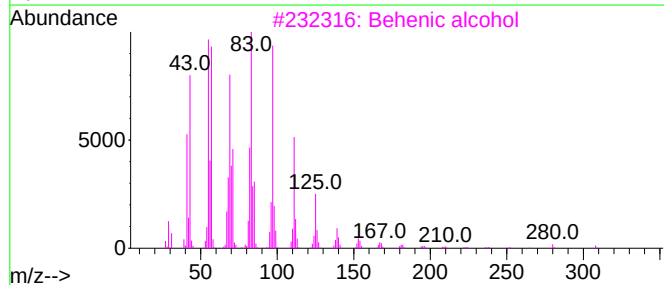
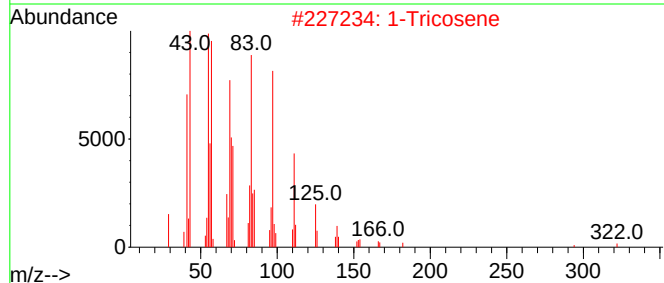
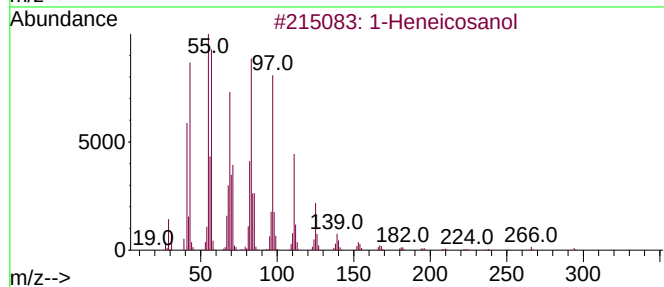
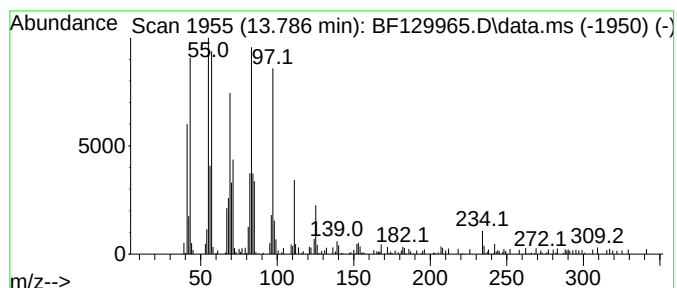
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Heneicosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.786	7.73 ng	303366	Chrysene-d12	13.951	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	1-Tricosene	322	C23H46	018835-32-0	94
3	Behenic alcohol	326	C22H46O	000661-19-8	91
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	90



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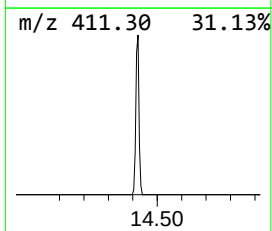
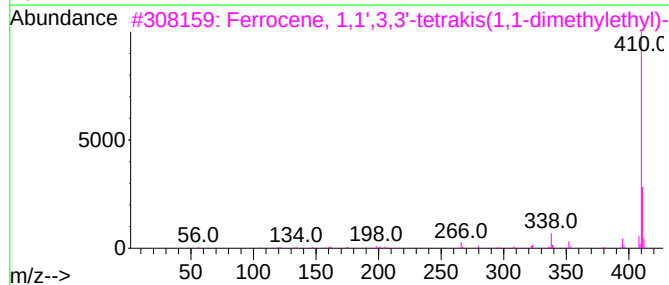
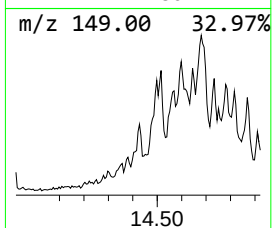
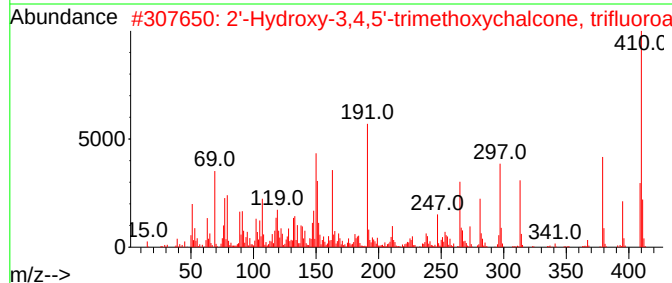
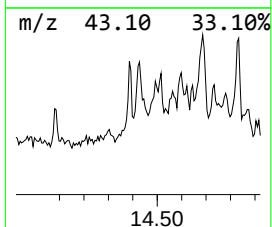
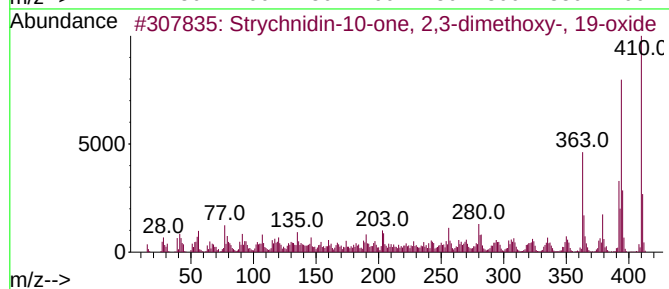
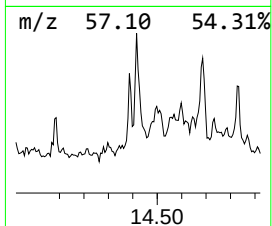
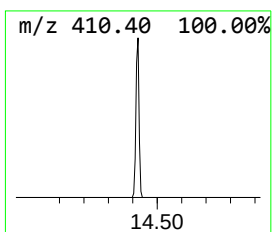
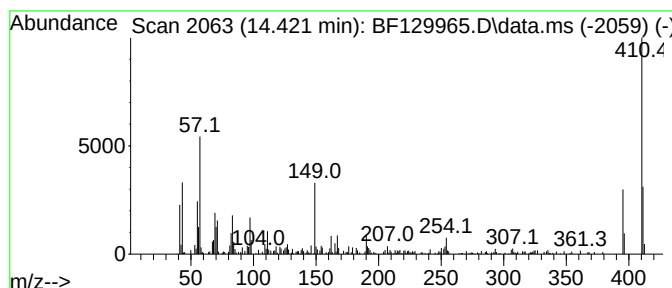
