

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080922\
 Data File : BF129676.D
 Acq On : 09 Aug 2022 20:36
 Operator : CG\JU
 Sample : N3963-16
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RVE-220

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-BF072522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129676.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.487	539	544	547	rBV	4128803	4241605	84.21%	10.941%
2	6.493	710	715	718	rBV	3937801	4258041	84.53%	10.984%
3	6.840	770	774	777	rBV	1358754	1108263	22.00%	2.859%
4	7.410	865	871	874	rBV	2717758	2802837	55.64%	7.230%
5	8.122	987	992	995	rBV	1735539	1426105	28.31%	3.679%
6	9.198	1169	1175	1178	rBV	5814498	5037028	100.00%	12.993%
7	9.875	1285	1290	1294	rBV	1626300	1502402	29.83%	3.875%
8	10.675	1421	1426	1429	rBV	2896964	2693360	53.47%	6.947%
9	11.369	1540	1544	1546	rBV	1509714	1231343	24.45%	3.176%
10	11.392	1546	1548	1553	rVB	216595	184144	3.66%	0.475%
11	11.886	1630	1632	1637	rVB2	108841	116644	2.32%	0.301%
12	11.980	1645	1648	1650	rBV2	64874	59439	1.18%	0.153%
13	12.580	1747	1750	1754	rBV	529076	477544	9.48%	1.232%
14	12.816	1783	1790	1792	rBV	494565	545946	10.84%	1.408%
15	12.951	1809	1813	1817	rBV	3640977	3451611	68.52%	8.903%
16	13.027	1822	1826	1830	rBV3	37789	60230	1.20%	0.155%
17	13.169	1847	1850	1855	rBV2	86865	93855	1.86%	0.242%
18	13.245	1859	1863	1865	rBV2	54193	63038	1.25%	0.163%
19	13.298	1865	1872	1873	rBV6	39338	77070	1.53%	0.199%
20	13.510	1905	1908	1911	rBV3	59974	63507	1.26%	0.164%
21	13.651	1930	1932	1937	rVB	72180	70254	1.39%	0.181%
22	13.857	1961	1967	1977	rVB5	401418	888265	17.63%	2.291%
23	13.980	1983	1988	1989	rBV3	59749	79704	1.58%	0.206%
24	14.016	1989	1994	1997	rVV2	1071930	1210255	24.03%	3.122%
25	14.039	1997	1998	2004	rVB	280036	193451	3.84%	0.499%
26	14.104	2004	2009	2014	rBV	384205	434327	8.62%	1.120%
27	14.157	2015	2018	2021	rBV2	64676	62635	1.24%	0.162%
28	14.280	2036	2039	2044	rBV5	57564	61396	1.22%	0.158%
29	14.463	2067	2070	2072	rBV	162480	139615	2.77%	0.360%
30	14.492	2072	2075	2083	rVB4	225487	439458	8.72%	1.134%
31	14.763	2119	2121	2124	rVB	61194	57141	1.13%	0.147%
32	14.839	2132	2134	2140	rVB	80444	78586	1.56%	0.203%
33	14.915	2143	2147	2151	rVB	403141	434381	8.62%	1.120%
34	15.057	2167	2171	2174	rBV	328083	453871	9.01%	1.171%
35	15.163	2184	2189	2200	rVB3	229349	569662	11.31%	1.469%
36	15.363	2220	2223	2229	rVB	198388	236997	4.71%	0.611%

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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-BF072522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.427	2230	2234	2238	rBV	239051	283625	5.63%	0.732%
38	15.492	2239	2245	2249	rBV	710396	954846	18.96%	2.463%
39	15.680	2273	2277	2285	rVB	253977	375046	7.45%	0.967%
40	15.910	2312	2316	2324	rVB	300178	452117	8.98%	1.166%
41	16.010	2329	2333	2334	rBV3	76386	99395	1.97%	0.256%
42	16.709	2447	2452	2458	rVB2	255414	473158	9.39%	1.221%
43	16.998	2492	2501	2508	rBV3	156094	518062	10.29%	1.336%
44	18.374	2728	2735	2751	rVB9	167632	707124	14.04%	1.824%

