

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070124\
 Data File : BF138399.D
 Acq On : 01 Jul 2024 13:09
 Operator : CG\JU
 Sample : P3119-06
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FB-20240627

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-BF062824.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138399.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.204	10	20	24	rVB	7968865	12329312	100.00%	28.835%
2	5.098	508	512	522	rVB	262867	320931	2.60%	0.751%
3	5.504	576	581	584	rBV	3284211	3144706	25.51%	7.355%
4	6.504	747	751	754	rBV	2477063	1983043	16.08%	4.638%
5	6.875	810	814	817	rVB	1360362	1153930	9.36%	2.699%
6	7.439	904	910	913	rBV	3655410	3856741	31.28%	9.020%
7	8.151	1027	1031	1035	rBV	1726369	1558879	12.64%	3.646%
8	9.233	1208	1215	1218	rBV	5915080	5880559	47.70%	13.753%
9	9.904	1324	1329	1333	rBV	1839003	1682523	13.65%	3.935%
10	10.698	1459	1464	1467	rBV	3394866	3110614	25.23%	7.275%
11	11.392	1578	1582	1585	rBV	1772136	1405975	11.40%	3.288%
12	11.910	1665	1670	1679	rBV2	143630	231257	1.88%	0.541%
13	12.621	1785	1791	1799	rBV	101750	136808	1.11%	0.320%
14	12.698	1799	1804	1816	rVV2	76855	144823	1.17%	0.339%
15	12.833	1818	1827	1838	rVB4	43206	151047	1.23%	0.353%
16	12.980	1847	1852	1855	rBV	4000462	3990025	32.36%	9.332%
17	13.786	1981	1989	1999	rBV2	62521	126657	1.03%	0.296%
