

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041823\
 Data File : BF132901.D
 Acq On : 18 Apr 2023 15:23
 Operator : CG\JU
 Sample : 02362-03
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HW-STONE-2-0414

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-BF041723.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132901.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.963	480	489	499	rBV	1855169	2702004	25.98%	4.007%
2	5.369	552	558	561	rBV	6808397	7818877	75.19%	11.595%
3	5.775	623	627	631	rVB	203580	193626	1.86%	0.287%
4	6.393	726	732	735	rBV	6951645	7959581	76.54%	11.804%
5	6.763	791	795	798	rBV	1923540	1462897	14.07%	2.169%
6	7.328	886	891	894	rBV	5408755	5079650	48.85%	7.533%
7	8.045	1010	1013	1016	rBV	2672476	1986899	19.11%	2.946%
8	9.128	1192	1197	1200	rBV	9943951	8683038	83.50%	12.876%
9	9.798	1308	1311	1315	rVB	2710620	2261403	21.75%	3.354%
10	10.516	1428	1433	1436	rBV	225584	188122	1.81%	0.279%
11	10.586	1441	1445	1448	rBV	5794432	5752249	55.31%	8.530%
12	11.280	1560	1563	1567	rVB	2969087	2368076	22.77%	3.512%
13	11.816	1640	1654	1659	rBV	537068	863795	8.31%	1.281%
14	12.286	1726	1734	1745	rBV4	53646	194979	1.87%	0.289%
15	12.604	1782	1788	1801	rVB	918227	1513680	14.56%	2.245%
16	12.874	1829	1834	1837	rBV	9642765	10399136	100.00%	15.421%
17	13.286	1896	1904	1912	rBV2	117992	282444	2.72%	0.419%
18	13.786	1984	1989	2004	rBV	387182	727744	7.00%	1.079%
19	13.916	2007	2011	2015	rBV	2622446	2300331	22.12%	3.411%
20	13.980	2017	2022	2026	rBV	143594	222960	2.14%	0.331%
21	14.104	2038	2043	2050	rVB	181149	180986	1.74%	0.268%
22	14.410	2090	2095	2098	rBV	250314	269632	2.59%	0.400%
23	14.527	2111	2115	2119	rBV	122801	211409	2.03%	0.314%
24	14.710	2141	2146	2152	rVB	235964	245768	2.36%	0.364%
25	15.039	2197	2202	2205	rBV	241859	301832	2.90%	0.448%
26	15.074	2205	2208	2213	rVB2	82342	135084	1.30%	0.200%
27	15.345	2237	2254	2260	rBV	1806837	2424260	23.31%	3.595%
28	15.404	2260	2264	2270	rVB2	192497	257673	2.48%	0.382%
29	15.698	2309	2314	2326	rVB3	58159	127835	1.23%	0.190%
30	15.827	2330	2336	2341	rBV	128056	192694	1.85%	0.286%
31	16.310	2413	2418	2427	rVB	70123	125112	1.20%	0.186%

