

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031324\
 Data File : BF137577.D
 Acq On : 13 Mar 2024 15:18
 Operator : CG\JU
 Sample : P1733-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-1

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: BF137577.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.311	26	38	53	rVB	1017143	1489790	22.70%	3.286%
2	5.593	591	596	599	rBV	5644069	5571015	84.88%	12.288%
3	6.563	755	761	764	rBV	5035557	5855367	89.21%	12.915%
4	6.916	817	821	838	rBV	1333229	1314172	20.02%	2.899%
5	7.475	911	916	931	rBV	3487163	3983657	60.69%	8.787%
6	8.181	1032	1036	1056	rBV	1963495	1815493	27.66%	4.004%
7	9.263	1214	1220	1223	rBV	6722707	6563728	100.00%	14.477%
8	9.939	1331	1335	1347	rBV	2463373	2098299	31.97%	4.628%
9	10.733	1466	1470	1489	rBV	3755850	4064964	61.93%	8.966%
10	11.433	1586	1589	1598	rBV	2303744	2027082	30.88%	4.471%
11	11.980	1678	1682	1692	rBV2	194485	276614	4.21%	0.610%
12	13.045	1858	1863	1866	rBV	5830534	6115579	93.17%	13.489%
13	13.533	1941	1946	1952	rBV	67195	88697	1.35%	0.196%
14	13.951	2014	2017	2028	rBV	297525	418477	6.38%	0.923%
15	14.098	2038	2042	2056	rBV	1447382	1439305	21.93%	3.175%
16	14.280	2067	2073	2091	rVB5	112036	300049	4.57%	0.662%
17	14.504	2102	2111	2122	rVV7	109952	358991	5.47%	0.792%
18	14.586	2122	2125	2137	rVB2	56544	91279	1.39%	0.201%
19	15.004	2192	2196	2201	rVB	79187	89046	1.36%	0.196%
20	15.657	2301	2307	2316	rBV	1028016	1376582	20.97%	3.036%

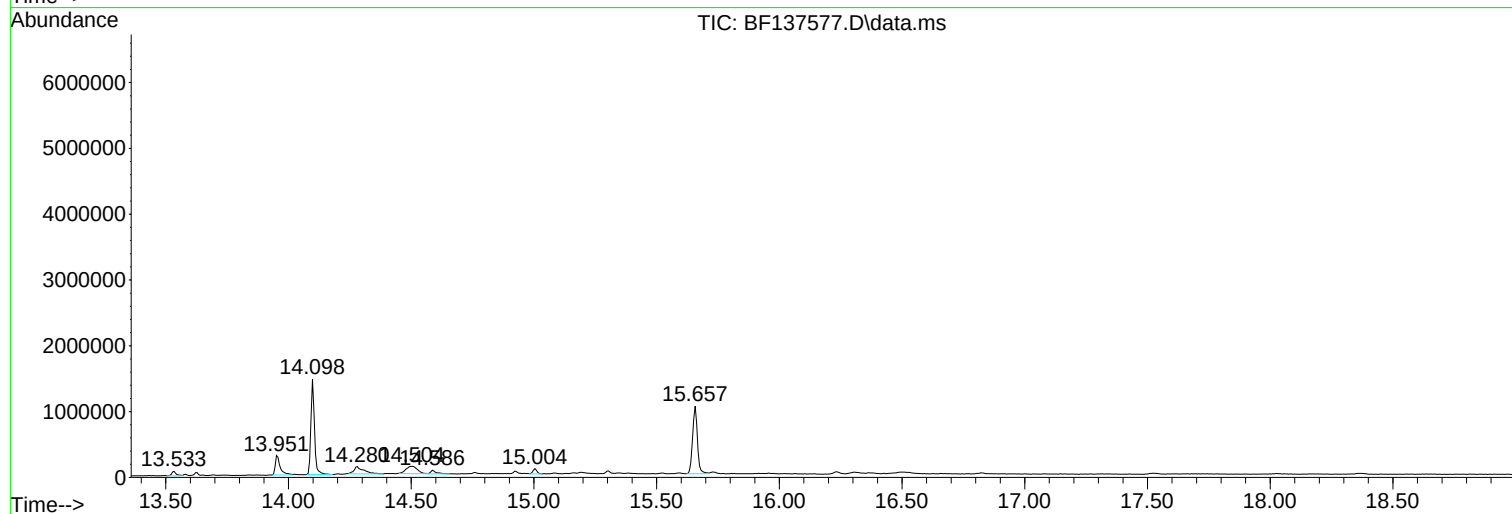