18	14.027	2026	2030	2034	rBV	987455	837610	6.79%	1.959%
19	15.492	2274	2279	2291	rBV	564794	713119	5.78%	1.668%

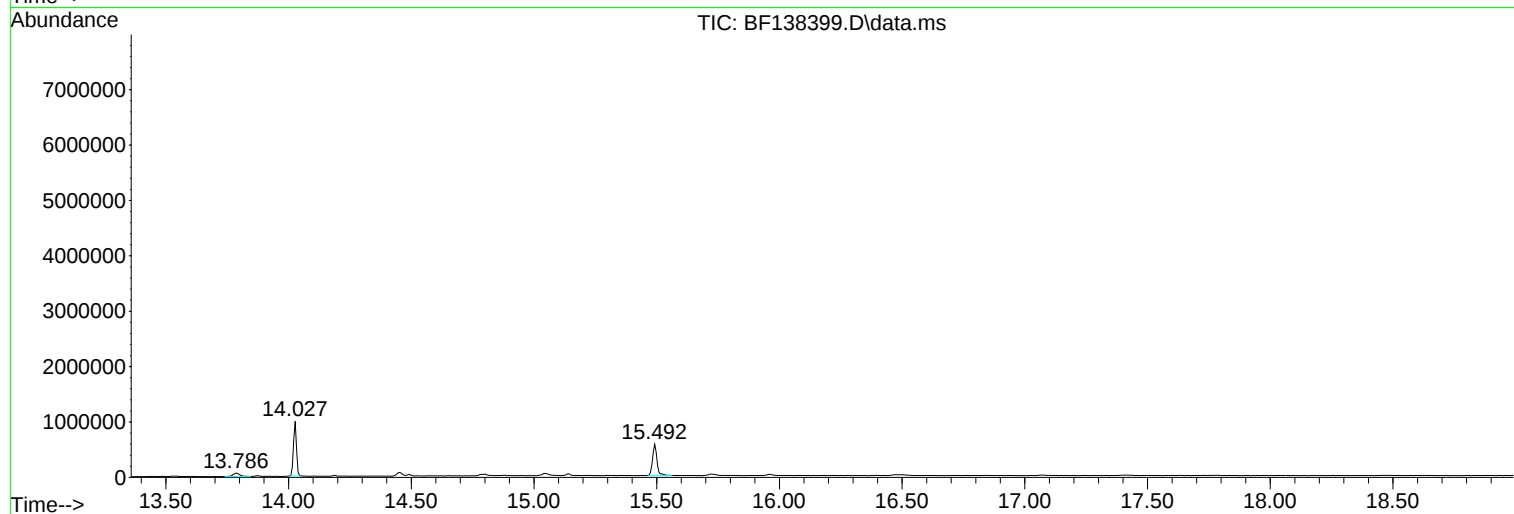
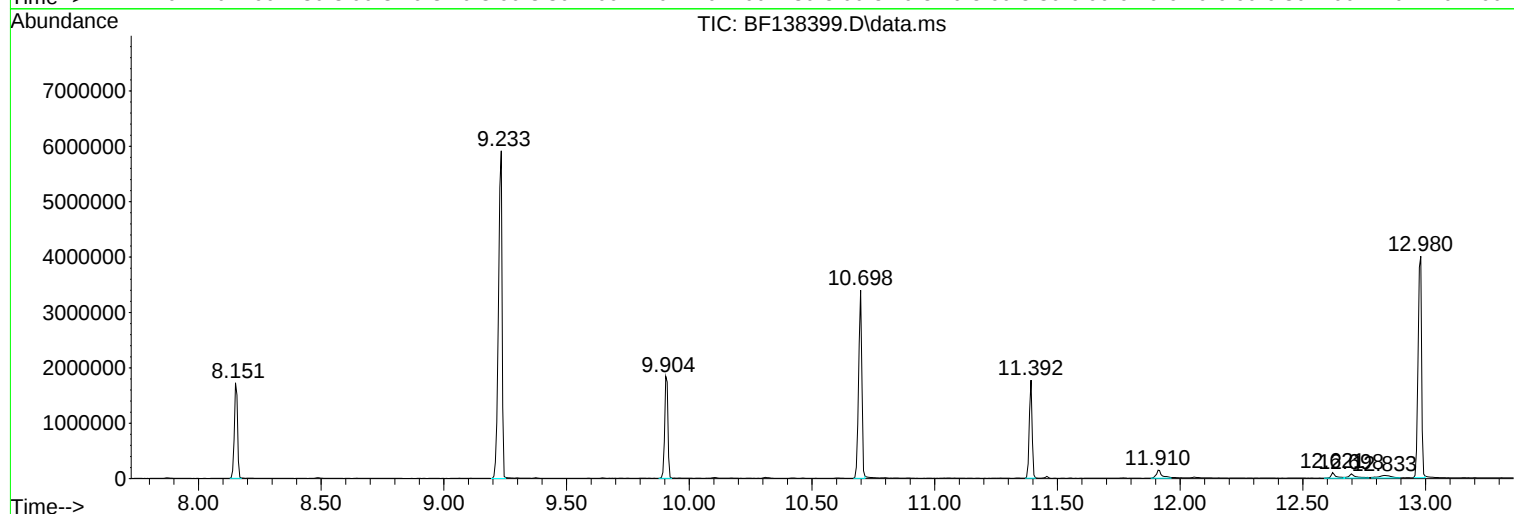
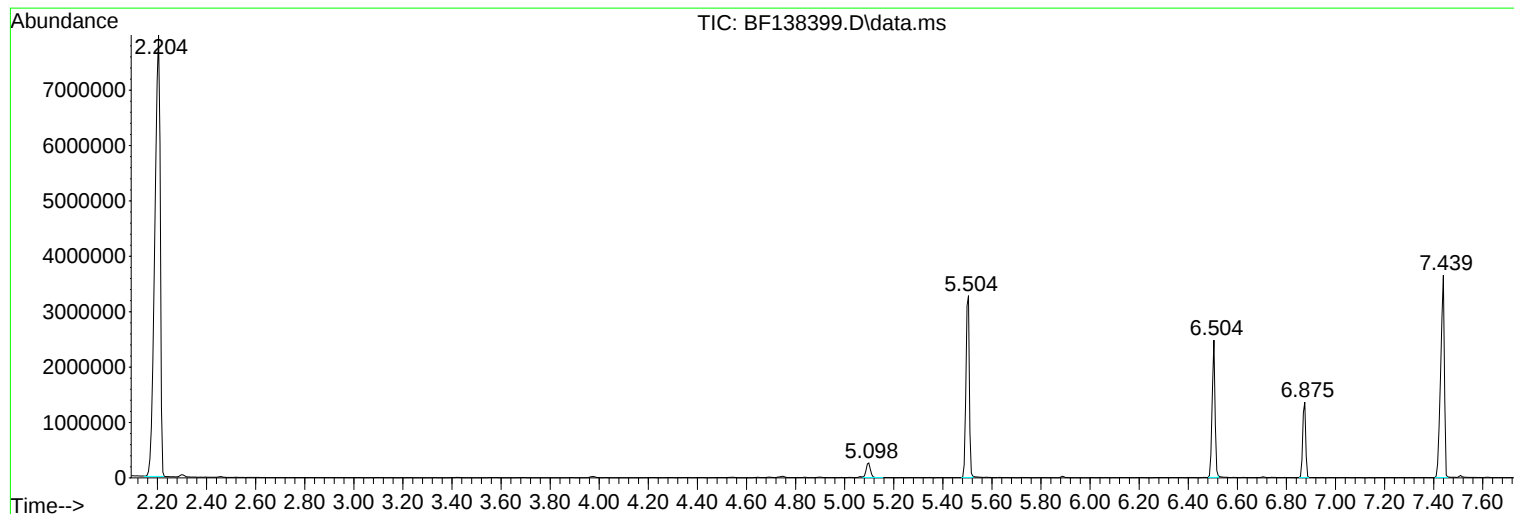
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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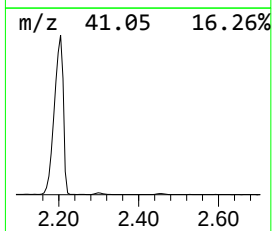
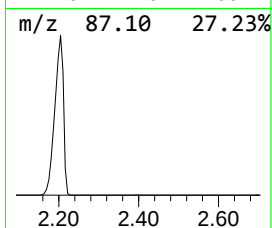
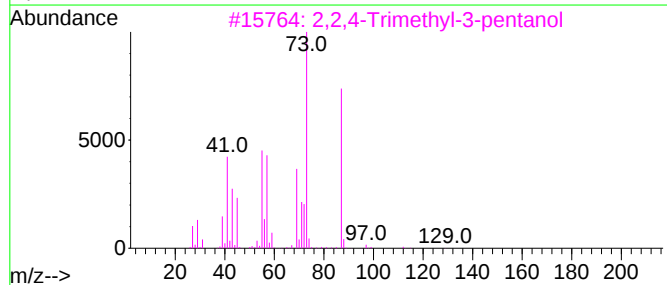
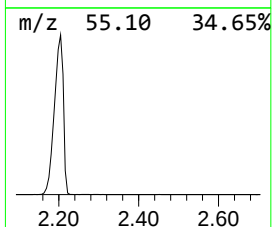
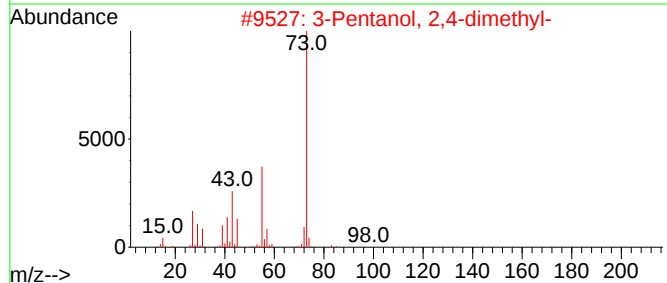
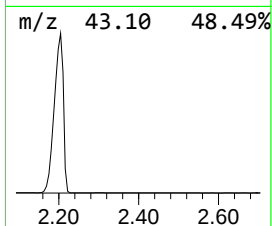
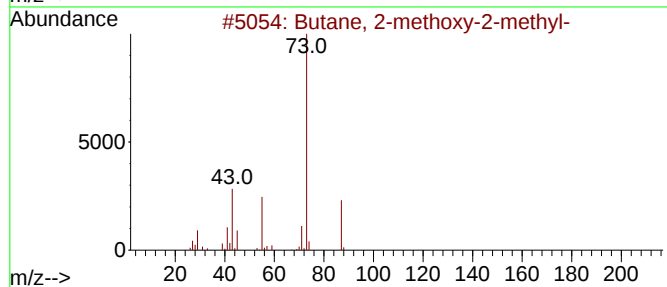
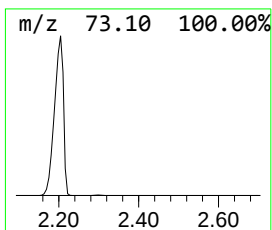