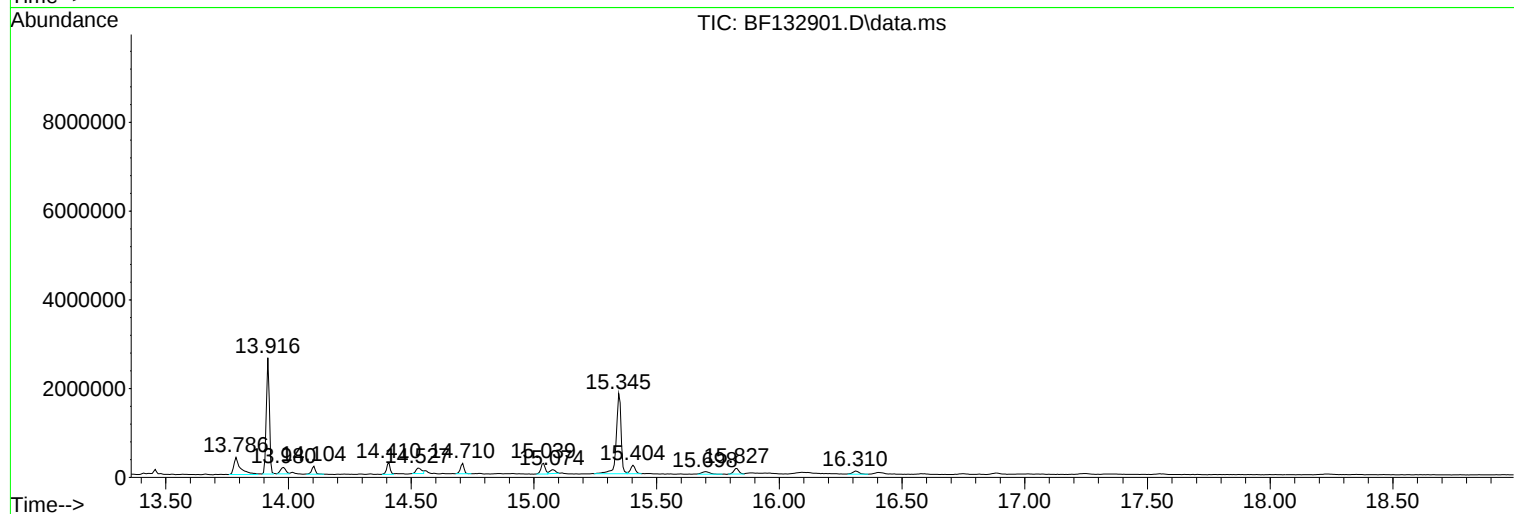
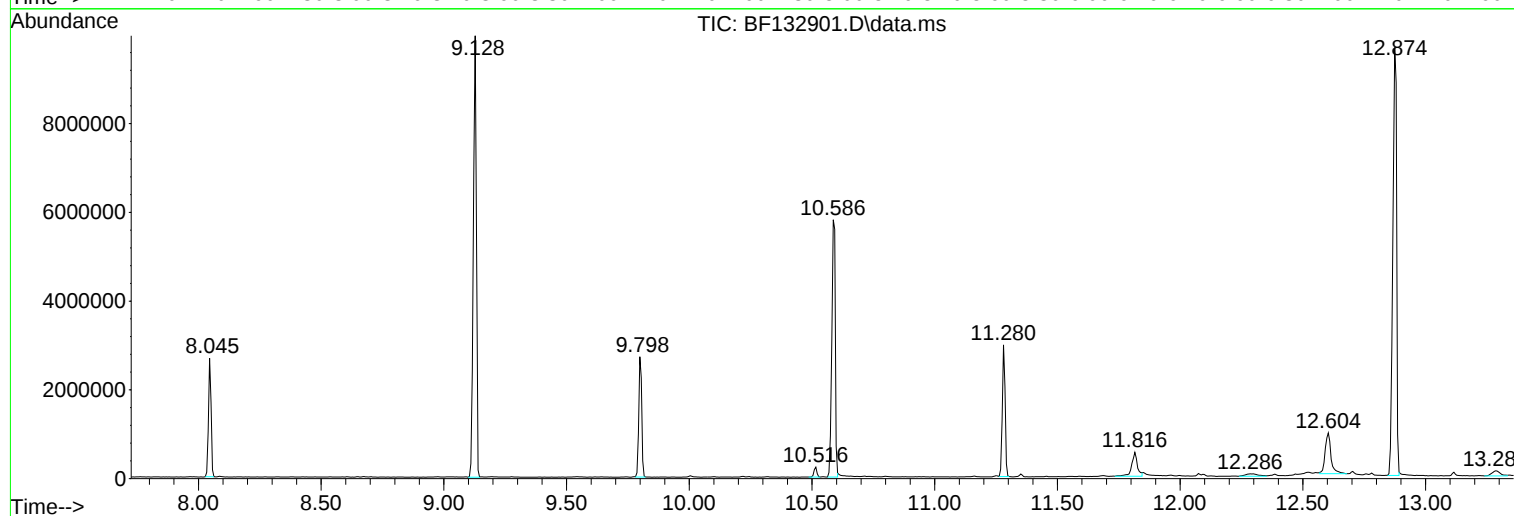
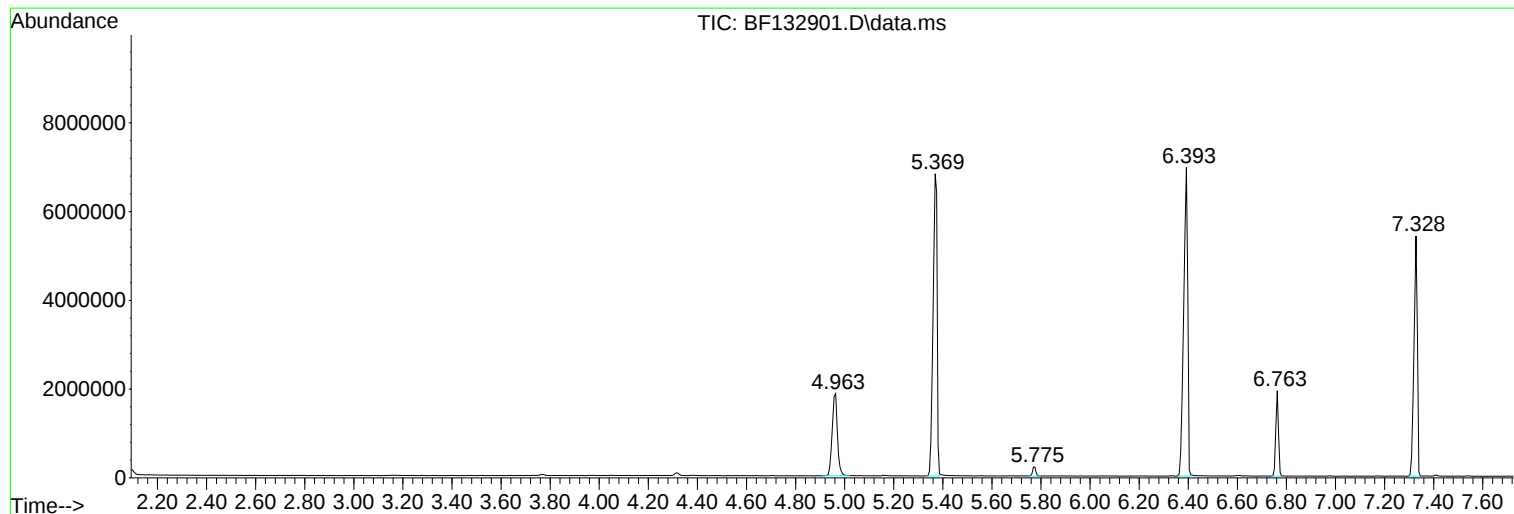
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF041723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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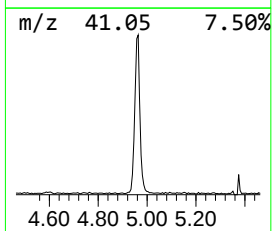
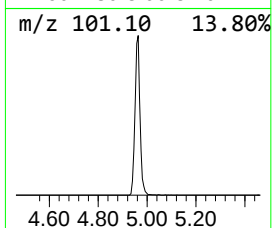
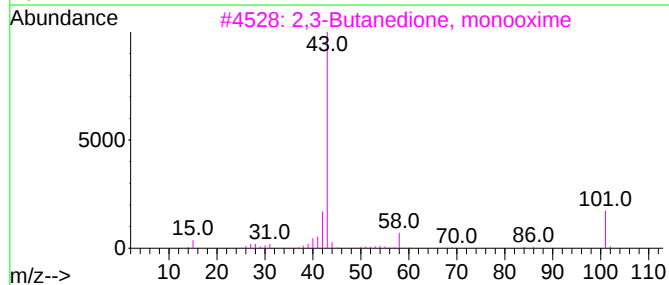
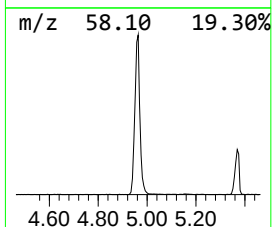
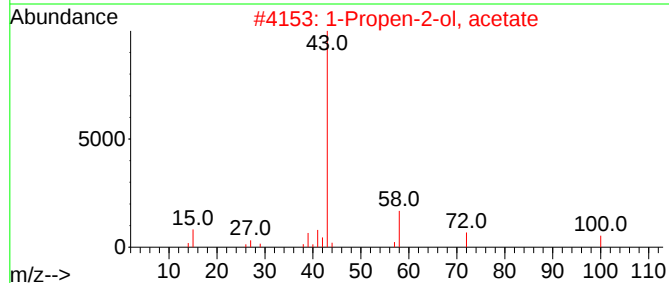
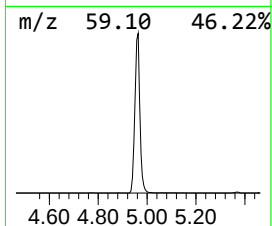
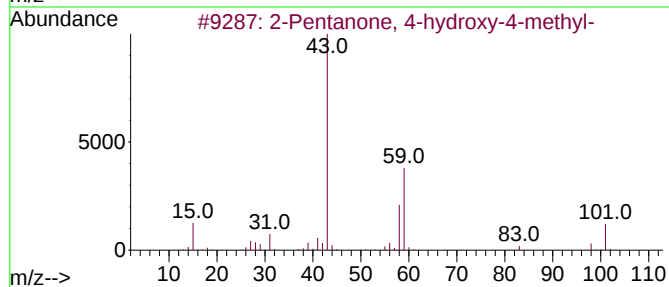
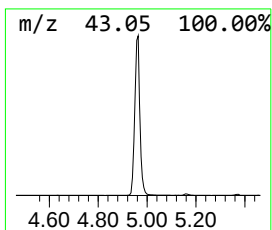
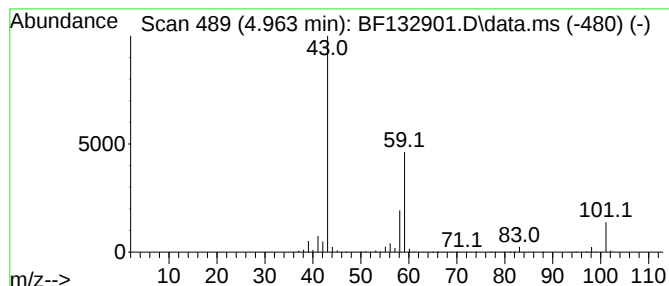
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF041723.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
4.963	36.94 ng	2702000	1,4-Dichlorobenzene-d4			6.763
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	83
2	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	16
3	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	12
4	Acetone		58	C3H6O	000067-64-1	9
5	Acetic acid, 1,1-dimethylethyl e...		116	C6H12O2	000540-88-5	9



