

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031124\
 Data File : BF137554.D
 Acq On : 11 Mar 2024 13:41
 Operator : CG\JU
 Sample : PB159519BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB159519BL

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: BF137554.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.328	35	41	47	rVB	79322	112397	1.34%	0.217%
2	2.452	58	62	72	rVB	65763	101826	1.22%	0.197%
3	5.210	528	531	543	rBV	203650	317351	3.79%	0.614%
4	5.581	589	594	597	rBV	6027607	6262029	74.74%	12.107%
5	6.551	753	759	762	rBV	5663631	6506866	77.66%	12.580%
6	6.904	815	819	837	rBV	1602938	1491900	17.81%	2.884%
7	7.463	909	914	944	rBV	4012562	4505956	53.78%	8.711%
8	8.175	1030	1035	1051	rBV	1860156	2047173	24.43%	3.958%
9	9.257	1213	1219	1222	rBV	6772023	7526004	89.83%	14.550%
10	9.933	1328	1334	1337	rBV	2456003	2375445	28.35%	4.593%
11	10.727	1464	1469	1495	rBV	4452098	4754936	56.75%	9.193%
12	11.427	1584	1588	1608	rBV	2765371	2536205	30.27%	4.903%
13	12.863	1828	1832	1836	rBV	260473	239402	2.86%	0.463%
14	13.039	1857	1862	1865	rBV	8116752	8378159	100.00%	16.198%
15	13.574	1949	1953	1957	rBV	207264	168880	2.02%	0.326%
16	14.092	2037	2041	2054	rBV	2090921	1968637	23.50%	3.806%
17	14.921	2175	2182	2191	rBV	103464	174536	2.08%	0.337%
18	15.292	2240	2245	2252	rBV	96102	123364	1.47%	0.239%
19	15.645	2300	2305	2313	rBV	1012676	1458997	17.41%	2.821%
20	15.721	2314	2318	2325	rVB	106258	157977	1.89%	0.305%
21	16.221	2398	2403	2410	rBV	79621	143346	1.71%	0.277%
