

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031324\
 Data File : BF137572.D
 Acq On : 13 Mar 2024 09:57
 Operator : CG\JU
 Sample : PB159549BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB159549BL

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: BF137572.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.316	34	39	50	rVB	72928	114688	1.49%	0.237%
2	2.440	56	60	68	rVB	63410	89963	1.17%	0.186%
3	5.210	527	531	543	rVB	197387	301575	3.93%	0.623%
4	5.581	589	594	597	rBV	6034624	6132954	79.87%	12.667%
5	6.551	754	759	762	rBV	5498233	6224059	81.06%	12.855%
6	6.904	815	819	836	rBV	1563154	1448385	18.86%	2.991%
7	7.463	909	914	917	rBV	3862212	4089190	53.25%	8.446%
8	8.175	1030	1035	1051	rBV	1805660	1967057	25.62%	4.063%
9	9.257	1213	1219	1222	rBV	6522068	7180266	93.51%	14.830%
10	9.927	1328	1333	1337	rBV	2295334	2222210	28.94%	4.590%
11	10.727	1465	1469	1472	rBV	4331245	4076414	53.09%	8.419%
12	11.427	1584	1588	1603	rBV	2518040	2266471	29.52%	4.681%
13	12.704	1801	1805	1808	rBV	94070	77315	1.01%	0.160%
