

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042723\
 Data File : BF133103.D
 Acq On : 27 Apr 2023 16:52
 Operator : CG\JU
 Sample : 02503-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TR-305A-COMP-01

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: BF133103.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.928	479	483	492	rVB	318656	401974	8.14%	1.137%
2	5.351	549	555	558	rBV	3656399	3871009	78.38%	10.953%
3	6.375	723	729	732	rBV	3875914	4010378	81.20%	11.348%
4	6.734	786	790	793	rBV	1477723	1130167	22.88%	3.198%
5	7.298	880	886	889	rBV	2837623	2562349	51.88%	7.250%
6	8.016	1004	1008	1012	rBV	1885744	1562167	31.63%	4.420%
7	9.092	1186	1191	1195	rBV	5007839	4668631	94.53%	13.210%
8	9.769	1302	1306	1309	rBV	2250533	1772660	35.89%	5.016%
9	10.480	1424	1427	1431	rVB	680923	508007	10.29%	1.437%
10	10.557	1435	1440	1443	rBV	3268623	2859347	57.90%	8.091%
11	10.786	1476	1479	1487	rVB	122324	98223	1.99%	0.278%
12	11.251	1554	1558	1561	rBV	2339273	1861673	37.70%	5.268%
13	11.322	1567	1570	1573	rVB	76037	60949	1.23%	0.172%
14	11.786	1645	1649	1659	rBV	539800	539601	10.93%	1.527%
15	12.569	1779	1782	1791	rBV	83928	107941	2.19%	0.305%
16	12.839	1823	1828	1831	rBV	5305011	4938615	100.00%	13.974%
