

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081922\
 Data File : BF129909.D
 Acq On : 19 Aug 2022 13:34
 Operator : CG\JU
 Sample : N4227-21
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-3

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-BF081422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129909.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.004	459	462	474	rBV	146929	186699	7.07%	0.969%
2	5.428	531	534	555	rBV	2164556	2191016	83.03%	11.374%
3	6.445	704	707	722	rBV	2321268	2165582	82.07%	11.242%
4	6.792	762	766	774	rBV	819302	657339	24.91%	3.412%
5	7.357	858	862	873	rBV	1503155	1405351	53.26%	7.296%
6	8.075	980	984	987	rBV	1062445	867549	32.88%	4.504%
7	9.151	1162	1167	1170	rBV	2954321	2638856	100.00%	13.699%
8	9.828	1279	1282	1286	rBV	997682	927844	35.16%	4.817%
9	10.628	1414	1418	1426	rBV	1559744	1346247	51.02%	6.989%
10	11.322	1533	1536	1539	rBV	946184	779150	29.53%	4.045%
11	12.545	1741	1744	1748	rVB	29435	30411	1.15%	0.158%
12	12.769	1778	1782	1785	rBV2	29457	34287	1.30%	0.178%
13	12.910	1802	1806	1809	rBV	2088006	1830306	69.36%	9.502%
14	13.121	1839	1842	1845	rVB2	32995	28184	1.07%	0.146%
15	13.668	1932	1935	1940	rVB	34307	35842	1.36%	0.186%
16	13.804	1953	1958	1970	rBV3	102240	264086	10.01%	1.371%