14	12.857	1827	1831	1837	rBV	272377	224980	2.93%	0.465%
15	13.039	1856	1862	1865	rBV	7131615	7678540	100.00%	15.859%
16	13.574	1949	1953	1957	rBV	168705	165238	2.15%	0.341%
17	14.092	2037	2041	2054	rBV	1912613	1803083	23.48%	3.724%
18	14.915	2177	2181	2191	rVB	104512	132473	1.73%	0.274%
19	15.292	2240	2245	2250	rBV	100804	131847	1.72%	0.272%
20	15.645	2299	2305	2313	rBV	937578	1324423	17.25%	2.735%
21	15.721	2313	2318	2325	rVB	121905	196167	2.55%	0.405%
22	16.221	2397	2403	2410	rVB	94372	158761	2.07%	0.328%
23	16.809	2495	2503	2512	rBV2	79733	179680	2.34%	0.371%
24	17.498	2613	2620	2629	rBV3	53953	150428	1.96%	0.311%
25	18.339	2756	2763	2764	rBV4	42186	82196	1.07%	0.170%

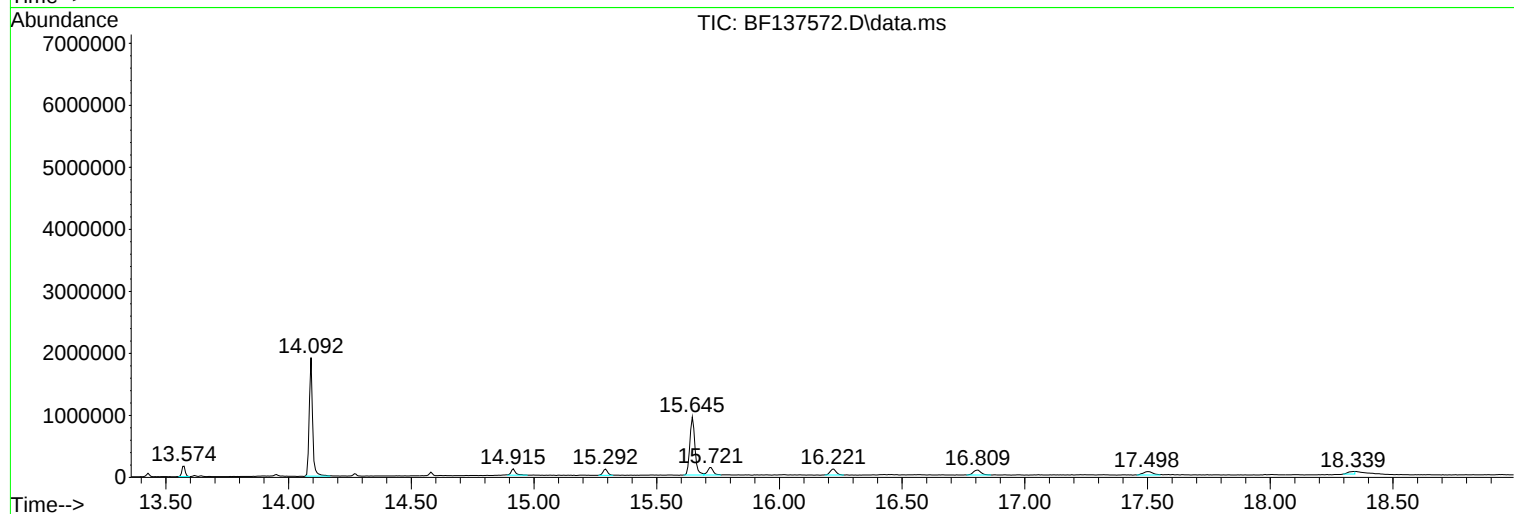
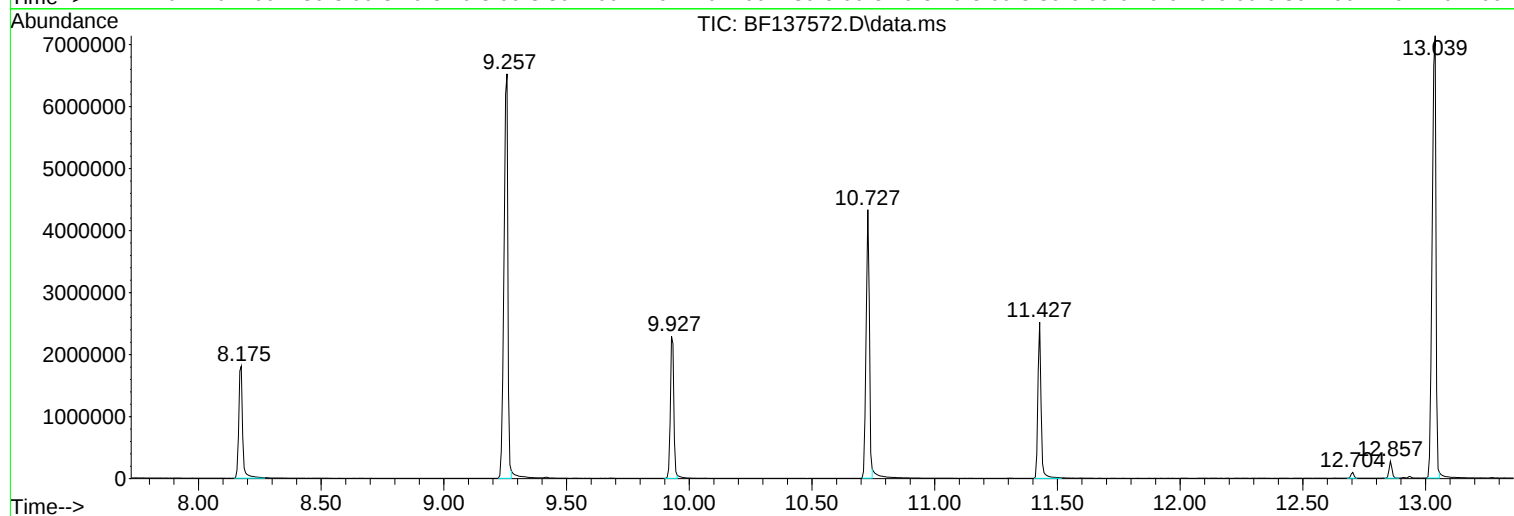
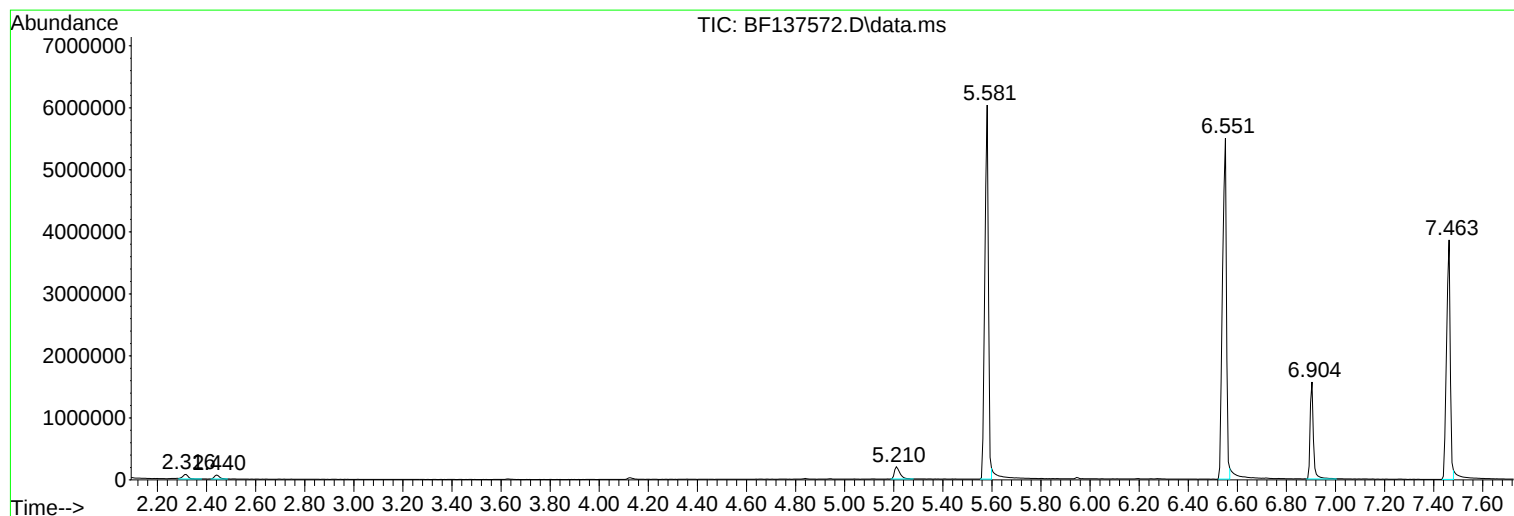
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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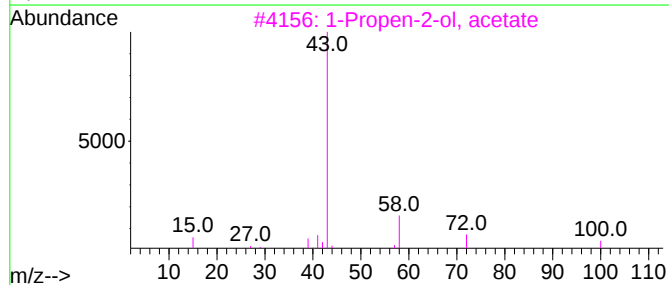
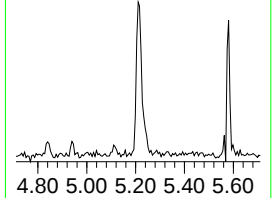
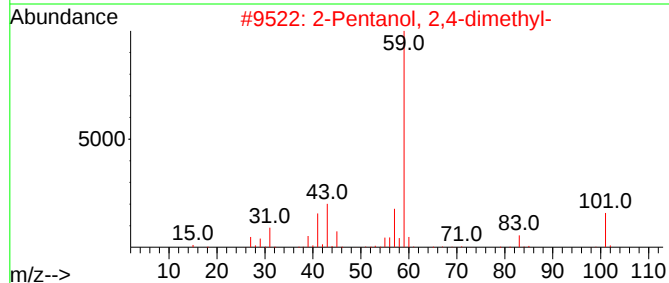