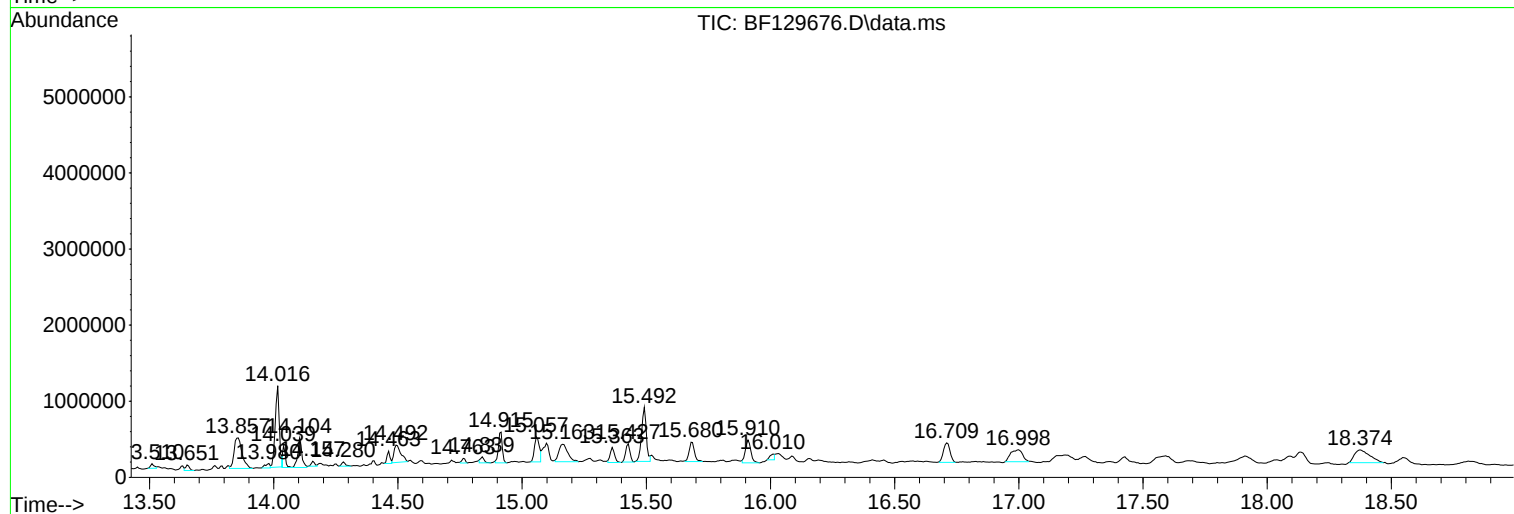
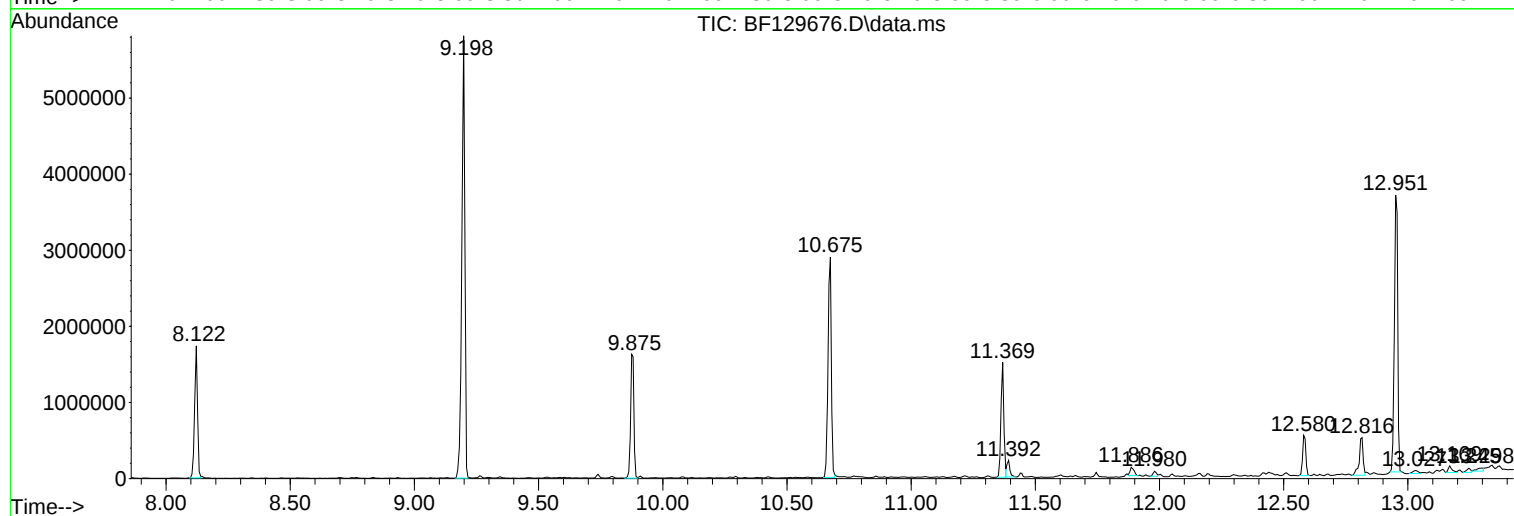
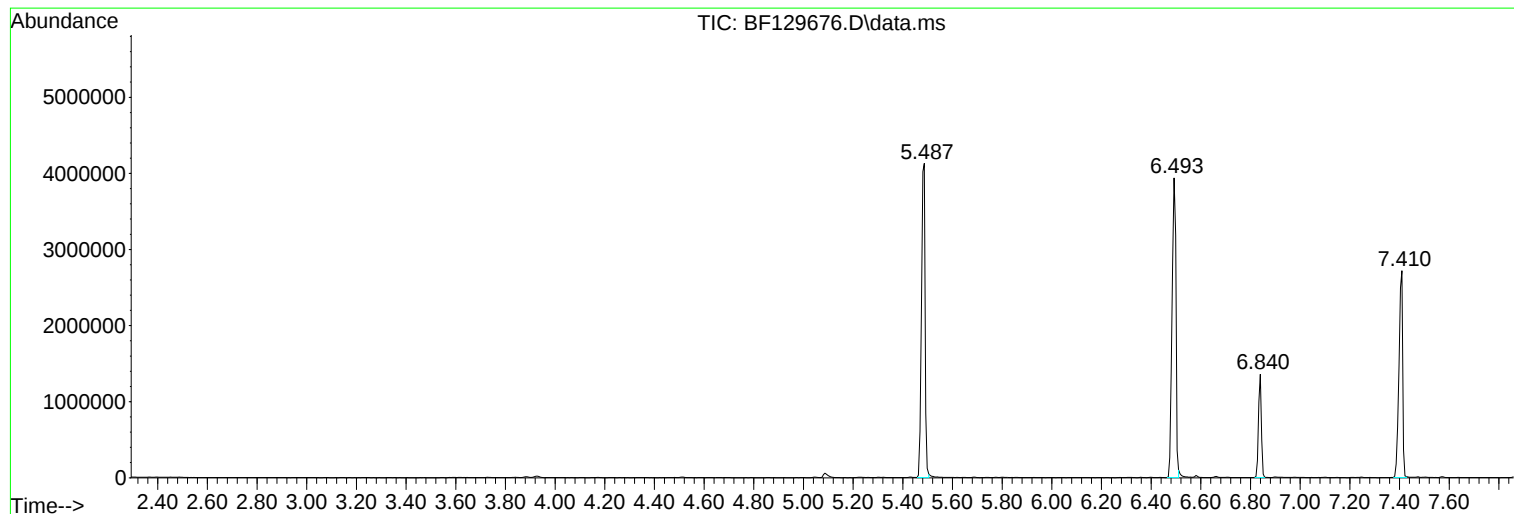
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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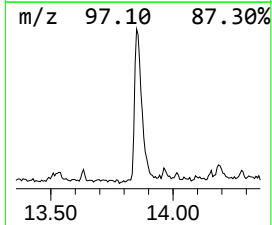
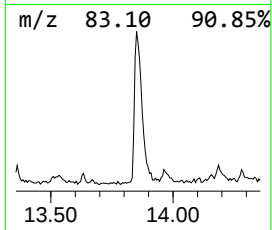
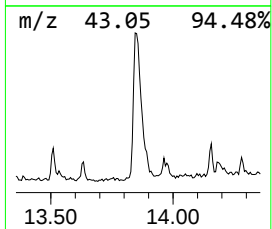
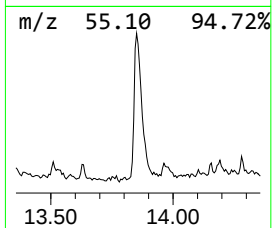
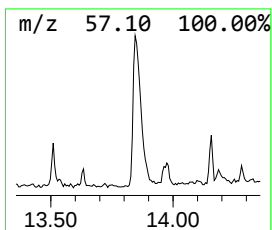
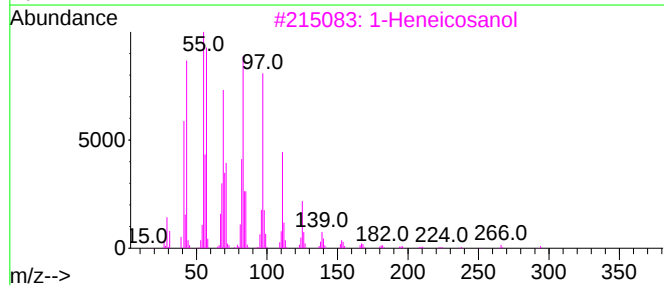
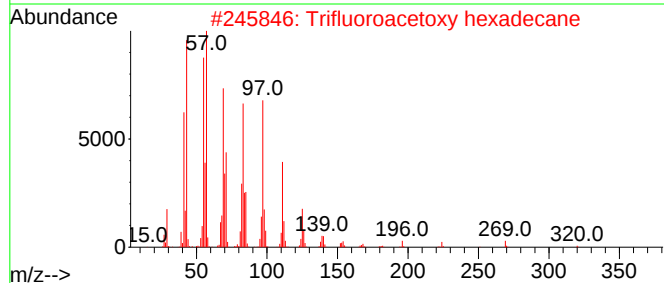
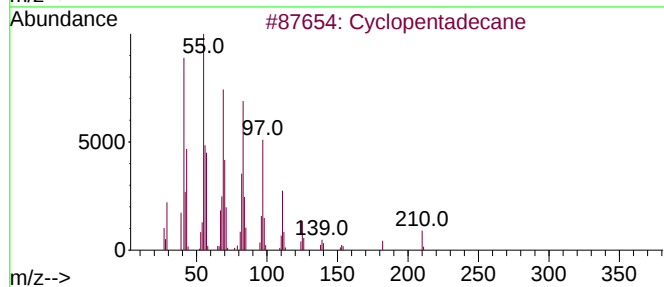
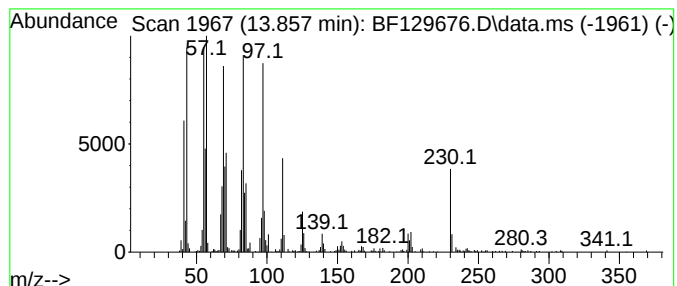
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Cyclopentadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	14.68 ng	888265	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	93
2			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
3			1-Heneicosanol	312	C21H44O	015594-90-8	93
4			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93



