

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031424\
 Data File : BF137594.D
 Acq On : 14 Mar 2024 16:59
 Operator : CG\JU
 Sample : PB159584BL
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB159584BL

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: BF137594.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.951	482	487	498	rBV	165357	272616	4.15%	0.637%
2	5.345	549	554	557	rBV	5258759	5767735	87.72%	13.467%
3	6.363	722	727	730	rBV	4711241	5878270	89.40%	13.725%
4	6.722	785	788	799	rBV	1382792	1339068	20.36%	3.126%
5	7.292	880	885	888	rBV	3717270	3775392	57.42%	8.815%
6	8.004	1002	1006	1036	rBV	1823461	1826511	27.78%	4.265%
7	9.086	1184	1190	1193	rBV	6232896	6575497	100.00%	15.353%
8	9.757	1299	1304	1323	rBV	2269129	2002183	30.45%	4.675%
9	10.545	1434	1438	1463	rBV	3528324	3687952	56.09%	8.611%
10	11.239	1552	1556	1576	rBV	2156469	1900117	28.90%	4.436%
11	12.651	1793	1796	1802	rBV	170043	149013	2.27%	0.348%
12	12.827	1822	1826	1830	rBV	5859930	6104694	92.84%	14.253%
13	13.357	1913	1916	1920	rBV	122344	101683	1.55%	0.237%
14	13.874	2000	2004	2019	rBV	1453048	1387636	21.10%	3.240%
15	14.651	2132	2136	2142	rBV	72857	73293	1.11%	0.171%
16	14.968	2186	2190	2196	rBV	101781	120384	1.83%	0.281%
17	15.298	2241	2246	2249	rBV	836228	1097942	16.70%	2.564%
18	15.333	2249	2252	2260	rVB	149888	213698	3.25%	0.499%
19	15.745	2316	2322	2330	rBV	113325	174502	2.65%	0.407%
20	16.215	2397	2402	2412	rVB	93058	165008	2.51%	0.385%