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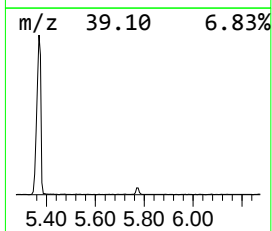
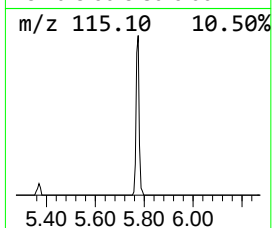
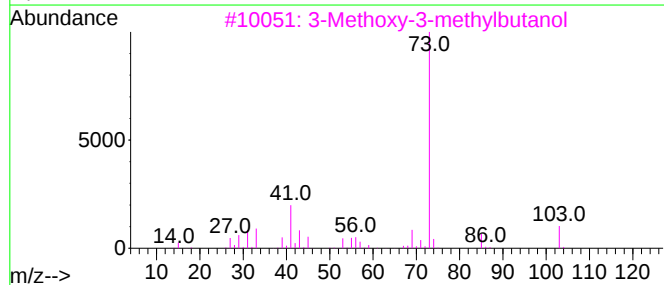
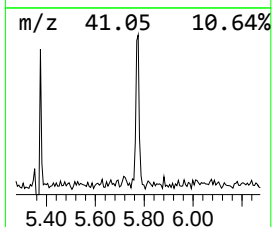
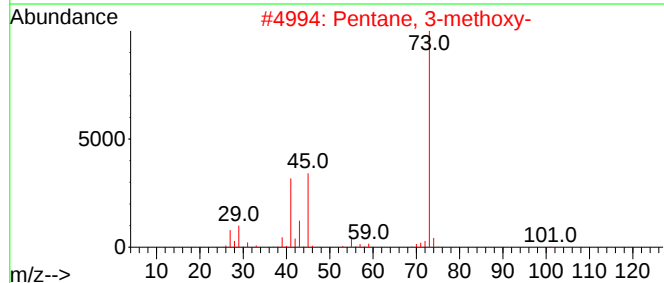
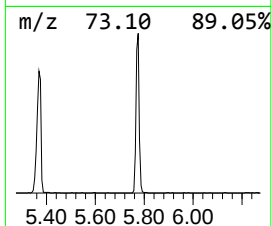
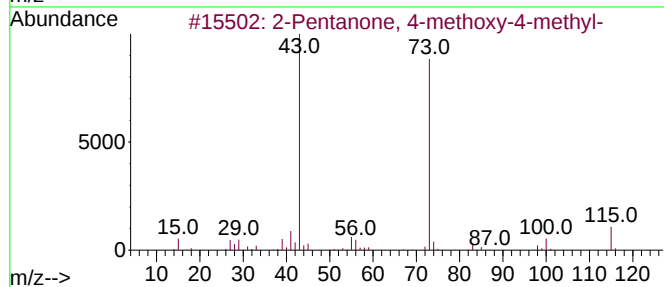
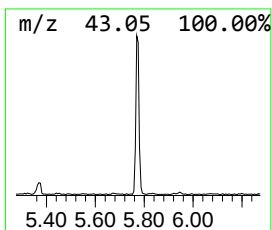
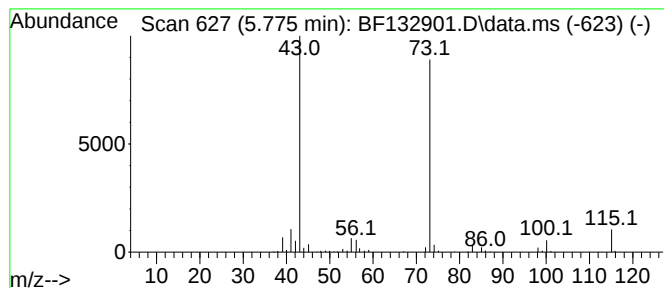
Instrument :
BNA_F
ClientSampleId :
HW-STONE-2-0414

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF041723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.775	2.65 ng	193626	1,4-Dichlorobenzene-d4			6.763
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-		130	C7H14O2	000107-70-0	90
2	Pentane, 3-methoxy-		102	C6H14O	036839-67-5	12
3	3-Methoxy-3-methylbutanol		118	C6H14O2	056539-66-3	10
4	1,3-Dioxolane, 2-(1-methylethyl)-		116	C6H12O2	000822-83-3	10
5	2-Pentanone, 3-ethyl-		114	C7H14O	006137-03-7	10