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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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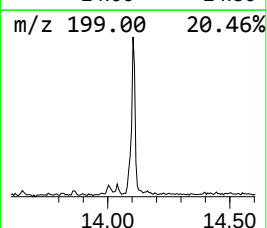
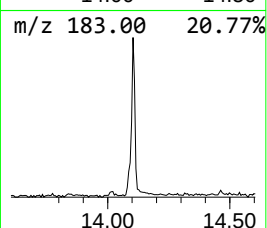
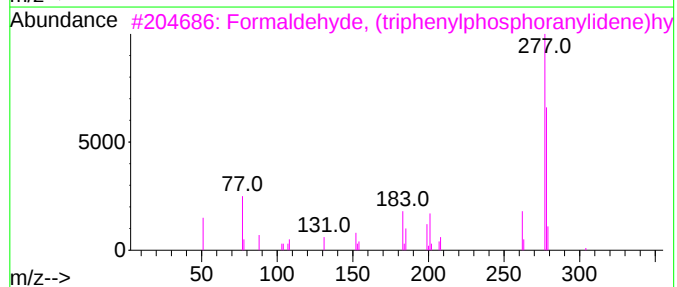
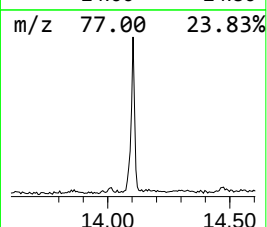
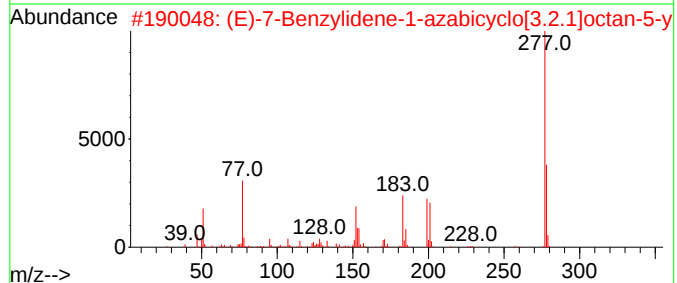
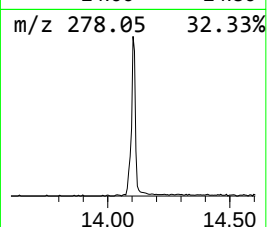
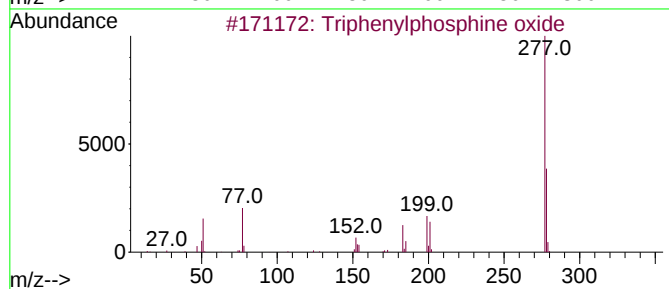
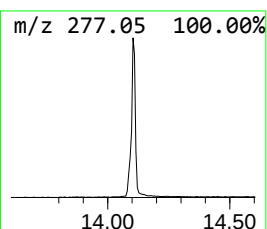
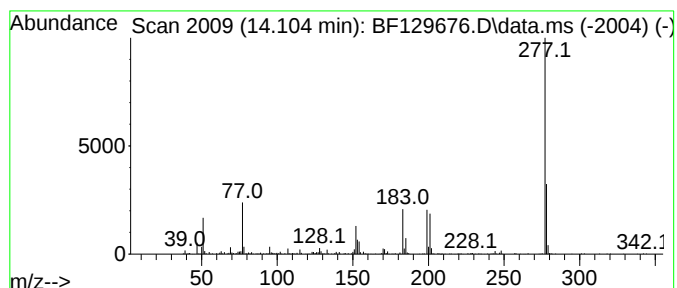
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Triphenylphosphine oxide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.104	7.18 ng	434327	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	94
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	76
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	50
4			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	50
5			2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	43



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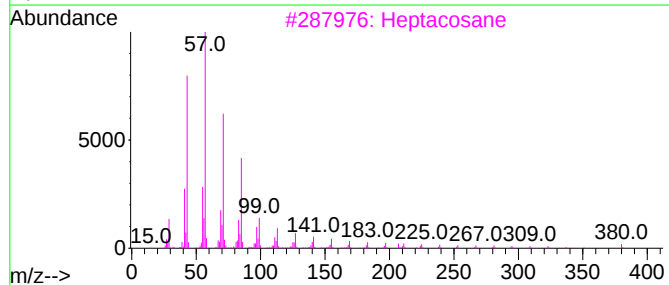
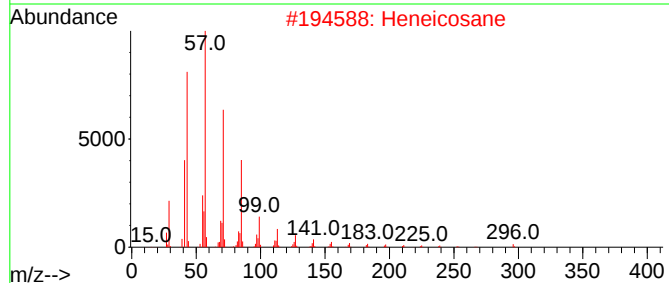
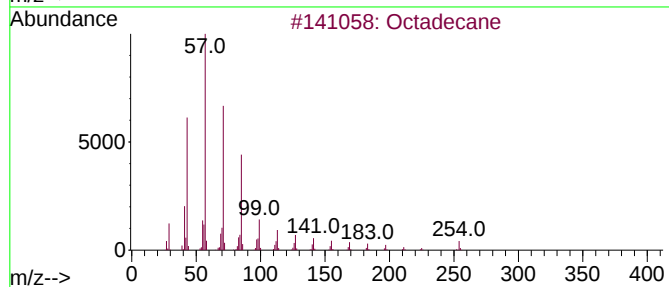
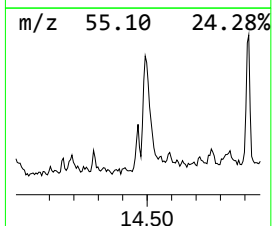
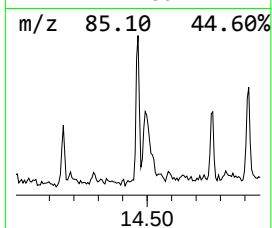
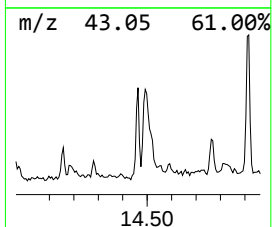
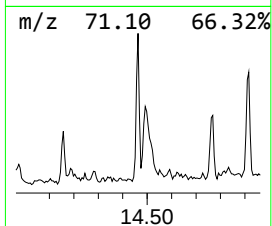
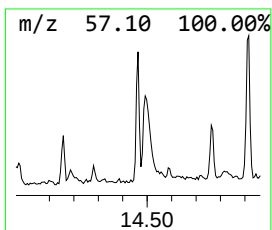
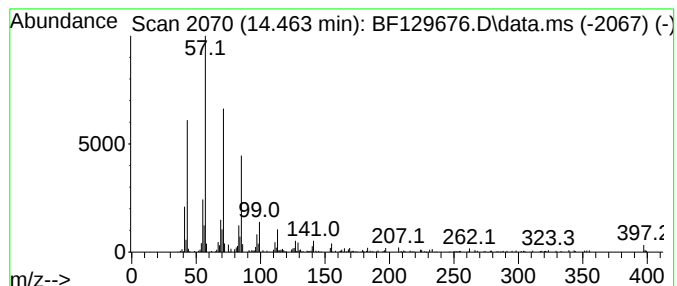
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Octadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.463	2.31 ng	139615	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	93
2			Heneicosane	296	C21H44	000629-94-7	90
3			Heptacosane	380	C27H56	000593-49-7	90
4			Hexacosane	366	C26H54	000630-01-3	90
5			Tridecane, 3-methyl-	198	C14H30	006418-41-3	89