21	16.774	2491	2497	2507	rVB	59717	123059	1.87%	0.287%
22	17.433	2603	2609	2620	rVB5	38491	93456	1.42%	0.218%

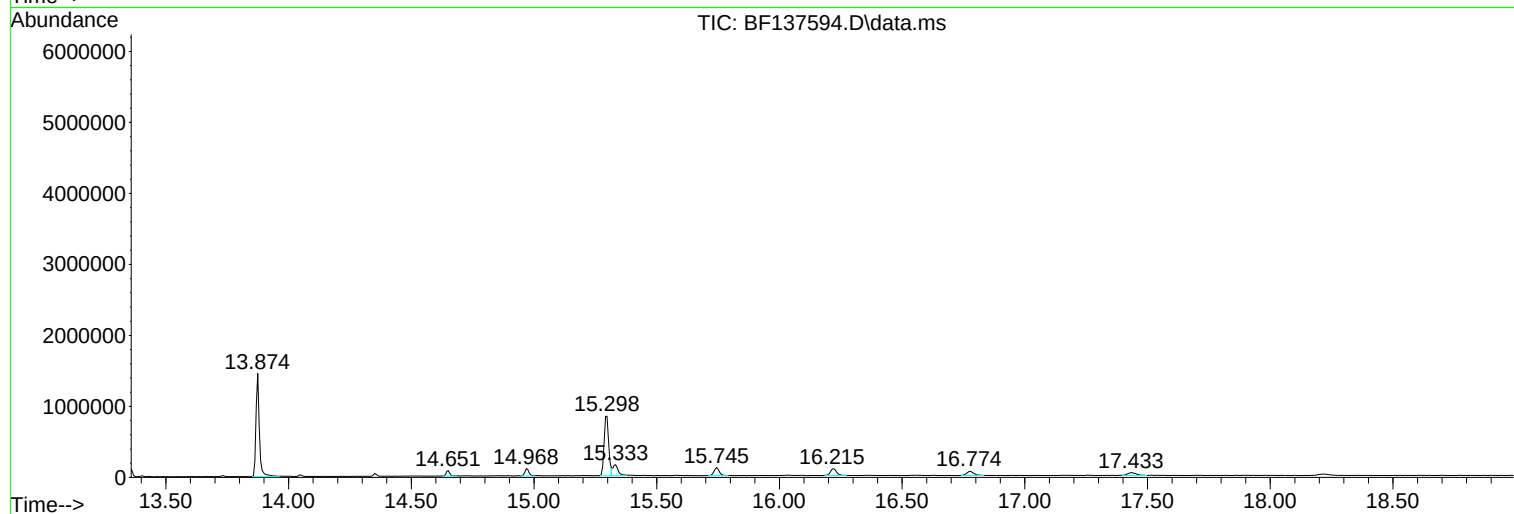
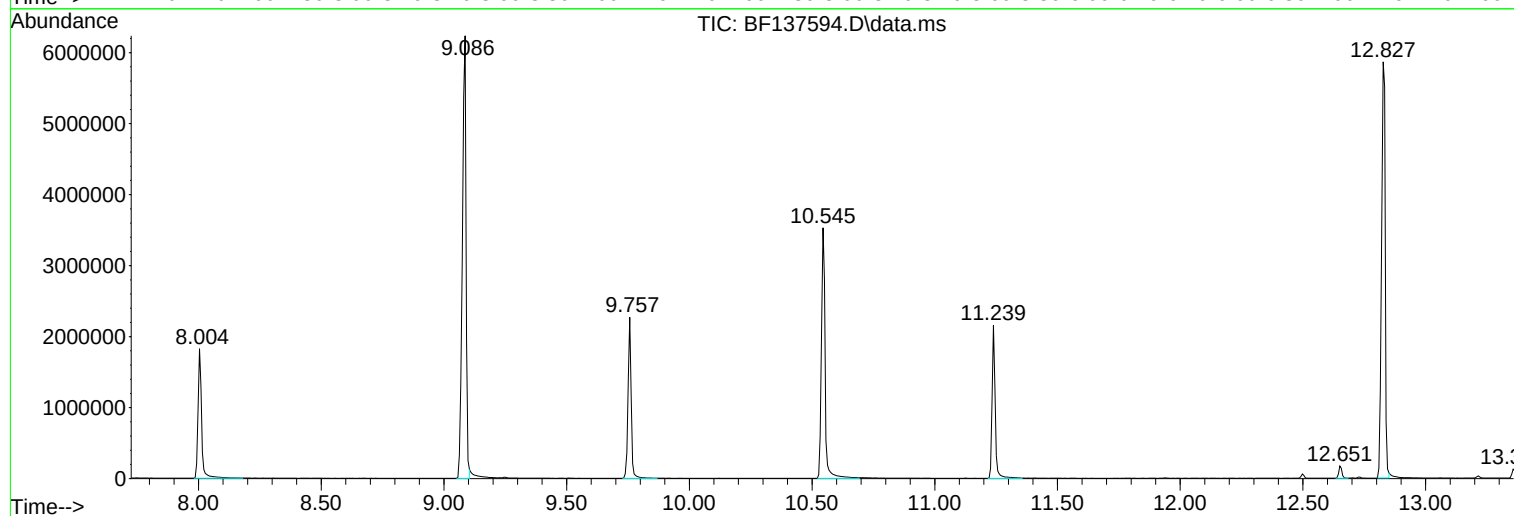
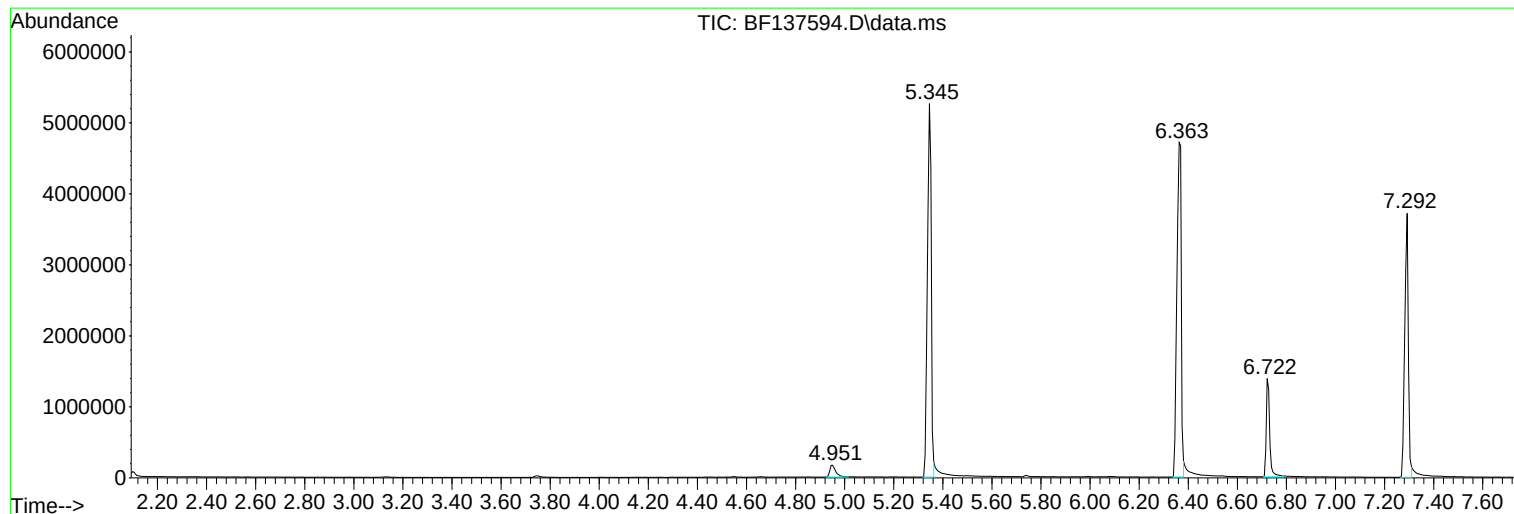
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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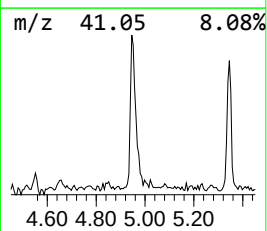
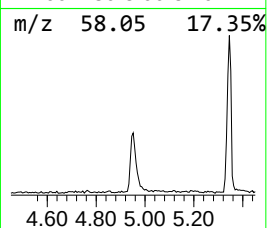
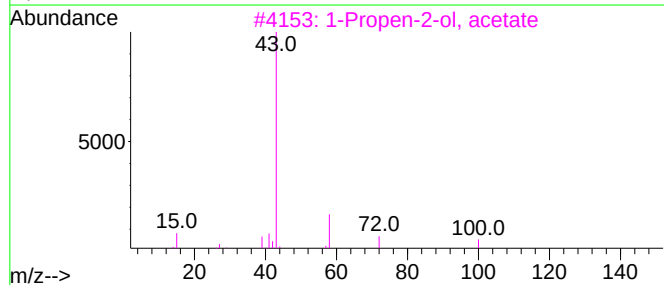
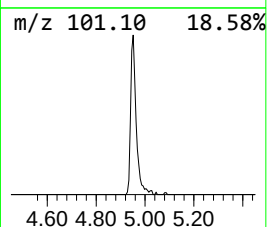
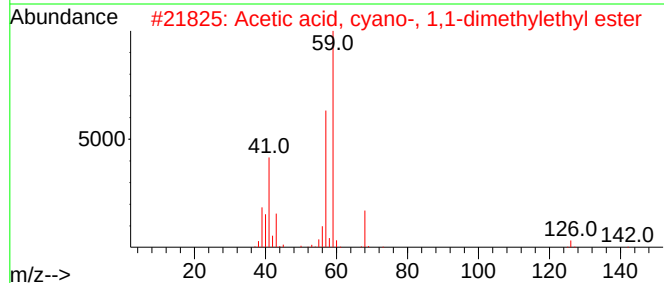
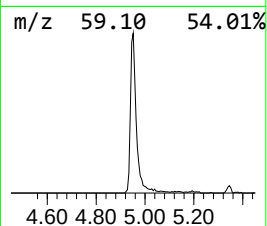
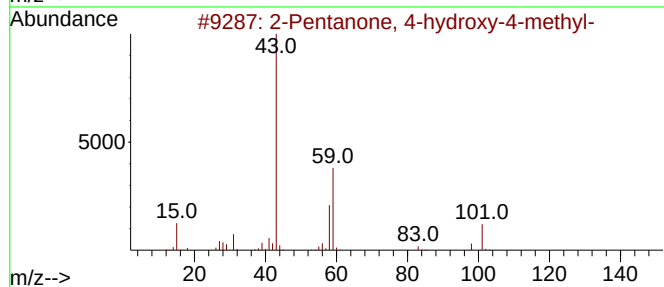
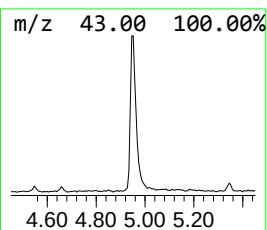
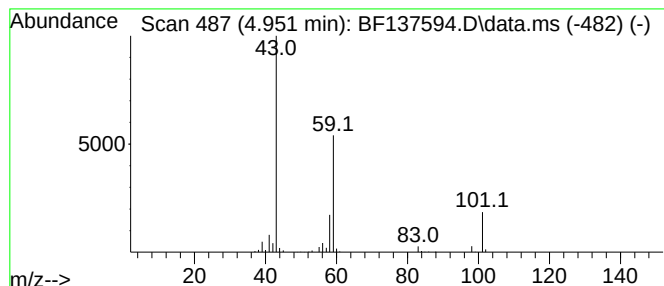
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.	