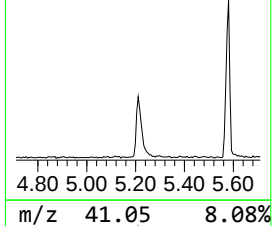
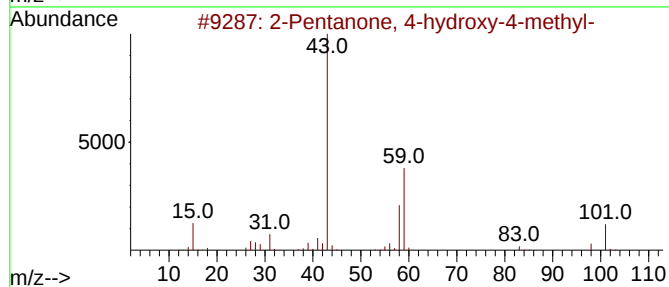
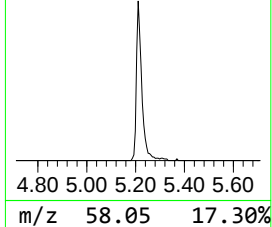
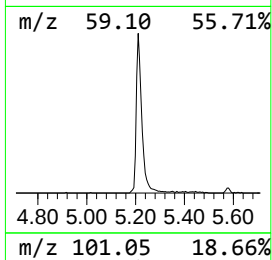
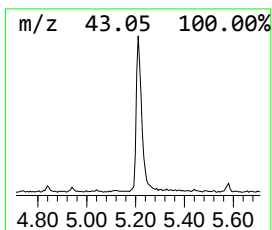
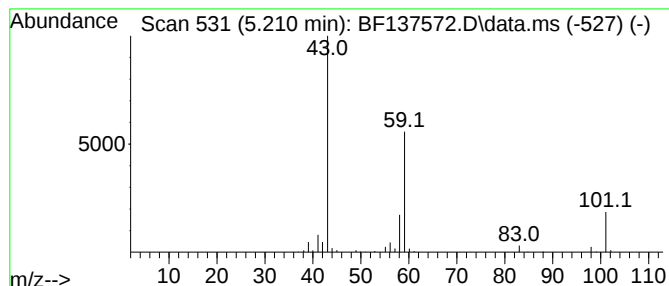
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.210	4.16 ng	301575	1,4-Dichlorobenzene-d4	6.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	28		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9		



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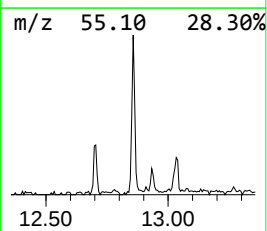
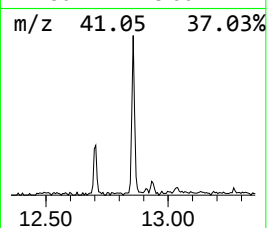
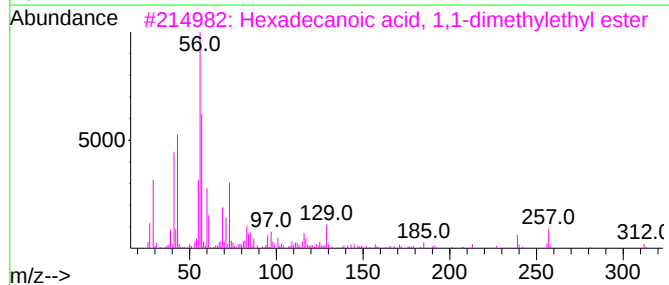
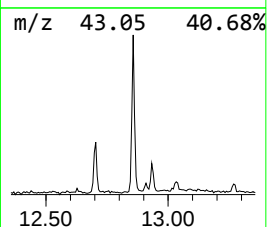
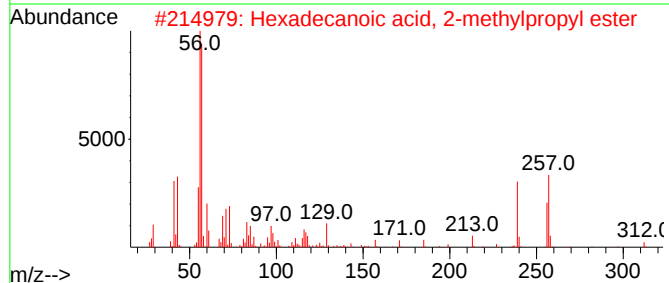
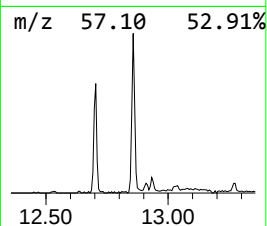
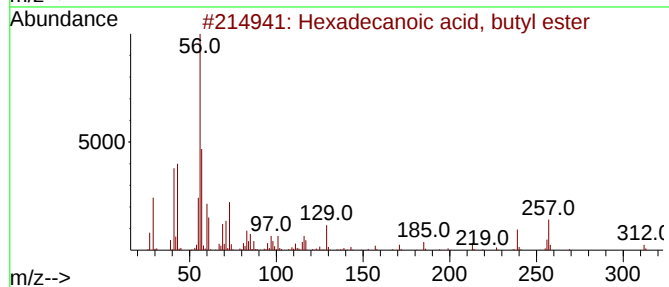
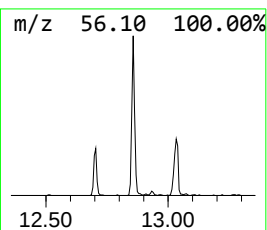
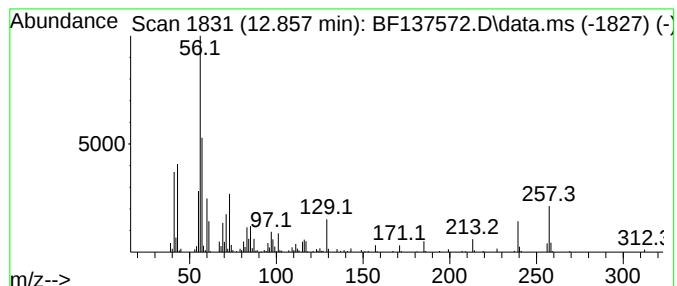
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.857	2.50 ng	224980	Chrysene-d12	14.092