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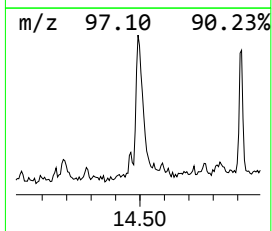
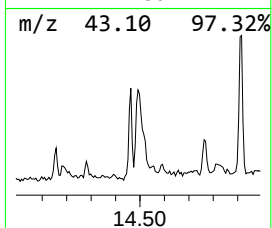
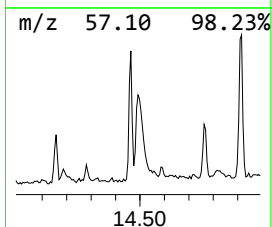
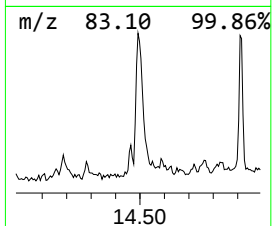
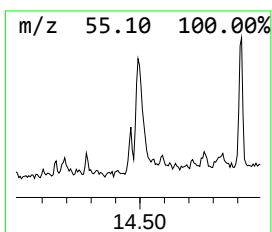
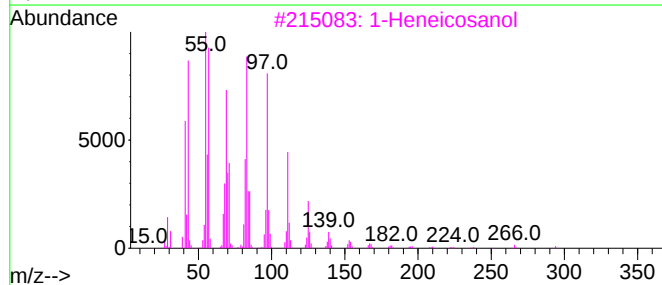
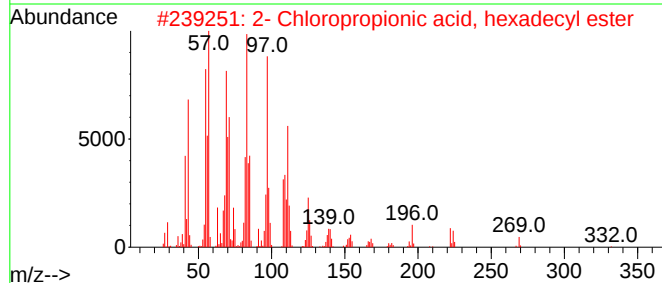
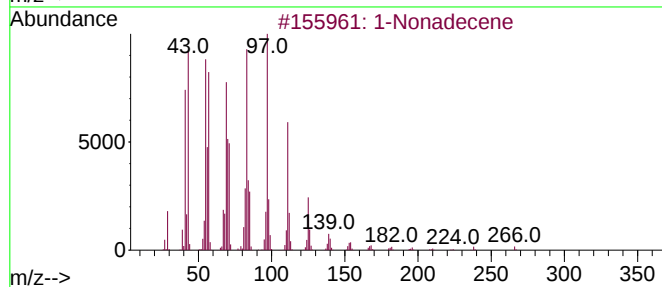
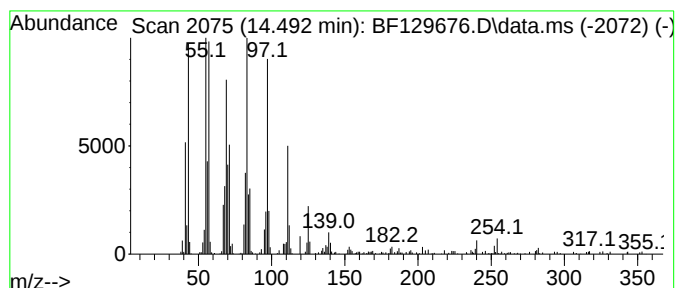
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 1-Nonadecene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.492	7.26 ng	439458	Chrysene-d12	14.015	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	95
2	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	94
4	1-Tetracosene	336	C24H48	010192-32-2	94
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	94



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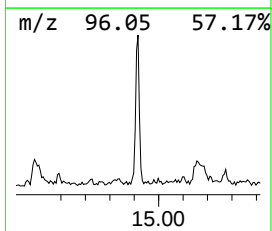
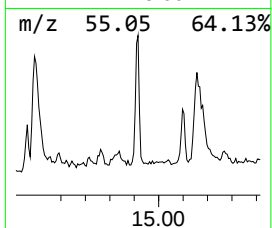
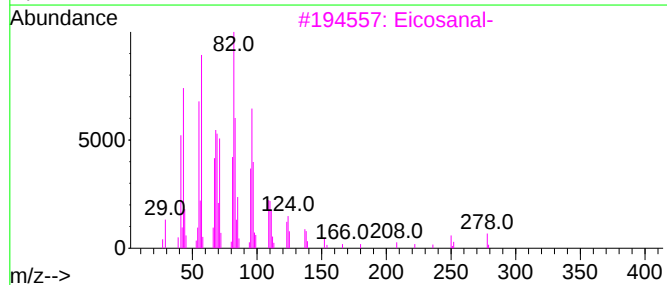
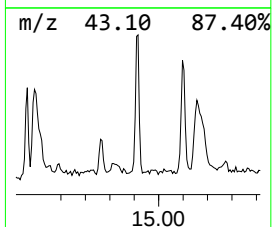
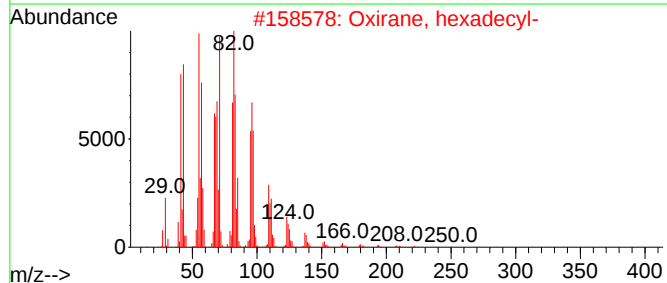
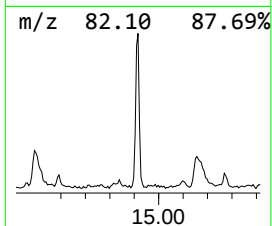
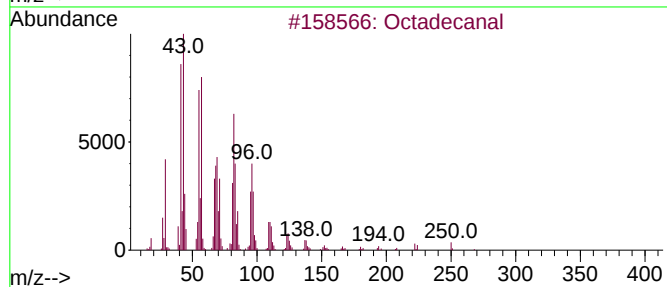
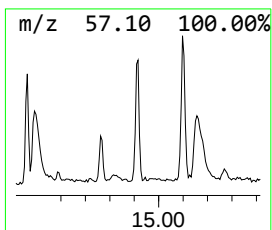
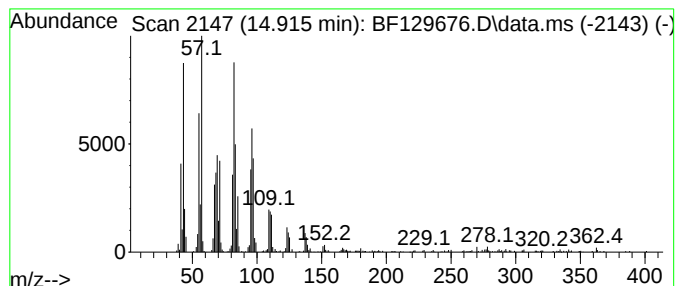
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.916	9.10 ng	434381	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanal	268	C18H36O	000638-66-4	91
2			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	87
3			Eicosanal-	296	C20H40O	002400-66-0	87
4			Hexacosanal	380	C26H52O	026627-85-0	83
5			(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	83