17	13.851	1987	2000	2001	rBV4	92962	270675	5.48%	0.766%
18	13.886	2001	2006	2009	rVB	1555408	1561214	31.61%	4.418%
19	13.980	2017	2022	2030	rVB	101779	128890	2.61%	0.365%
20	14.368	2084	2088	2093	rBV	46630	52900	1.07%	0.150%
21	14.739	2148	2151	2155	rBV	142490	134845	2.73%	0.382%
22	14.992	2191	2194	2198	rVB	75017	79692	1.61%	0.225%
23	15.304	2242	2247	2252	rBV2	1066986	1215439	24.61%	3.439%
24	15.357	2252	2256	2260	rVB	94658	119823	2.43%	0.339%
25	15.762	2321	2325	2333	rVB	117843	174777	3.54%	0.495%
26	16.245	2401	2407	2413	rBV2	103623	183894	3.72%	0.520%
27	16.804	2496	2502	2509	rVB	82604	164754	3.34%	0.466%
28	17.462	2608	2614	2624	rVB	74677	171257	3.47%	0.485%
29	18.239	2741	2746	2758	rVB4	46720	129562	2.62%	0.367%

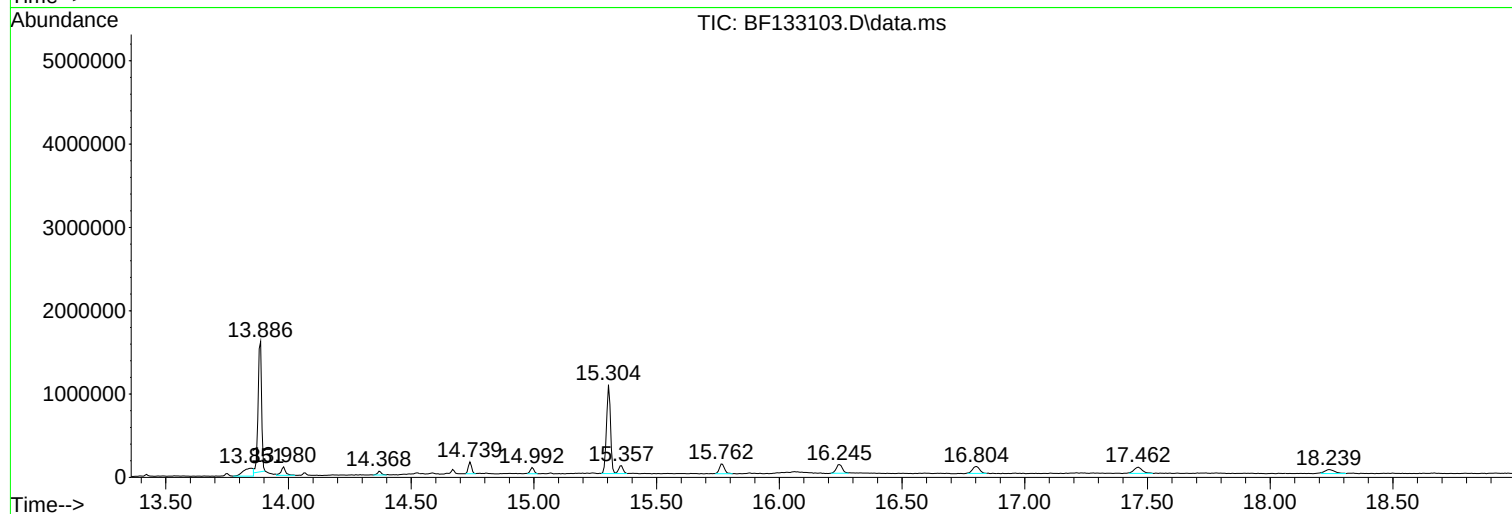
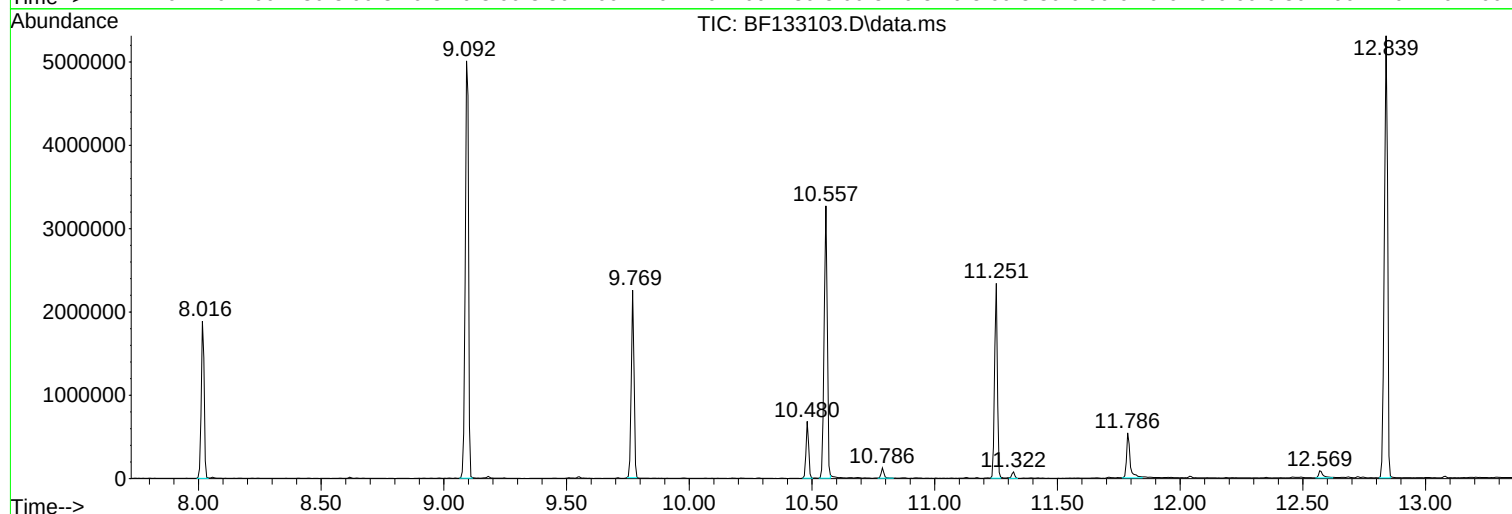
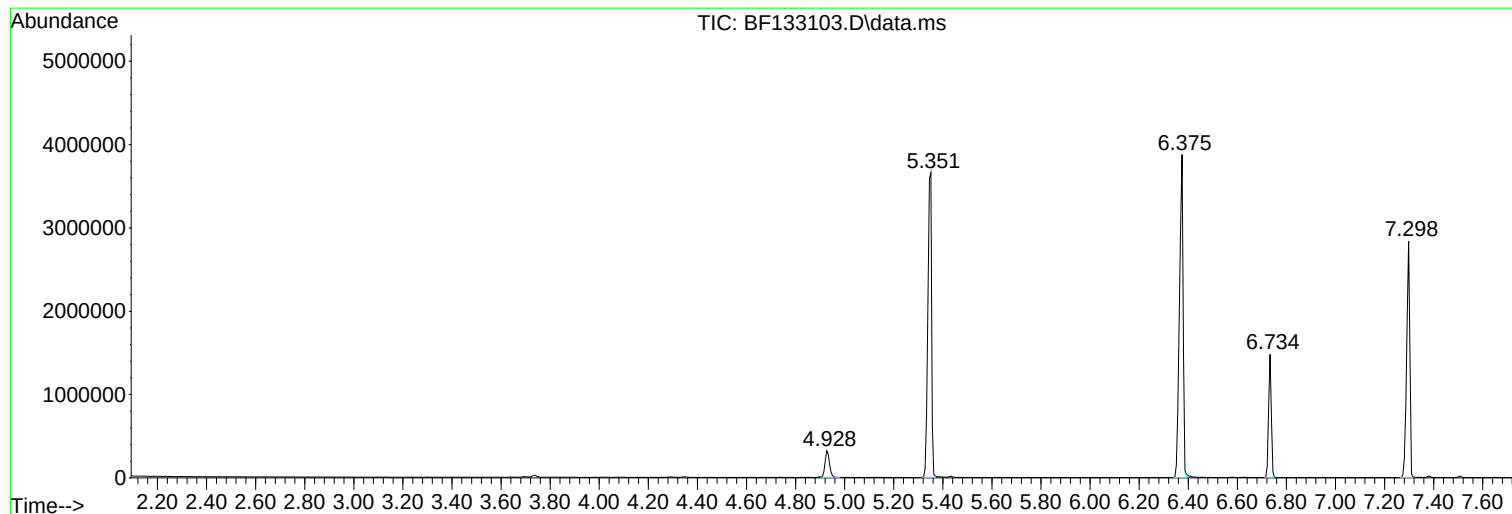
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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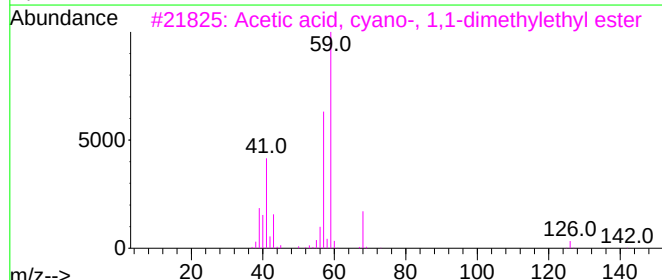
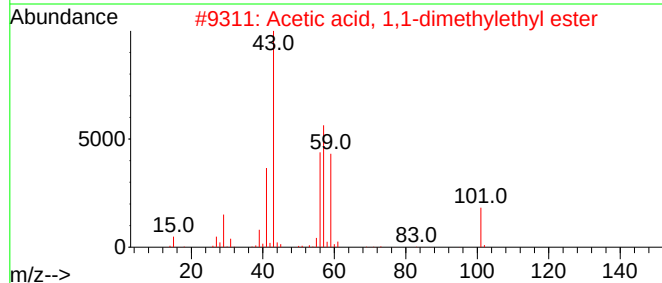
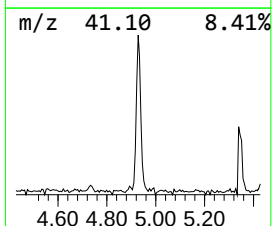
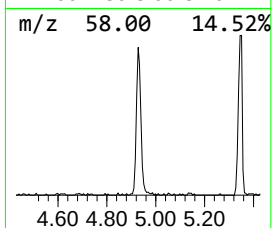
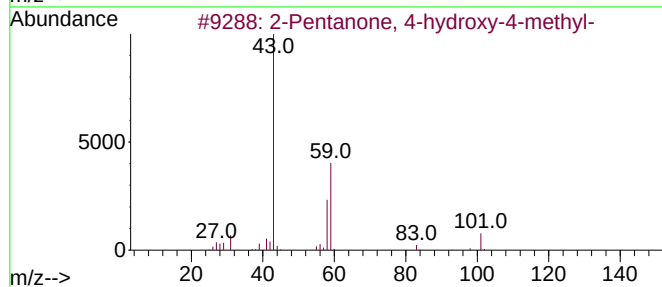
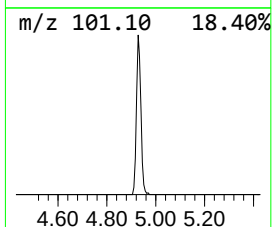
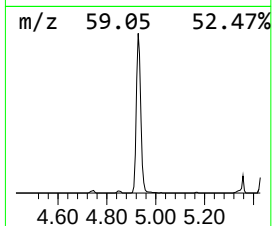