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2			Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	55
3			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	43
4			Trifluoroacetic acid, 4-methylpe...	198	C8H13F3O2	000327-71-9	38
5			Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	35



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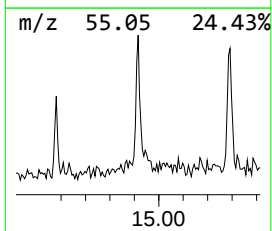
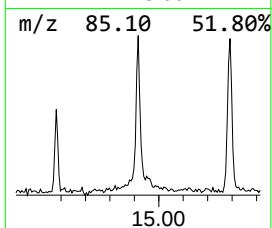
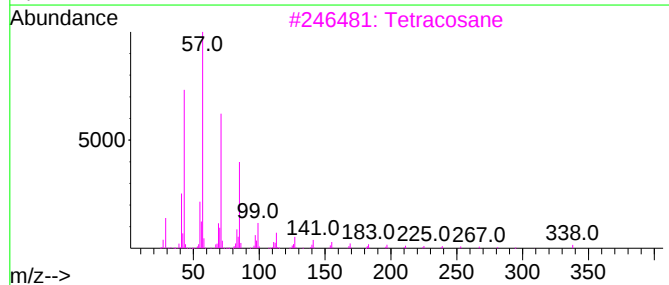
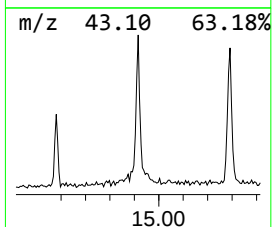
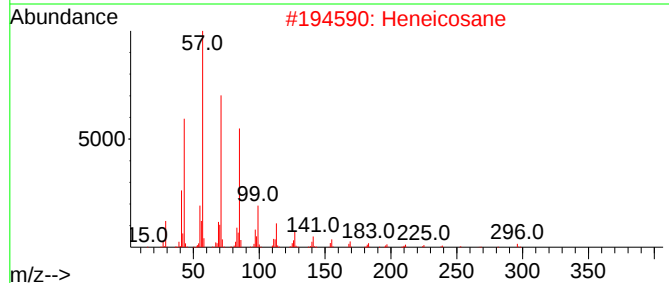
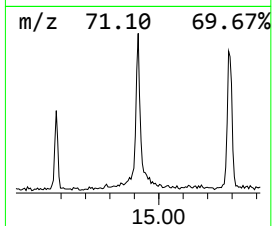
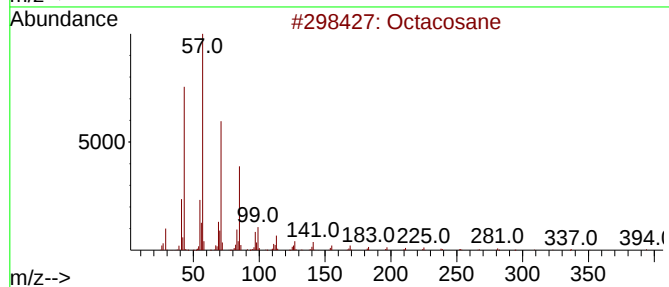
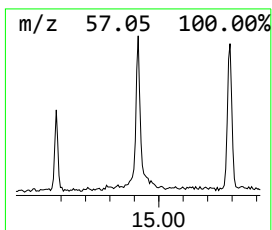
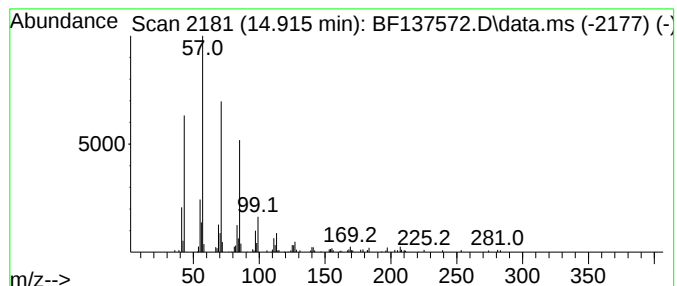
Instrument :
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.915	2.00 ng	132473	Perylene-d12	15.645	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	87
2	Heneicosane	296	C21H44	000629-94-7	86
3	Tetracosane	338	C24H50	000646-31-1	86
4	Nonadecane	268	C19H40	000629-92-5	86
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	86