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Acq On : 09 Aug 2022 20:36
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Sample : N3963-16
Misc :
ALS Vial : 10 Sample Multiplier: 1

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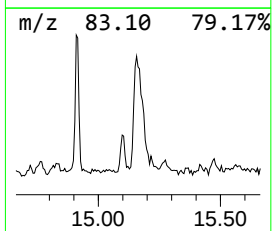
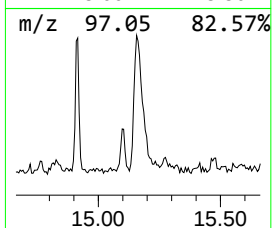
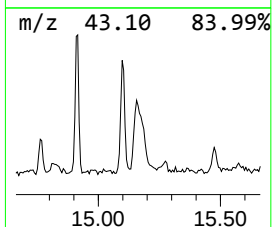
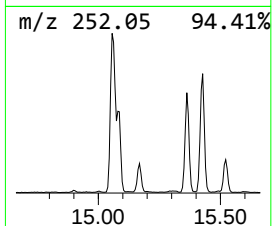
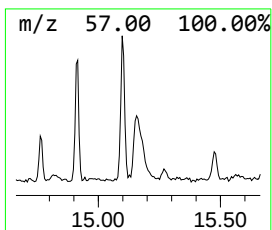
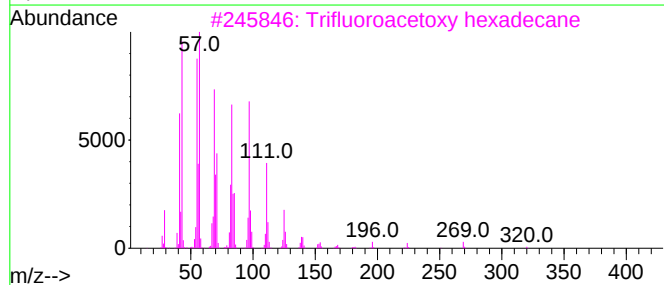
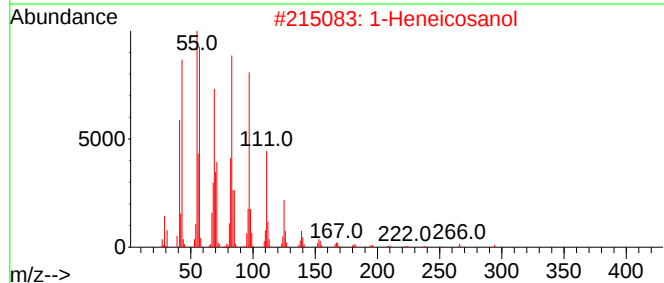
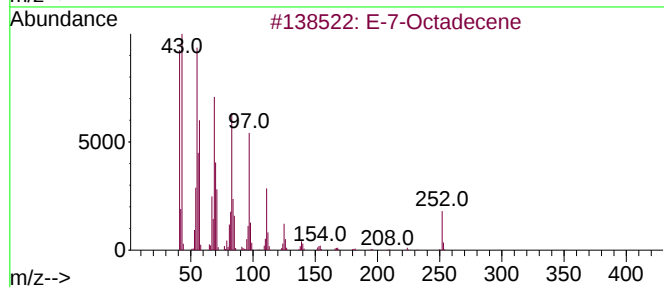
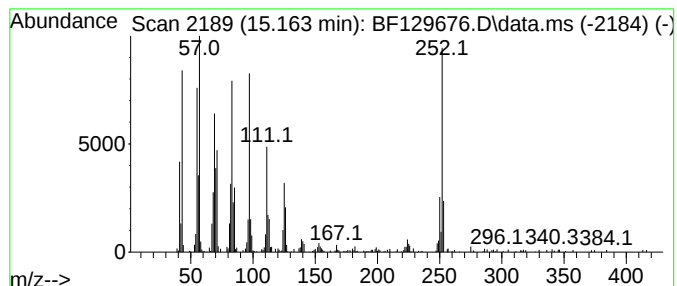
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 E-7-Octadecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.163	11.93 ng	569662	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			E-7-Octadecene	252	C18H36	1000130-92-0	81
2			1-Heneicosanol	312	C21H44O	015594-90-8	70
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	60
4			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	60
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080922\
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ClientSampleId :
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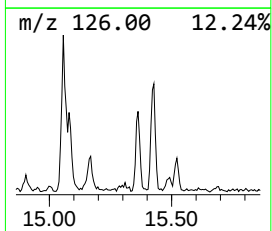
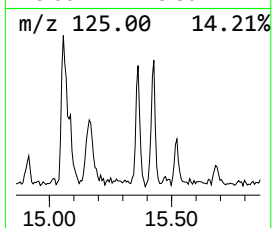
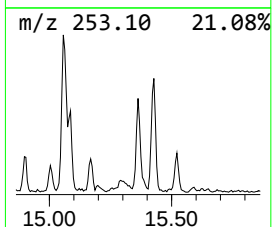
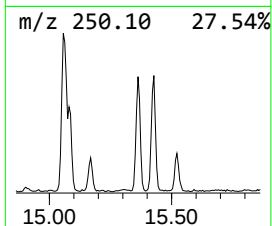
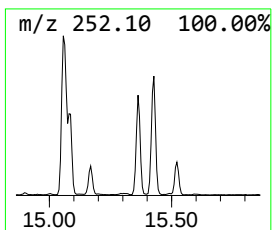
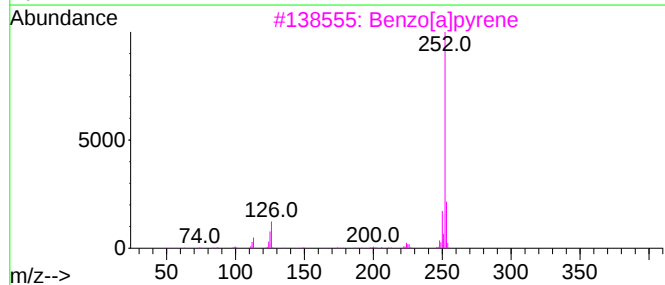
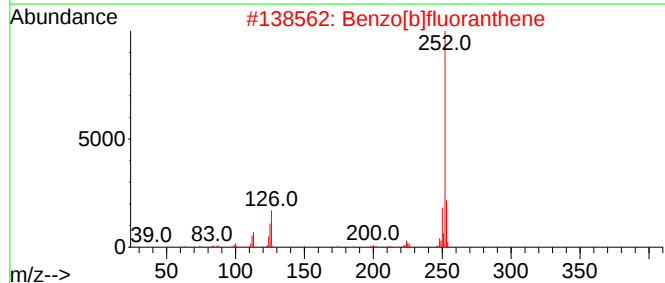
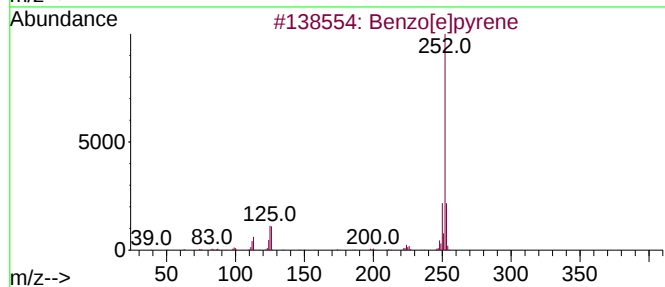
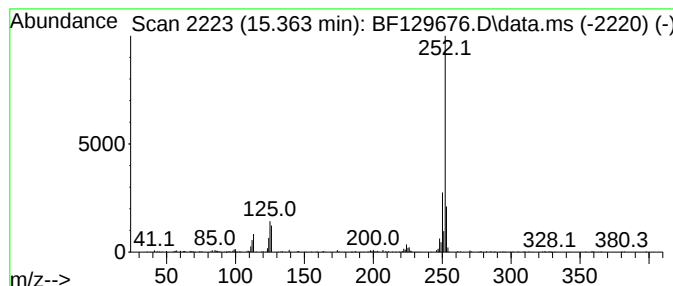
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[e]pyrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.363	4.96 ng	236997	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	99
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	97
3			Benzo[a]pyrene	252	C20H12	000050-32-8	96
4			Benzo[j]fluoranthene	252	C20H12	000205-82-3	95
5			Perylene	252	C20H12	000198-55-0	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080922\
Data File : BF129676.D
Acq On : 09 Aug 2022 20:36
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Sample : N3963-16
Misc :
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Instrument :
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ClientSampleId :
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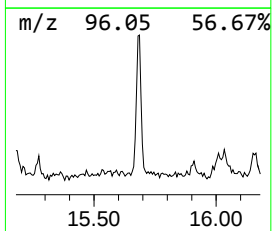
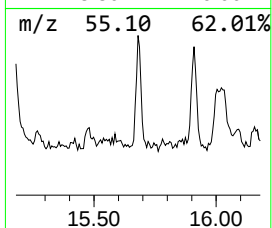
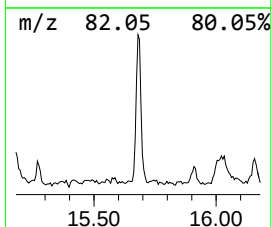
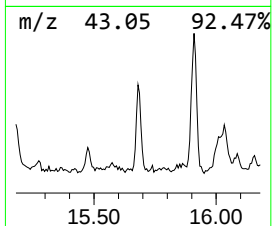
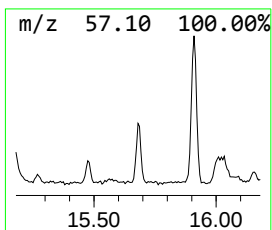
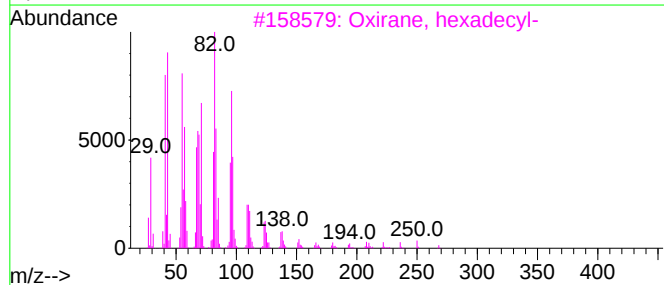
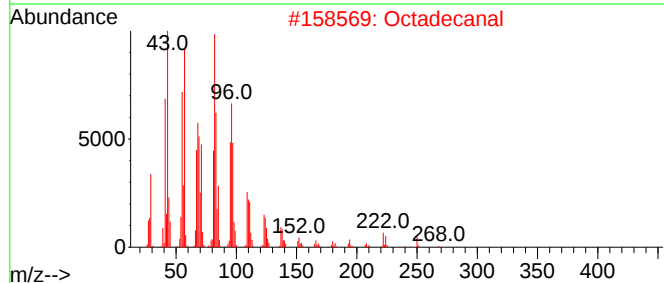
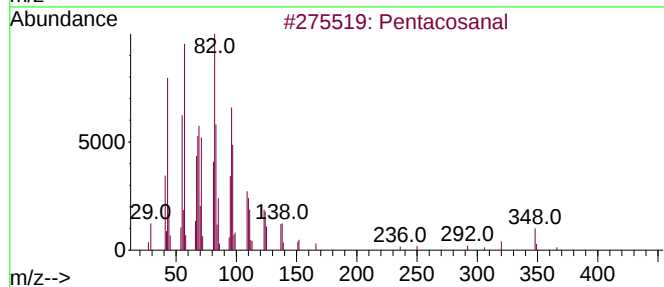
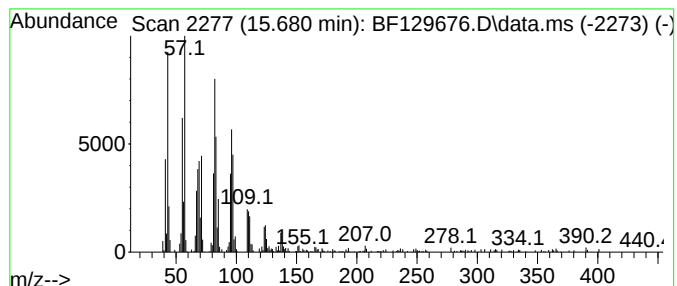
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentacosanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.680	7.86 ng	375046	Perylene-d12	15.492