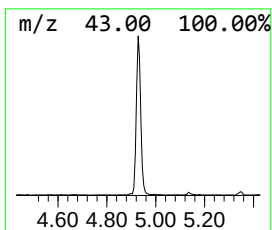
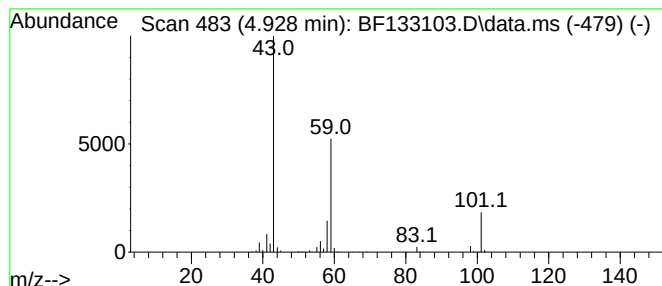
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.928	7.11 ng	401974	1,4-Dichlorobenzene-d4	6.734

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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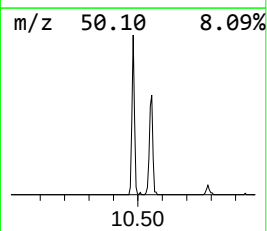
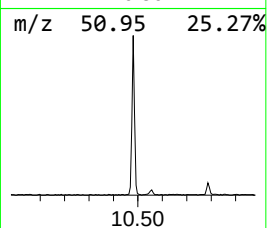
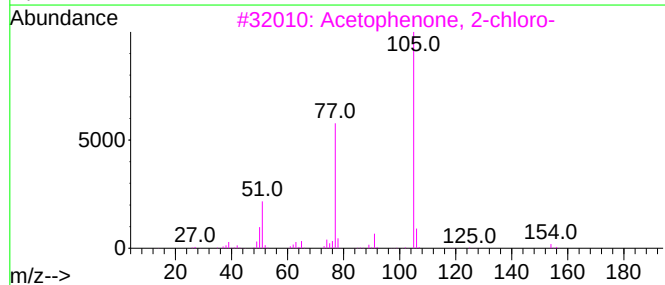
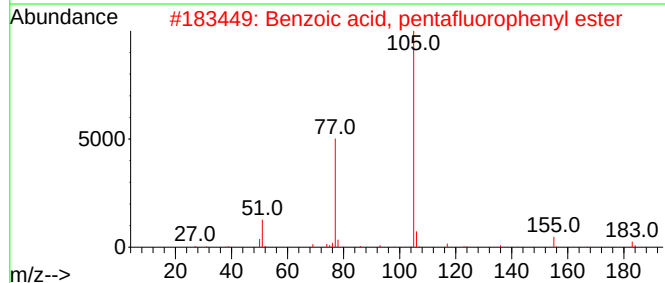
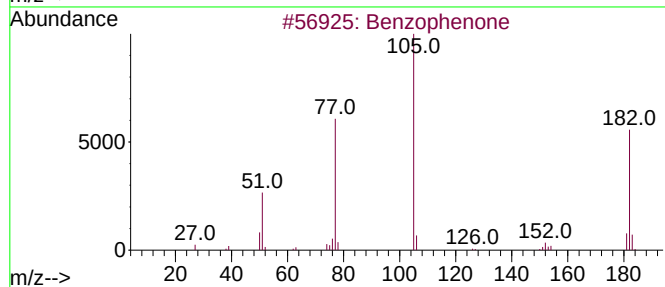
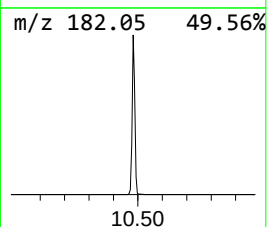
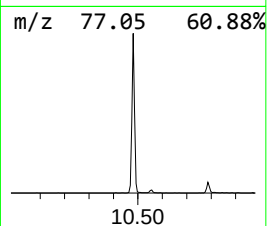
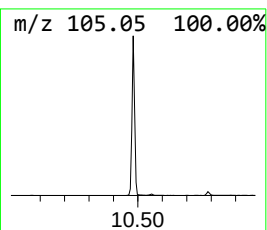
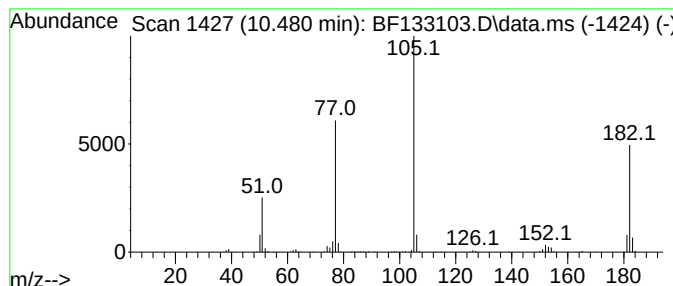
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.480	5.73 ng	508007	Acenaphthene-d10	9.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	50
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
5			Vinyl benzoate	148	C9H8O2	000769-78-8	47



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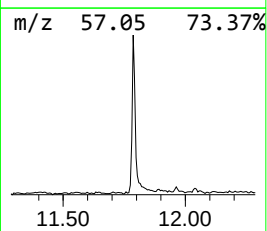
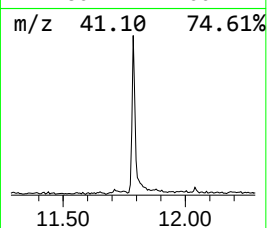
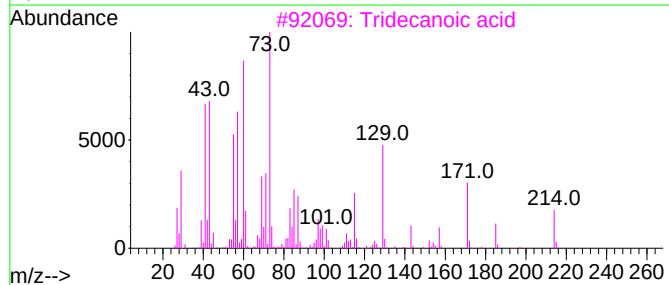
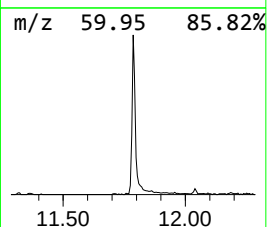
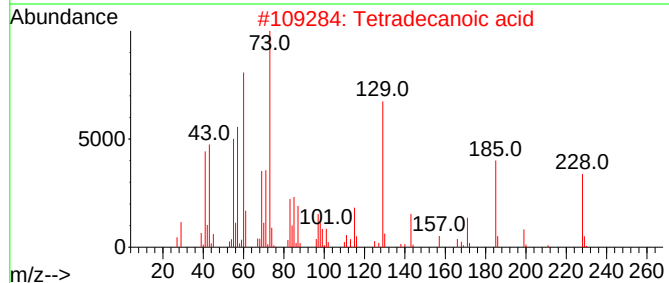
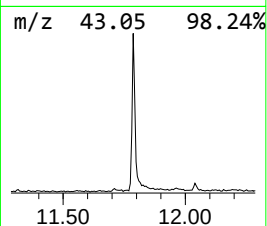