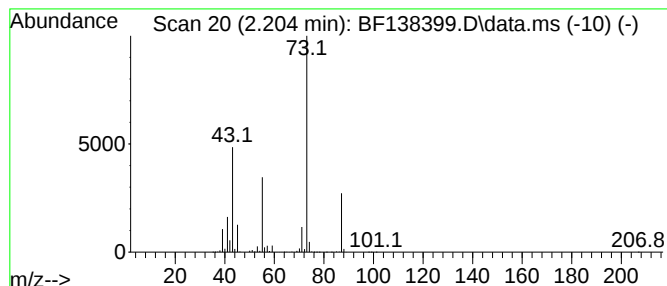
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.204	213.69 ng	12329300	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	25



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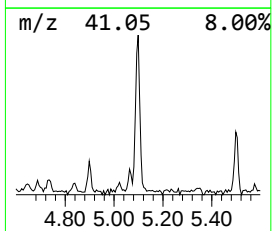
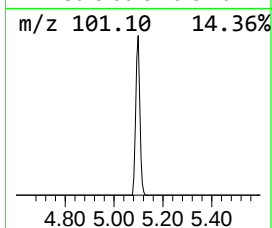
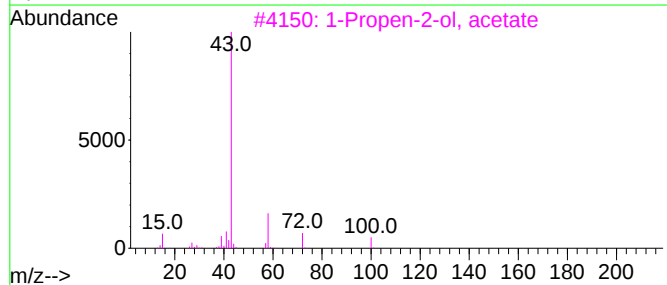
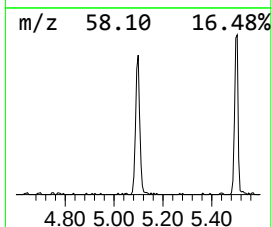
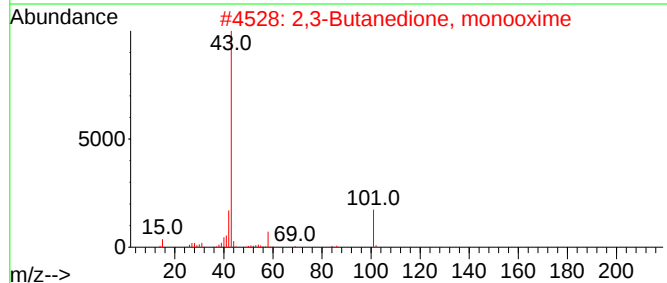
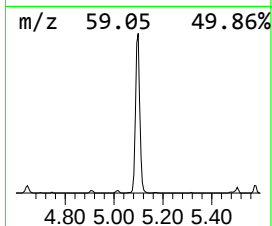
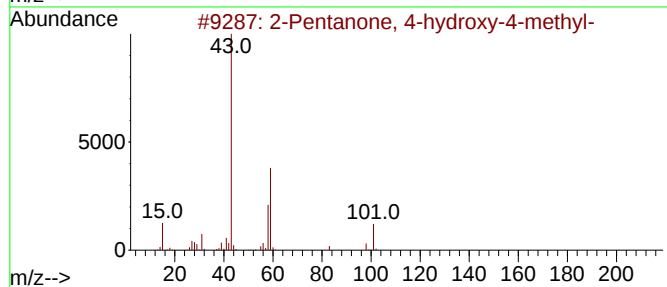
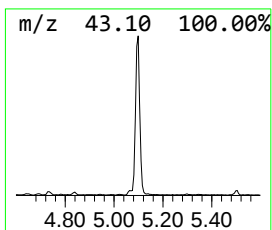
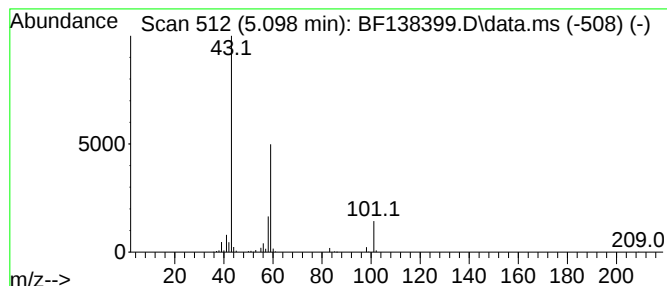
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD		R.T.	