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Strychnidin-10-one, 2,3-dim... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.421	5.11 ng	200674	Chrysene-d12		13.951	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Strychnidin-10-one, 2,3-dimethox...		410	C23H26N2O5	017301-81-4	58
2	2'-Hydroxy-3,4,5'-trimethoxychal...		410	C20H17F3O6	1000449-43-5	55
3	Ferrocene, 1,1',3,3'-tetrakis(1,...		410	C26H42Fe	001317-17-5	38
4	3-Acetyl-1-(3,4-dimethoxyphenyl)...		410	C23H26N2O5	090140-65-1	38
5	6,9-Methanobenzo[h]pentaphene-5,...		410	C27H22O4	057427-50-6	37



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Operator : CG\JU
Sample : N4292-01
Misc :
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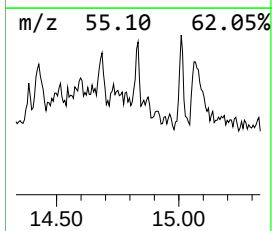
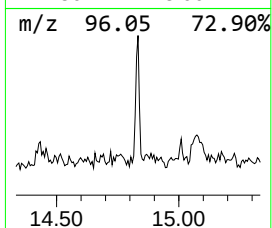
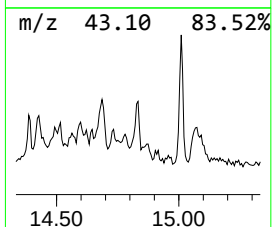
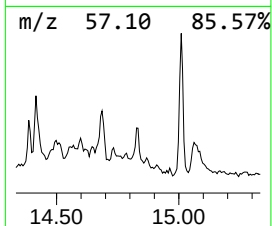
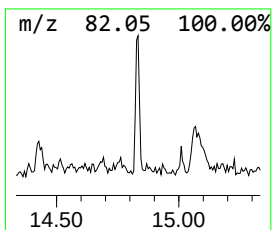
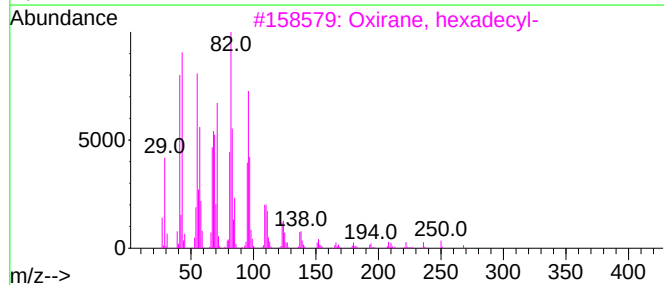
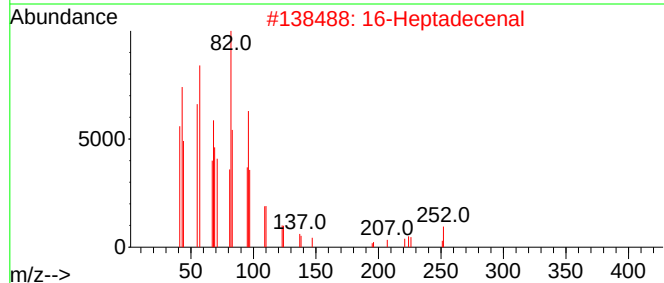
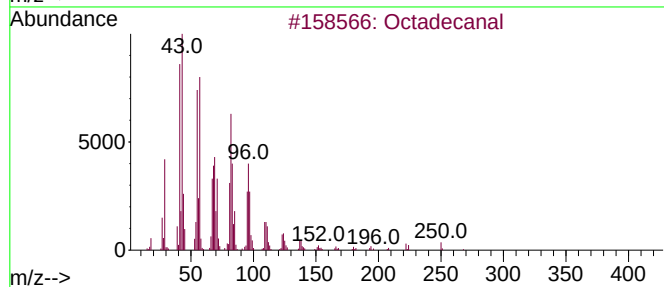
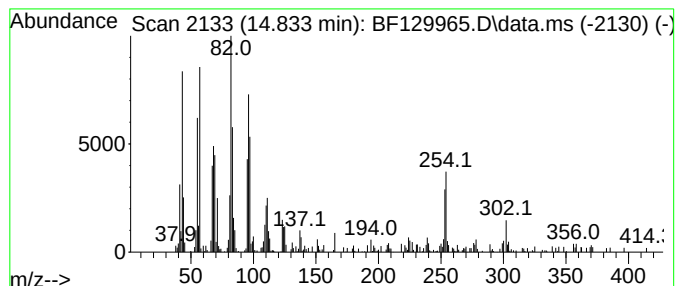