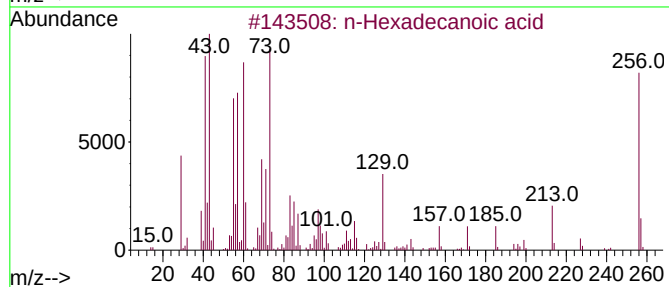
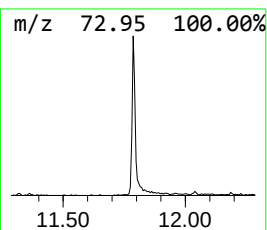
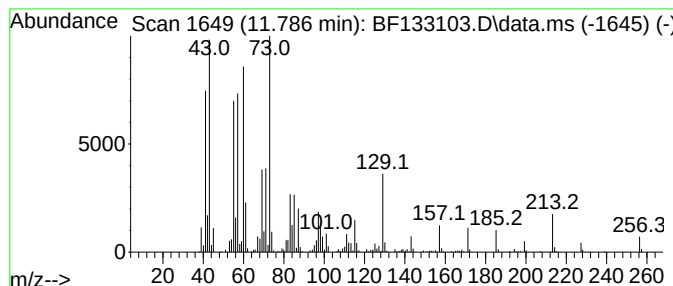
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.786	5.80 ng	539601	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	95
3			Tridecanoic acid	214	C13H26O2	000638-53-9	95
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60



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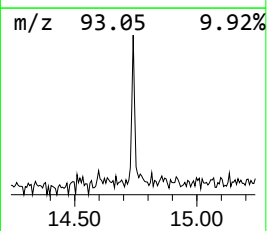
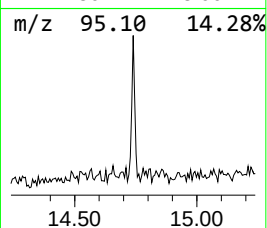
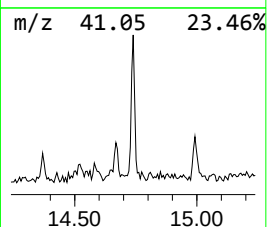
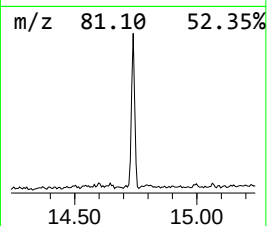
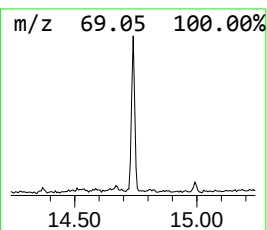
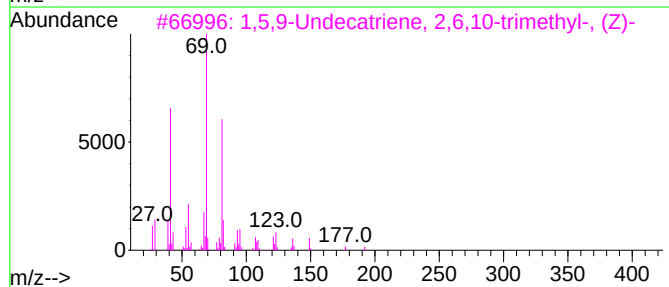
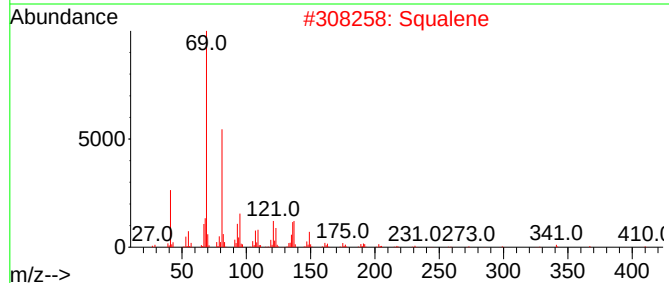
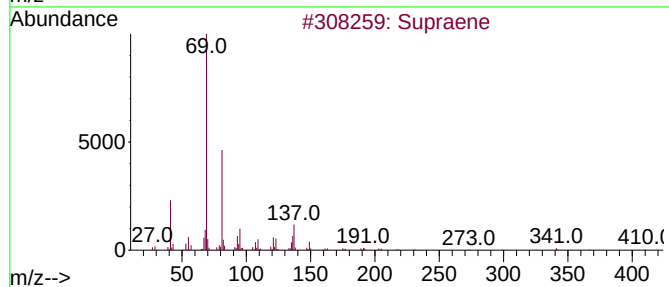
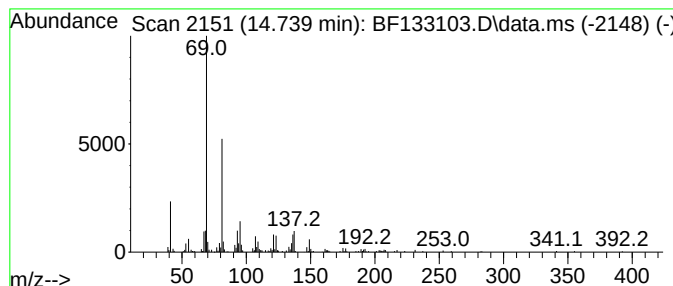
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Supraene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.739	2.22 ng	134845	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			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	87
4			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
5			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	83



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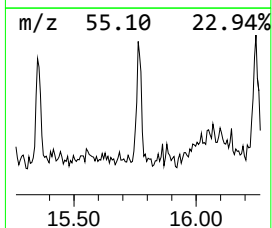