5.098	5.56 ng	320931	1,4-Dichlorobenzene-d4		6.875	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	59
2	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	27
3	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	9
4	5-Aminovaleric acid		117	C5H11NO2	000660-88-8	9
5	Formamide, N,N-diethyl-		101	C5H11NO	000617-84-5	7



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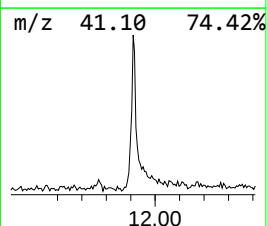
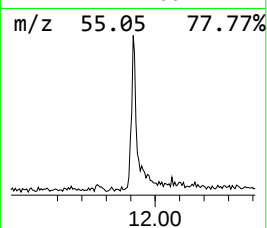
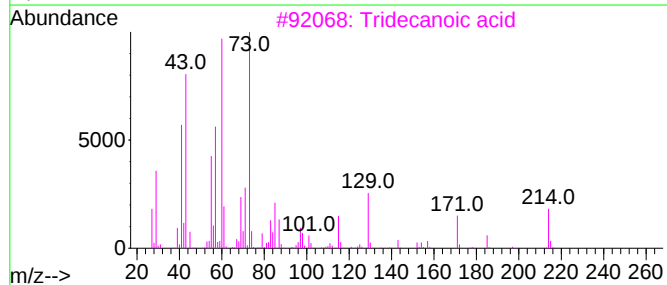
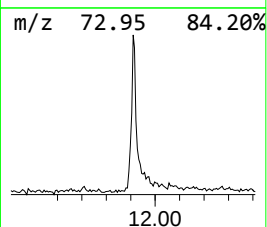
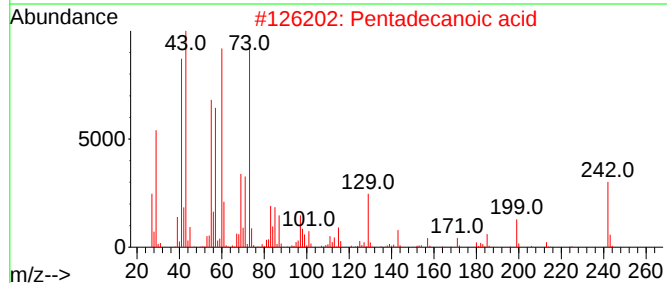
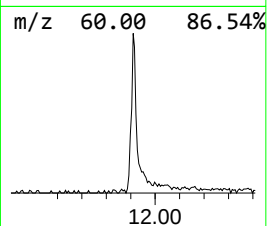
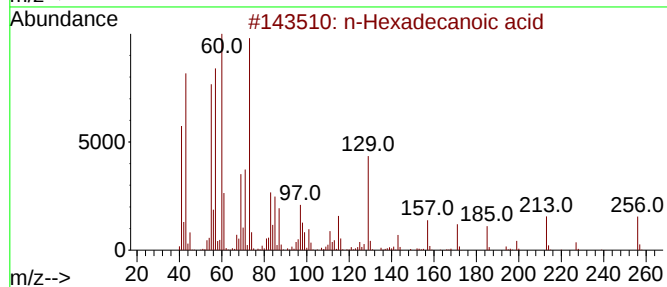
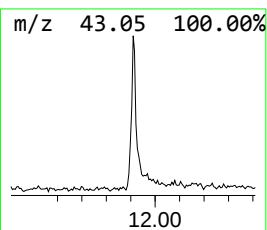
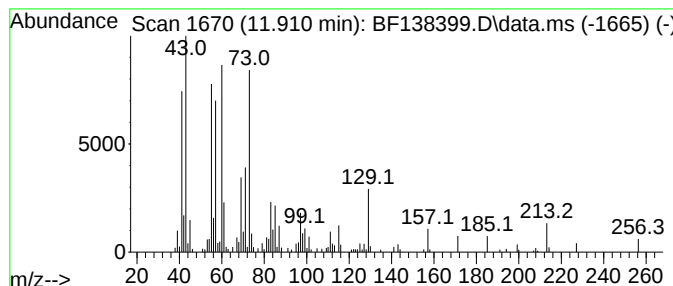
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	3.29 ng	231257	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3			Tridecanoic acid	214	C13H26O2	000638-53-9	60
