

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031924\
 Data File : BF137642.D
 Acq On : 19 Mar 2024 12:13
 Operator : CG\JU
 Sample : PB159643BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB159643BL

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-BF022924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137642.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.945	481	486	500	rBV	162705	270894	4.33%	0.657%
2	5.351	550	555	558	rBV	4852818	5450233	87.13%	13.222%
3	6.369	723	728	731	rBV	4812752	5509007	88.07%	13.365%
4	6.722	785	788	799	rBV	1275771	1269197	20.29%	3.079%
5	7.292	880	885	888	rBV	3508141	3582646	57.27%	8.691%
6	8.004	1002	1006	1024	rBV	1787292	1707670	27.30%	4.143%
7	9.086	1184	1190	1193	rBV	6524554	6255454	100.00%	15.175%
8	9.757	1300	1304	1323	rBV	2220732	1915734	30.63%	4.647%
9	10.551	1434	1439	1464	rBV	3444070	3683624	58.89%	8.936%
10	11.239	1552	1556	1572	rBV	1997640	1854321	29.64%	4.498%
11	12.651	1793	1796	1800	rBV	195223	157316	2.51%	0.382%
12	12.827	1822	1826	1830	rBV	5819689	6090982	97.37%	14.776%
13	13.357	1913	1916	1921	rBV	146250	128192	2.05%	0.311%
14	13.874	2000	2004	2016	rBV	1409103	1323559	21.16%	3.211%
15	14.645	2132	2135	2139	rVB	84610	81587	1.30%	0.198%
16	14.968	2186	2190	2194	rBV	117500	118412	1.89%	0.287%
17	15.298	2241	2246	2249	rBV	845243	1022960	16.35%	2.482%
18	15.327	2249	2251	2267	rVB	162702	229696	3.67%	0.557%
19	15.739	2316	2321	2328	rBV	115123	159591	2.55%	0.387%
20	16.215	2397	2402	2410	rBV2	97095	168244	2.69%	0.408%
21	16.774	2491	2497	2504	rBV3	67789	124525	1.99%	0.302%
22	17.427	2600	2608	2619	rBV2	45462	117197	1.87%	0.284%