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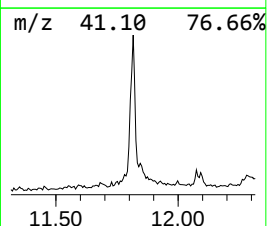
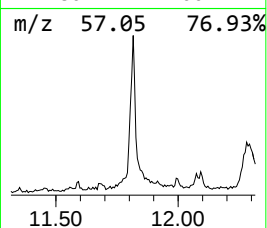
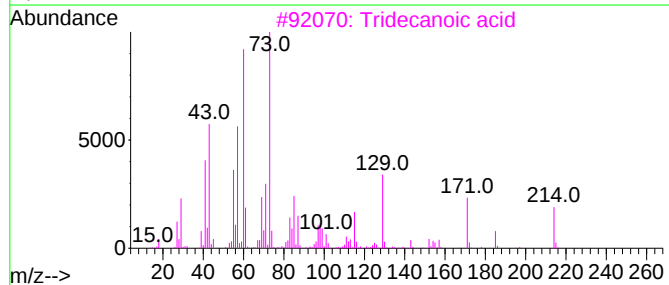
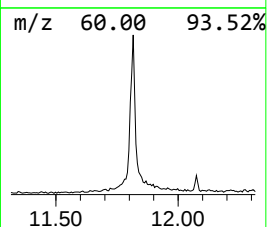
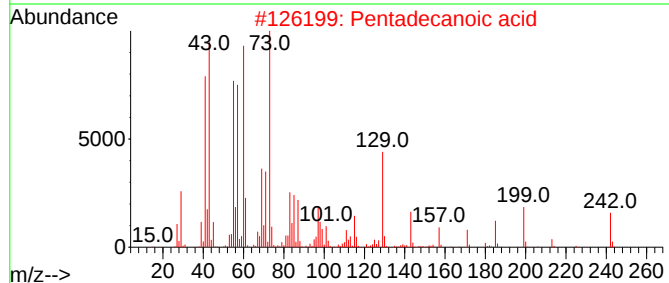
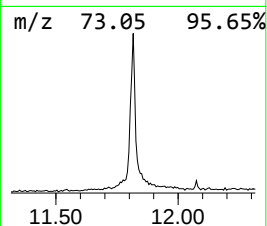
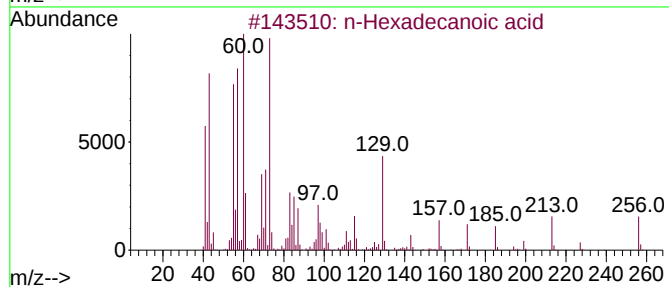
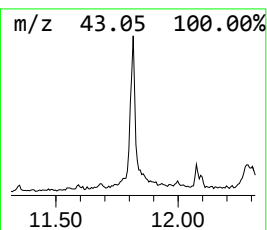
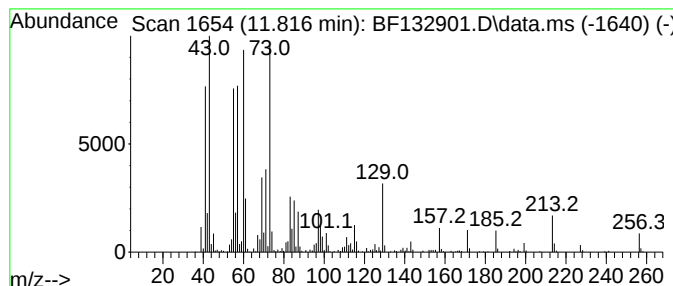
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.816	7.30 ng	863795	Phenanthrene-d10	11.280

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	58



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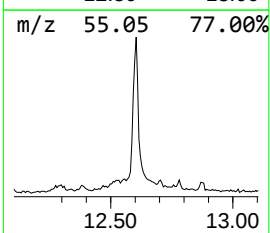
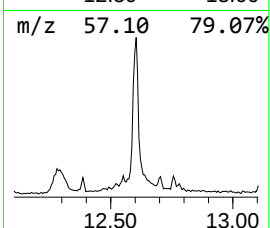
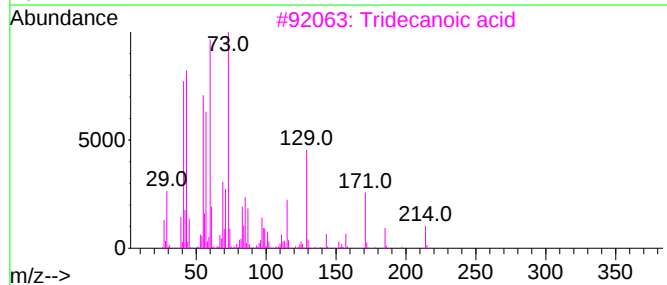
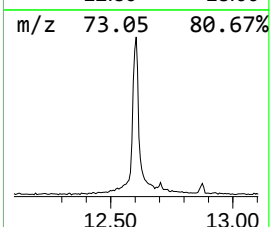
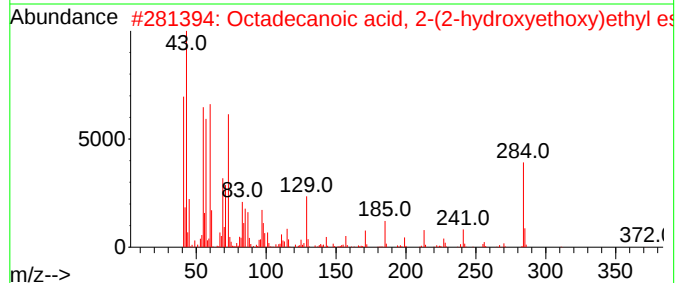
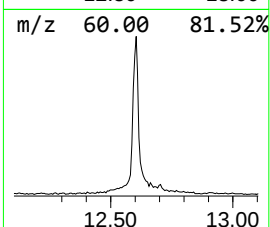
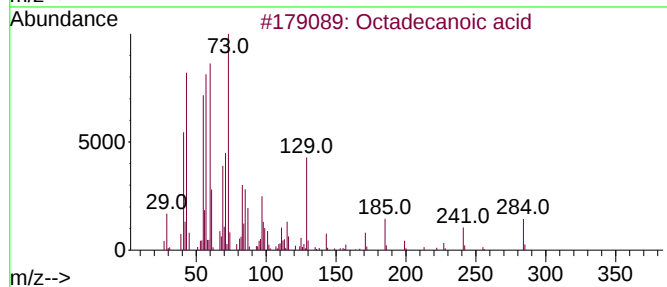
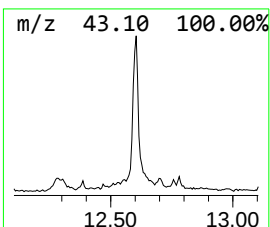
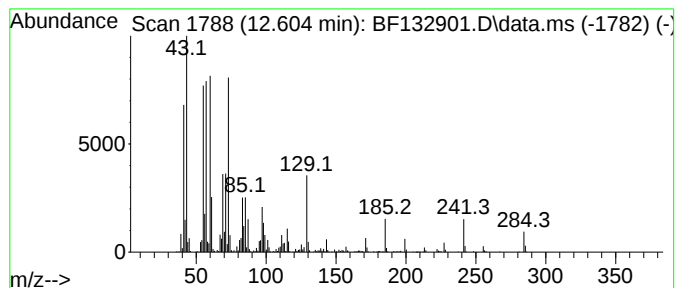
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Peak Number 4 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.604	13.16 ng	1513680	Chrysene-d12	13.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
3			Tridecanoic acid	214	C13H26O2	000638-53-9	68
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
5			Dodecanoic acid	200	C12H24O2	000143-07-7	58