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5			Octanoic acid	144	C8H16O2	000124-07-2	49



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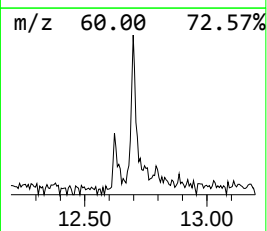
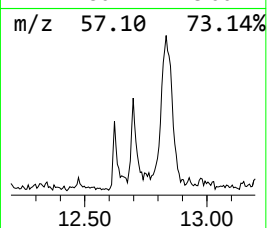
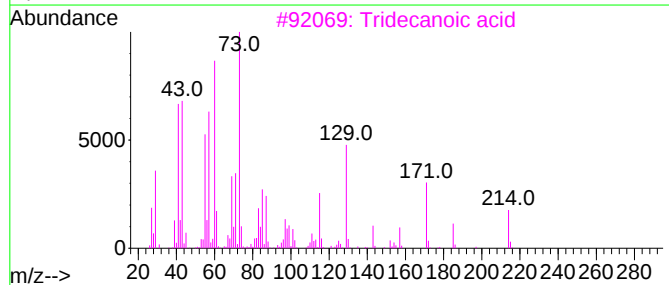
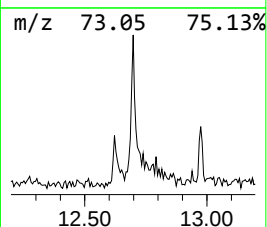
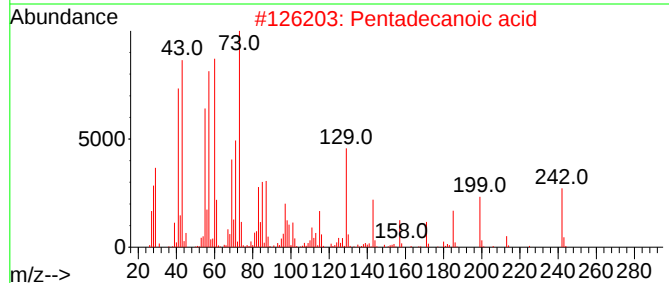
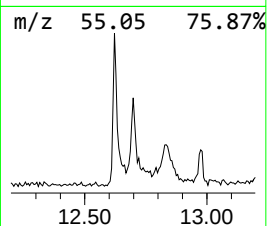
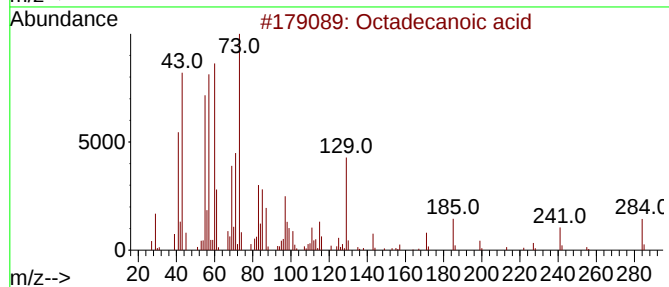
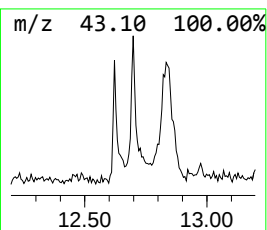
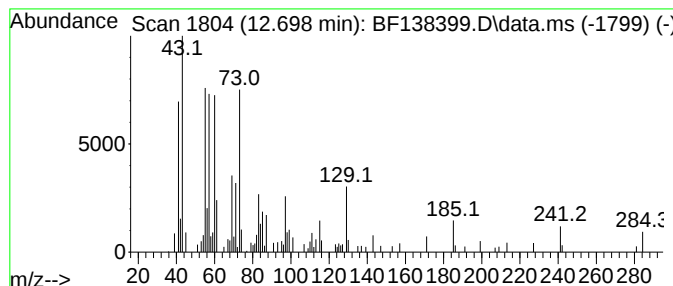
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.698	2.06 ng	144823	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
3			Tridecanoic acid	214	C13H26O2	000638-53-9	58
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	58



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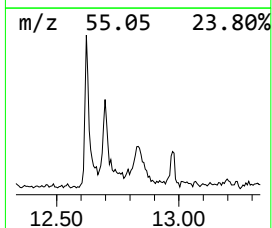
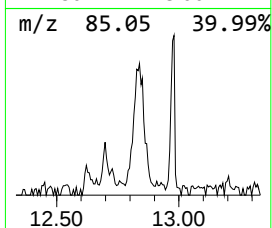
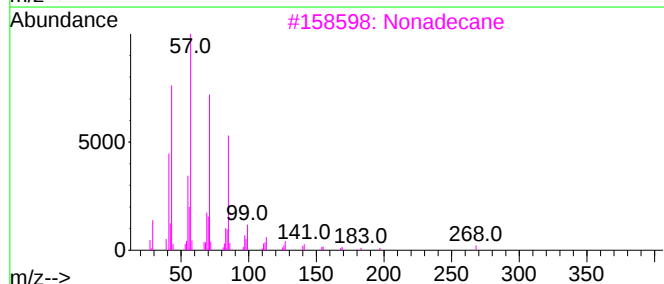
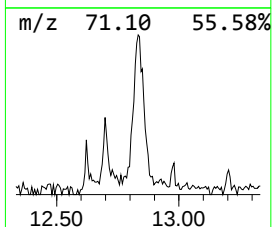
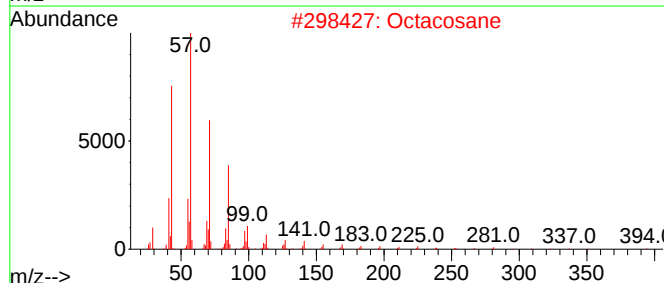