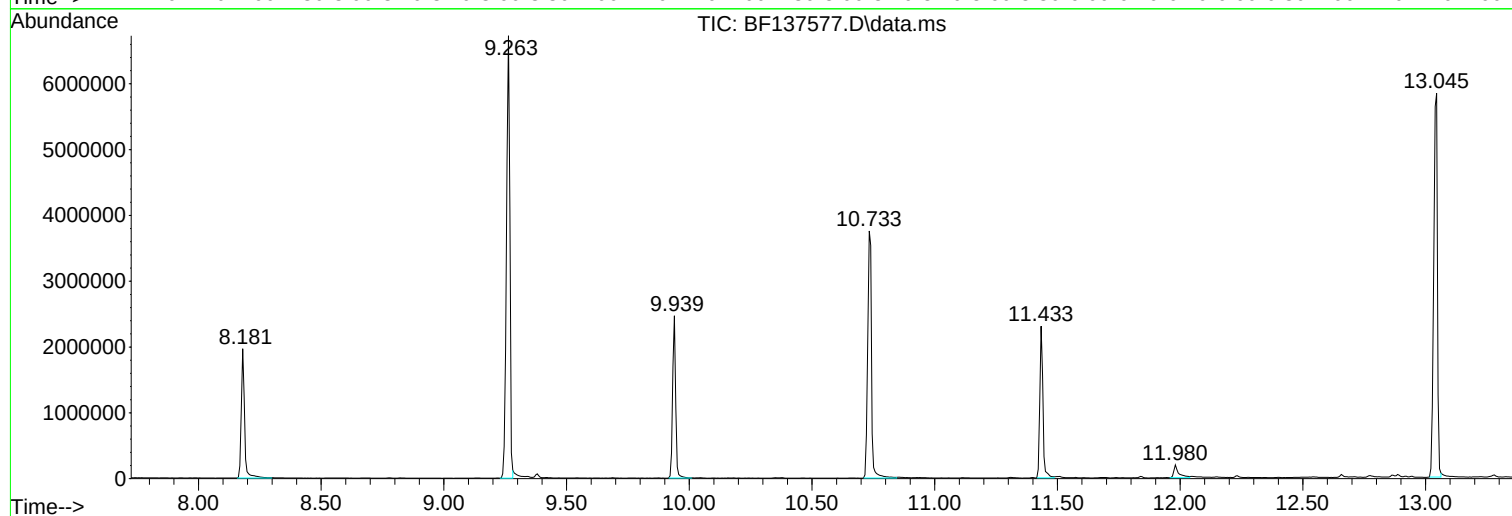
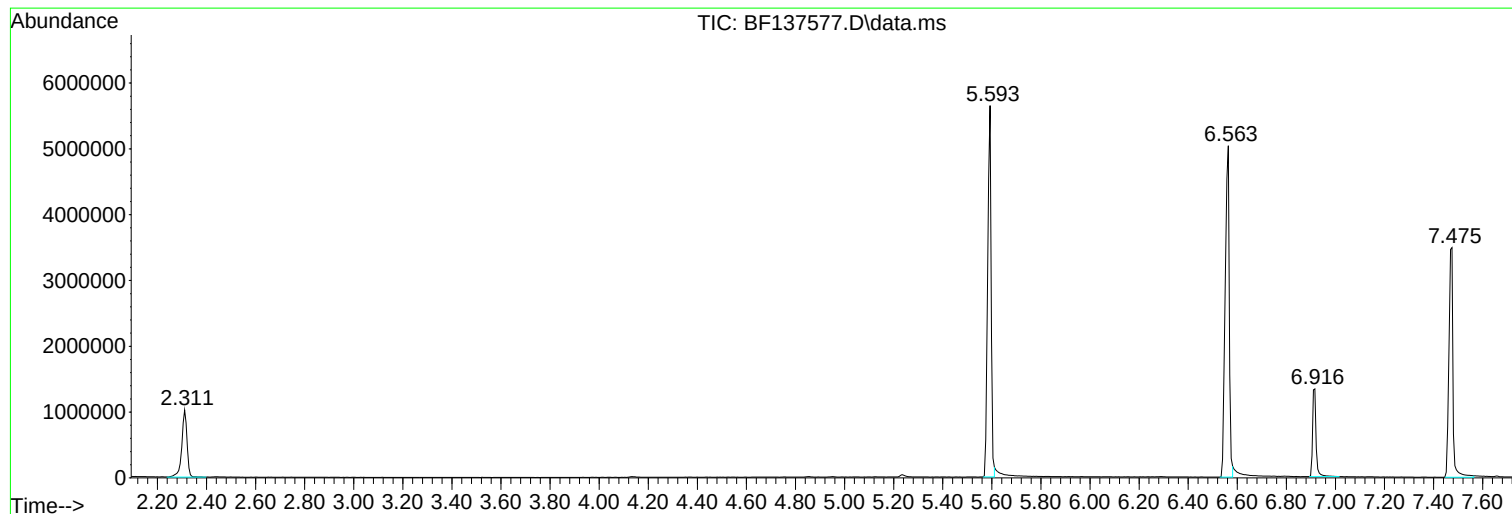
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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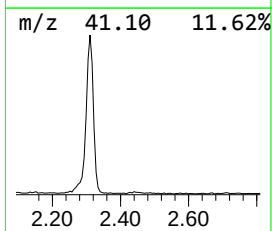
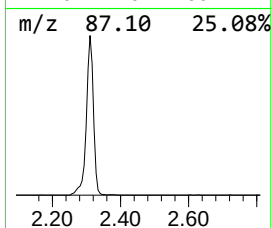
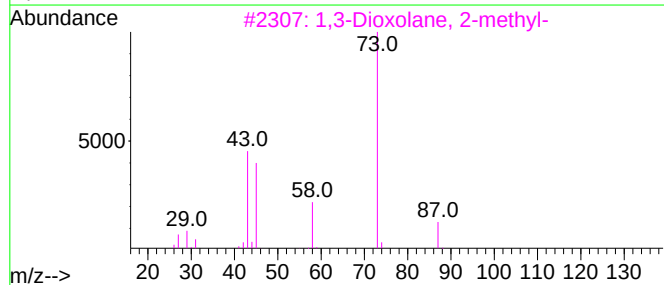
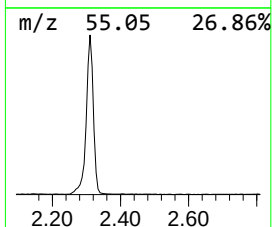
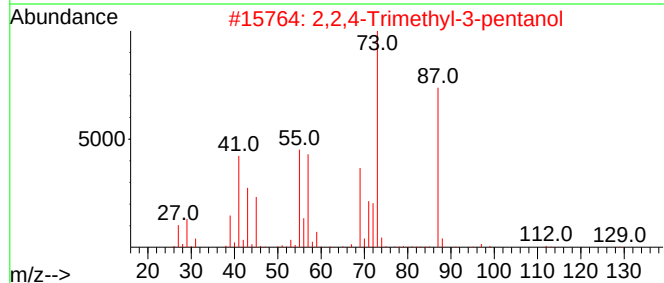
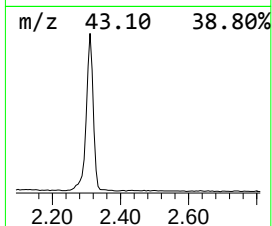
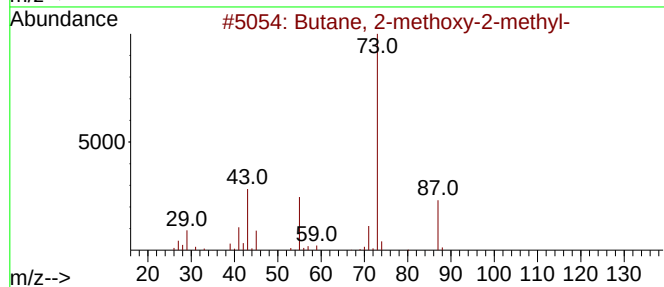
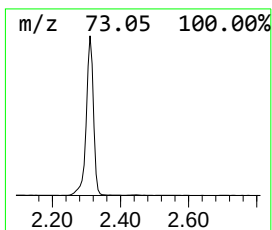
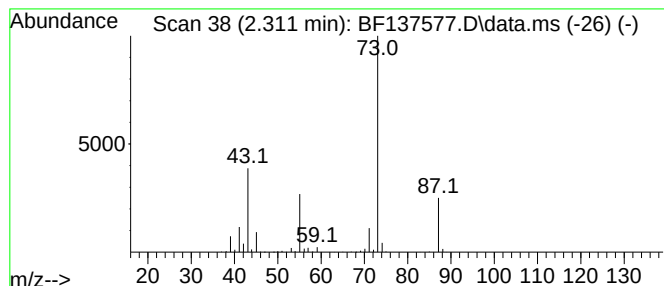
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.311	22.67 ng	1489790	1,4-Dichlorobenzene-d4	6.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	10