17	13.974	1983	1987	1991	rBV	601992	590590	22.38%	3.066%
18	14.063	1997	2002	2007	rBV	174965	188727	7.15%	0.980%
19	14.415	2058	2062	2064	rBV	48040	48347	1.83%	0.251%
20	14.445	2064	2067	2076	rVB7	33510	78091	2.96%	0.405%
21	14.863	2134	2138	2141	rBV3	30592	34331	1.30%	0.178%
22	15.045	2165	2169	2172	rVB	66765	74572	2.83%	0.387%
23	15.439	2230	2236	2241	rVB	534504	718297	27.22%	3.729%
24	15.615	2263	2266	2273	rVB6	32944	47044	1.78%	0.244%
25	15.833	2298	2303	2309	rBV	103951	153914	5.83%	0.799%
26	16.615	2433	2436	2443	rVB5	31195	52785	2.00%	0.274%
27	16.904	2481	2485	2493	rVB5	41686	88535	3.36%	0.460%
28	16.998	2494	2501	2509	rBV	768339	1489360	56.44%	7.732%
29	17.998	2669	2671	2683	rVB5	39436	91734	3.48%	0.476%
30	18.151	2691	2697	2706	rVB5	85713	218027	8.26%	1.132%

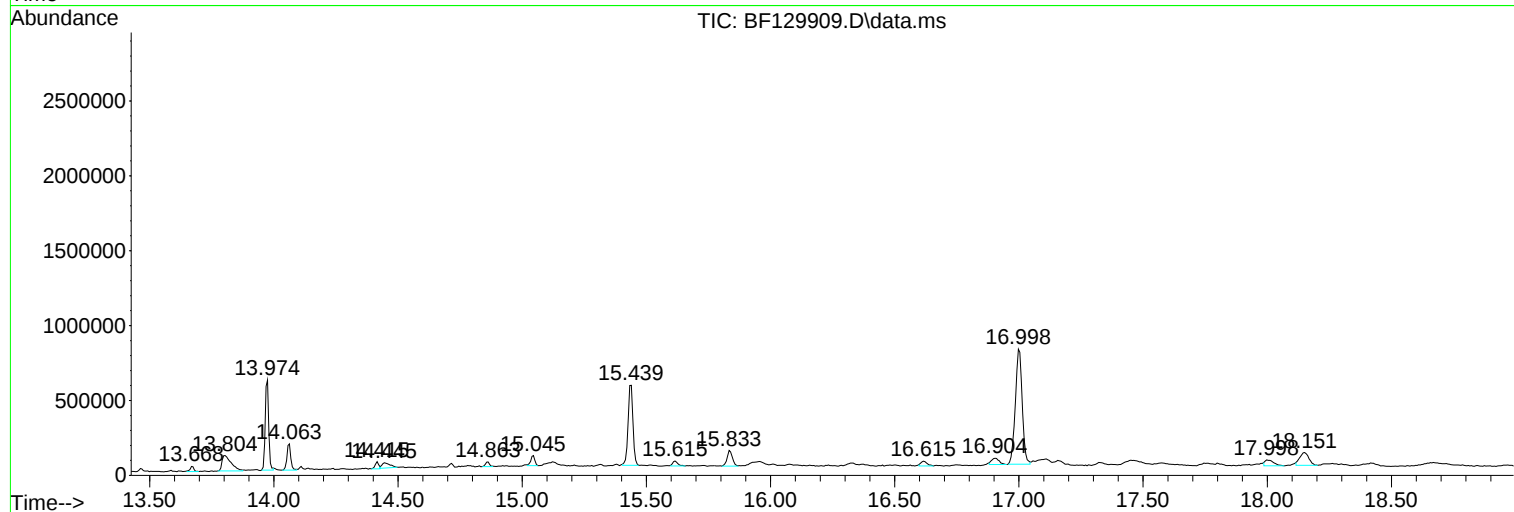
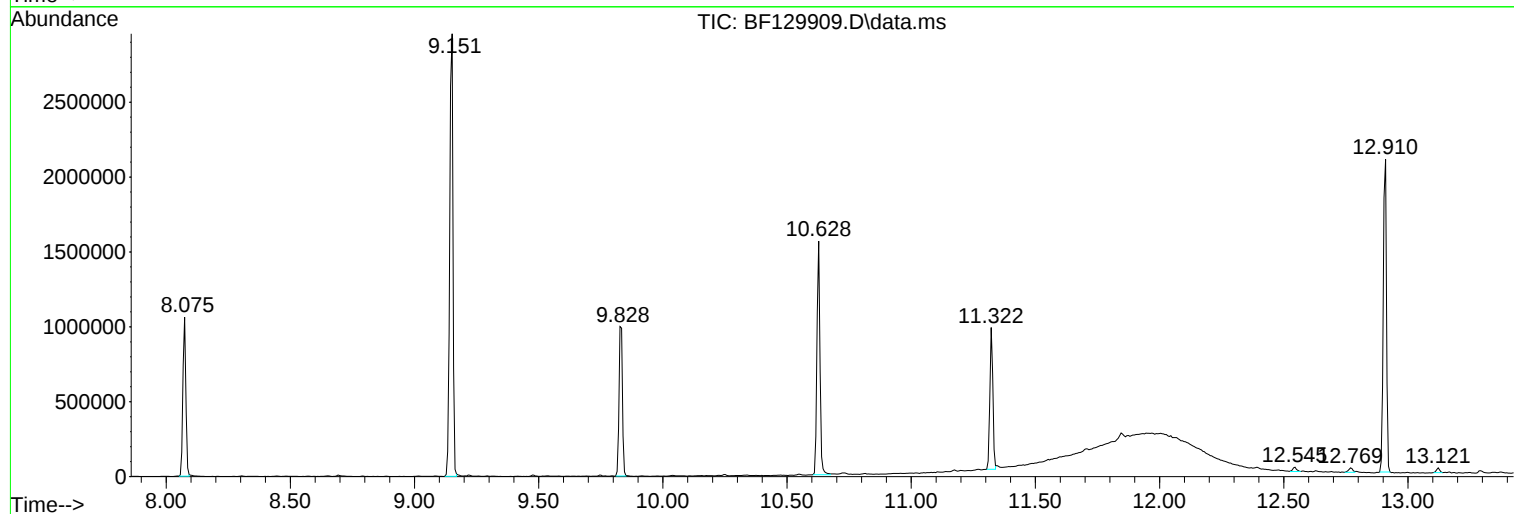
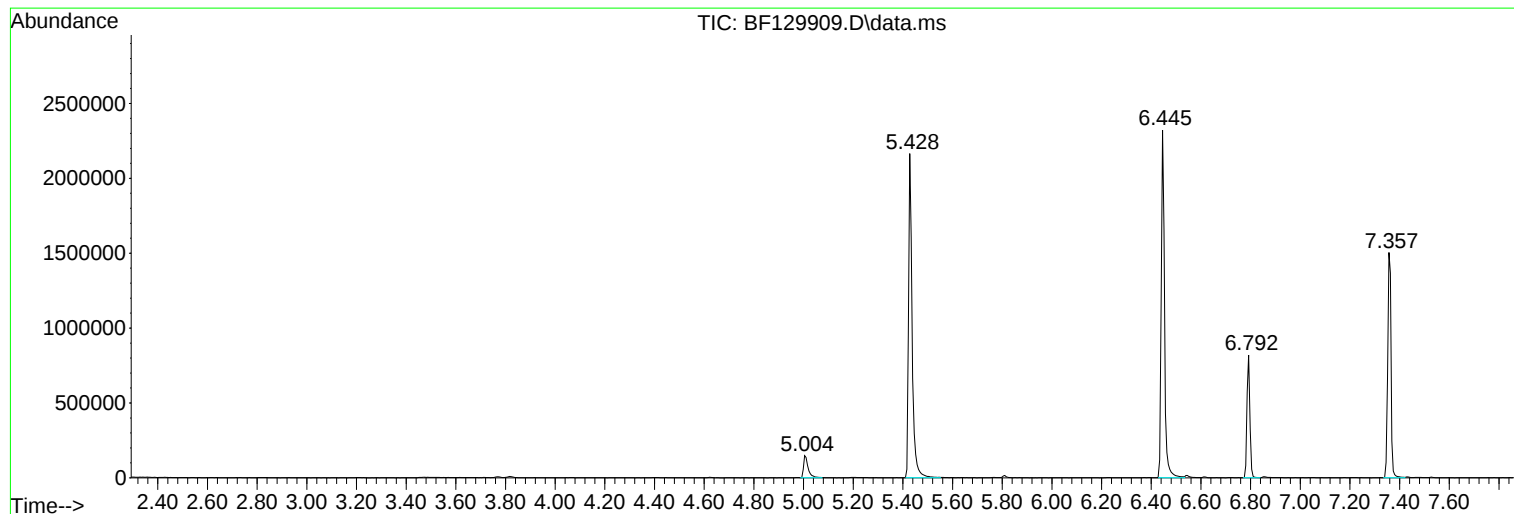
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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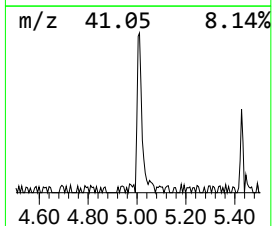
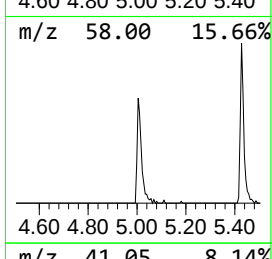
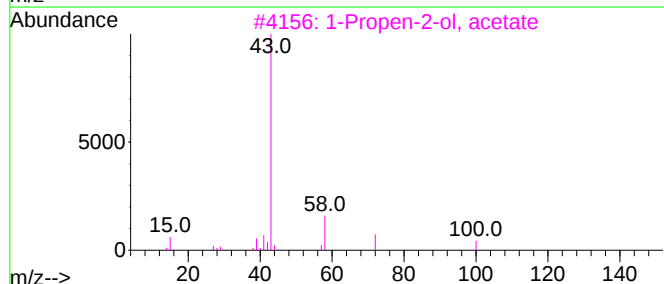
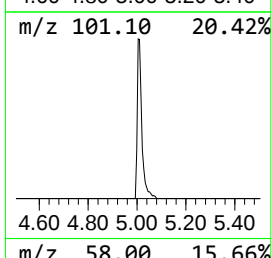
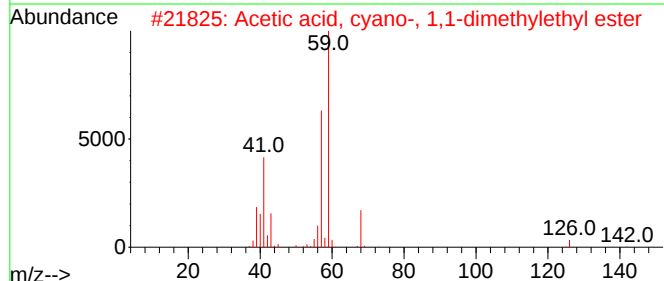