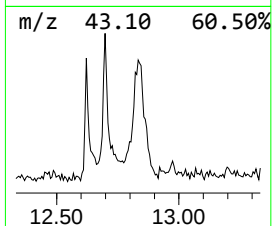
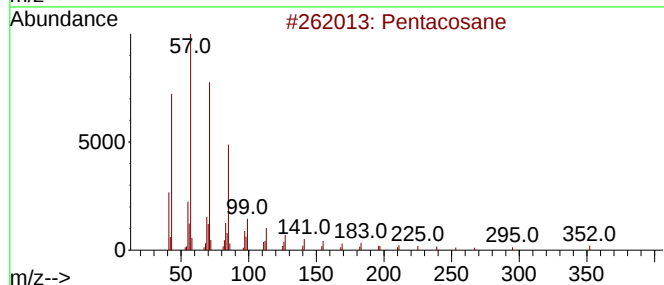
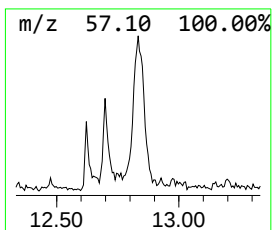
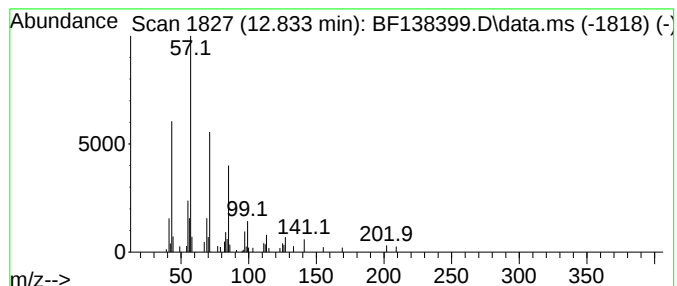
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Pentacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.833	3.61 ng	151047	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	90
2			Octacosane	394	C28H58	000630-02-4	86
3			Nonadecane	268	C19H40	000629-92-5	86
4			Heptacosane	380	C27H56	000593-49-7	86
5			Tetracosane	338	C24H50	000646-31-1	86



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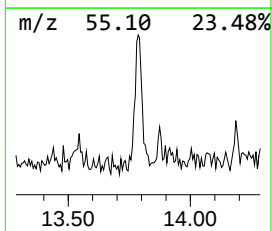
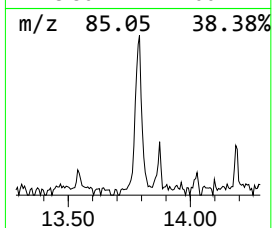
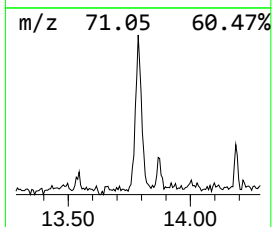
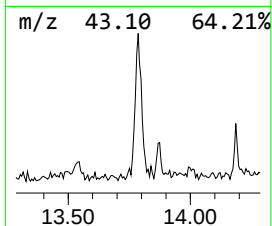
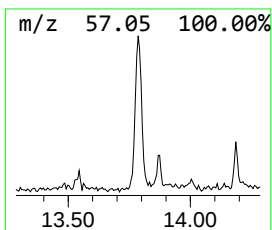
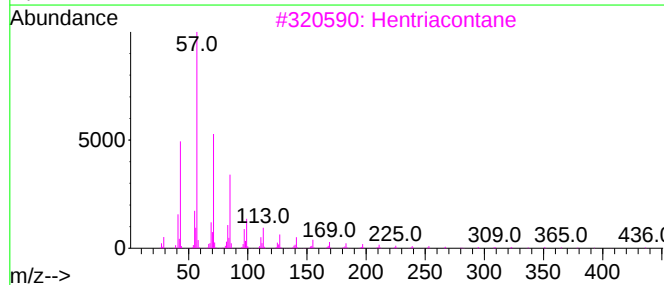
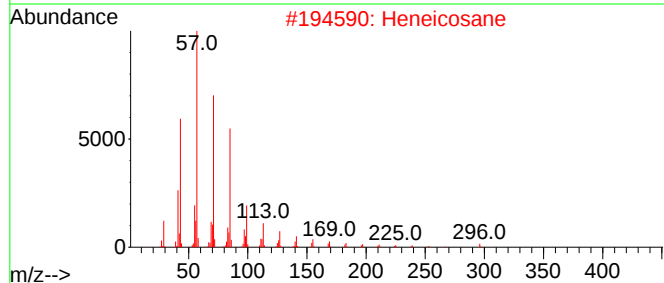
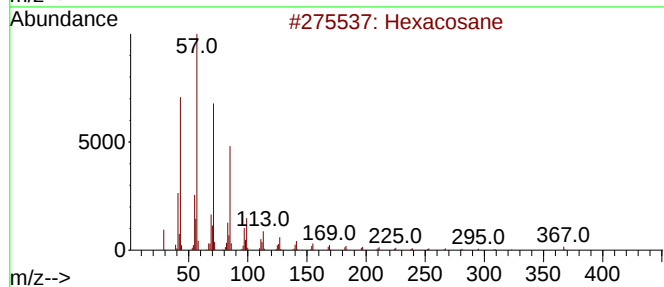
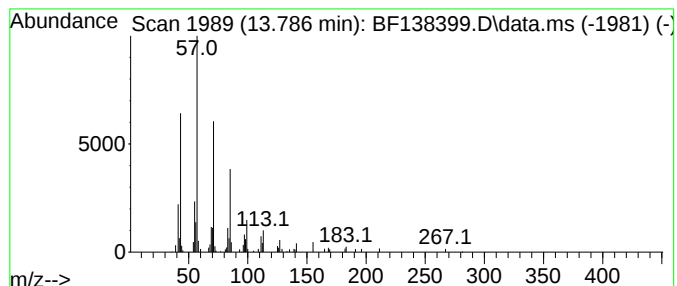
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.786	3.02 ng	126657	Chrysene-d12	14.027

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexacosane	366	C26H54	000630-01-3	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Hentriacontane	437	C31H64	000630-04-6	91
4		Octadecane	254	C18H38	000593-45-3	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070124\
Data File : BF138399.D
Acq On : 01 Jul 2024 13:09
Operator : CG\JU
Sample : P3119-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FB-20240627

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.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
Butane, 2-metho...	2.204	213.7	ng	12329300	1	6.875	1153930	20.0
2-Pentanone, 4-...	5.098	5.6	ng	320931	1	6.875	1153930	20.0
n-Hexadecanoic ...	11.910	3.3	ng	231257	4	11.392	1405980	20.0
Octadecanoic acid	12.698	2.1	ng	144823	4	11.392	1405980	20.0
Pentacosane	12.833	3.6	ng	151047	5	14.027	837610	20.0
Hexacosane	13.786	3.0	ng	126657	5	14.027	837610	20.0