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentacosanal	366	C25H50O	058196-28-4	92
2		Octadecanal	268	C18H36O	000638-66-4	91
3		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
4		Tricosanal	338	C23H46O	072934-02-2	91
5		Docosanal	324	C22H44O	057402-36-5	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080922\
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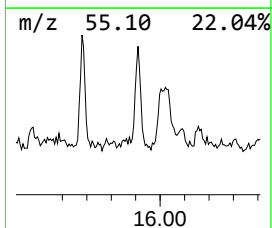
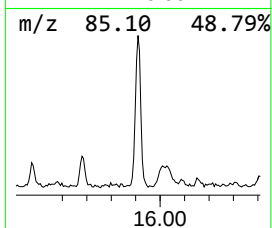
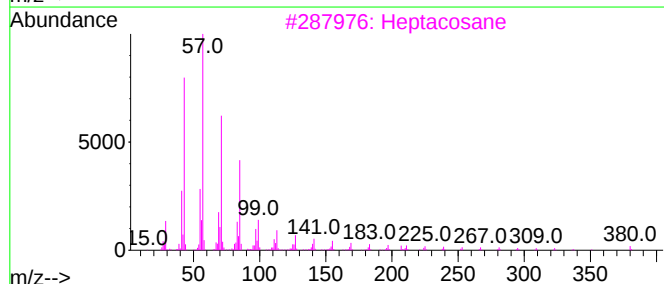
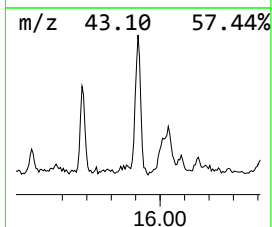
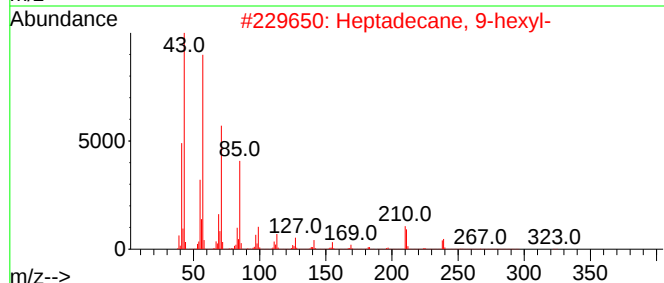
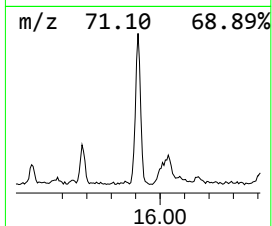
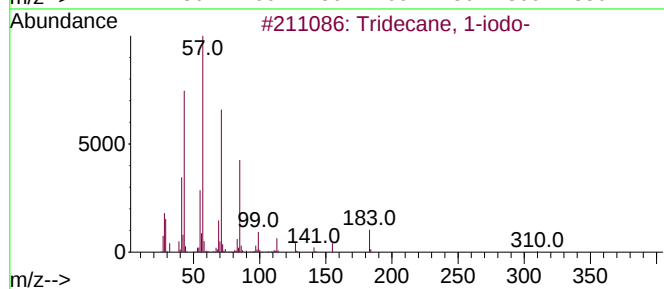
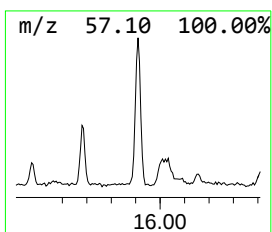
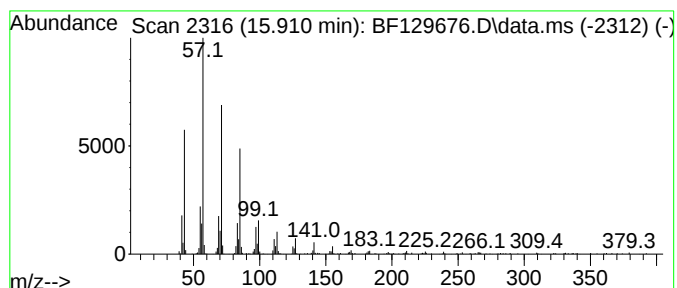
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tridecane, 1-iodo- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.910	9.47 ng	452117	Perylene-d12	15.492	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	93
2	Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	93
3	Heptacosane	380	C27H56	000593-49-7	91
4	Tetratetracontane	619	C44H90	007098-22-8	91
5	Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080922\
Data File : BF129676.D
Acq On : 09 Aug 2022 20:36
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Misc :
ALS Vial : 10 Sample Multiplier: 1