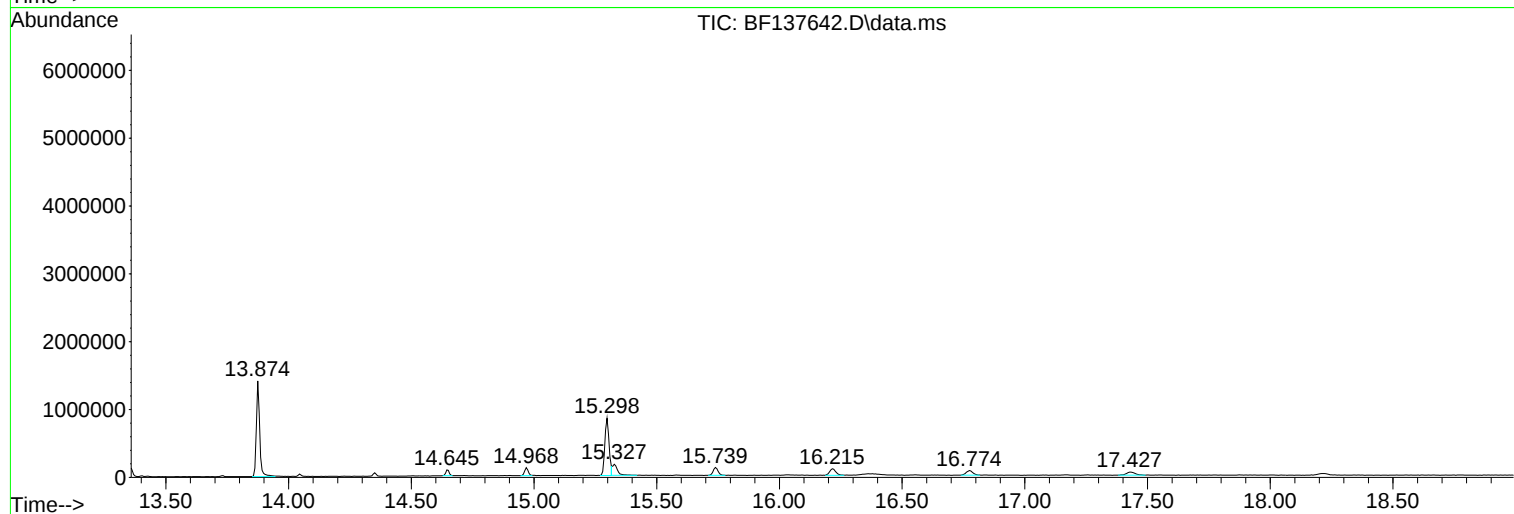
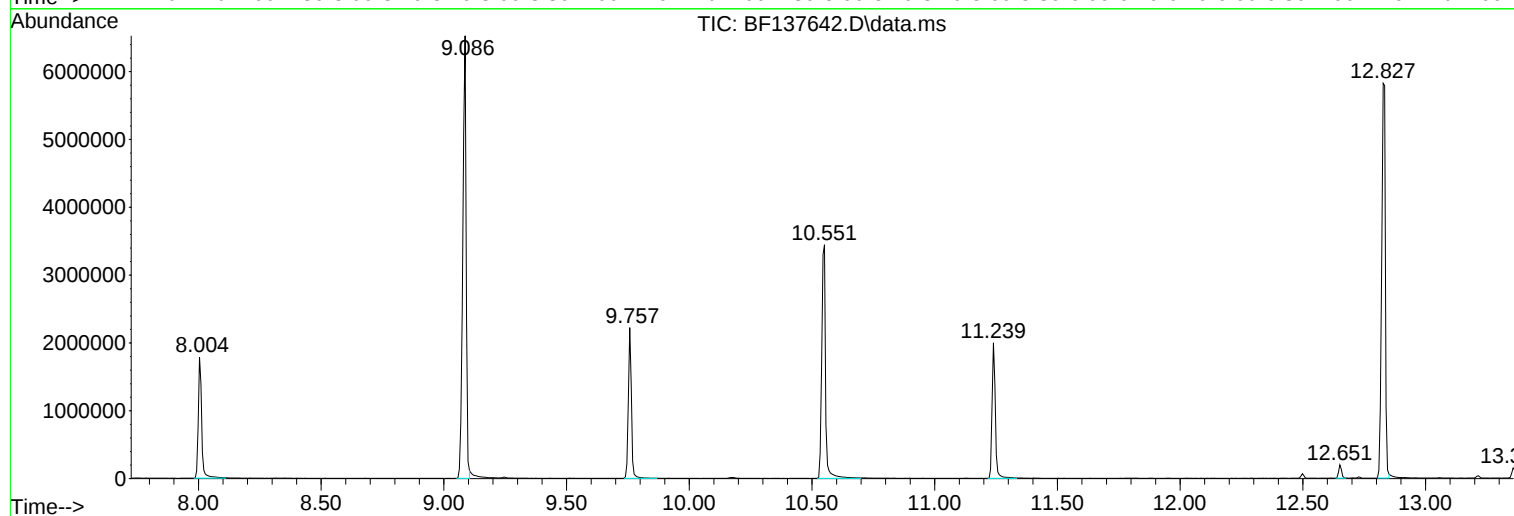
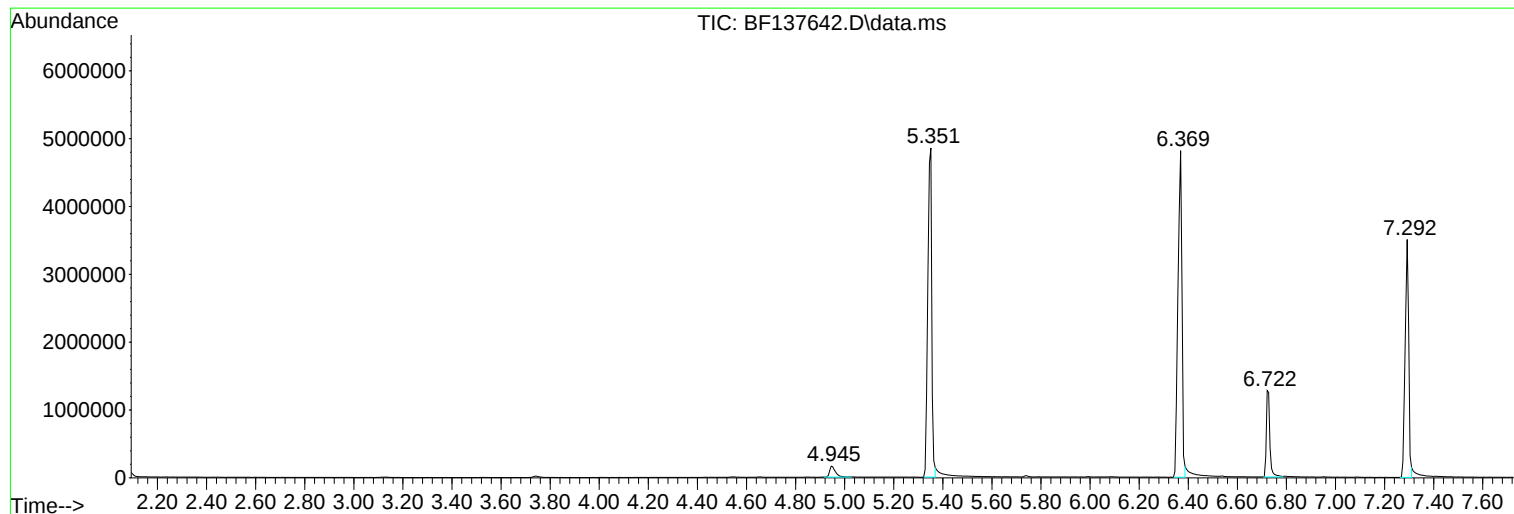
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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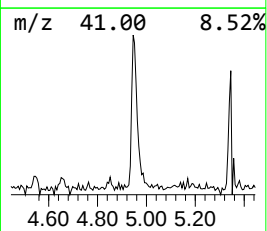
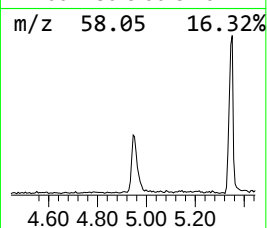
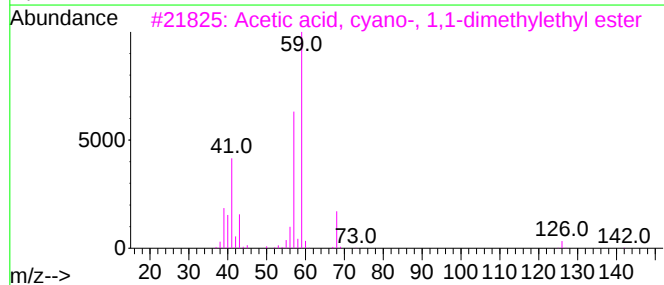
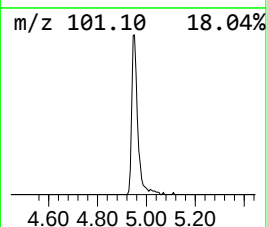
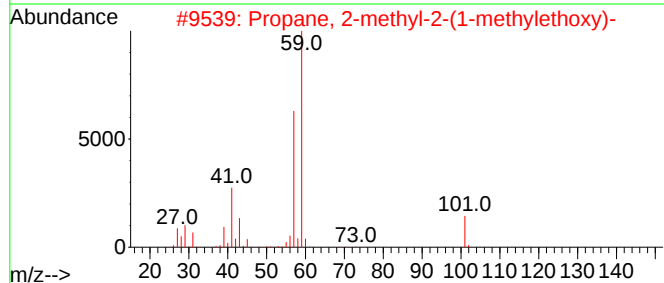
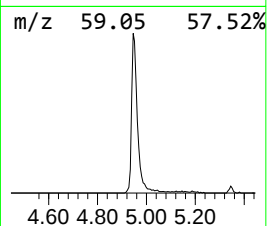
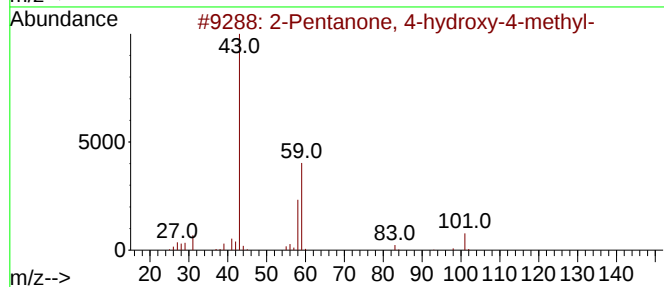
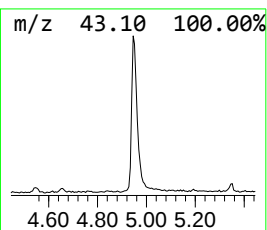
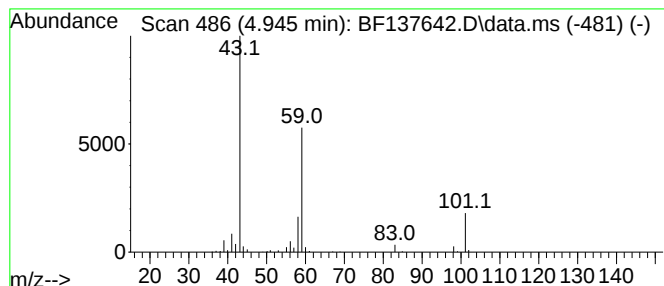
Instrument :
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ClientSampleId :
PB159643BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.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.