4.951	4.07 ng	272616	1,4-Dichlorobenzene-d4	6.722	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	5-Hexen-2-one	98	C6H10O	000109-49-9	10
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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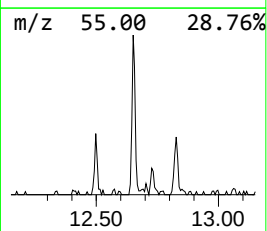
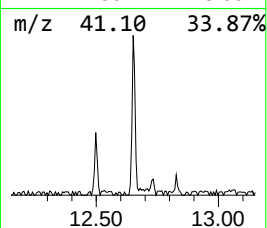
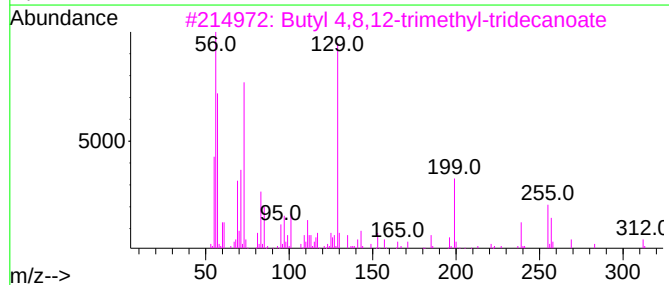
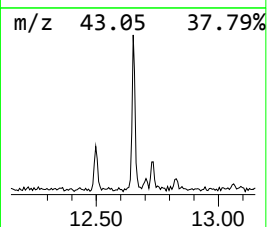
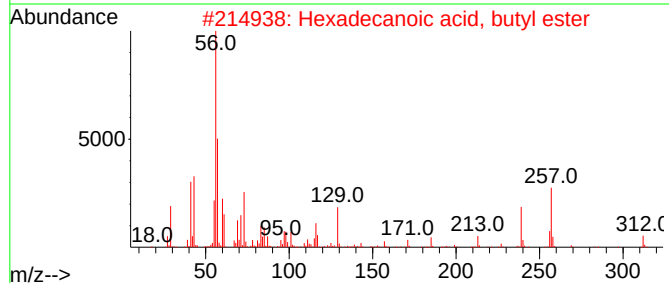
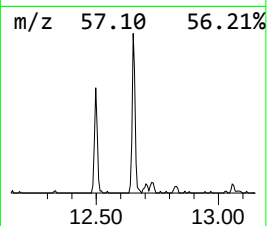
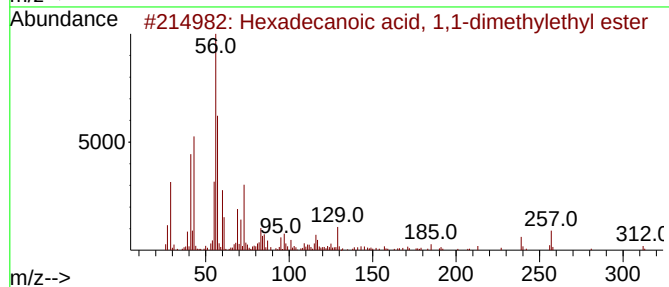
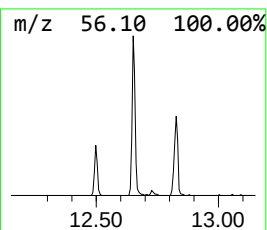
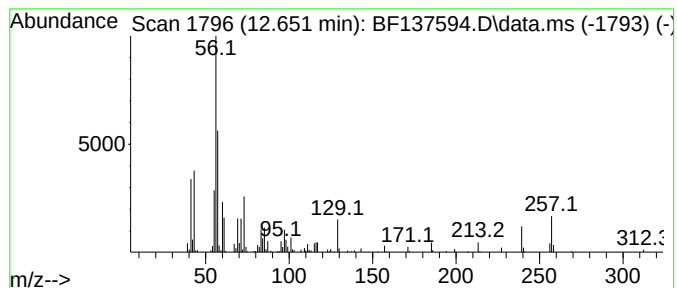
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Hexadecanoic acid, 1,1-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.651	2.15 ng	149013	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	92
2			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
3			Butyl 4,8,12-trimethyl-tridecanoate	312	C20H40O2	1000336-63-2	64
4			Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	38