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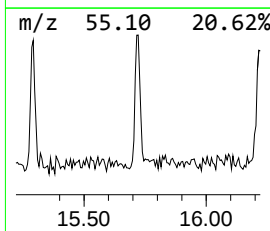
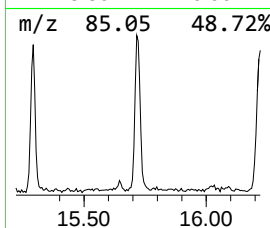
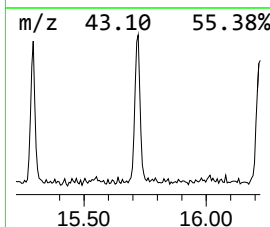
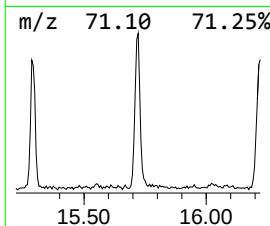
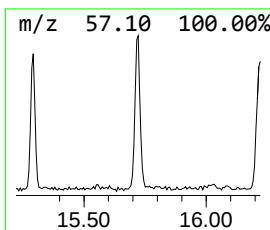
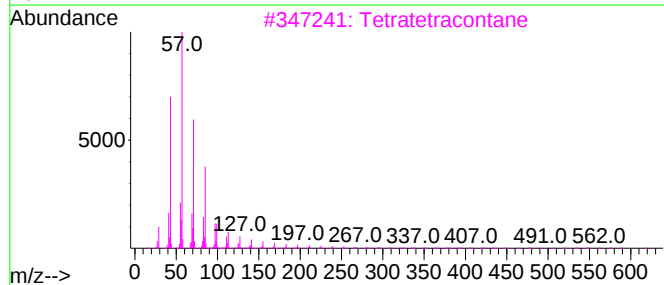
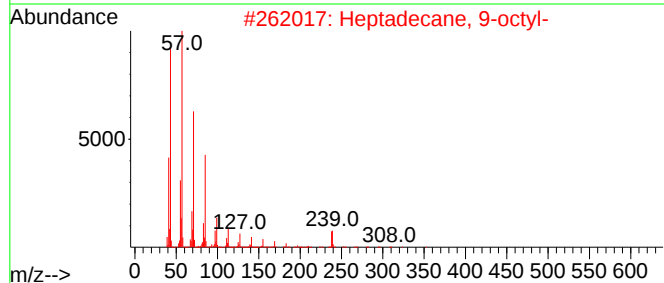
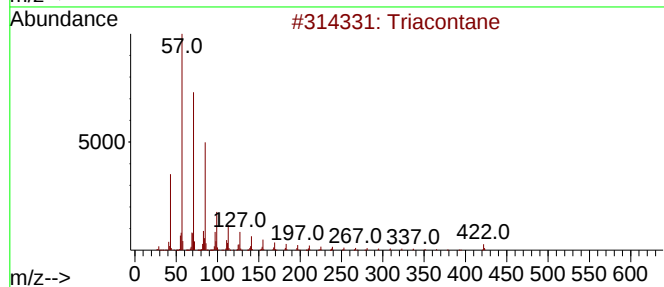
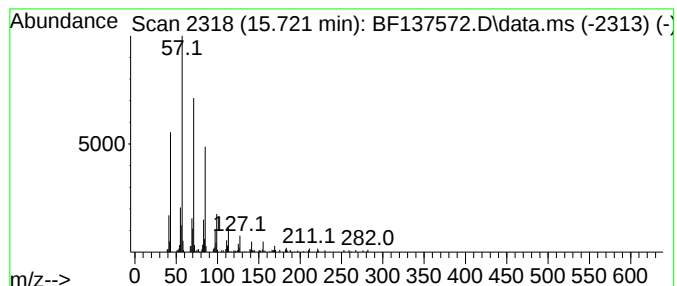
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Triacontane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.721	2.96 ng	196167	Perylene-d12	15.645

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triacontane	422	C30H62	000638-68-6	91
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3			Tetratetracontane	619	C44H90	007098-22-8	91
4			Heneicosane	296	C21H44	000629-94-7	91
5			Heptacosane	380	C27H56	000593-49-7	91



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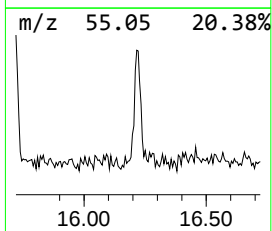
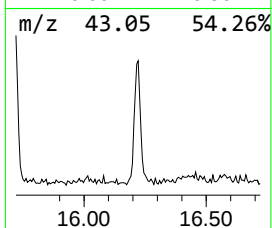
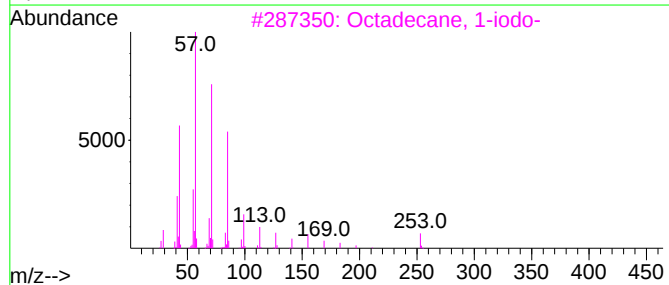