4.945	4.27 ng	270894	1,4-Dichlorobenzene-d4			6.728
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...		116	C7H16O	017348-59-3	42
3	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	25
4	N,N'-Bis(2-methyl-2-nitrosopenta...		258	C12H22N2O4	094514-30-4	10
5	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	10



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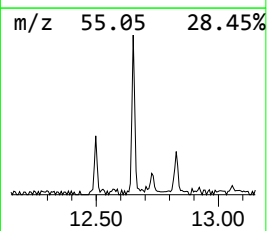
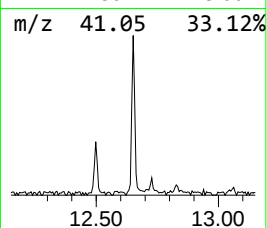
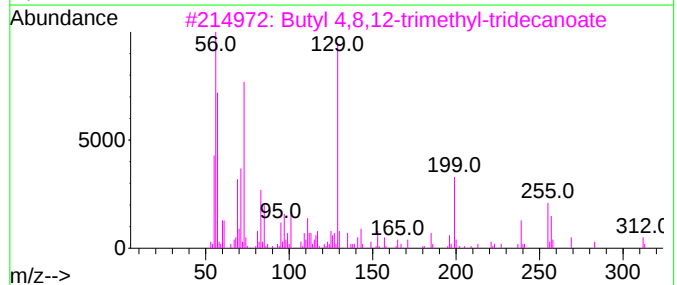
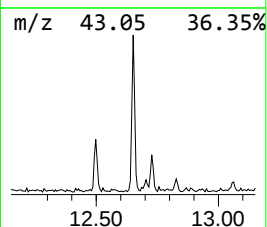
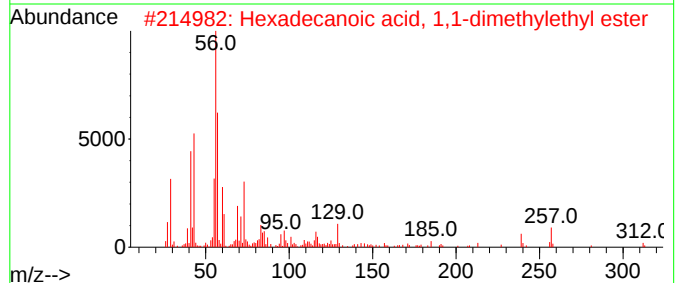
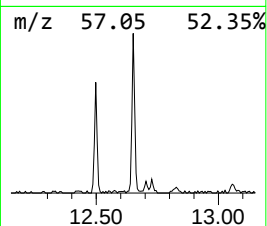
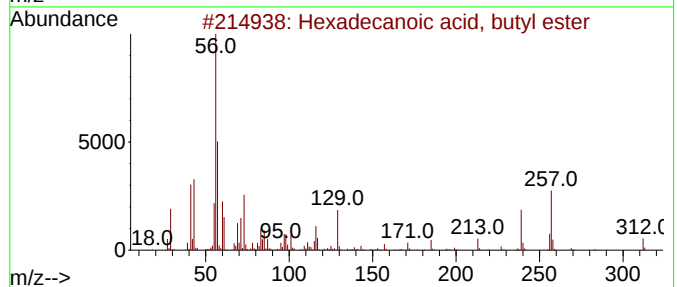
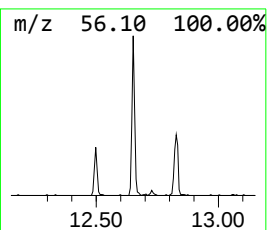
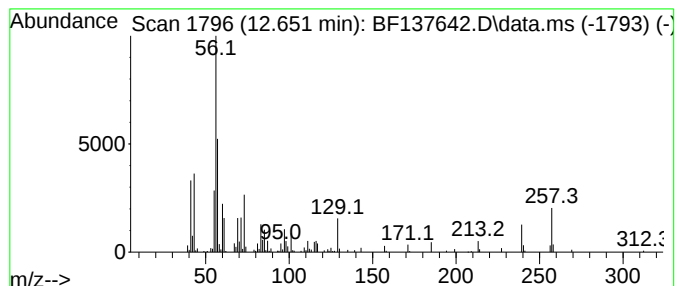
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.651	2.38 ng	157316	Chrysene-d12	13.874	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	80
3	Butyl 4,8,12-trimethyl-tridecanoate	312	C20H40O2	1000336-63-2	45
4	1,3-Hexanediol, 2-ethyl- (isomer 1)	146	C8H18O2	1000484-18-2	37
5	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35



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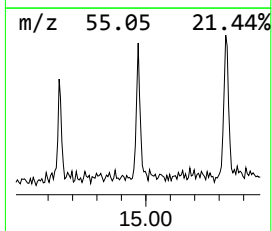