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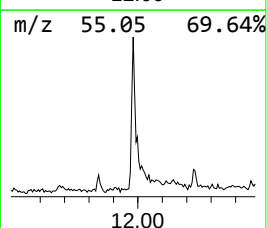
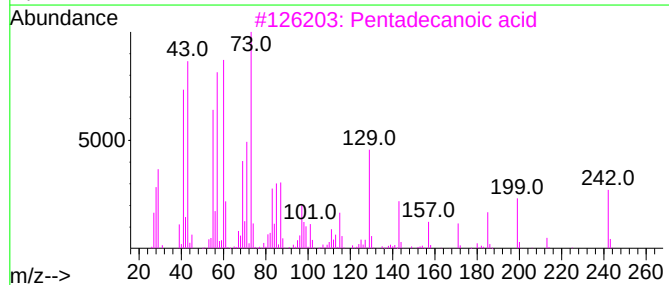
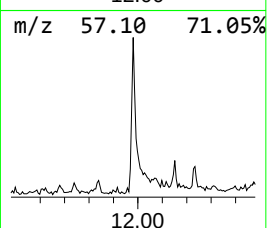
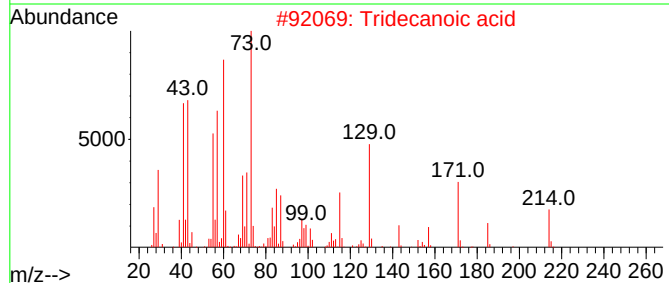
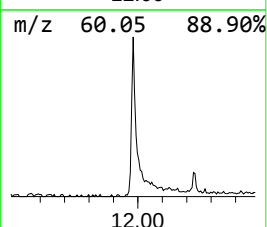
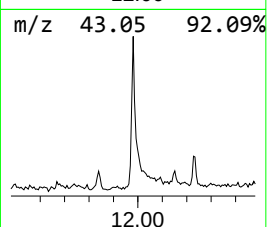
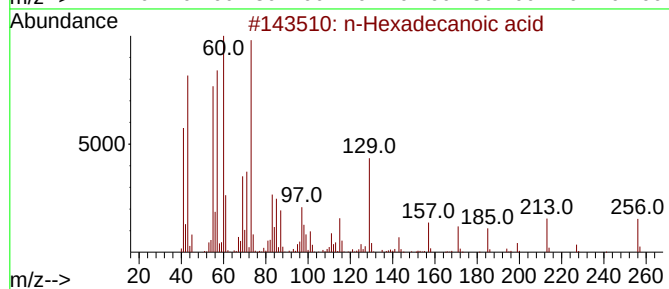
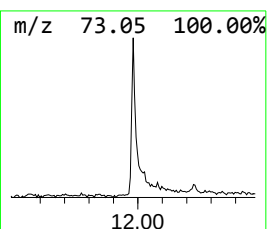
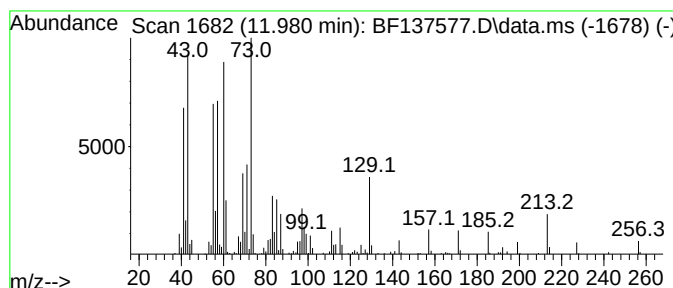
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.980	2.73 ng	276614	Phenanthrene-d10	11.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	83
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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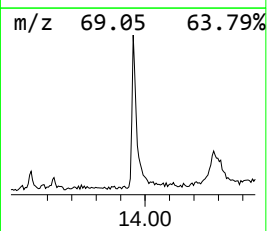
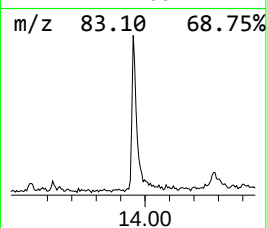