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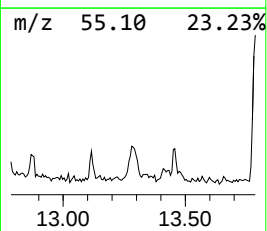
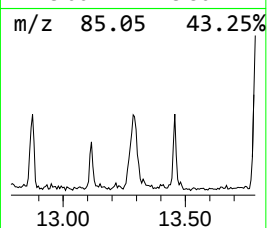
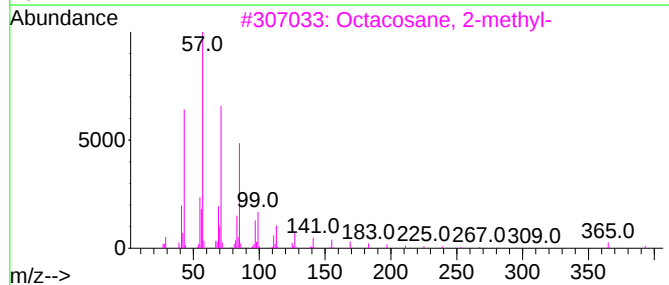
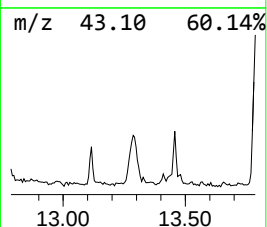
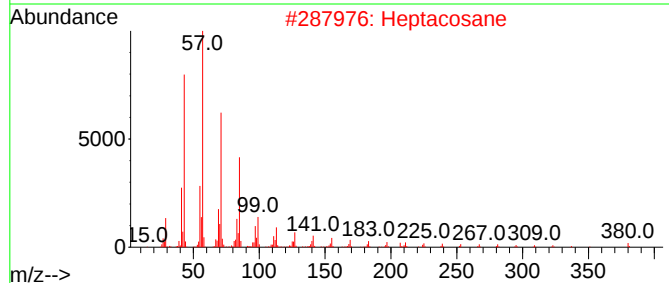
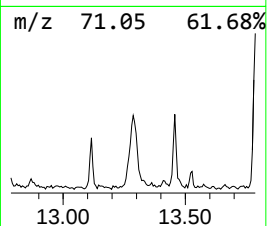
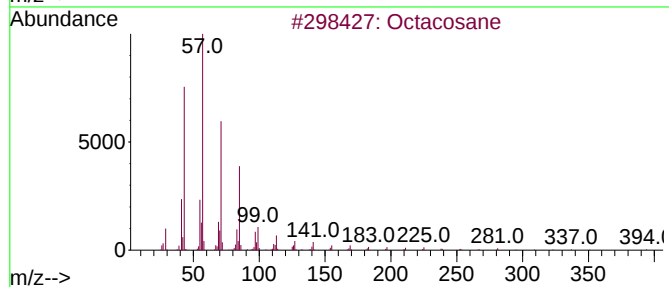
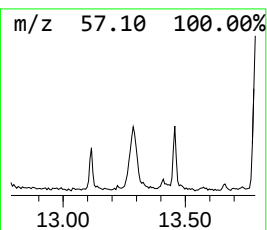
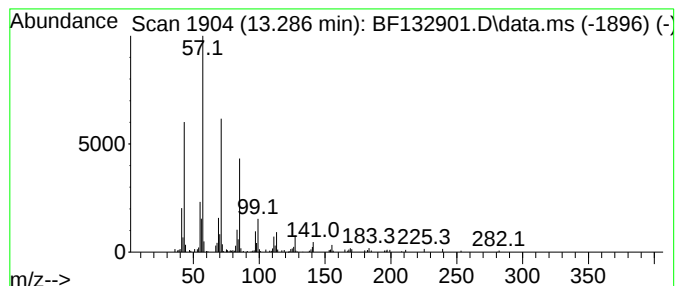
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.286	2.46 ng	282444	Chrysene-d12	13.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Heptacosane	380	C27H56	000593-49-7	91
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4			Heneicosane	296	C21H44	000629-94-7	91
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