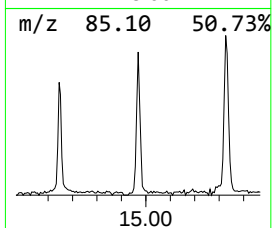
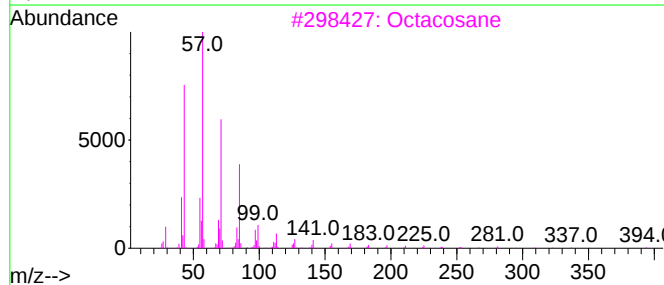
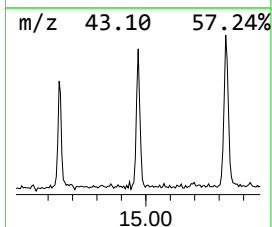
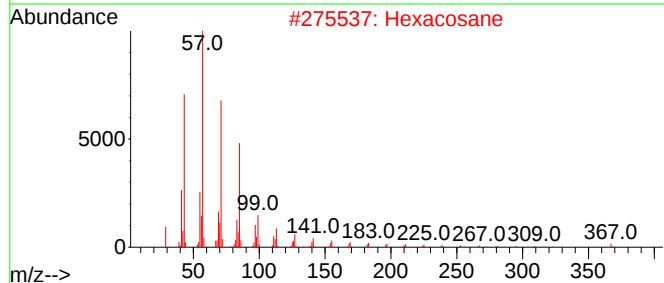
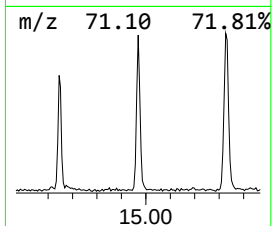
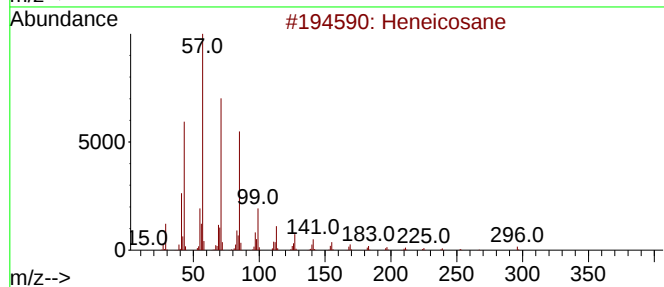
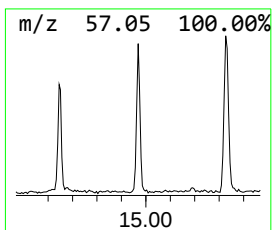
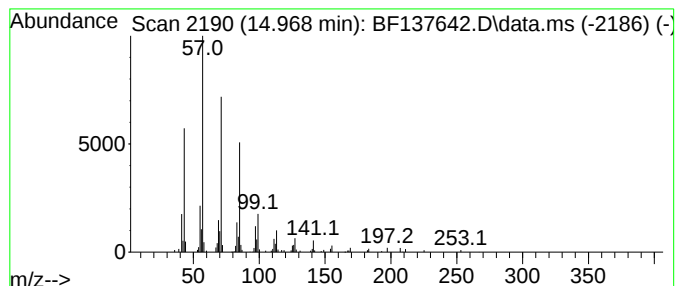
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.968	2.32 ng	118412	Perylene-d12	15.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Hexacosane	366	C26H54	000630-01-3	91
3			Octacosane	394	C28H58	000630-02-4	91
4			Heptadecane	240	C17H36	000629-78-7	91
5			Hexadecane	226	C16H34	000544-76-3	87



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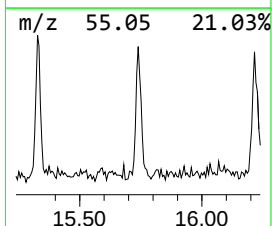
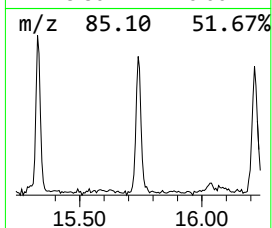
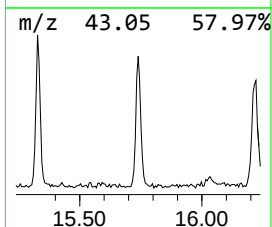
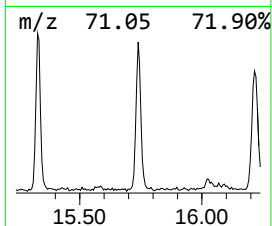
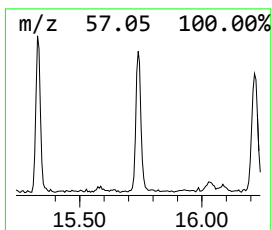
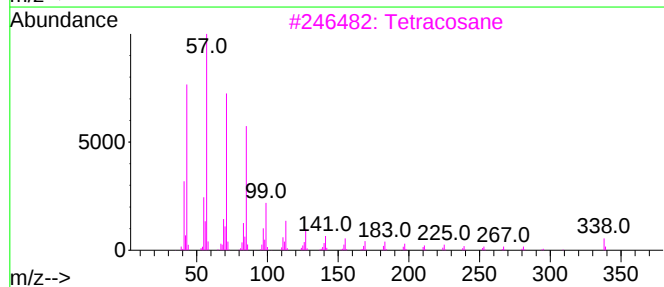
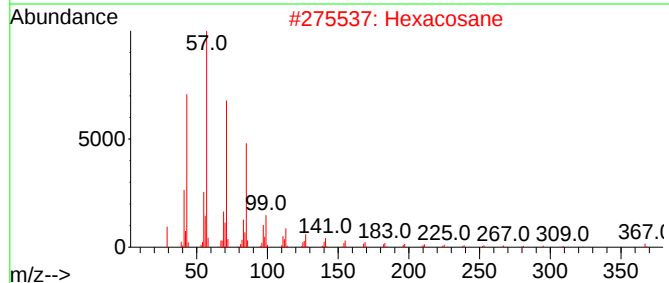
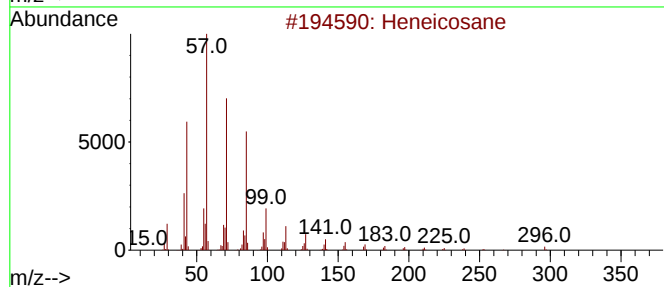
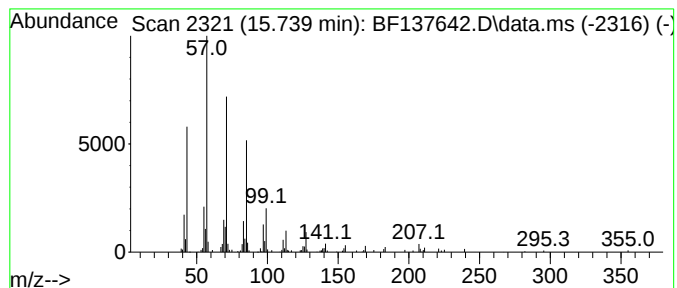