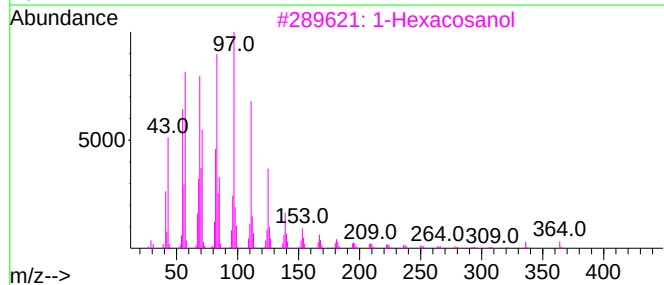
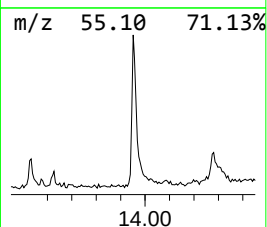
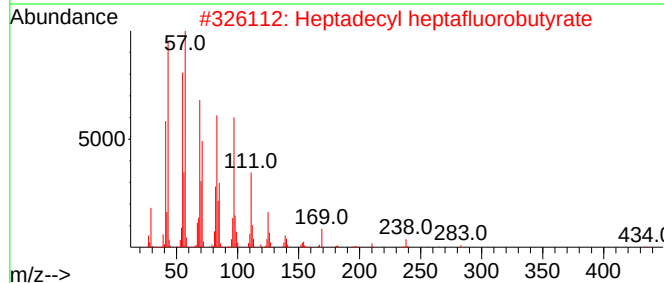
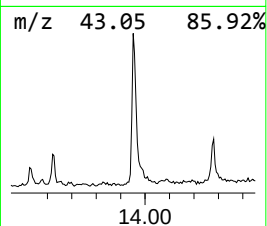
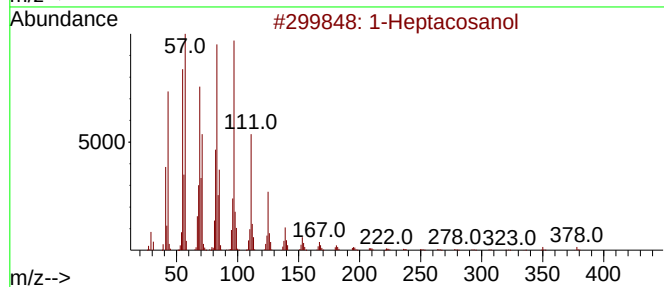
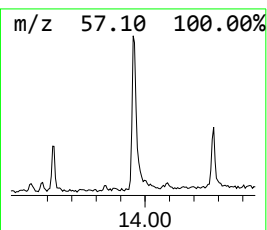
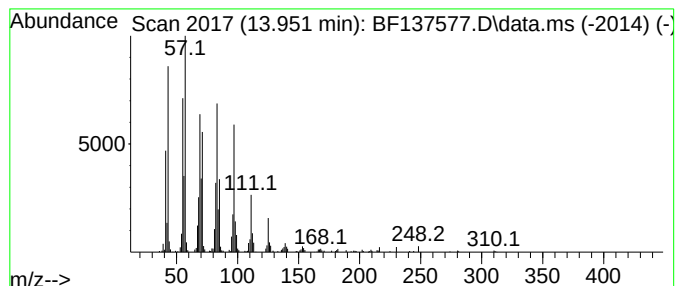
Instrument :
BNA_F
ClientSampleId :
WC-1

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 3 1-Heptacosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.951	5.81 ng	418477	Chrysene-d12	14.098	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	91
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
3	1-Hexacosanol	382	C26H54O	000506-52-5	91
4	Pentafluoropropionic acid, octadecyl ester	416	C21H37F5O2	959261-25-7	91