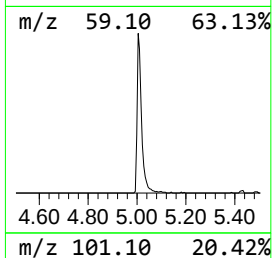
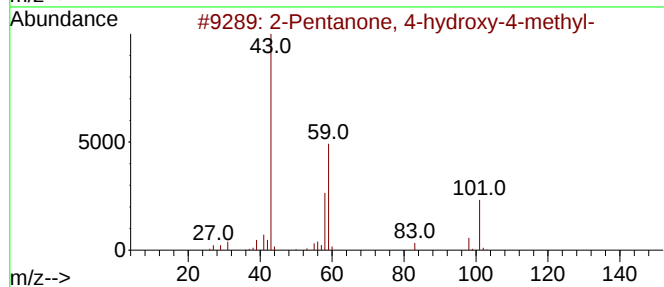
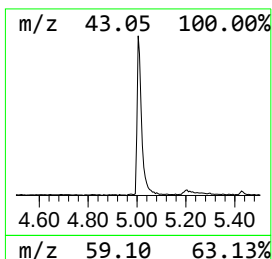
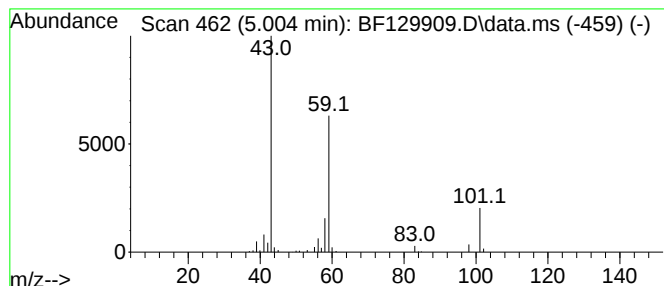
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.004	5.68 ng	186699	1,4-Dichlorobenzene-d4	6.792

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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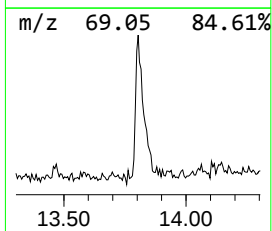
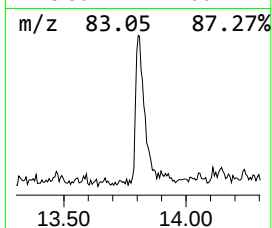
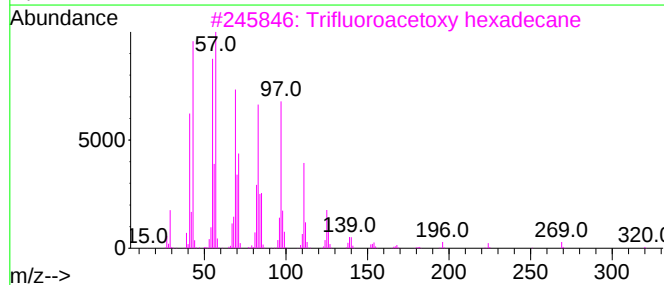
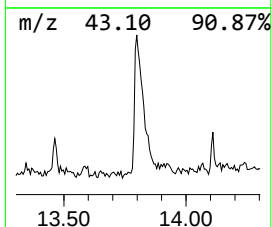
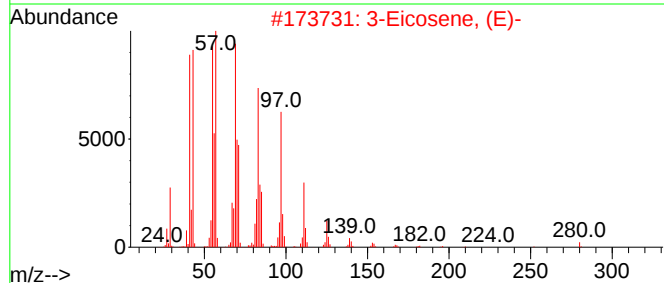
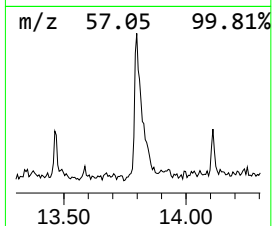
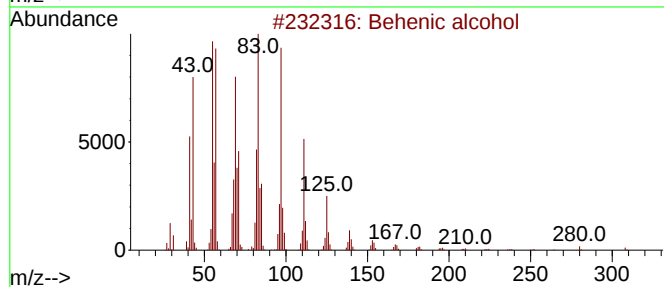
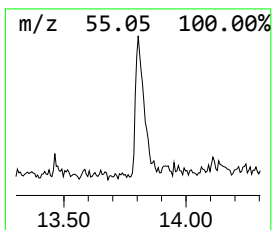
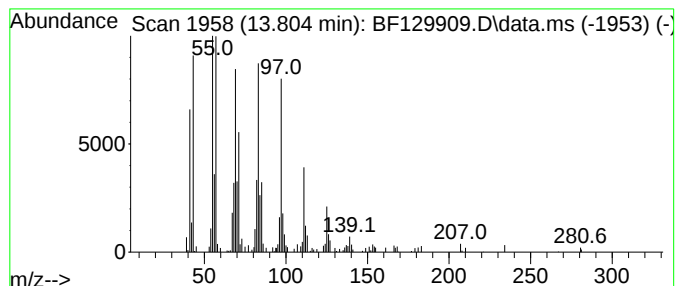
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Peak Number 2 Behenic alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.804	8.94 ng	264086	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	95
2			3-Eicosene, (E)-	280	C20H40	074685-33-9	94
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94



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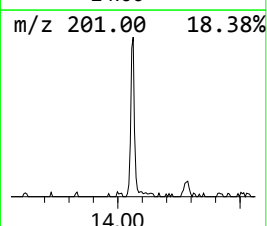
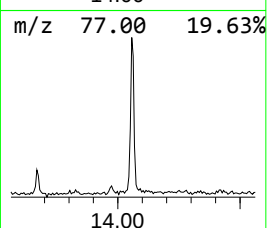
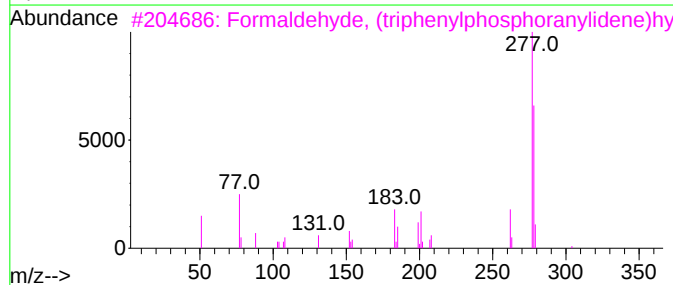