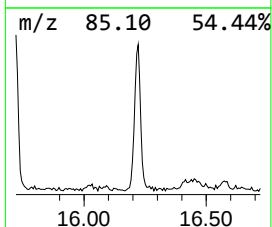
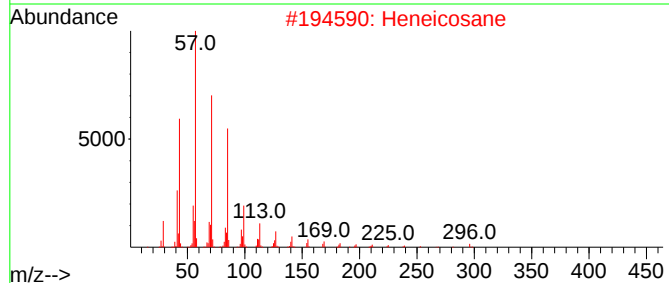
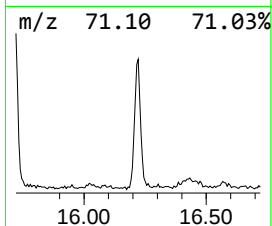
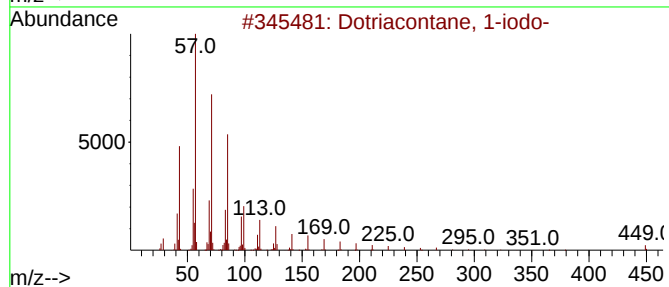
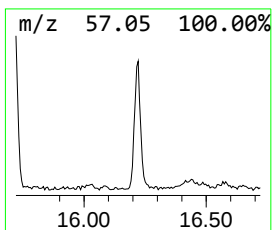
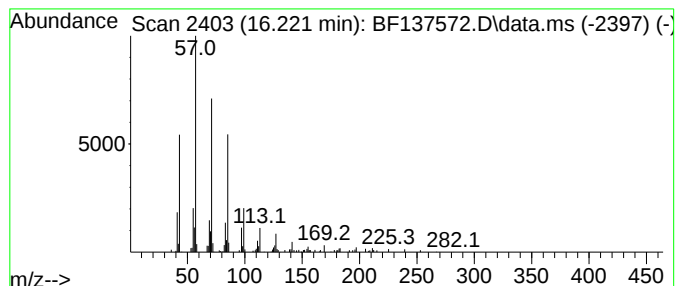
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Dotriacontane, 1-iodo- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.221	2.40 ng	158761	Perylene-d12	15.645	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
2	Heneicosane	296	C21H44	000629-94-7	90
3	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87
4	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	86
5	2-Bromotetradecane	276	C14H29Br	074036-95-6	86



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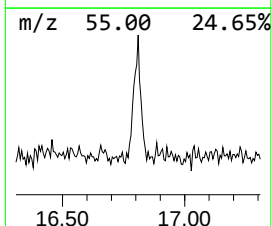
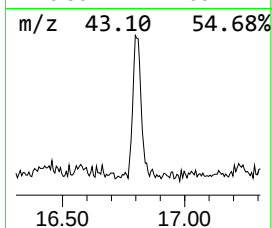
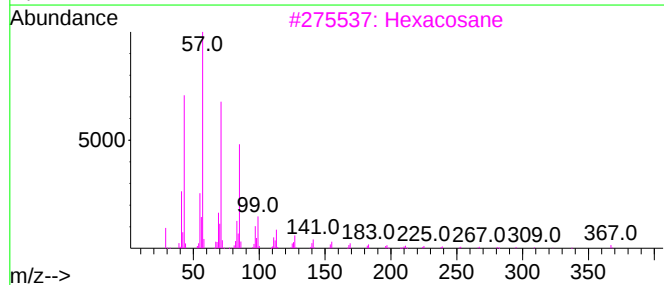
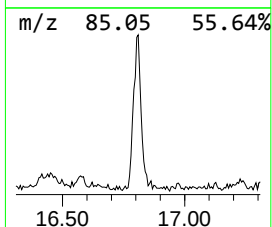
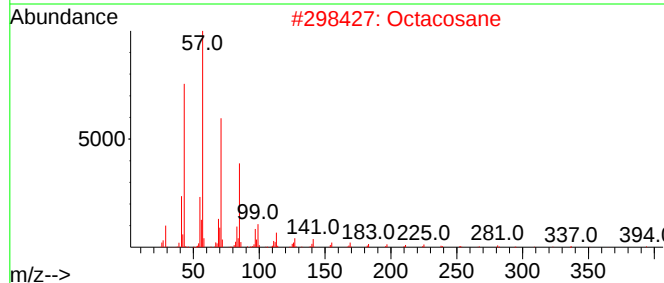
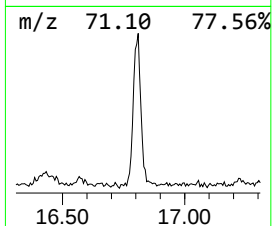
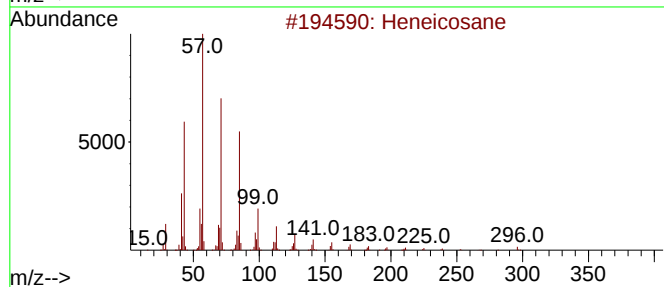
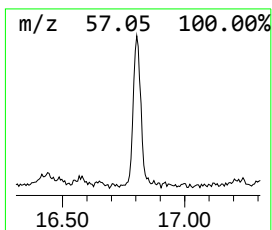