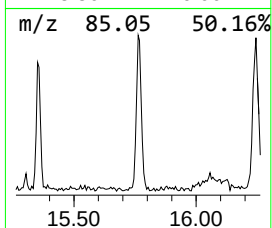
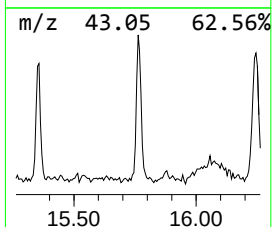
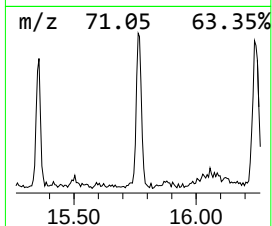
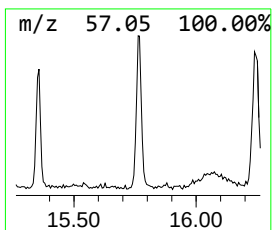
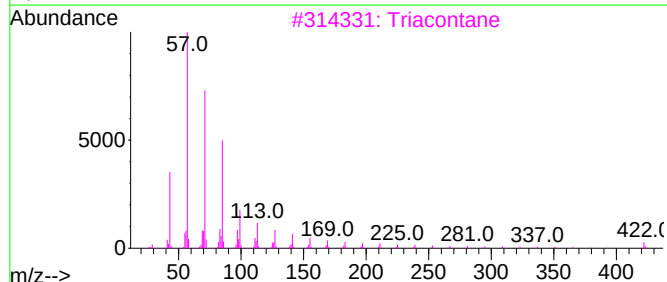
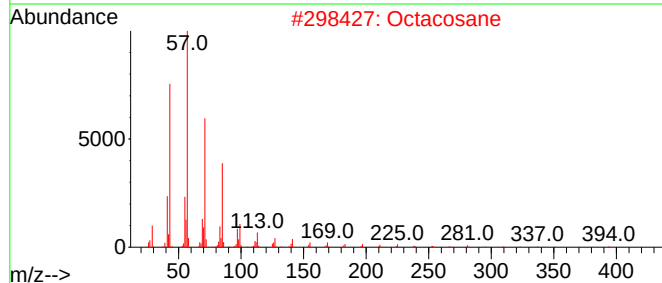
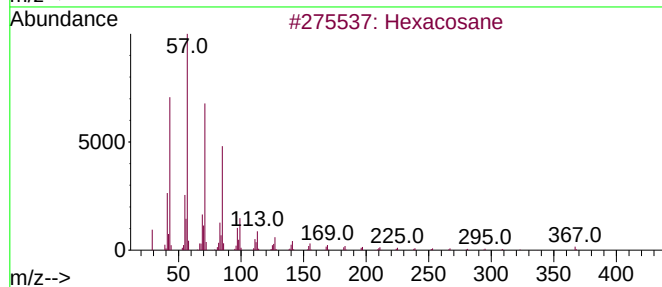
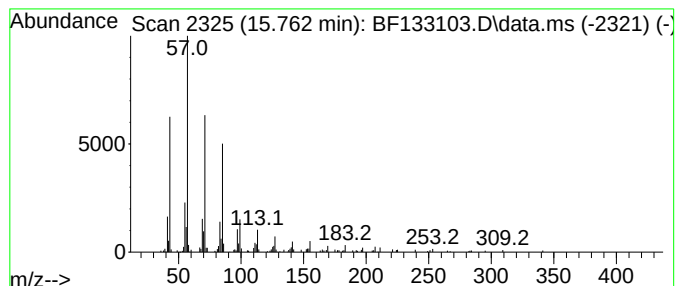
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.762	2.88 ng	174777	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			Octacosane	394	C28H58	000630-02-4	91
3			Triacontane	422	C30H62	000638-68-6	91
4			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	91
5			Tetracosane	338	C24H50	000646-31-1	91



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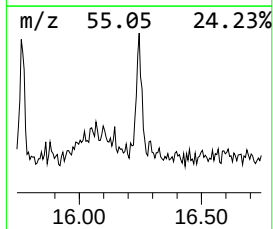
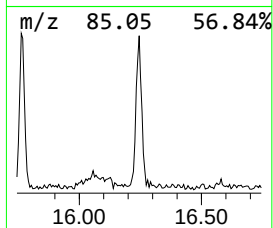
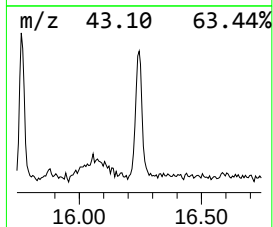
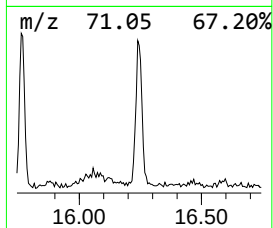
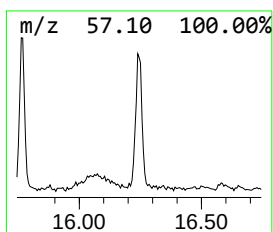
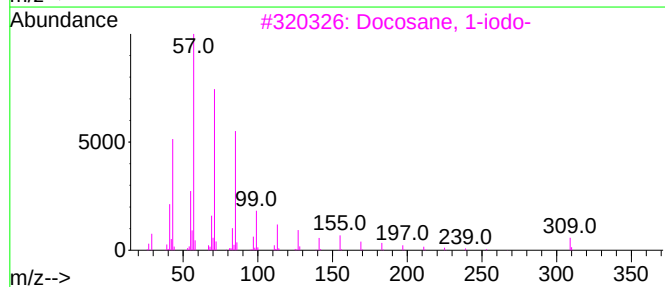
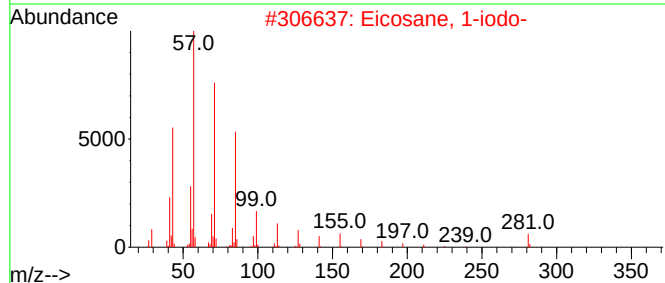
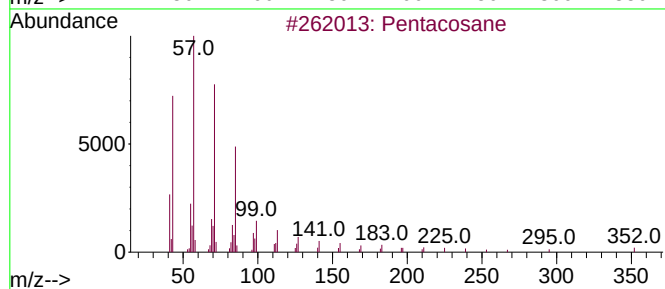
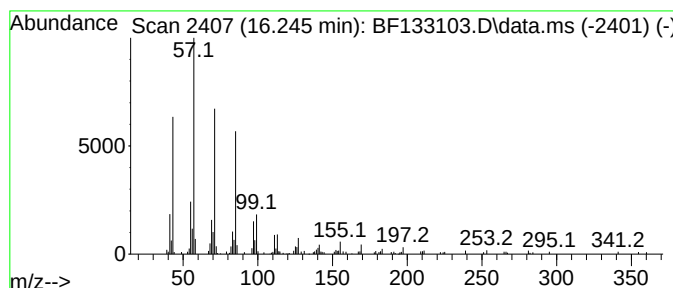
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.245	3.03 ng	183894	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	91
2			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	90