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.739	3.12 ng	159591	Perylene-d12	15.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Hexacosane	366	C26H54	000630-01-3	90
3			Tetracosane	338	C24H50	000646-31-1	90
4			Heptadecane	240	C17H36	000629-78-7	87
5			Nonadecane, 2-methyl-	282	C20H42	001560-86-7	86



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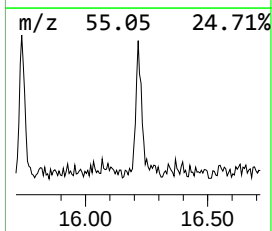
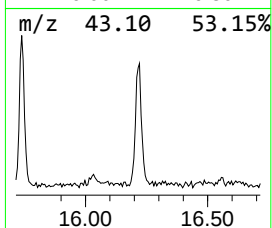
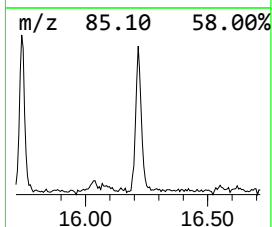
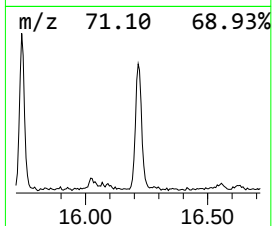
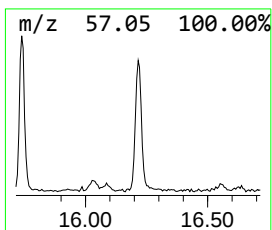
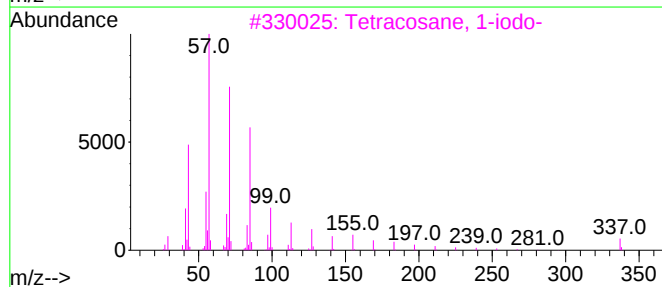
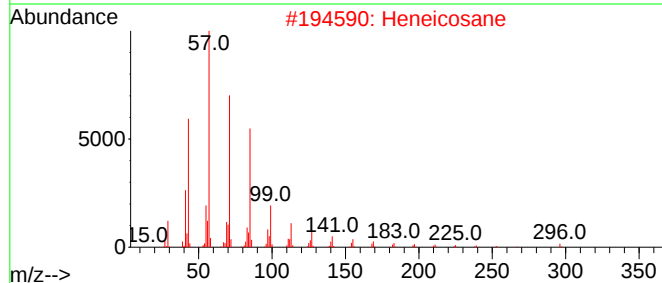
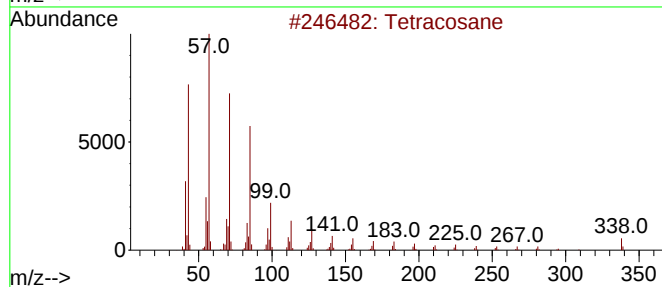
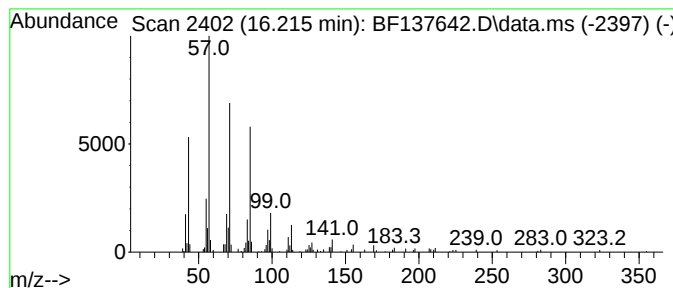
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tetracosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.215	3.29 ng	168244	Perylene-d12	15.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	90
2			Heneicosane	296	C21H44	000629-94-7	90
3			Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	86
4			Nonadecane	268	C19H40	000629-92-5	83
5			Tetratetracontane	619	C44H90	007098-22-8	81



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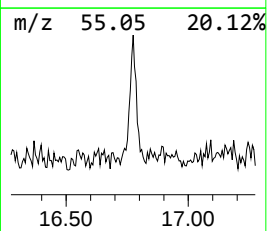