22	16.809	2497	2503	2511	rVB	72966	148607	1.77%	0.287%
23	17.509	2615	2622	2633	rBV3	48668	113842	1.36%	0.220%
24	18.350	2756	2765	2766	rBV4	55230	110529	1.32%	0.214%

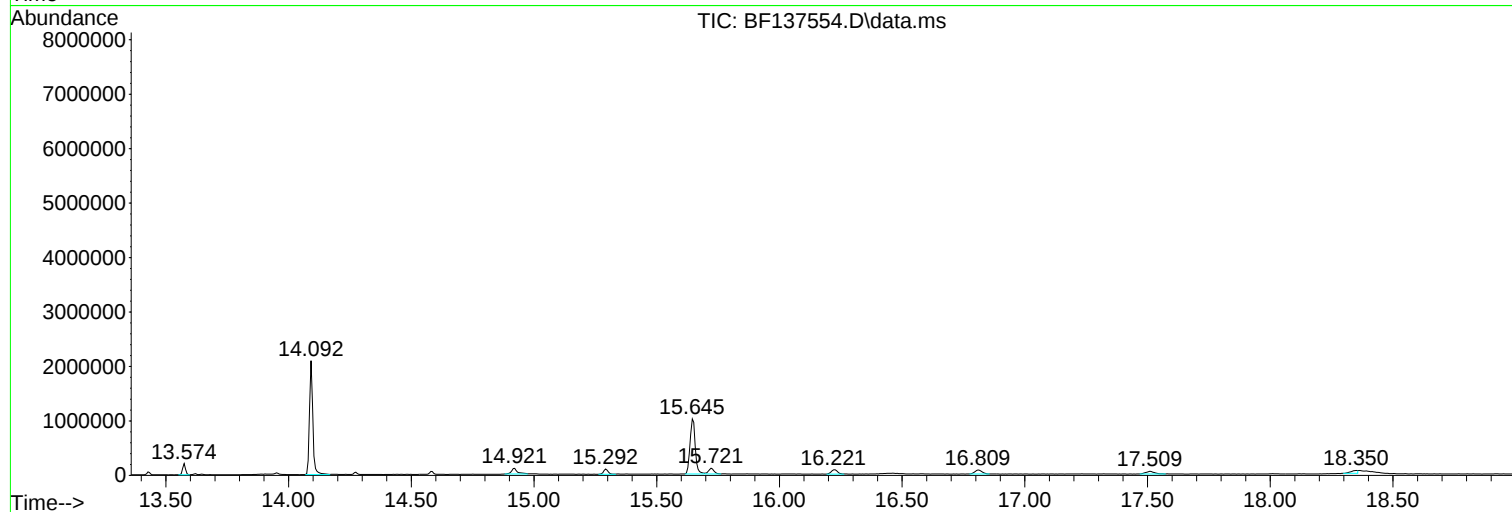
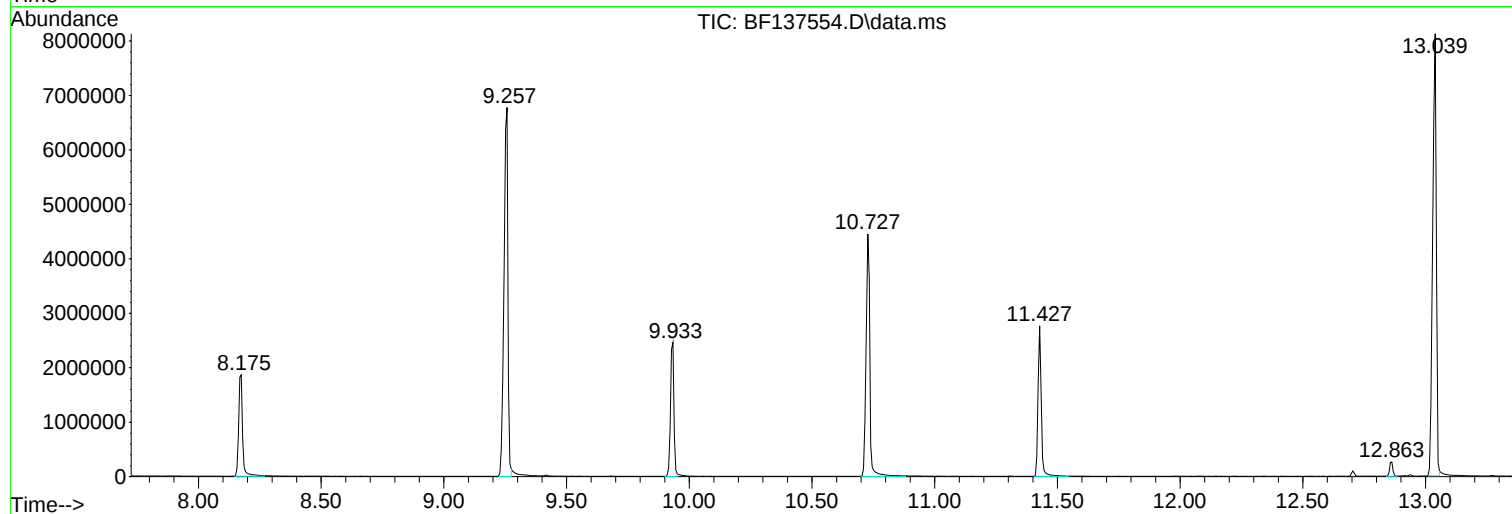
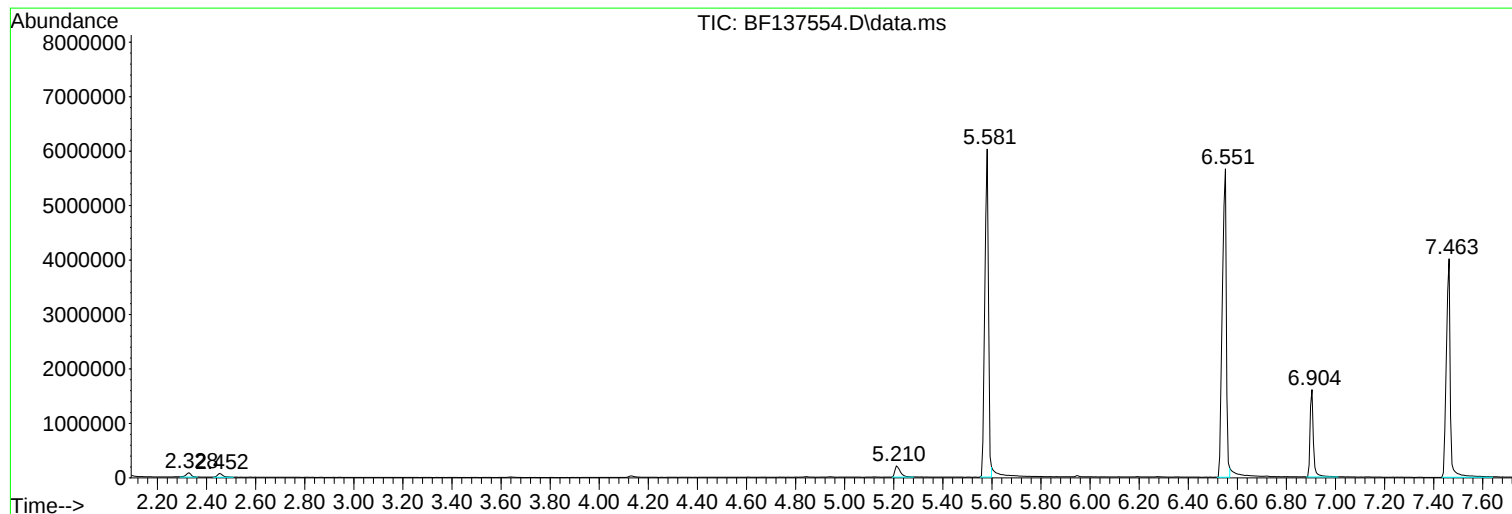
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Instrument :
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ClientSampleId :
PB159519BL

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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Misc :
ALS Vial : 3 Sample Multiplier: 1

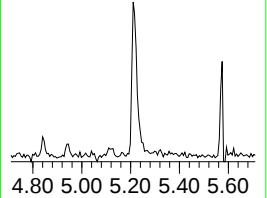
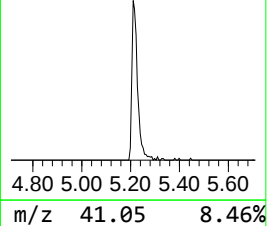
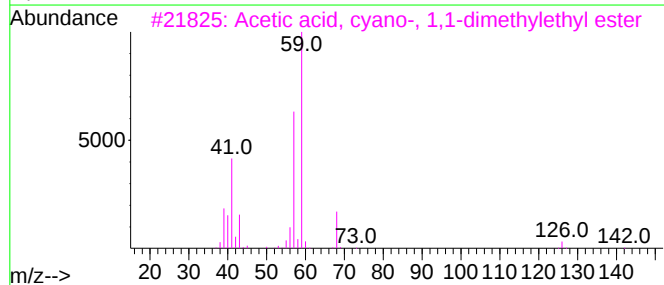
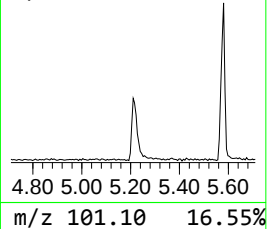