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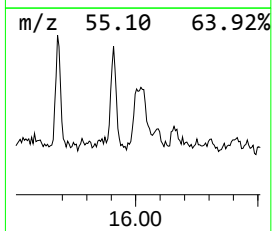
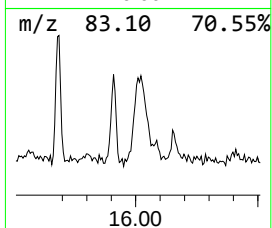
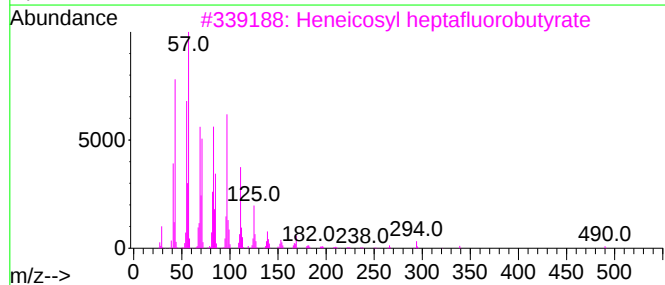
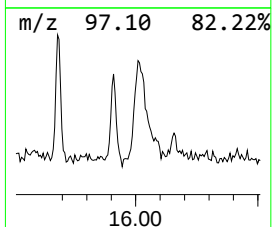
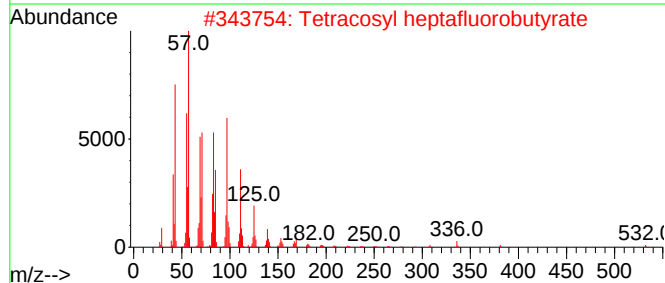
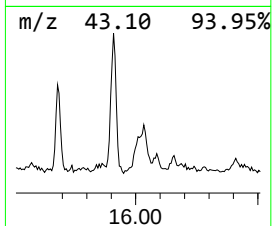
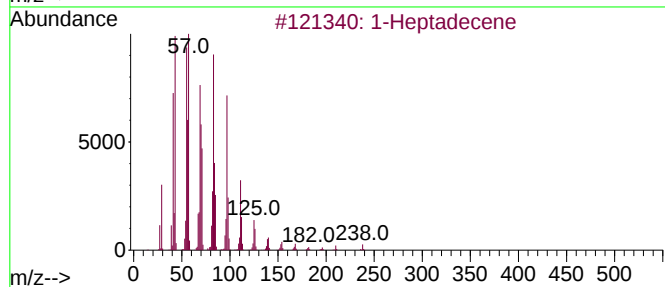
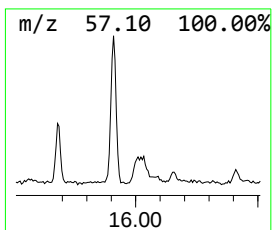
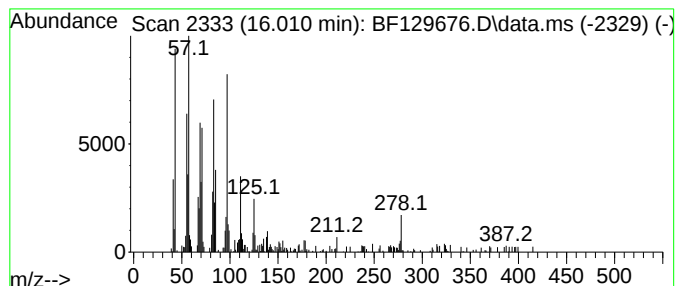
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 1-Heptadecene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.009	2.08 ng	99395	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptadecene	238	C17H34	006765-39-5	95
2			Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	94
3			Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	94
4			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	94
5			Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080922\
Data File : BF129676.D
Acq On : 09 Aug 2022 20:36
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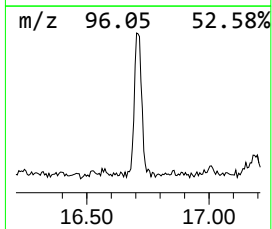
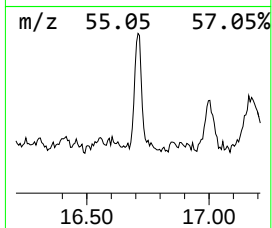
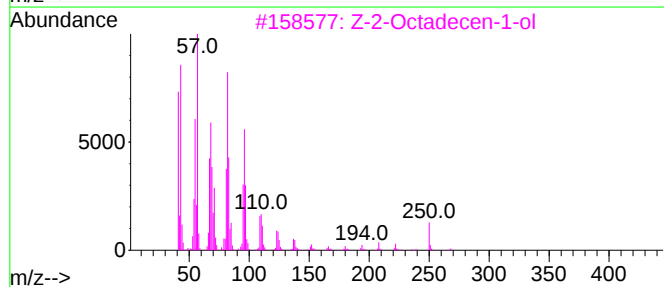
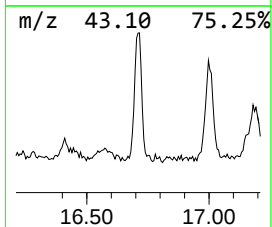
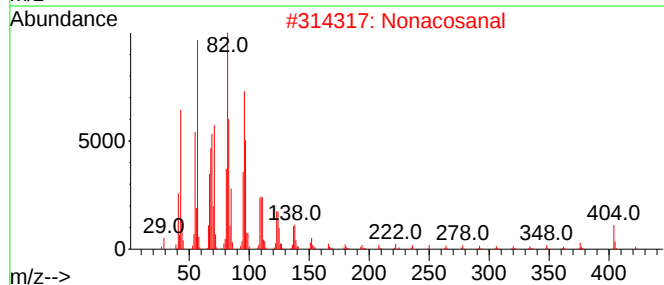
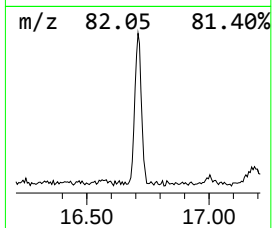
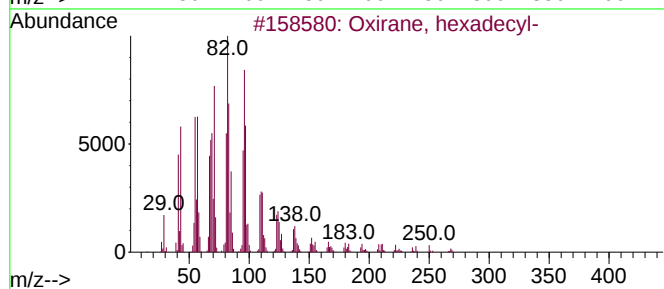
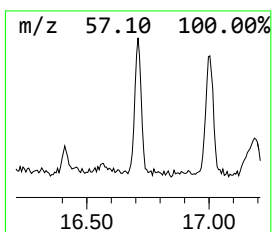
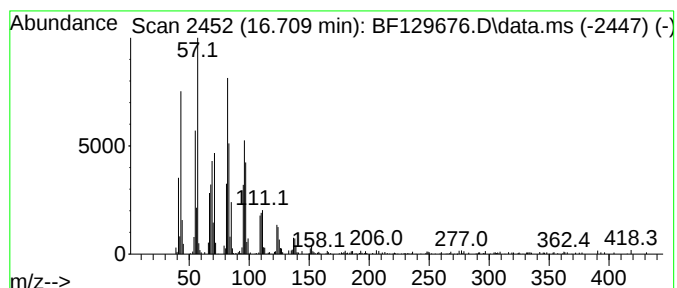
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Oxirane, hexadecyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.709	9.91 ng	473158	Perylene-d12	15.492