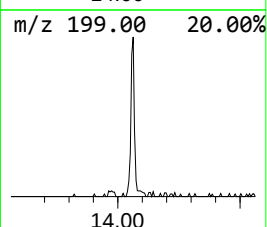
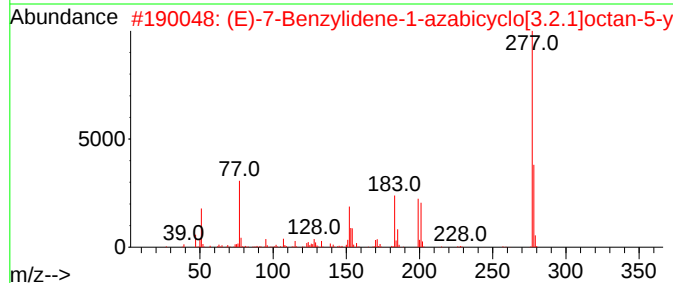
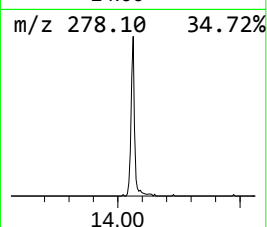
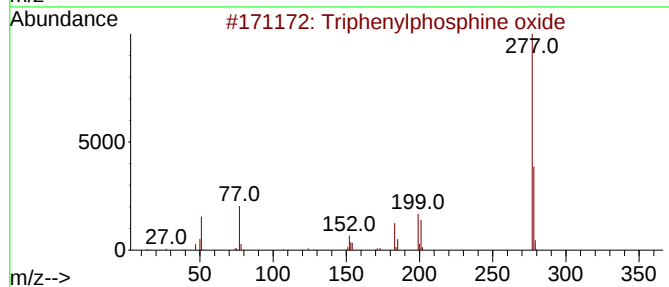
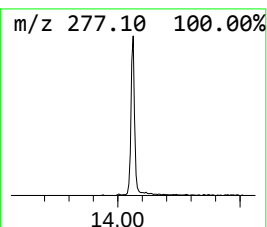
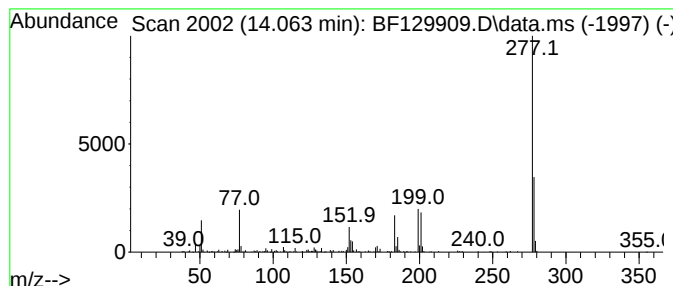
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.063	6.39 ng	188727	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	98
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	38
4			5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	33
5			1H-Indole-3-acetic acid, 5-[(tri...]	277	C14H19NO3Si	072101-35-0	23



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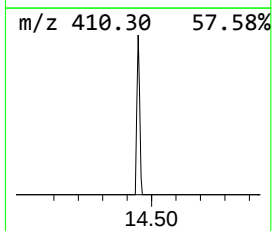
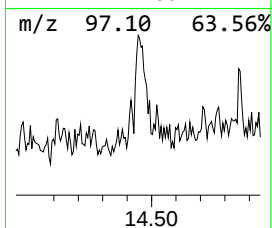
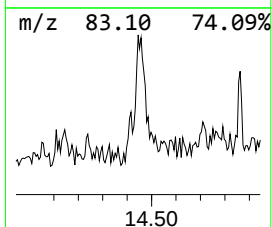
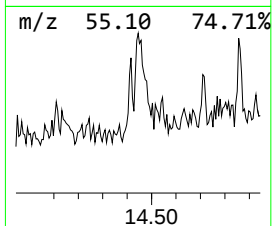
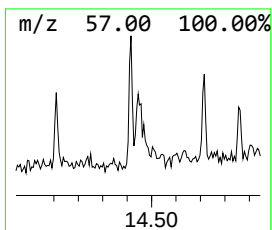
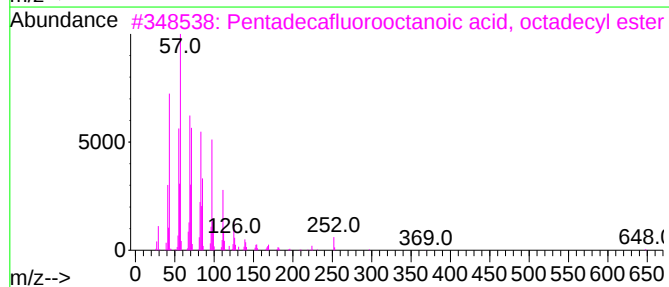
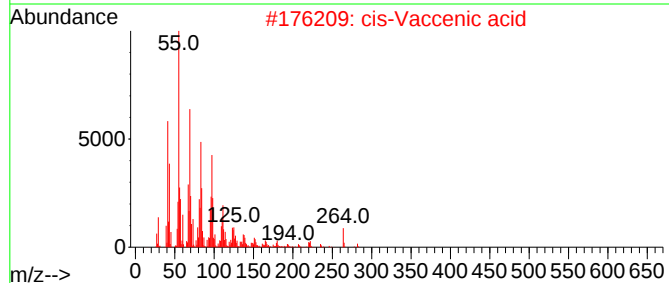
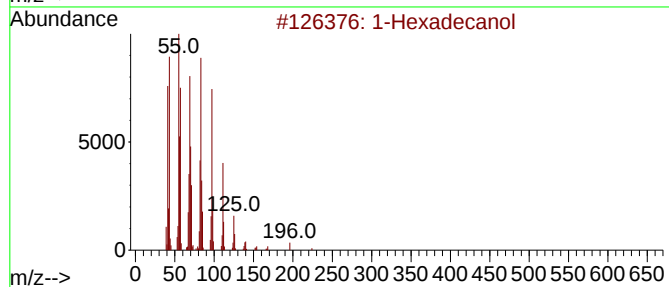
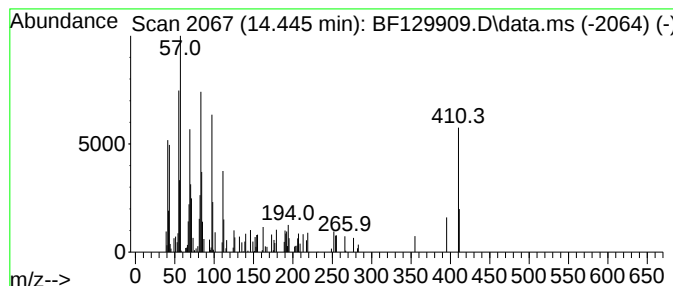
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Peak Number 4 1-Hexadecanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.445	2.64 ng	78091	Chrysene-d12	13.974	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	55
2	cis-Vaccenic acid	282	C18H34O2	000506-17-2	53