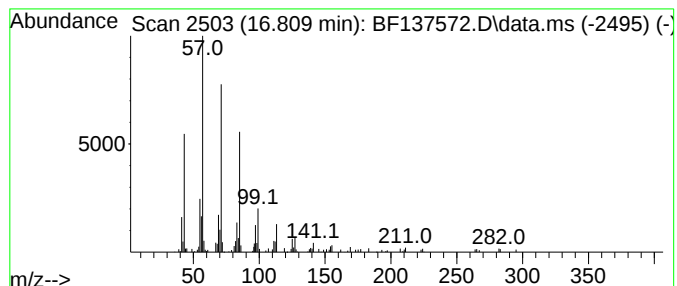
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.809	2.71 ng	179680	Perylene-d12	15.645

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Octacosane	394	C28H58	000630-02-4	90
3			Hexacosane	366	C26H54	000630-01-3	90
4			Heptadecane	240	C17H36	000629-78-7	90
5			2-Bromotetradecane	276	C14H29Br	074036-95-6	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031324\
Data File : BF137572.D
Acq On : 13 Mar 2024 09:57
Operator : CG\JU
Sample : PB159549BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

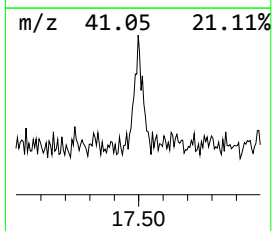
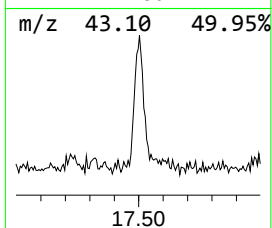
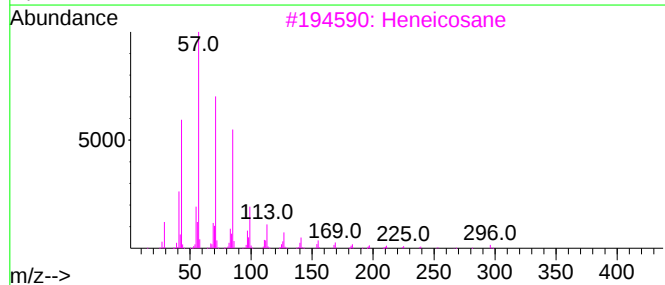
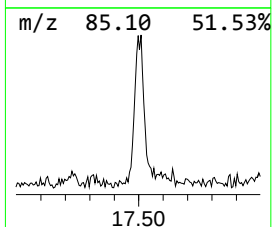
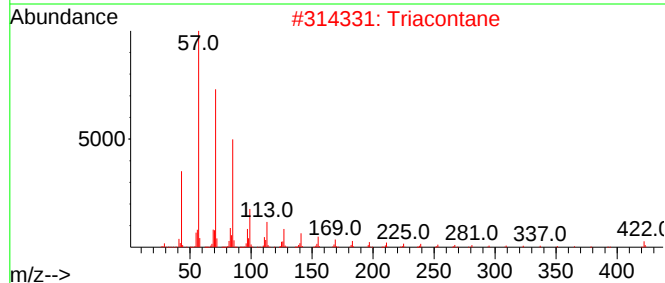
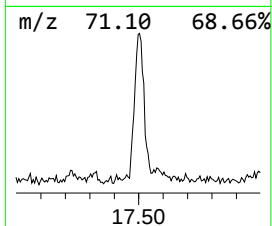
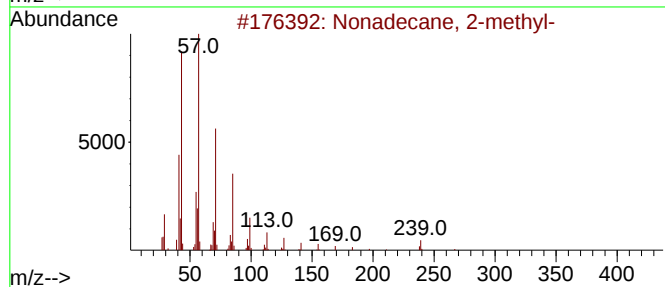
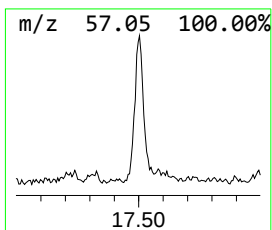
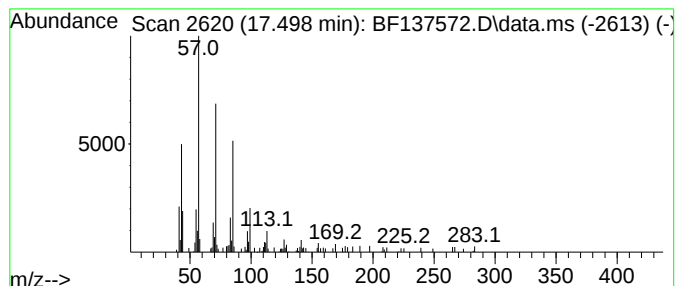
Instrument :
BNA_F
ClientSampleId :
PB159549BL

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 7 Nonadecane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
17.498	2.27 ng	150428	Perylene-d12		15.645	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Nonadecane, 2-methyl-		282	C20H42	001560-86-7	72
2	Triacontane		422	C30H62	000638-68-6	68
3	Heneicosane		296	C21H44	000629-94-7	68
4	Docosane		310	C22H46	000629-97-0	68
5	Eicosane, 1-iodo-		408	C20H41I	1000406-31-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031324\
Data File : BF137572.D
Acq On : 13 Mar 2024 09:57
Operator : CG\JU
Sample : PB159549BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB159549BL

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-...	5.210	4.2	ng	301575	1	6.904	1448390	20.0
Hexadecanoic ac...	12.857	2.5	ng	224980	5	14.092	1803080	20.0
Octacosane	14.915	2.0	ng	132473	6	15.645	1324420	20.0
Triacontane	15.721	3.0	ng	196167	6	15.645	1324420	20.0
Dotriacontane, ...	16.221	2.4	ng	158761	6	15.645	1324420	20.0
Heneicosane	16.809	2.7	ng	179680	6	15.645	1324420	20.0
Nonadecane, 2-m...	17.498	2.3	ng	150428	6	15.645	1324420	20.0