5			Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38



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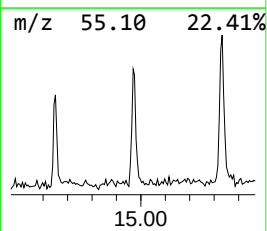
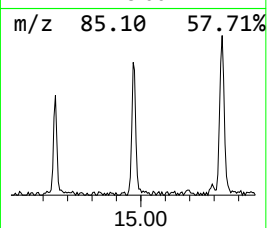
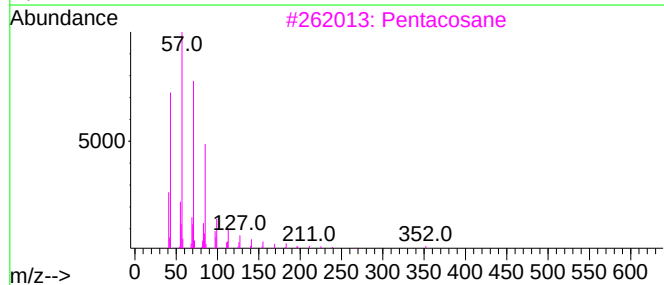
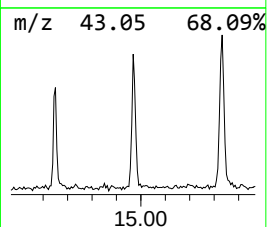
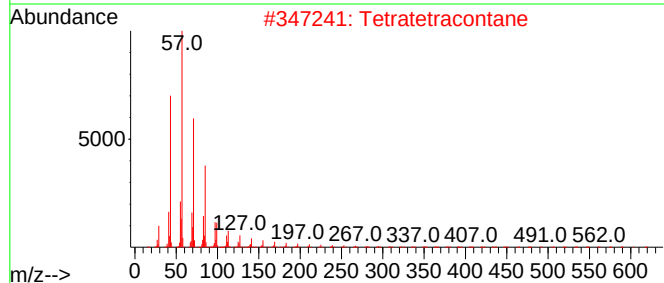
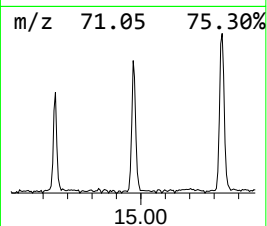
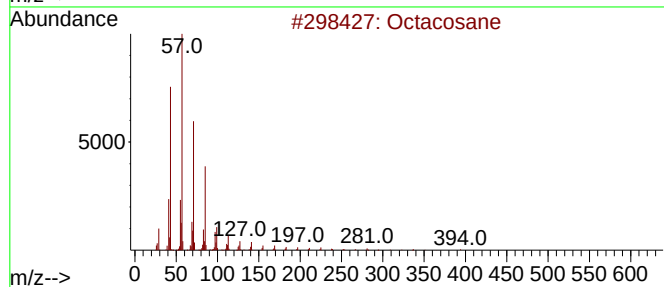
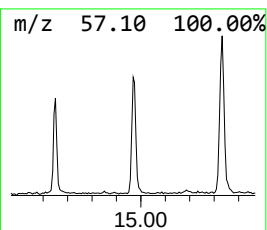
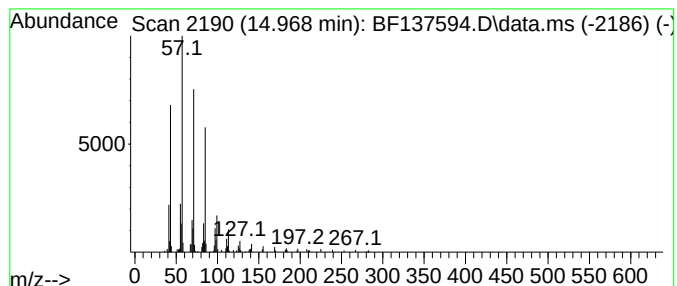
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Peak Number 3 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.968	2.19 ng	120384	Perylene-d12	15.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	87
2			Tetratetracontane	619	C44H90	007098-22-8	87
3			Pentacosane	352	C25H52	000629-99-2	83
4			Hexadecane, 5-butyl-	282	C20H42	006912-07-8	83
5			Tetracosane	338	C24H50	000646-31-1	80



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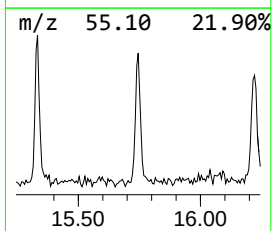