3	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	53
4	5-Octadecene, (E)-	252	C18H36	007206-21-5	52
5	Chloroacetic acid, dodecyl ester	262	C14H27ClO2	006316-04-7	49



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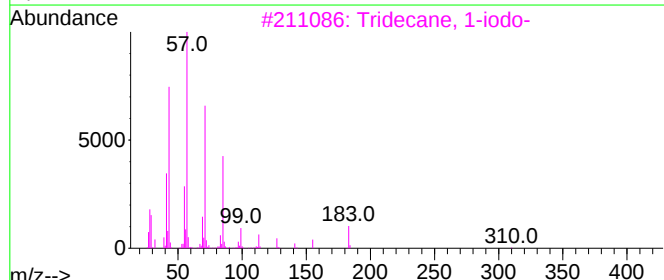
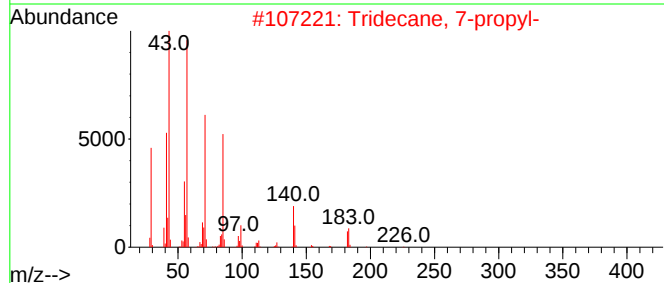
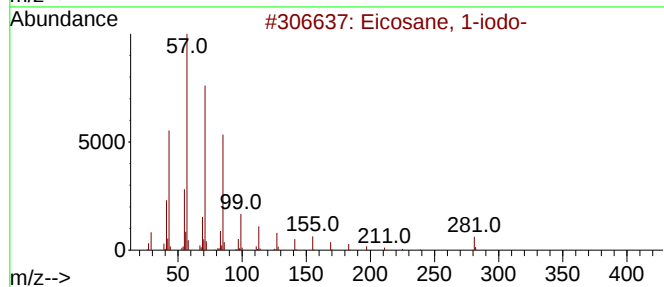
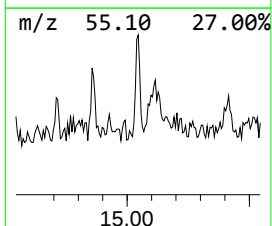
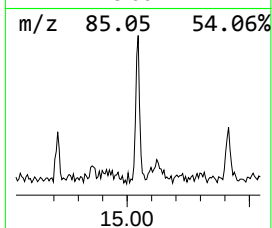
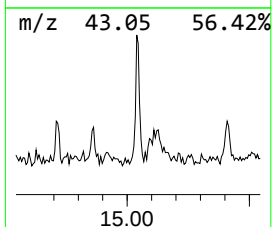
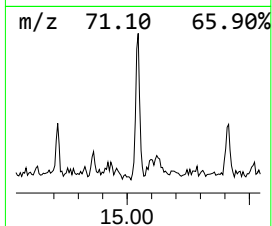
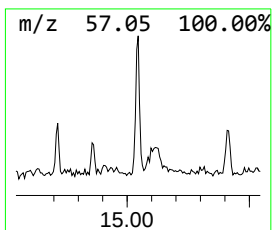
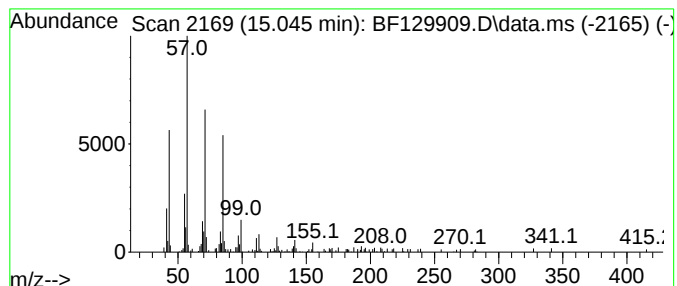
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Peak Number 5 Eicosane, 1-iodo- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.045	2.08 ng	74572	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	86
2			Tridecane, 7-propyl-	226	C16H34	055045-09-5	83
3			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80
4			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	80
5			Tridecane, 6-propyl-	226	C16H34	055045-10-8	80



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SP-3

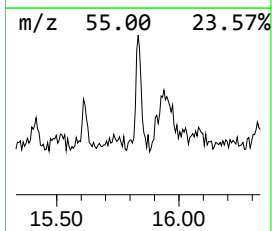
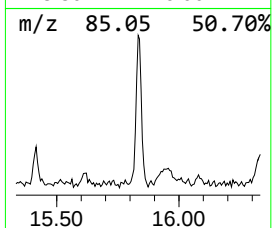
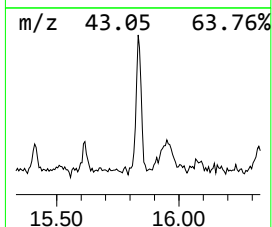