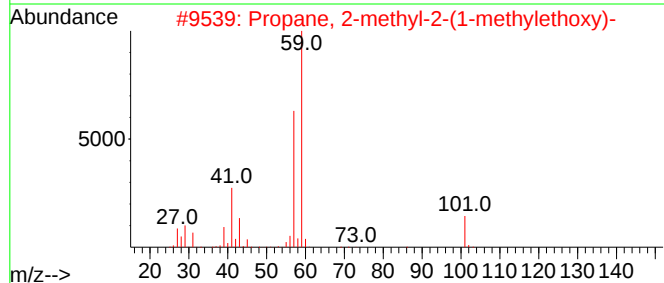
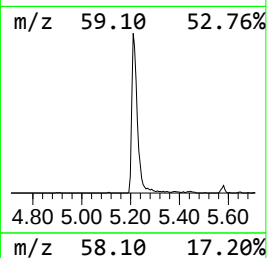
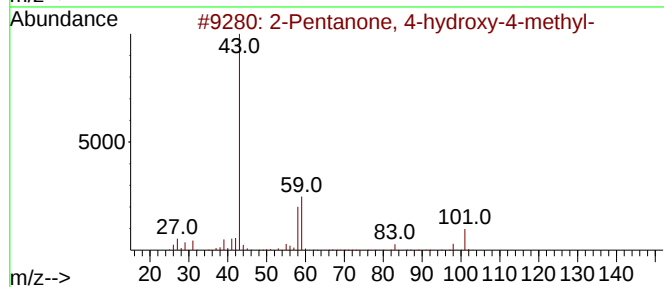
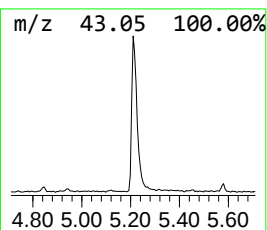
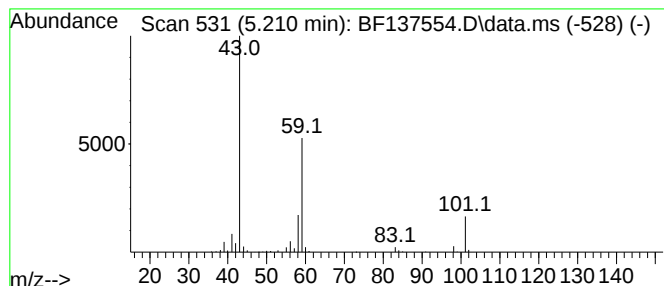
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.210	4.25 ng	317351	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	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12



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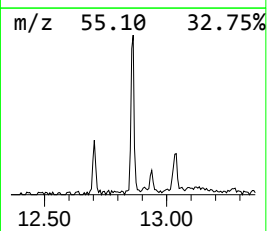
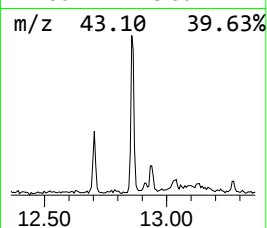
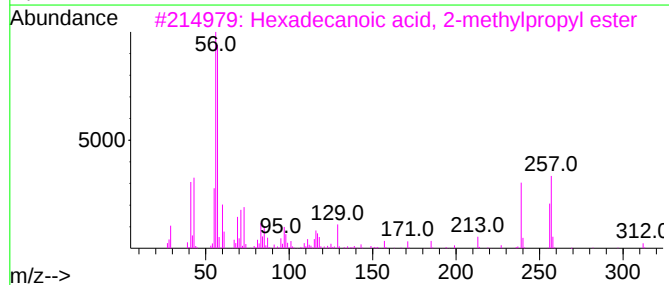
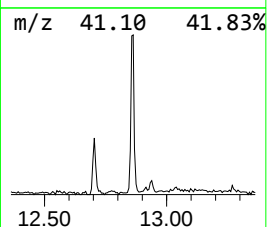
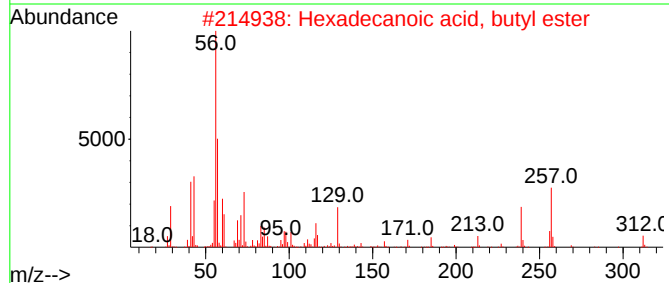
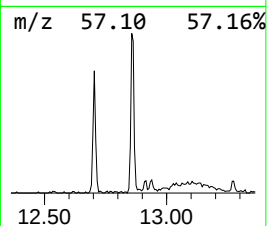
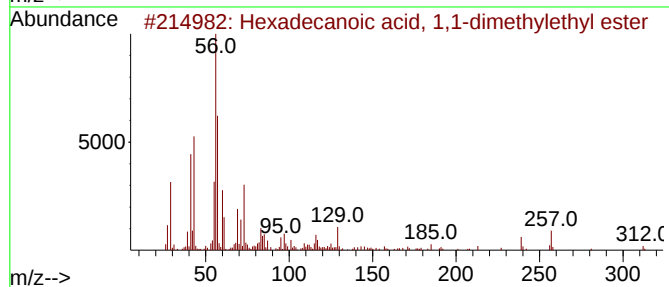
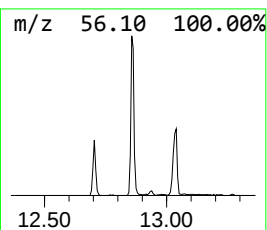