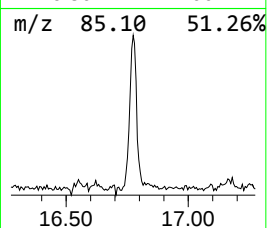
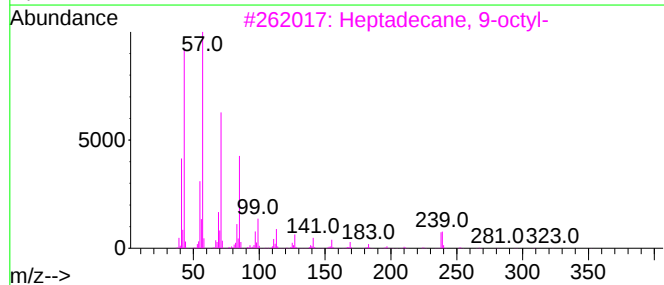
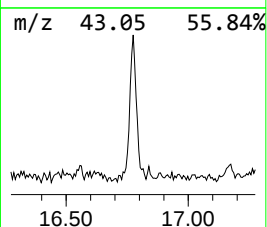
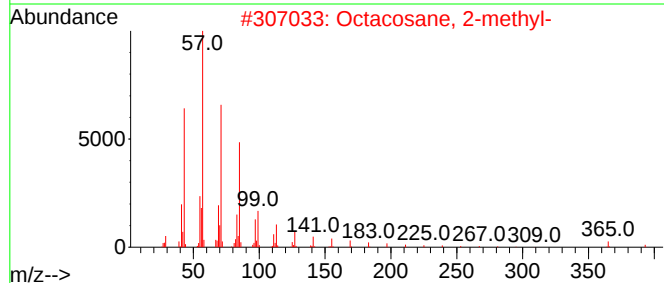
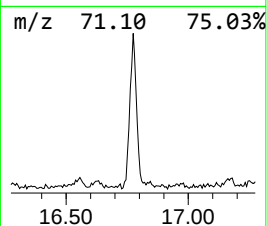
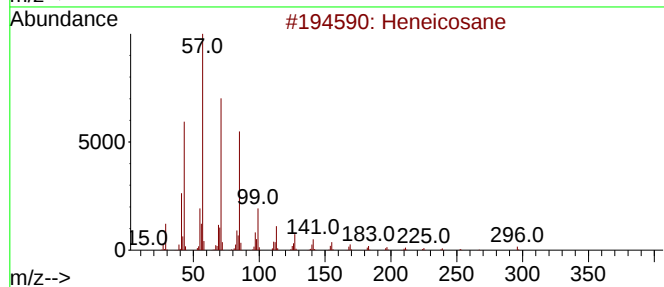
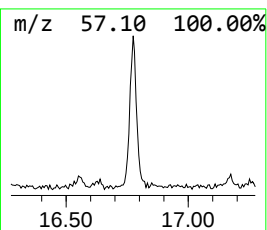
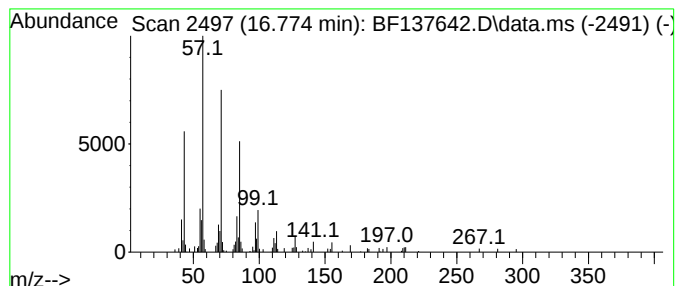
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octacosane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.774	2.43 ng	124525	Perylene-d12	15.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
5			Octacosane	394	C28H58	000630-02-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031924\
Data File : BF137642.D
Acq On : 19 Mar 2024 12:13
Operator : CG\JU
Sample : PB159643BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

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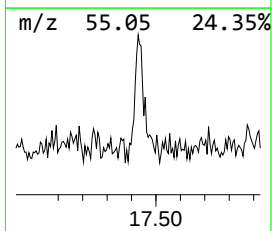
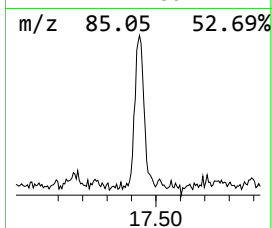
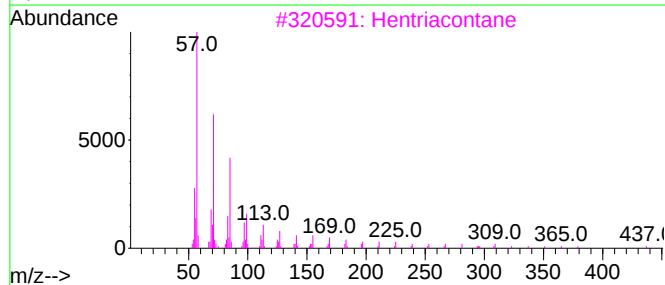
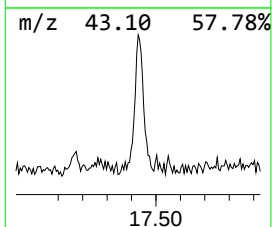
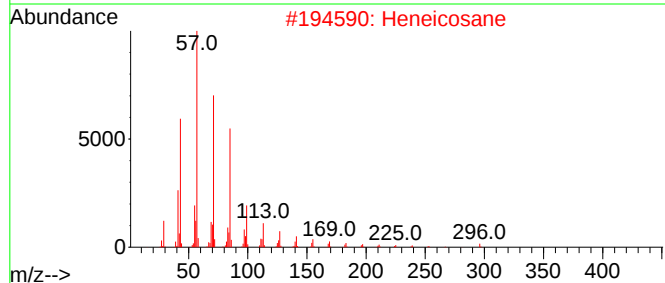
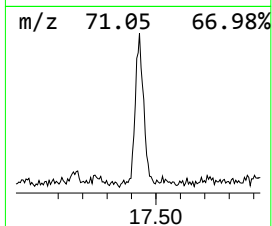
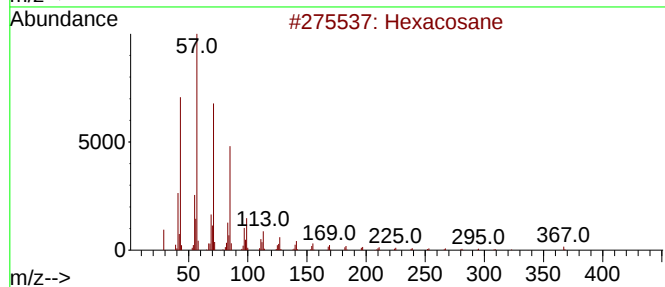
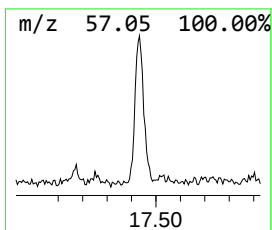