3			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	90
4			Heptadecane	240	C17H36	000629-78-7	87
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042723\
Data File : BF133103.D
Acq On : 27 Apr 2023 16:52
Operator : CG\JU
Sample : 02503-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-305A-COMP-01

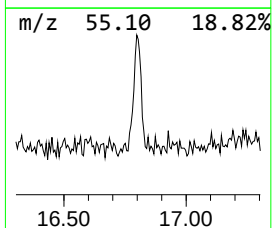
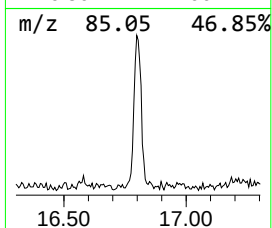
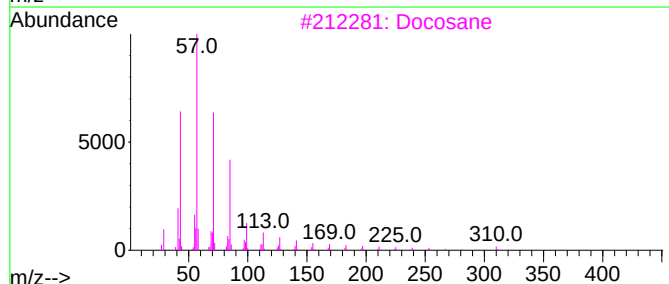
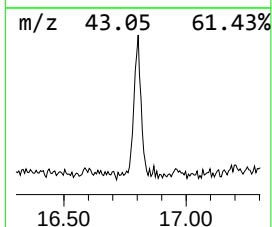
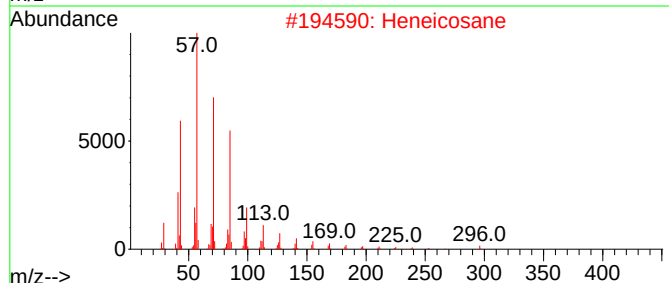
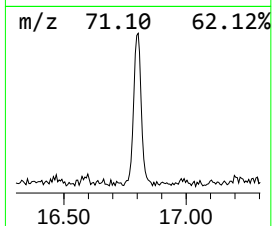
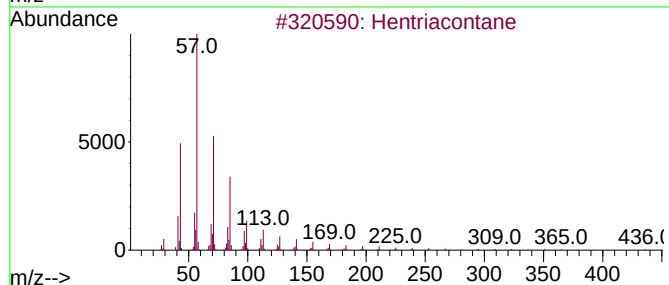
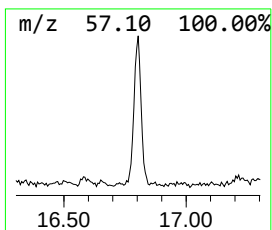
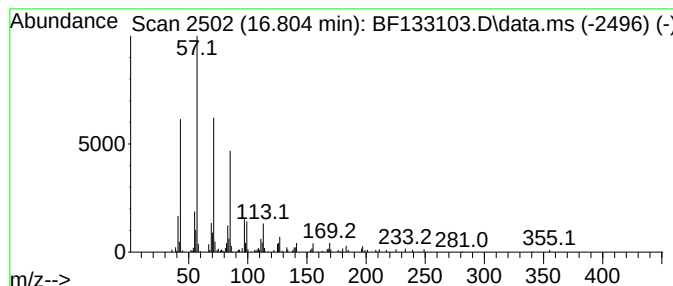
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hentriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.804	2.71 ng	164754	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	90
2			Heneicosane	296	C21H44	000629-94-7	90
3			Docosane	310	C22H46	000629-97-0	90
4			Octadecane	254	C18H38	000593-45-3	90
5			Pentacosane	352	C25H52	000629-99-2	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042723\
Data File : BF133103.D
Acq On : 27 Apr 2023 16:52
Operator : CG\JU
Sample : 02503-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-305A-COMP-01