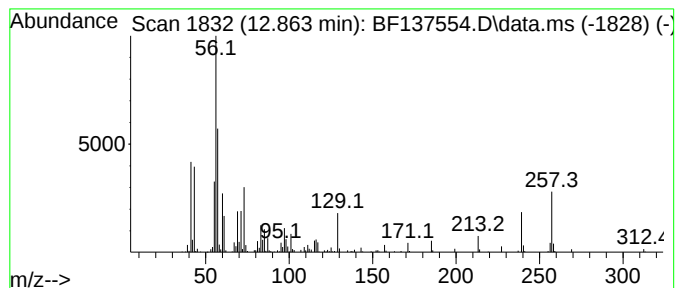
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.863	2.43 ng	239402	Chrysene-d12	14.092	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	96
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	90
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	87
4	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
5	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	35



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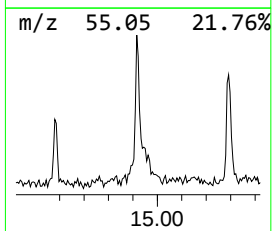
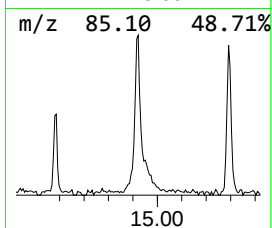
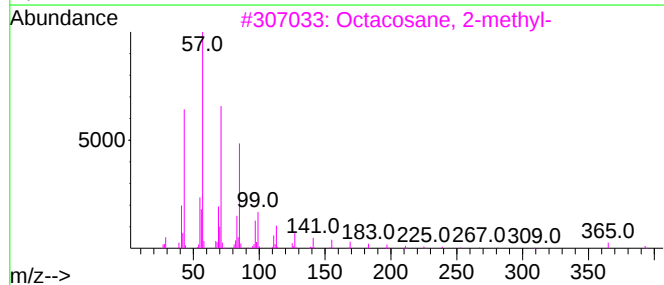
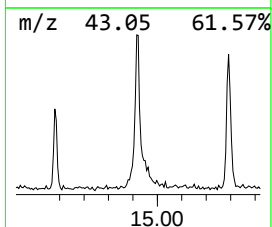
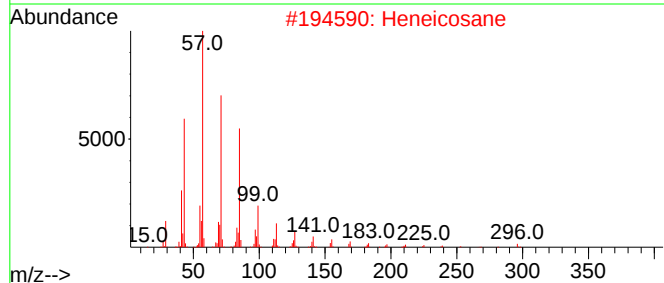
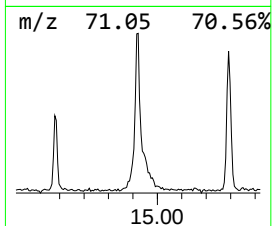
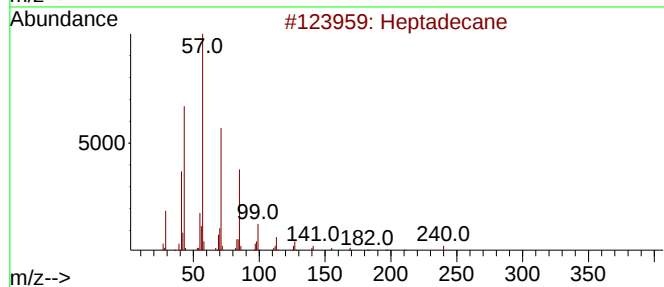