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HW-STONE-2-0414

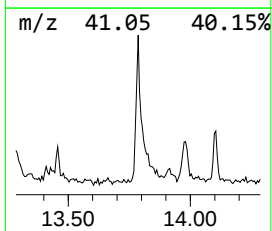
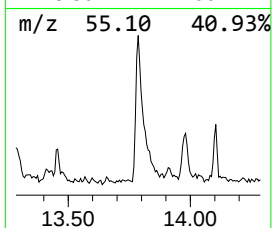
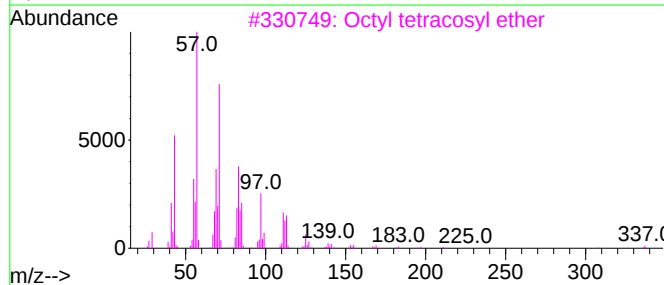
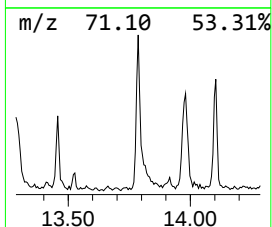
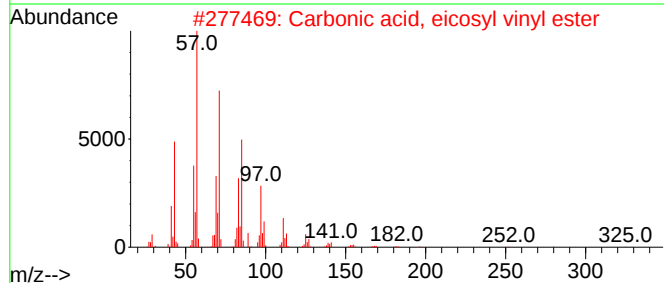
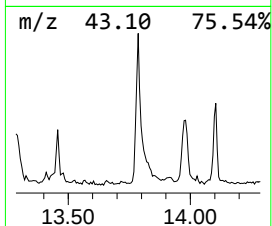
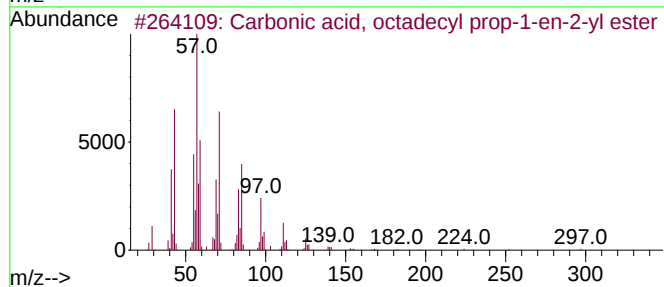
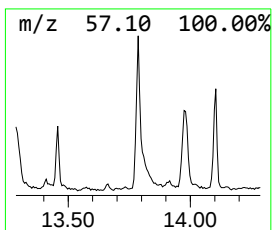
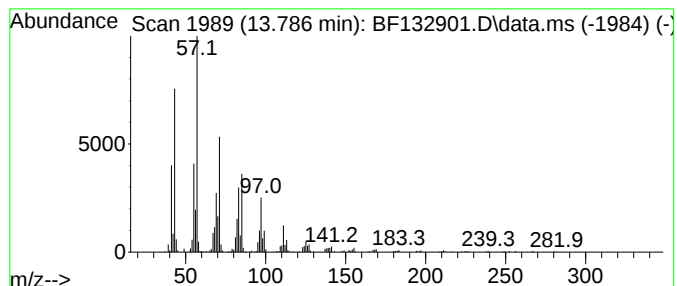
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Carbonic acid, octadecyl pr... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.786	6.33 ng	727744	Chrysene-d12	13.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	91
2			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	90
3			Octyl tetracosyl ether	467	C32H66O	1000406-39-0	87
4			Docosyl octyl ether	438	C30H62O	1000406-38-9	87
5			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041823\
Data File : BF132901.D
Acq On : 18 Apr 2023 15:23
Operator : CG\JU
Sample : 02362-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HW-STONE-2-0414

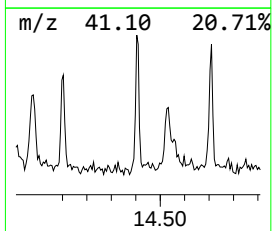
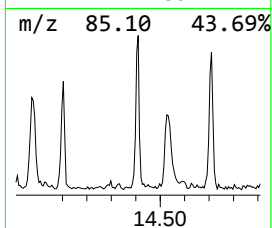
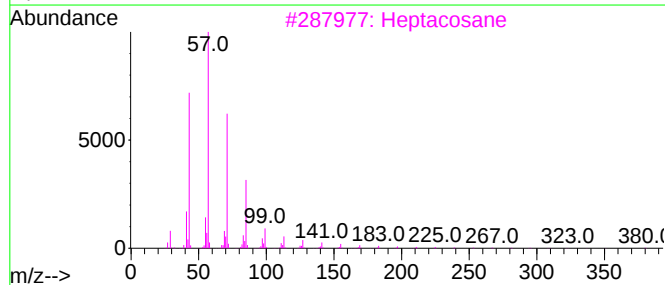
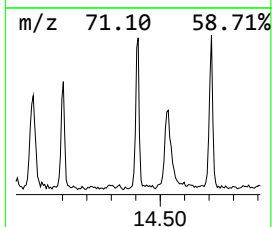
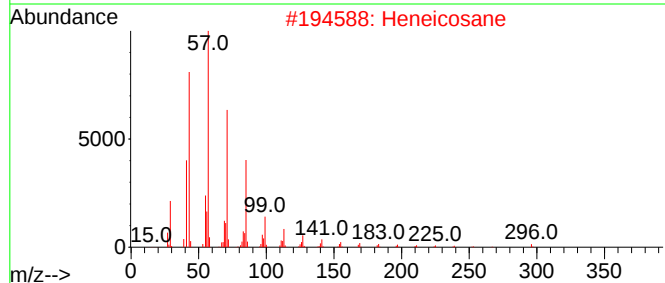
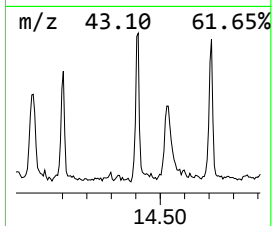
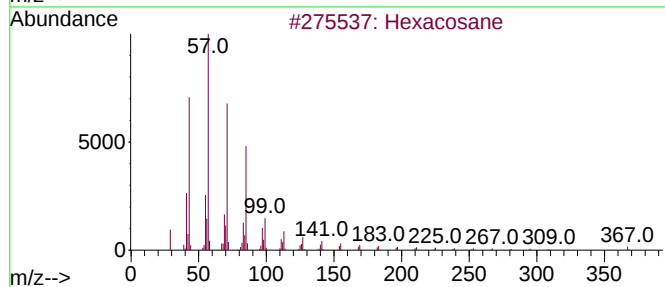
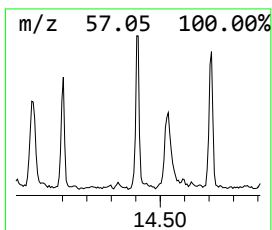
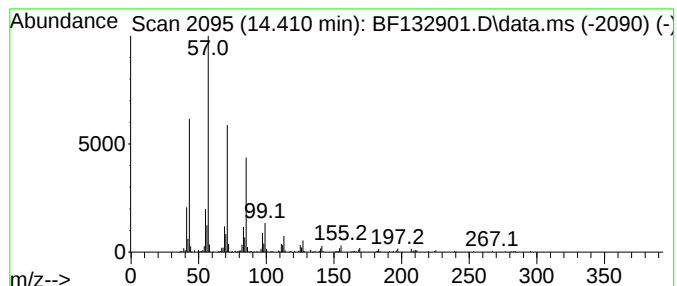
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.410	2.34 ng	269632	Chrysene-d12	13.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	94
2			Heneicosane	296	C21H44	000629-94-7	91
3			Heptacosane	380	C27H56	000593-49-7	91
4			Octadecane	254	C18H38	000593-45-3	91
5			Pentadecane	212	C15H32	000629-62-9	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041823\
Data File : BF132901.D
Acq On : 18 Apr 2023 15:23
Operator : CG\JU
Sample : 02362-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HW-STONE-2-0414