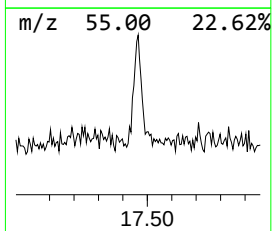
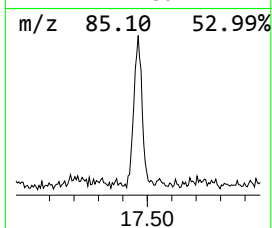
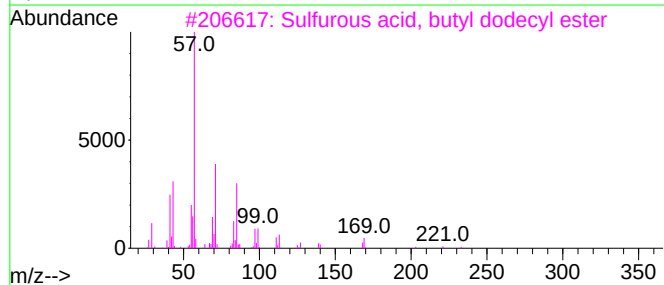
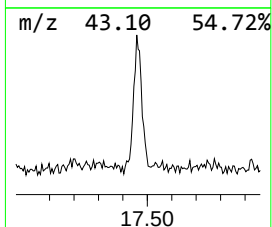
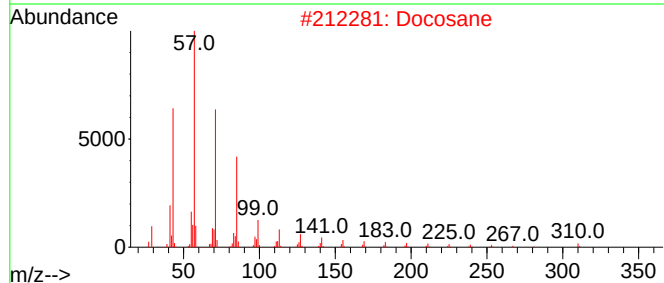
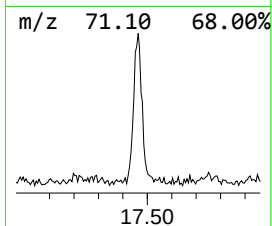
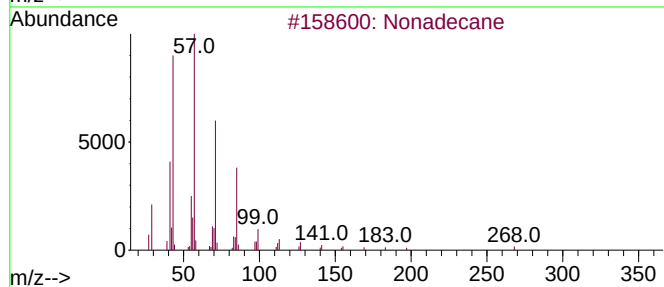
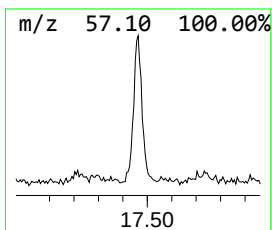
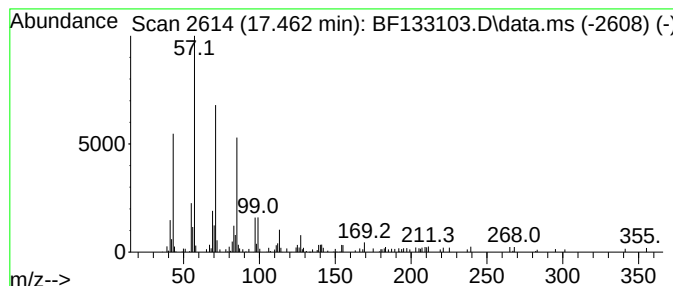
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.462	2.82 ng	171257	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	93
2			Docosane	310	C22H46	000629-97-0	87
3			Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	87
4			Heneicosane	296	C21H44	000629-94-7	87
5			Octacosane	394	C28H58	000630-02-4	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042723\
Data File : BF133103.D
Acq On : 27 Apr 2023 16:52
Operator : CG\JU
Sample : 02503-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-305A-COMP-01

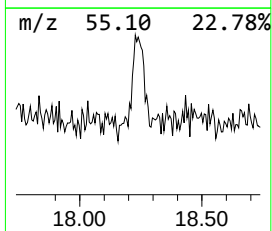
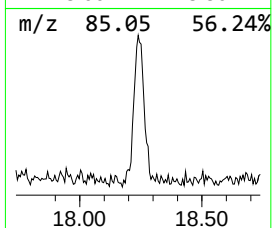
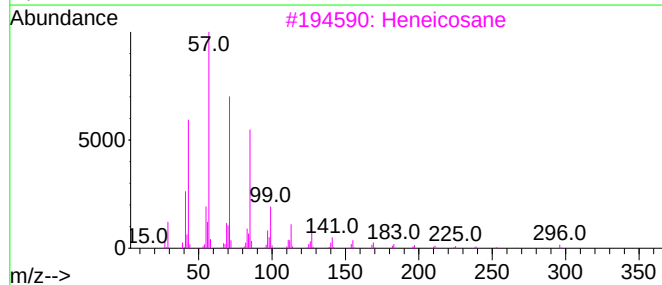
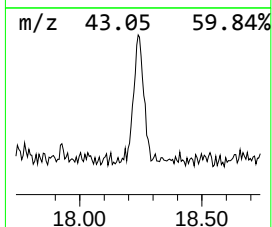
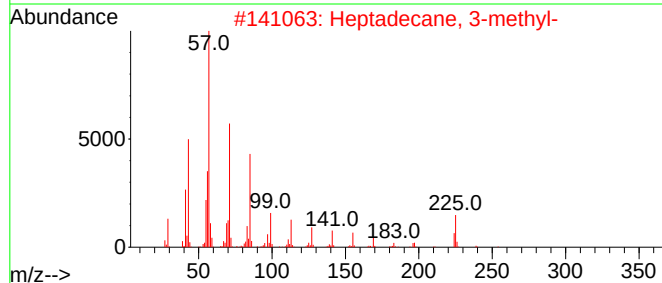
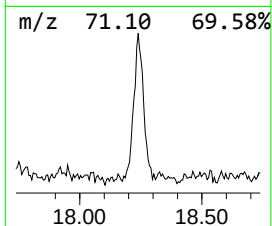
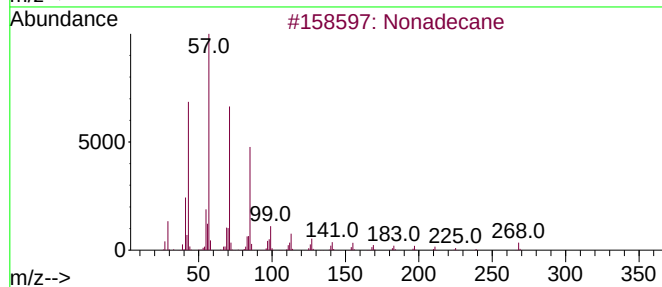
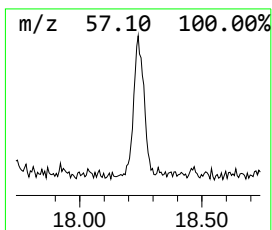