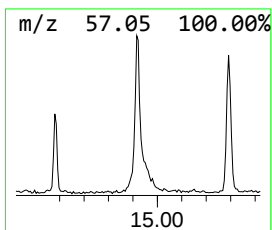
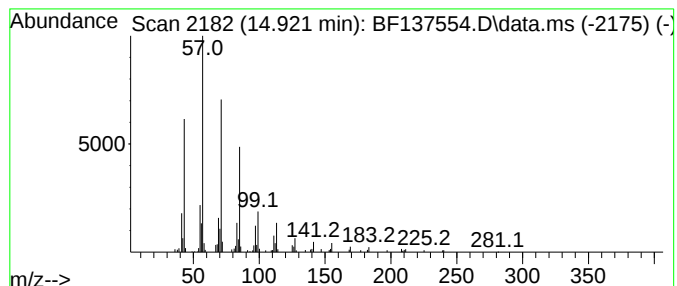
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Heptadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.921	2.39 ng	174536	Perylene-d12	15.645

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	94
2			Heneicosane	296	C21H44	000629-94-7	91
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4			Tetratetracontane	619	C44H90	007098-22-8	91
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



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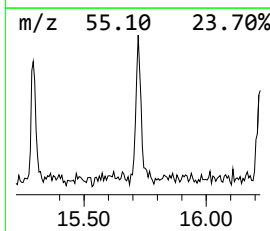
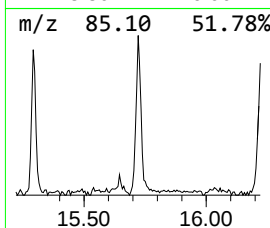
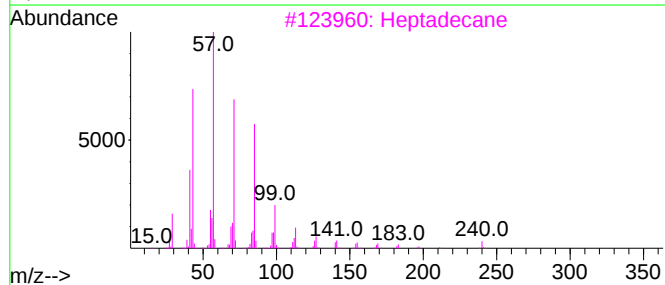
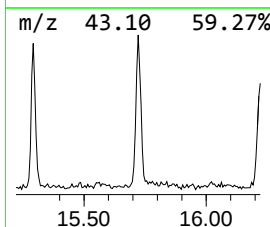
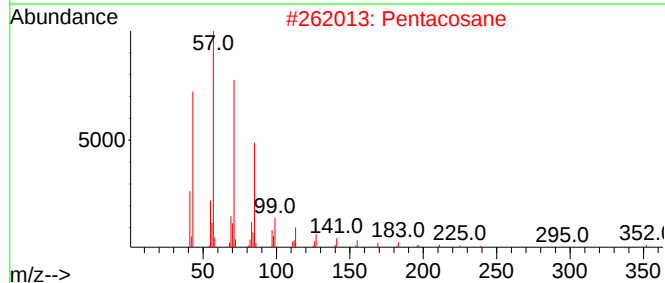