5	Pentafluoropropionic acid, heptadecyl ester	402	C20H35F5O2	959218-78-1	91



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ALS Vial : 13 Sample Multiplier: 1

Instrument :
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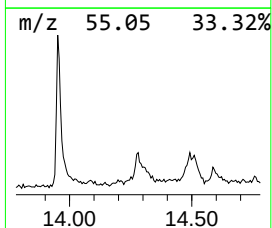
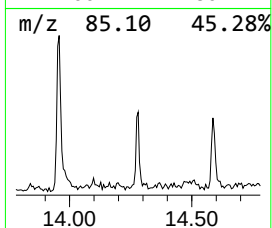
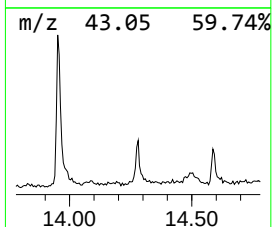
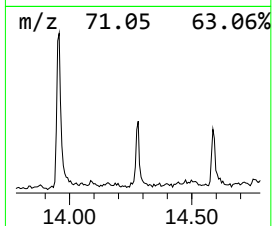
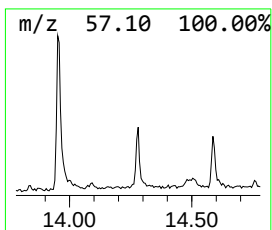
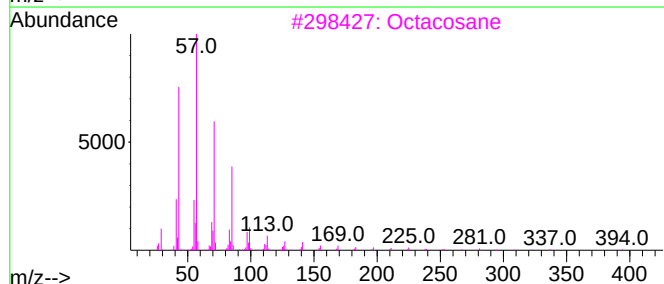
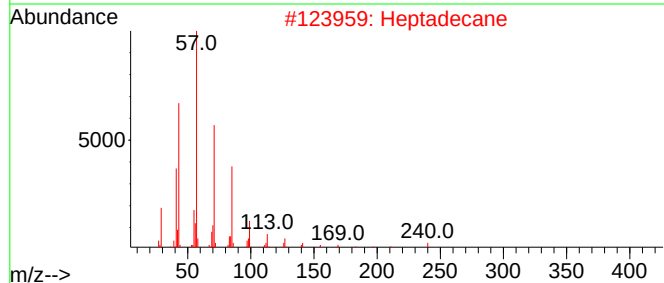
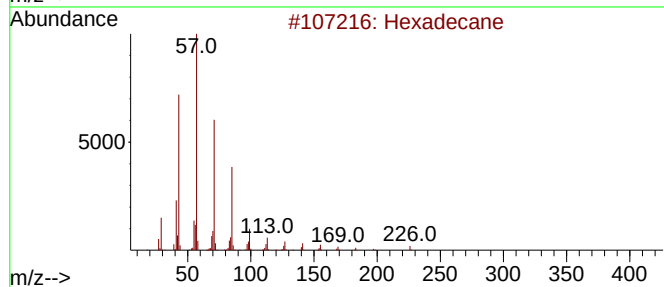
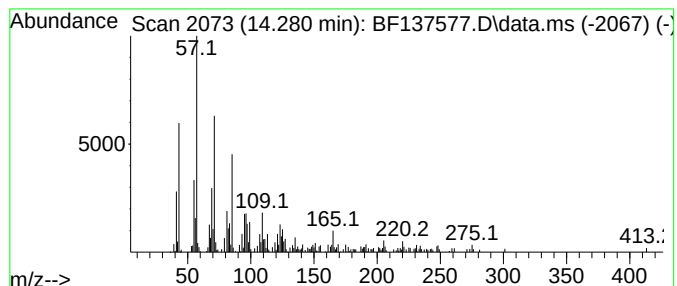
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.280	4.17 ng	300049	Chrysene-d12	14.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	78