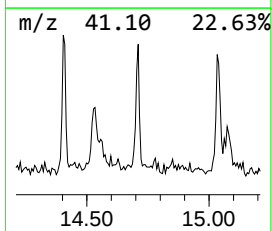
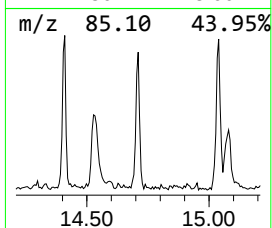
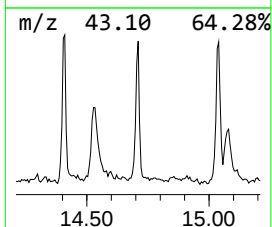
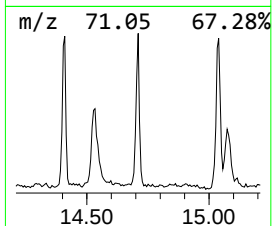
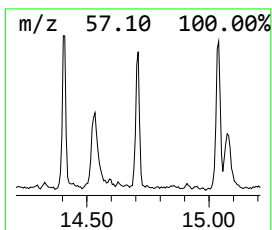
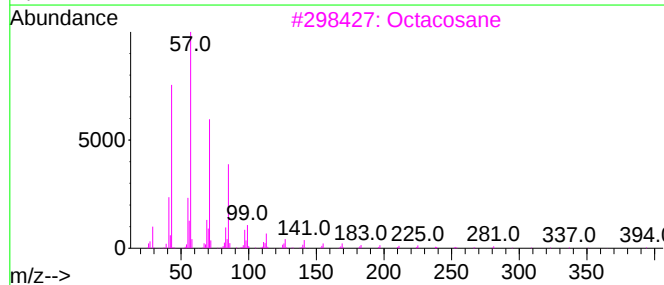
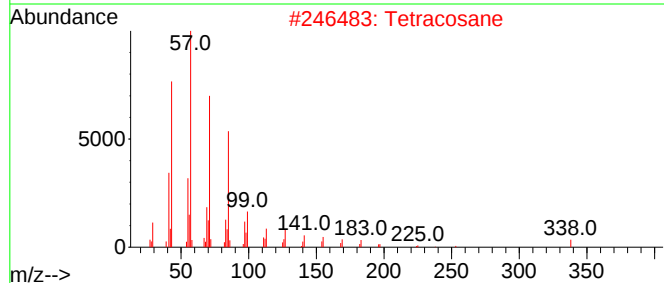
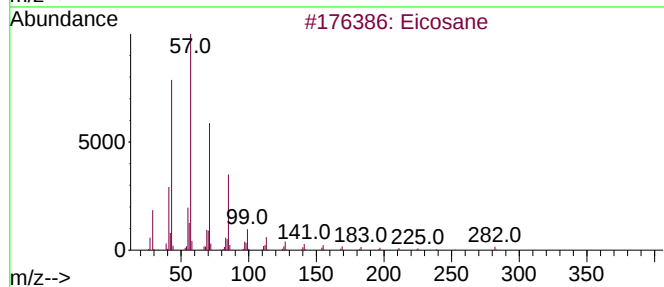
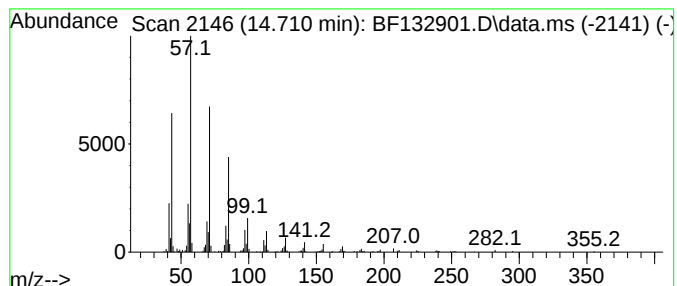
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.710	2.03 ng	245768	Perylene-d12	15.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	94
2			Tetracosane	338	C24H50	000646-31-1	91
3			Octacosane	394	C28H58	000630-02-4	91
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5			Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041823\
Data File : BF132901.D
Acq On : 18 Apr 2023 15:23
Operator : CG\JU
Sample : 02362-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

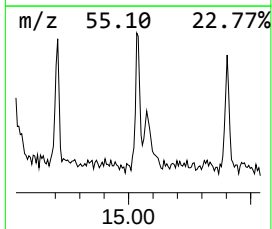
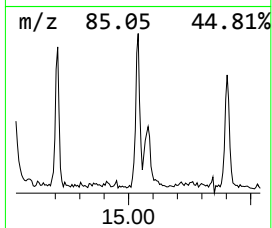
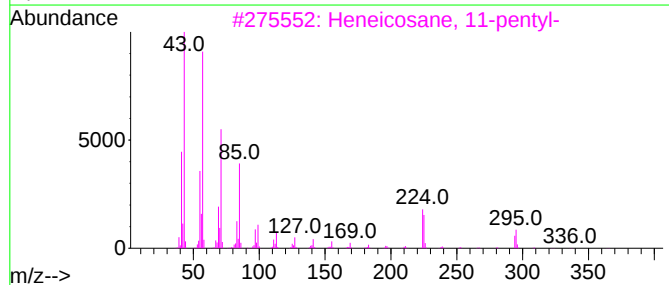
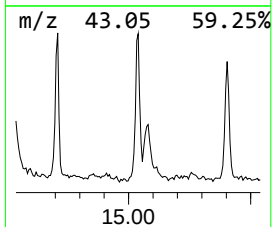
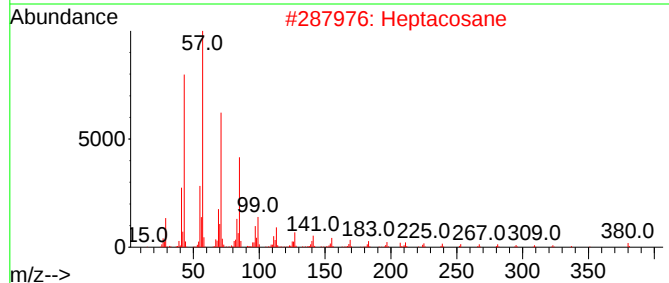
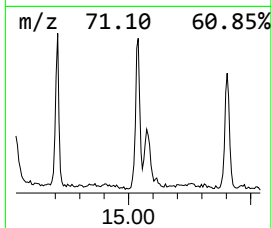
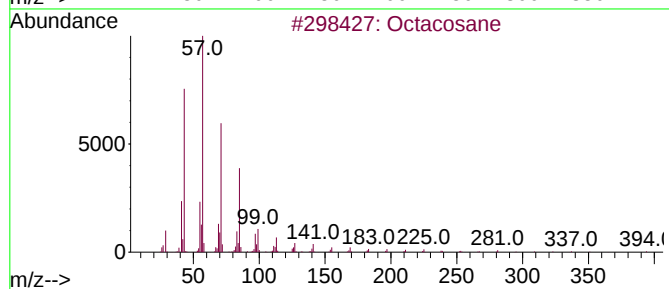
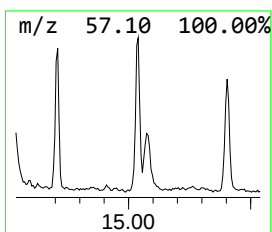
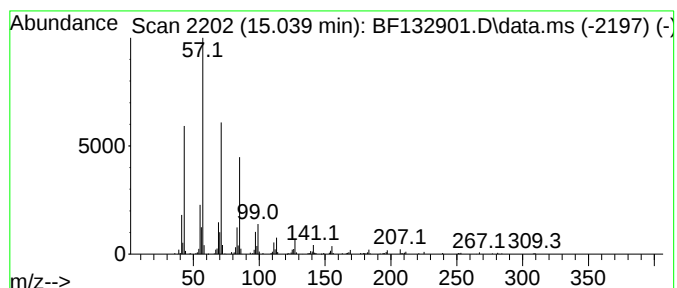
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HW-STONE-2-0414