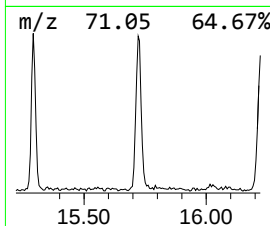
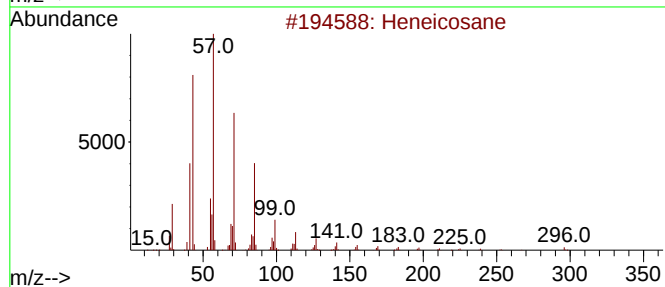
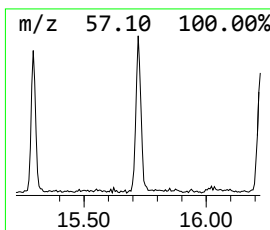
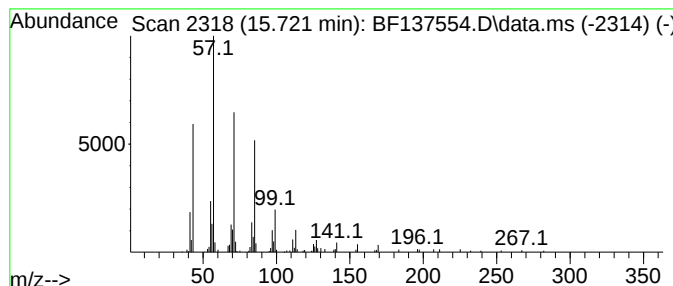
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.721	2.17 ng	157977	Perylene-d12	15.645

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Pentacosane	352	C25H52	000629-99-2	87
3			Heptadecane	240	C17H36	000629-78-7	87
4			Hexacosane	366	C26H54	000630-01-3	83
5			Hexadecane	226	C16H34	000544-76-3	80



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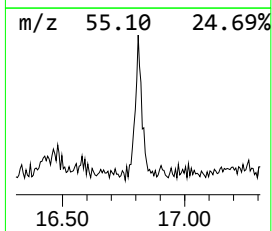
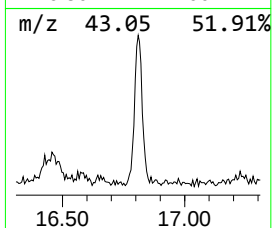
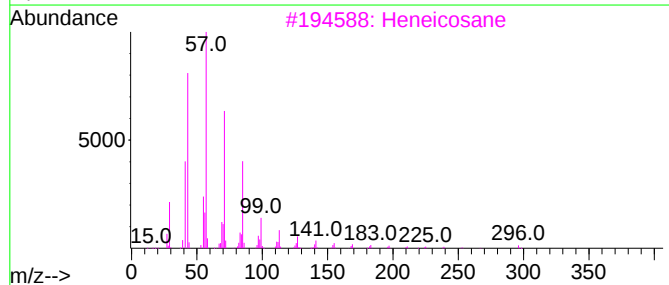
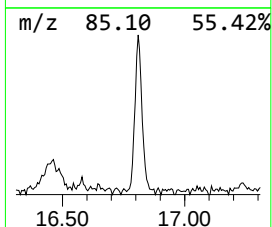
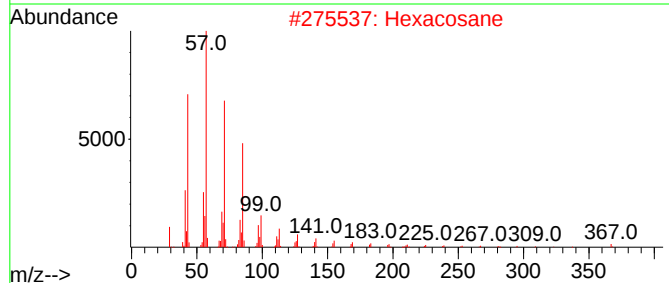