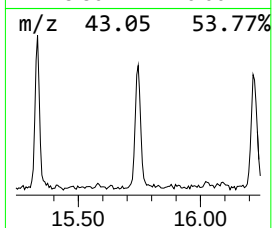
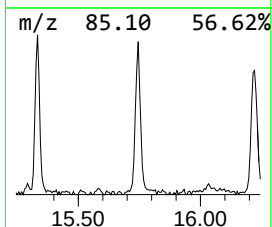
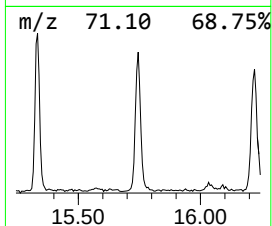
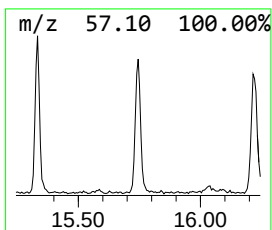
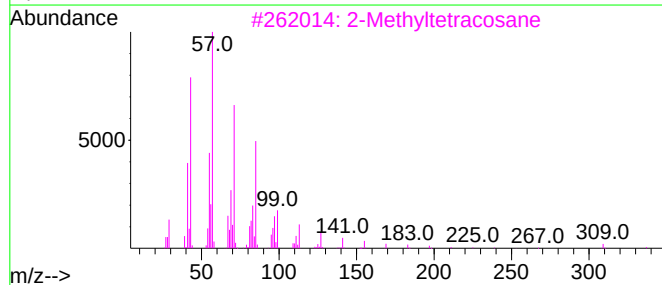
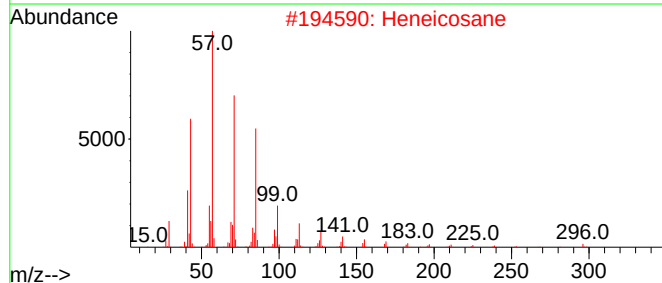
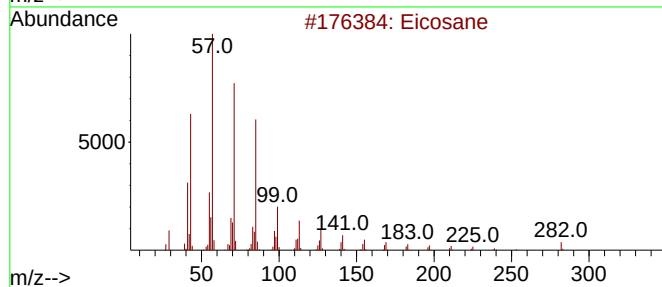
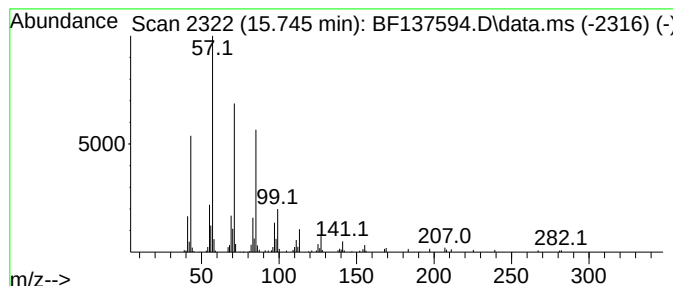
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Peak Number 4 Eicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.745	3.18 ng	174502	Perylene-d12	15.298	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Heneicosane	296	C21H44	000629-94-7	91
3	2-Methyltetracosane	352	C25H52	001560-78-7	90
4	Hexacosane	366	C26H54	000630-01-3	87
5	2-Bromotetradecane	276	C14H29Br	074036-95-6	86



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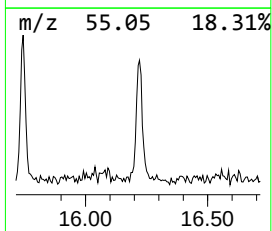
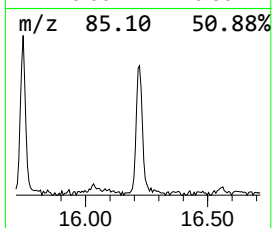
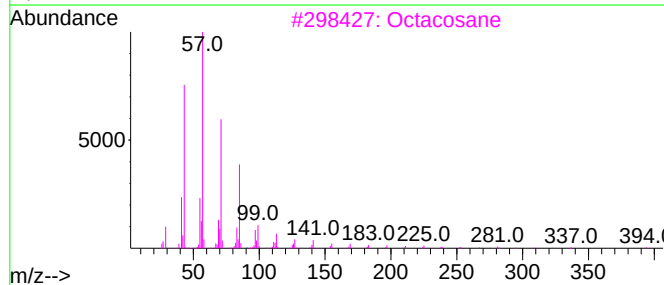
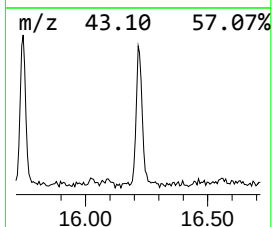
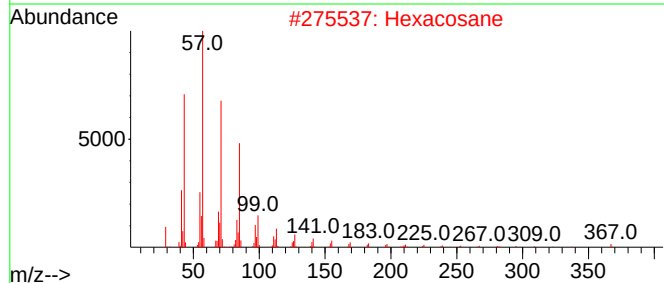