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.833	3.82 ng	122757	Perylene-d12	15.404	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	90
2	16-Heptadecenal	252	C17H32O	1010144-57-9	89
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	81
4	Bicyclo[10.8.0]eicosane, cis-	278	C20H38	1000155-82-2	78
5	Docosanal	324	C22H44O	057402-36-5	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082322\
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Acq On : 23 Aug 2022 22:04
Operator : CG\JU
Sample : N4292-01
Misc :
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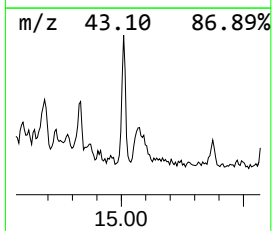
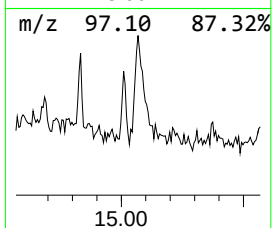
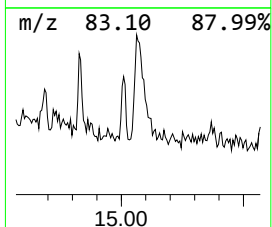
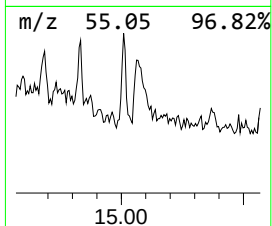
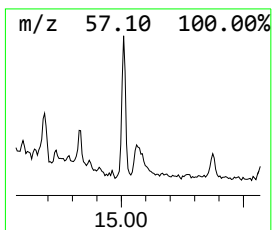
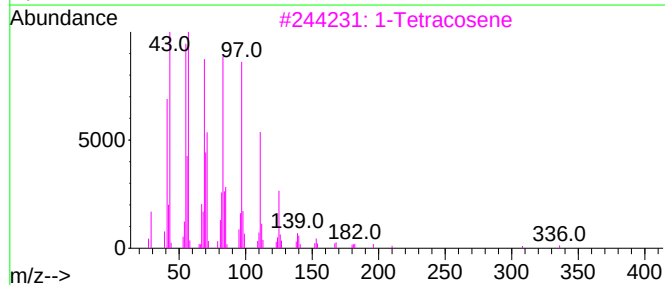
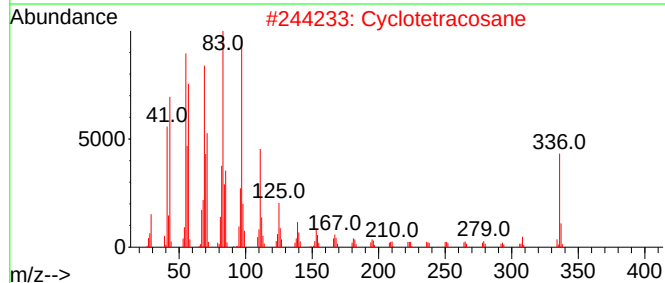
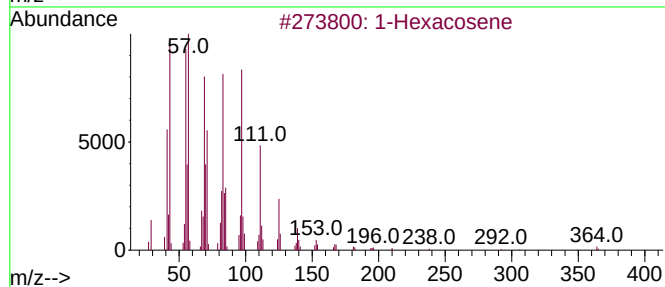
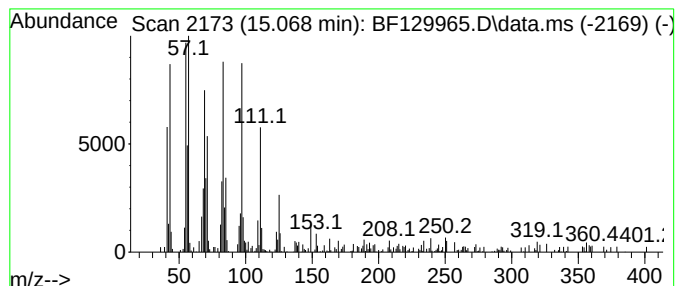