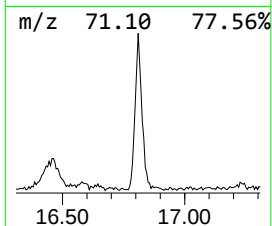
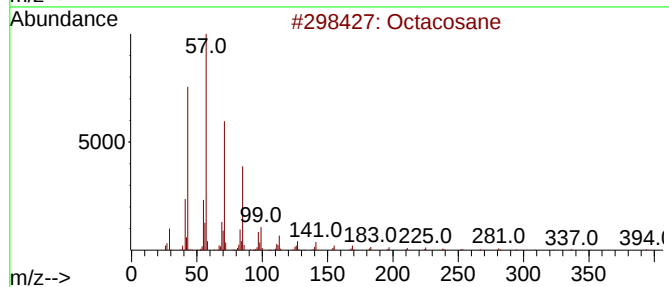
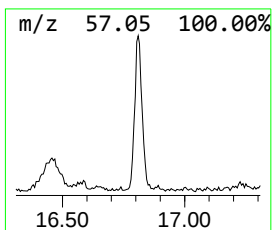
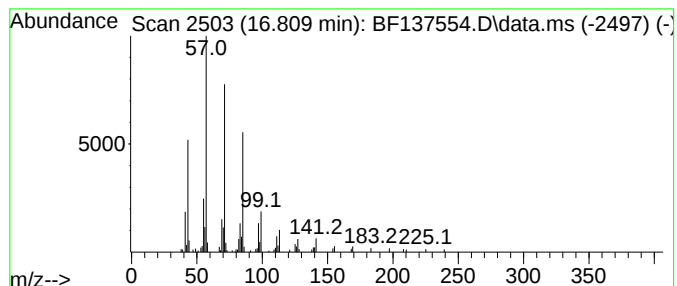
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.809	2.04 ng	148607	Perylene-d12	15.645

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Hexacosane	366	C26H54	000630-01-3	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Tetracosane	338	C24H50	000646-31-1	91
5			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.210	4.3	ng	317351	1	6.904	1491900	20.0
Hexadecanoic ac...	12.863	2.4	ng	239402	5	14.092	1968640	20.0
Heptadecane	14.921	2.4	ng	174536	6	15.645	1459000	20.0
Heneicosane	15.721	2.2	ng	157977	6	15.645	1459000	20.0
Octacosane	16.809	2.0	ng	148607	6	15.645	1459000	20.0