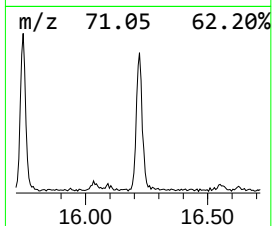
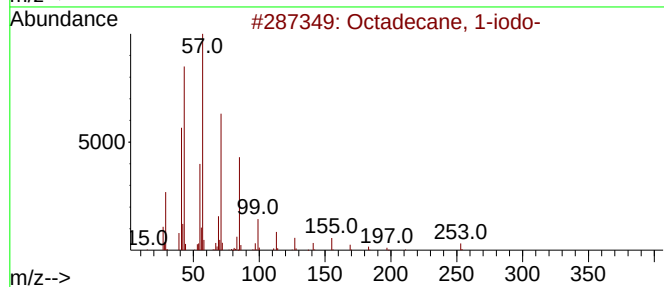
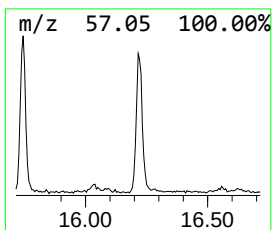
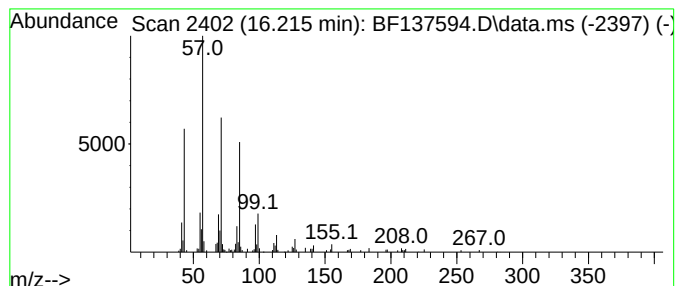
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecane, 1-iodo- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.215	3.01 ng	165008	Perylene-d12	15.298

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	83
2		Hexacosane	366	C26H54	000630-01-3	76
3		Octacosane	394	C28H58	000630-02-4	74
4		Heneicosane	296	C21H44	000629-94-7	74
5		Hentriacontane	437	C31H64	000630-04-6	72



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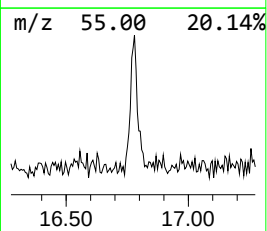
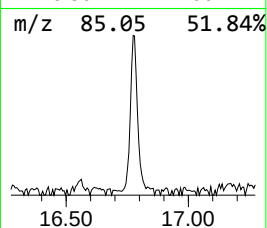
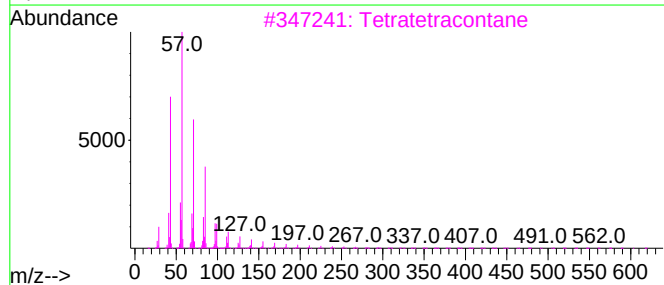
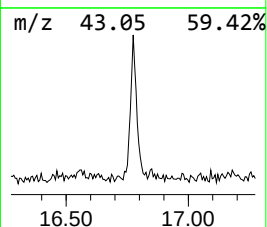
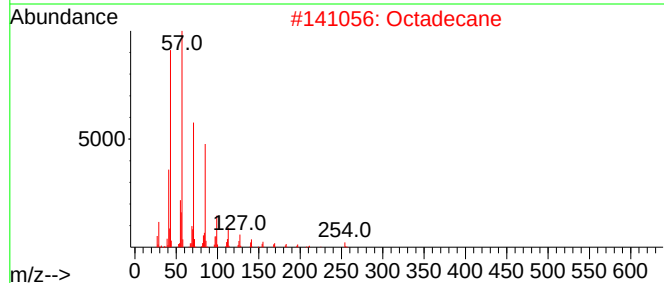
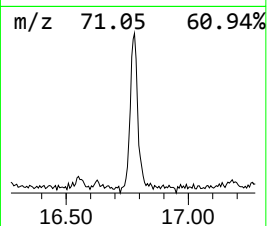
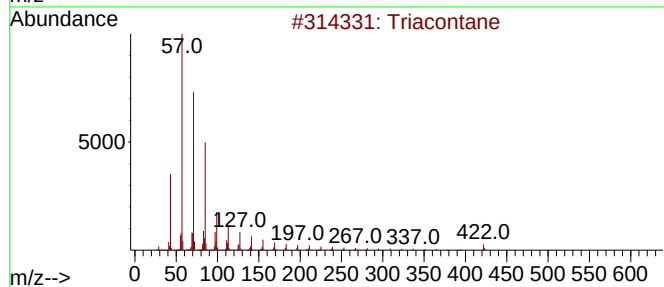
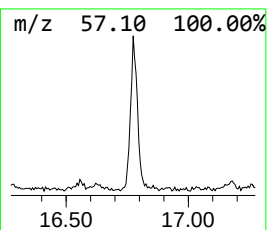
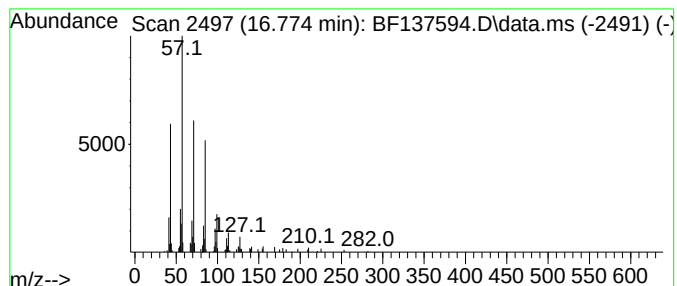
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triacontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.774	2.24 ng	123059	Perylene-d12	15.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triacontane	422	C30H62	000638-68-6	90
2			Octadecane	254	C18H38	000593-45-3	86
3			Tetratetracontane	619	C44H90	007098-22-8	83
4			Hentriacontane	437	C31H64	000630-04-6	72
5			Hexacosane	366	C26H54	000630-01-3	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031424\
Data File : BF137594.D
Acq On : 14 Mar 2024 16:59
Operator : CG\JU
Sample : PB159584BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB159584BL

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.951	4.1	ng	272616	1	6.722	1339070	20.0
Hexadecanoic ac...	12.651	2.1	ng	149013	5	13.874	1387640	20.0
Octacosane	14.968	2.2	ng	120384	6	15.298	1097940	20.0
Eicosane	15.745	3.2	ng	174502	6	15.298	1097940	20.0
Octadecane, 1-i...	16.215	3.0	ng	165008	6	15.298	1097940	20.0
triacontane	16.774	2.2	ng	123059	6	15.298	1097940	20.0