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	96
2		Nonacosanal	422	C29H58O	072934-04-4	95
3		Z-2-Octadecen-1-ol	268	C18H36O	1000131-11-0	90
4		Pentacosanal	366	C25H50O	058196-28-4	87
5		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080922\
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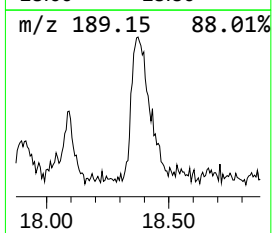
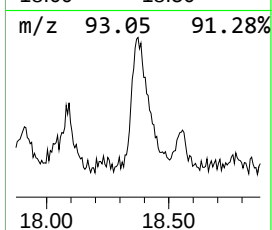
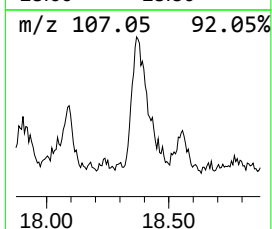
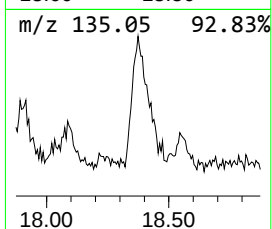
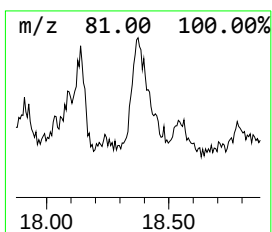
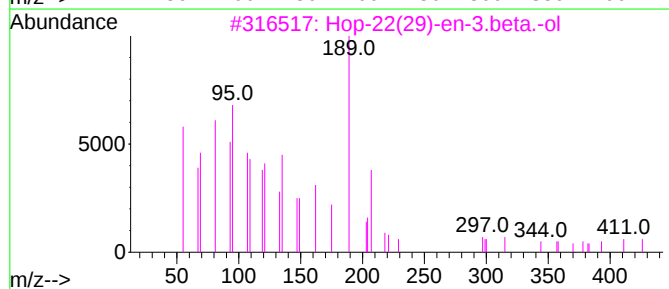
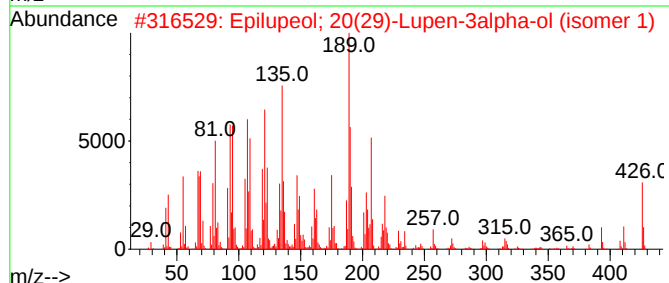
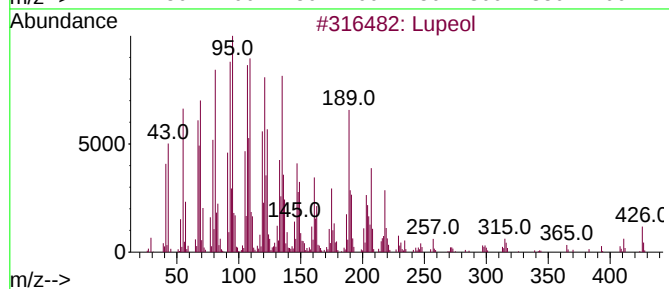
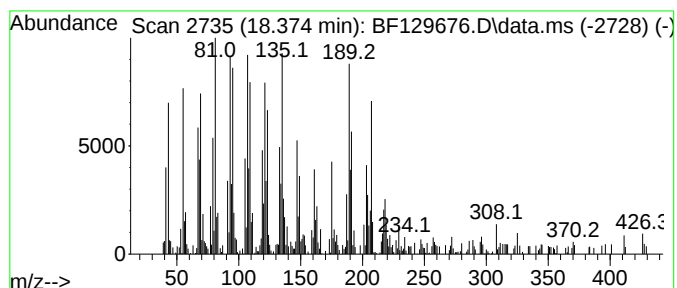
Instrument :
BNA_F
ClientSampleId :
RVE-220

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Lupeol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.374	14.81 ng	707124	Perylene-d12	15.492
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		Lupeol	426 C30H50O	000545-47-1 98
2		Epilupeol; 20(29)-Lupen-3alpha-o...	426 C30H50O	1000513-01-3 90
3		Hop-22(29)-en-3.beta.-ol	426 C30H50O	058801-23-3 64
4		Epilupeol; 20(29)-Lupen-3alpha-o...	426 C30H50O	1000513-01-4 62
5		1,2-Pentanediol, 5-(6-bromodecah...	486 C24H39BrO5	115334-14-0 62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080922\
Data File : BF129676.D
Acq On : 09 Aug 2022 20:36
Operator : CG\JU
Sample : N3963-16
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-220

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.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
Cyclopentadecane	13.857	14.7	ng	888265	5	14.015	1210260	20.0
Triphenylphosph...	14.104	7.2	ng	434327	5	14.015	1210260	20.0
Octadecane	14.463	2.3	ng	139615	5	14.015	1210260	20.0
1-Nonadecene	14.492	7.3	ng	439458	5	14.015	1210260	20.0
Octadecanal	14.916	9.1	ng	434381	6	15.492	954846	20.0
E-7-Octadecene	15.163	11.9	ng	569662	6	15.492	954846	20.0
Benzo[e]pyrene	15.363	5.0	ng	236997	6	15.492	954846	20.0
Pentacosanal	15.680	7.9	ng	375046	6	15.492	954846	20.0
Tridecane, 1-iodo-	15.910	9.5	ng	452117	6	15.492	954846	20.0
1-Heptadecene	16.009	2.1	ng	99395	6	15.492	954846	20.0
Oxirane, hexade...	16.709	9.9	ng	473158	6	15.492	954846	20.0
Lupeol	18.374	14.8	ng	707124	6	15.492	954846	20.0