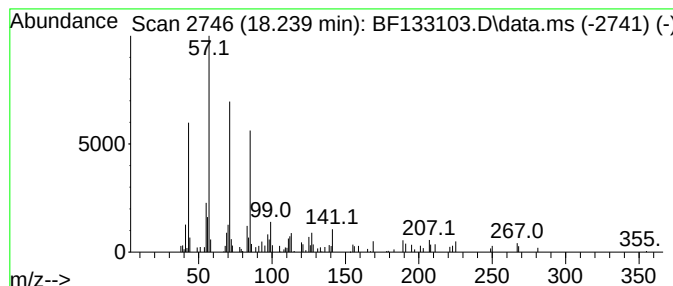
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecane, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.239	2.13 ng	129562	Perylene-d12	15.304

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Nonadecane	268	C19H40	000629-92-5	93
2		Heptadecane, 3-methyl-	254	C18H38	006418-44-6	80
3		Heneicosane	296	C21H44	000629-94-7	74
4		Tetracosane	338	C24H50	000646-31-1	74
5		Heptadecane	240	C17H36	000629-78-7	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042723\
Data File : BF133103.D
Acq On : 27 Apr 2023 16:52
Operator : CG\JU
Sample : 02503-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-305A-COMP-01

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
2-Pentanone, 4-...	4.928	7.1	ng	401974	1	6.734	1130170	20.0
Benzophenone	10.480	5.7	ng	508007	3	9.769	1772660	20.0
n-Hexadecanoic ...	11.786	5.8	ng	539601	4	11.251	1861670	20.0
Supraene	14.739	2.2	ng	134845	6	15.304	1215440	20.0
Hexacosane	15.762	2.9	ng	174777	6	15.304	1215440	20.0
Pentacosane	16.245	3.0	ng	183894	6	15.304	1215440	20.0
Hentriacontane	16.804	2.7	ng	164754	6	15.304	1215440	20.0
Nonadecane	17.462	2.8	ng	171257	6	15.304	1215440	20.0
Heptadecane, 3-...	18.239	2.1	ng	129562	6	15.304	1215440	20.0