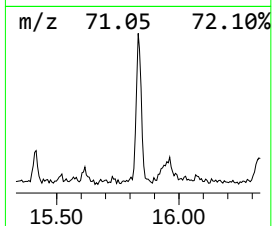
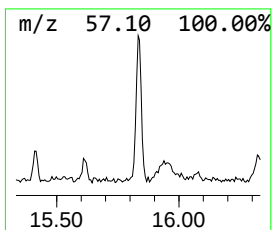
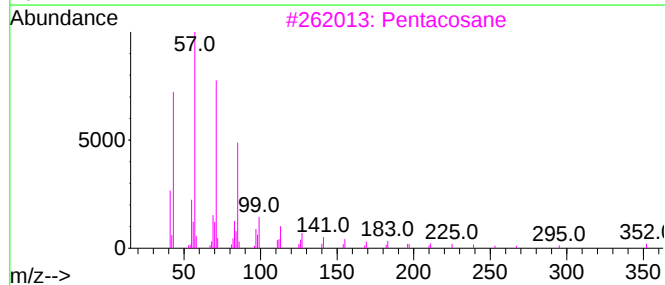
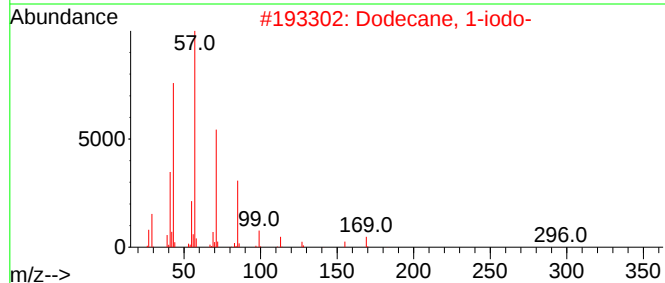
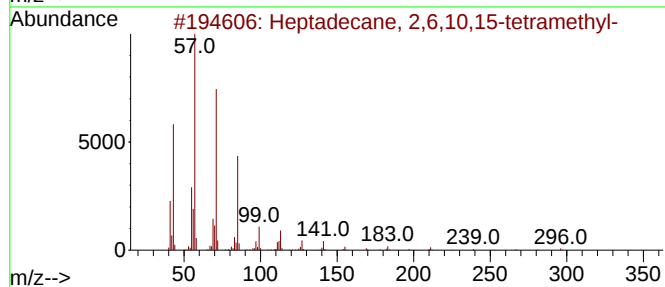
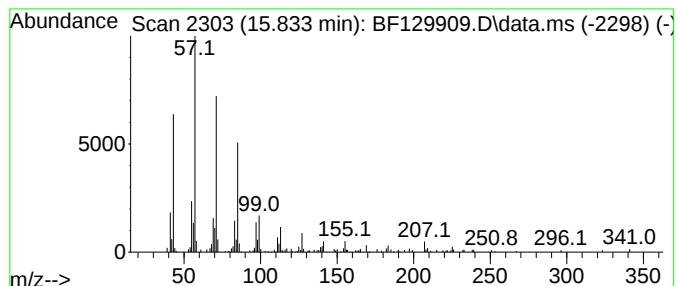
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptadecane, 2,6,10,15-tetr... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.833	4.29 ng	153914	Perylene-d12	15.439

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
2		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	91
3		Pentacosane	352	C25H52	000629-99-2	90
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
5		Tetratetracontane	619	C44H90	007098-22-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081922\
Data File : BF129909.D
Acq On : 19 Aug 2022 13:34
Operator : CG\JU
Sample : N4227-21
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-3

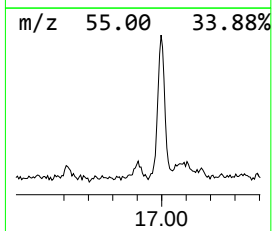
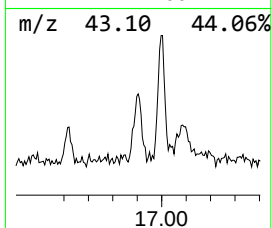
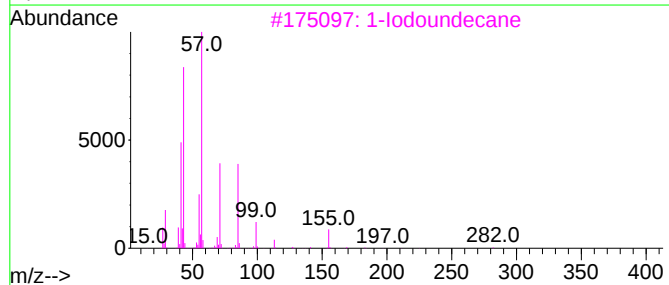
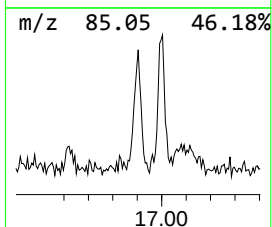
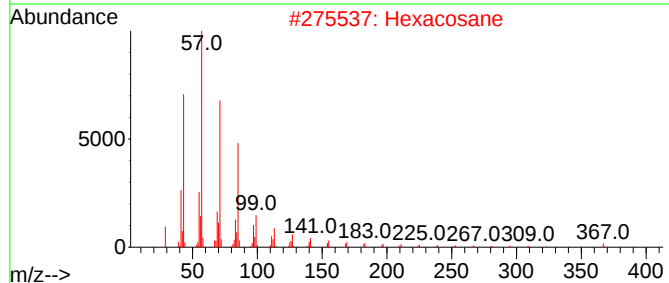
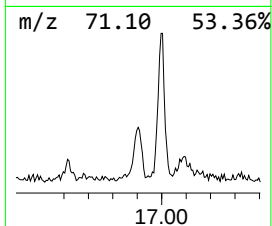
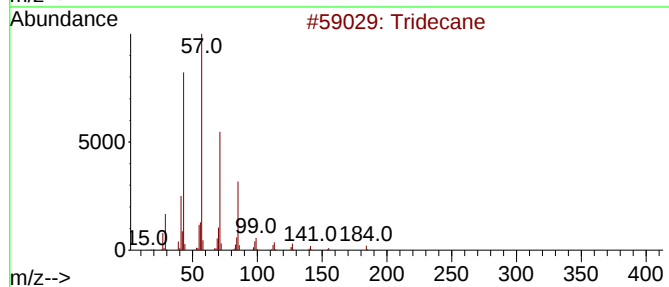
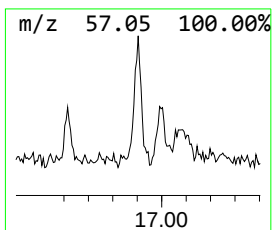
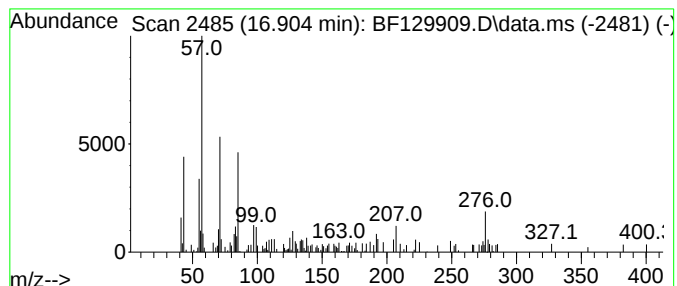