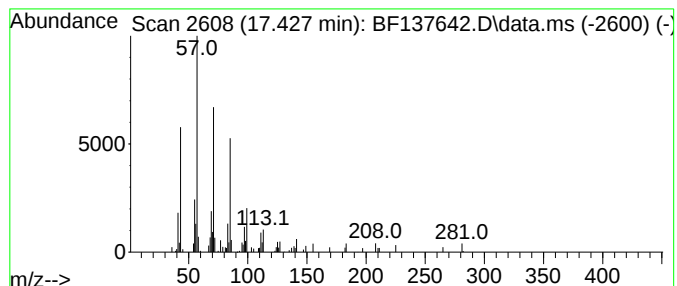
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hentriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.427	2.29 ng	117197	Perylene-d12	15.298

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexacosane	366	C26H54	000630-01-3	87
2		Heneicosane	296	C21H44	000629-94-7	87
3		Hentriacontane	437	C31H64	000630-04-6	87
4		Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
5		10-Methylnonadecane	282	C20H42	056862-62-5	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031924\
Data File : BF137642.D
Acq On : 19 Mar 2024 12:13
Operator : CG\JU
Sample : PB159643BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB159643BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.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-...	4.945	4.3	ng	270894	1	6.728	1269200	20.0
Hexadecanoic ac...	12.651	2.4	ng	157316	5	13.874	1323560	20.0
Heneicosane	14.968	2.3	ng	118412	6	15.298	1022960	20.0
Hexacosane	15.739	3.1	ng	159591	6	15.298	1022960	20.0
Tetracosane	16.215	3.3	ng	168244	6	15.298	1022960	20.0
Octacosane, 2-m...	16.774	2.4	ng	124525	6	15.298	1022960	20.0
Hentriacontane	17.427	2.3	ng	117197	6	15.298	1022960	20.0