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Hexacosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.068	4.52 ng	145544	Perylene-d12	15.404	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	94
2	Cyclotetracosane	336	C24H48	000297-03-0	93
3	1-Tetracosene	336	C24H48	010192-32-2	89
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	87
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082322\
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Sample : N4292-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

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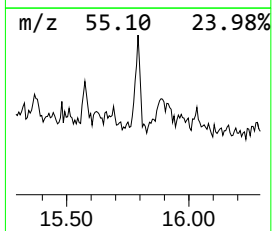
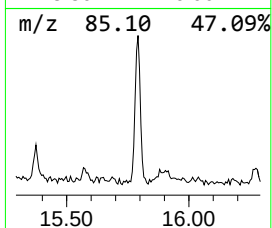
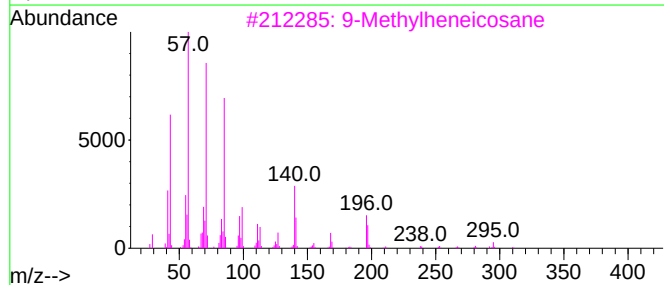
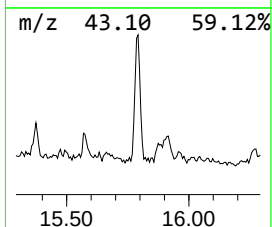
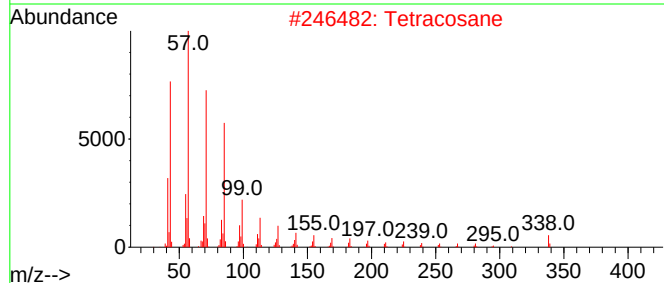
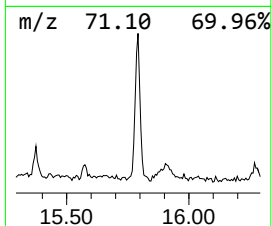
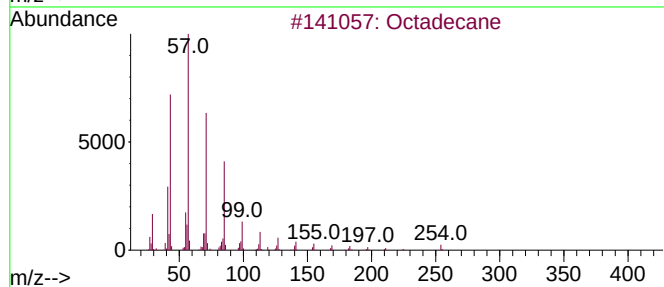
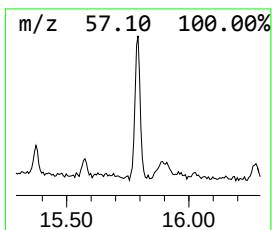
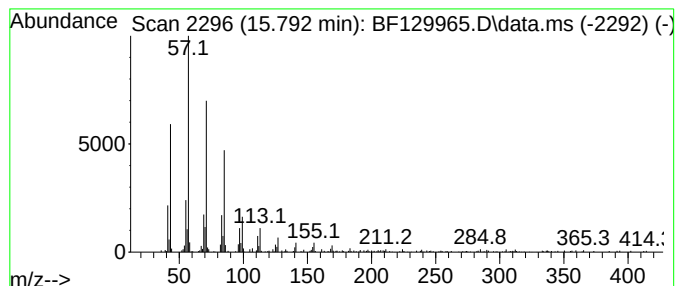
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.792	7.15 ng	230149	Perylene-d12	15.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	95
2			Tetracosane	338	C24H50	000646-31-1	95
3			9-Methylheneicosane	310	C22H46	070475-51-3	91
4			Docosane, 2,21-dimethyl-	338	C24H50	077536-31-3	90
5			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	87



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Acq On : 23 Aug 2022 22:04
Operator : CG\JU
Sample : N4292-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-04-082222

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.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
2-Pentanone, 4-...	4.998	10.2	ng	467443	1	6.775	914909	20.0
n-Hexadecanoic ...	11.822	3.4	ng	154288	4	11.298	896635	20.0
Octadecanoic acid	12.610	2.1	ng	96263	4	11.298	896635	20.0
1-Heneicosanol	13.786	7.7	ng	303366	5	13.951	785057	20.0
Strychnidin-10-...	14.421	5.1	ng	200674	5	13.951	785057	20.0
Octadecanal	14.833	3.8	ng	122757	6	15.404	643360	20.0
1-Hexacosene	15.068	4.5	ng	145544	6	15.404	643360	20.0
Octadecane	15.792	7.2	ng	230149	6	15.404	643360	20.0