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tridecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.904	2.47 ng	88535	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	53
2			Hexacosane	366	C26H54	000630-01-3	49
3			1-Iodoundecane	282	C11H23I	004282-44-4	49
4			3-Hexanone, 2,4-dimethyl-	128	C8H16O	018641-70-8	47
5			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081922\
Data File : BF129909.D
Acq On : 19 Aug 2022 13:34
Operator : CG\JU
Sample : N4227-21
Misc :
ALS Vial : 10 Sample Multiplier: 1

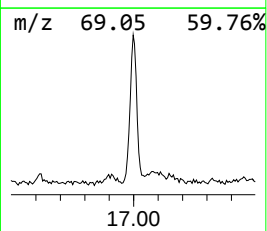
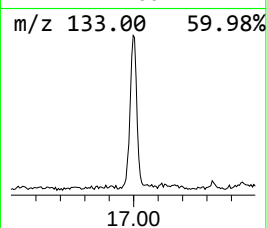
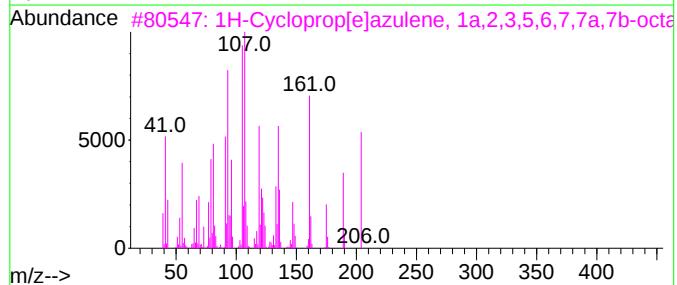
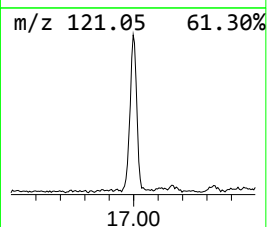
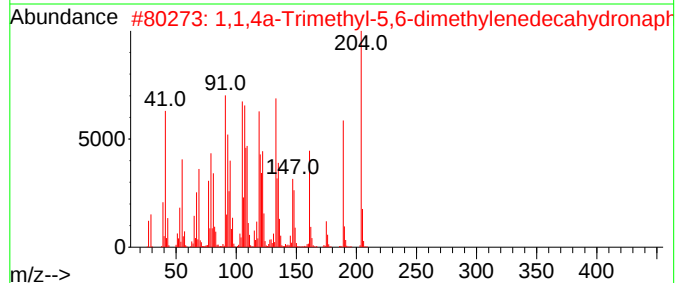
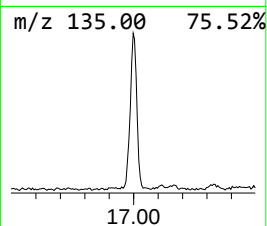
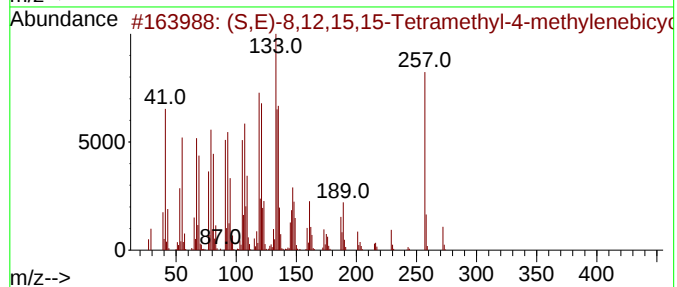
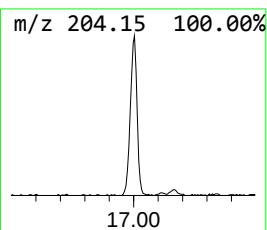
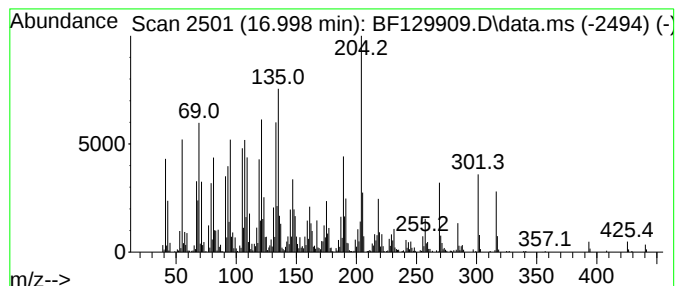
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 (S,E)-8,12,15,15-Tetramethy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.998	41.47 ng	1489360	Perylene-d12	15.439	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S,E)-8,12,15,15-Tetramethyl-4-m...	272	C20H32	386223-19-4	55
2	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	53