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF041723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.039	2.49 ng	301832	Perylene-d12	15.345	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	90
4	Triacontane	422	C30H62	000638-68-6	90
5	Heneicosane	296	C21H44	000629-94-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041823\
Data File : BF132901.D
Acq On : 18 Apr 2023 15:23
Operator : CG\JU
Sample : 02362-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HW-STONE-2-0414

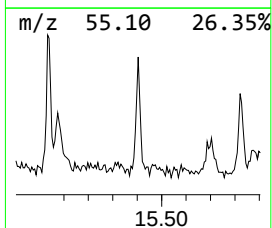
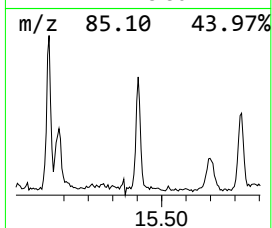
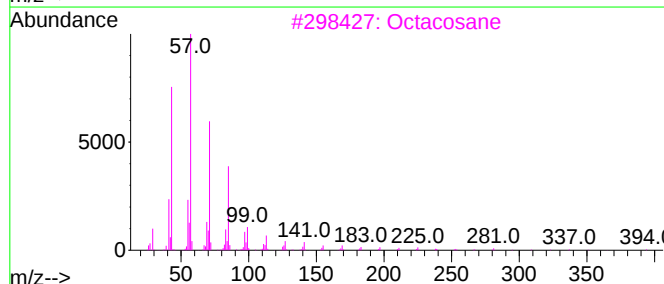
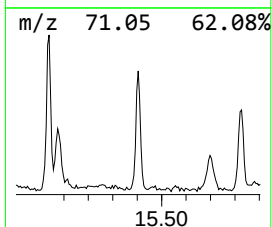
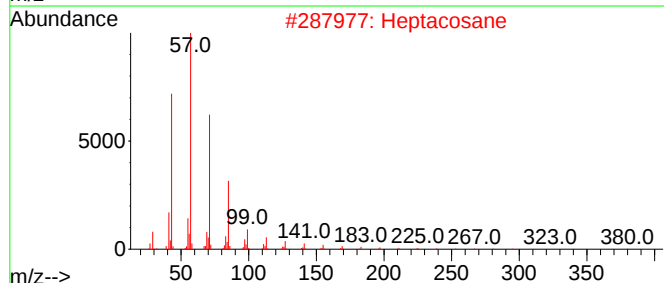
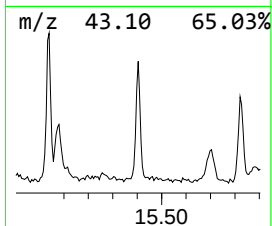
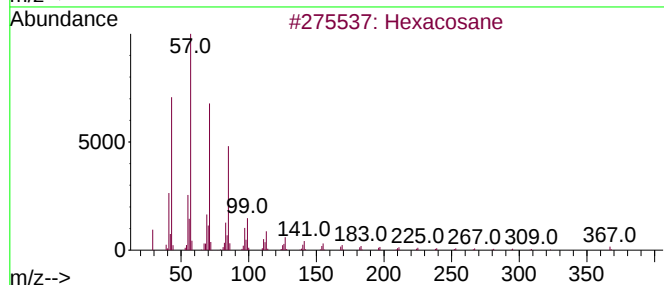
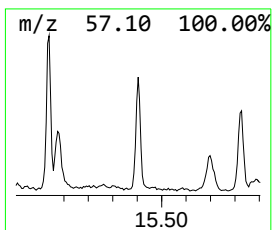
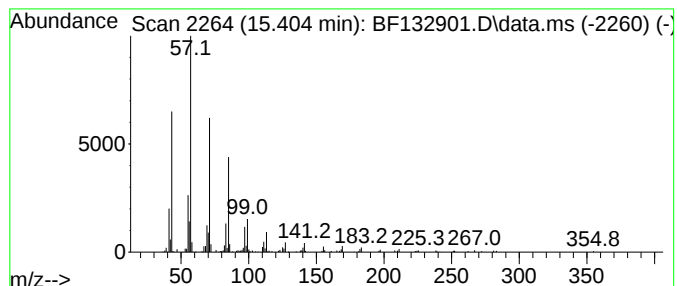
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.404	2.13 ng	257673	Perylene-d12	15.345

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexacosane	366	C26H54	000630-01-3	91
2		Heptacosane	380	C27H56	000593-49-7	91
3		Octacosane	394	C28H58	000630-02-4	90
4		Heptadecane	240	C17H36	000629-78-7	90
5		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041823\
Data File : BF132901.D
Acq On : 18 Apr 2023 15:23
Operator : CG\JU
Sample : 02362-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HW-STONE-2-0414

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF041723.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
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2-Pentanone, 4-...	5.775	2.6	ng	193626	1	6.763	1462900	20.0
n-Hexadecanoic ...	11.816	7.3	ng	863795	4	11.280	2368080	20.0
Octadecanoic acid	12.604	13.2	ng	1513680	5	13.916	2300330	20.0
Octacosane	13.286	2.5	ng	282444	5	13.916	2300330	20.0
Carbonic acid, ...	13.786	6.3	ng	727744	5	13.916	2300330	20.0
Hexacosane	14.410	2.3	ng	269632	5	13.916	2300330	20.0
Eicosane	14.710	2.0	ng	245768	6	15.345	2424260	20.0
Heptacosane	15.039	2.5	ng	301832	6	15.345	2424260	20.0
Heptadecane	15.404	2.1	ng	257673	6	15.345	2424260	20.0