2			Heptadecane	240	C17H36	000629-78-7	60
3			Octacosane	394	C28H58	000630-02-4	60
4			Tetratetracontane	619	C44H90	007098-22-8	60
5			Pentacosane	352	C25H52	000629-99-2	53



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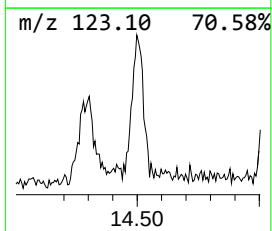
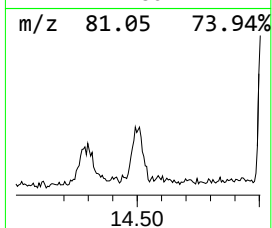
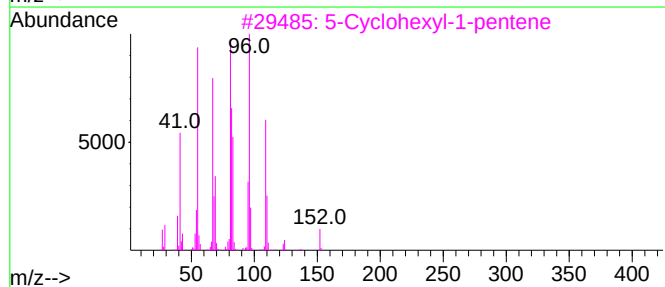
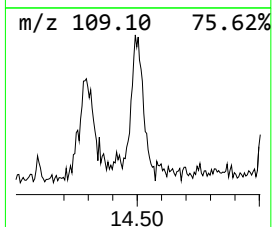
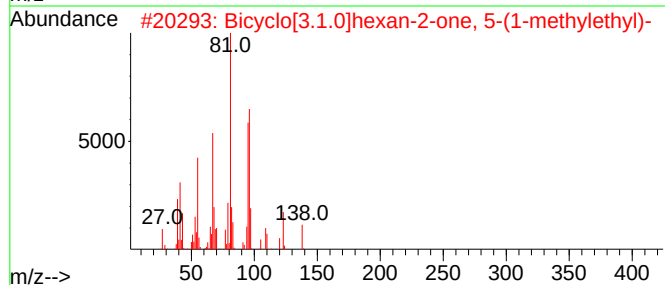
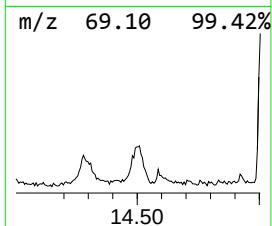
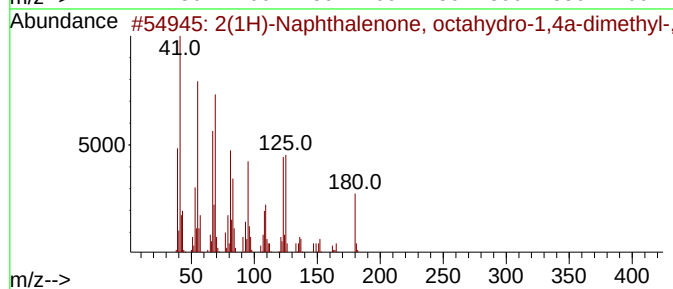
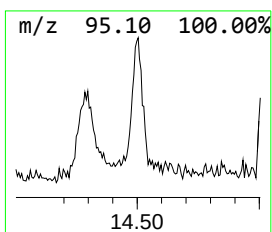
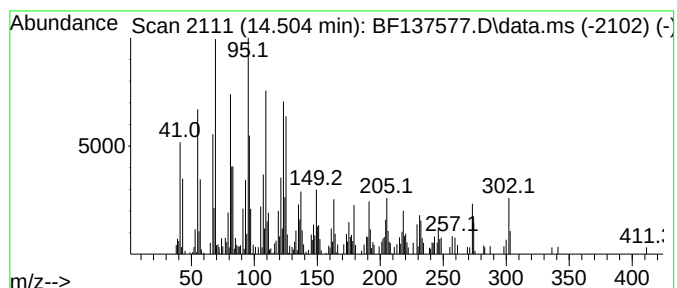
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown14.504 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.504	4.99 ng	358991	Chrysene-d12	14.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Naphthalenone, octahydro-1...	180	C12H20O	022738-31-4	38		
2	Bicyclo[3.1.0]hexan-2-one, 5-(1-...	138	C9H14O	000513-20-2	38		
3	5-Cyclohexyl-1-pentene	152	C11H20	005729-54-4	35		
4	1H-Indene, octahydro-, cis-	124	C9H16	004551-51-3	25		
5	Tricyclo[5.1.0.0(3,5)]octane-2,6...	192	C12H16O2	016650-33-2	25		



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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...	2.311	22.7	ng	1489790	1	6.916	1314170	20.0
n-Hexadecanoic ...	11.980	2.7	ng	276614	4	11.433	2027080	20.0
1-Heptacosanol	13.951	5.8	ng	418477	5	14.098	1439310	20.0
Hexadecane	14.280	4.2	ng	300049	5	14.098	1439310	20.0
unknown14.504	14.504	5.0	ng	358991	5	14.098	1439310	20.0