3	1H-Cycloprop[e]azulene, 1a,2,3,5...	204	C15H24	021747-46-6	50
4	1-Naphthalenecarboxylic acid, de...	316	C21H32O2	001235-39-8	49
5	1H-3a,7-Methanoazulene, 2,3,6,7,...	204	C15H24	000560-32-7	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081922\
Data File : BF129909.D
Acq On : 19 Aug 2022 13:34
Operator : CG\JU
Sample : N4227-21
Misc :
ALS Vial : 10 Sample Multiplier: 1

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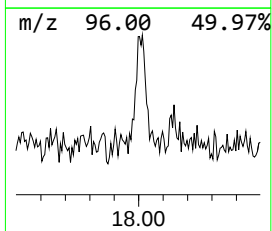
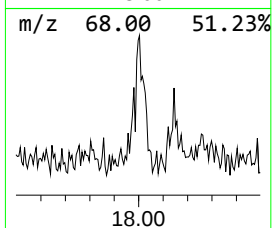
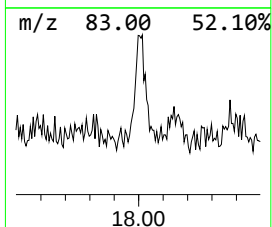
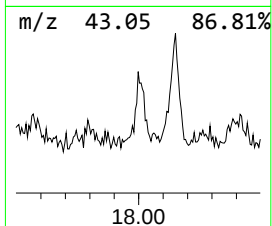
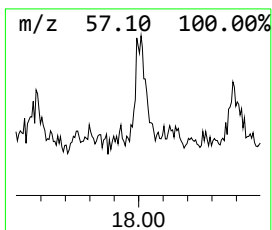
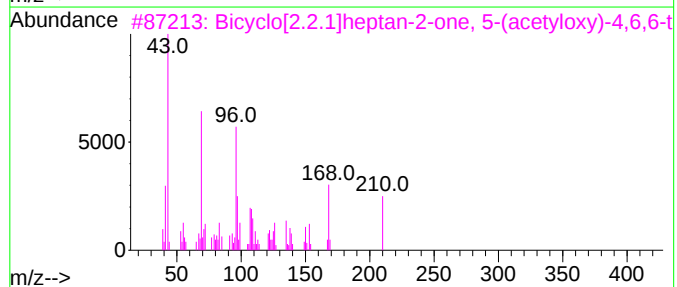
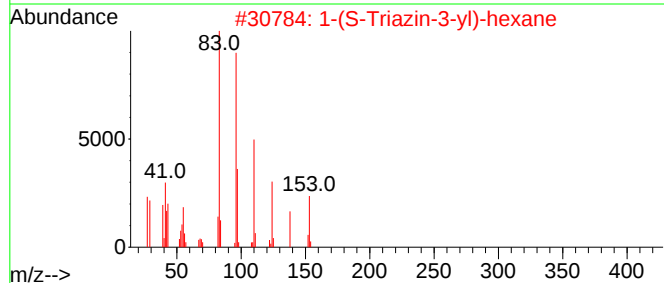
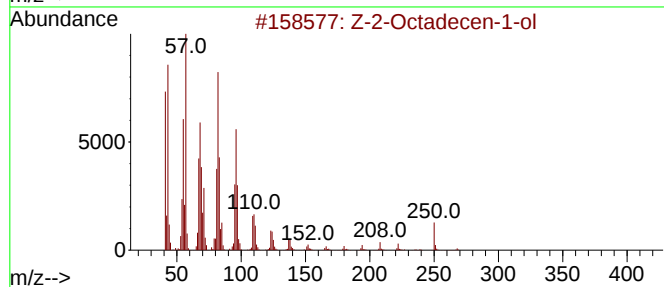
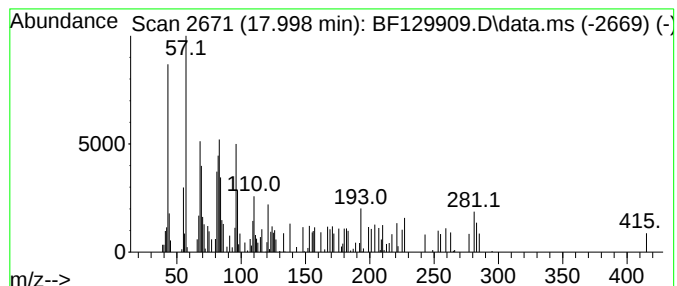
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown17.998 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.998	2.55 ng	91734	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Z-2-Octadecen-1-ol	268	C18H36O	1000131-11-0	35
2			1-(S-Triazin-3-yl)-hexane	153	C8H15N3	067646-18-8	35
3			Bicyclo[2.2.1]heptan-2-one, 5-(a...	210	C12H18O3	055590-78-8	27
4			Tropine, TBDMS derivative	255	C14H29NOSi	1000364-41-5	27
5			Tridecanal	198	C13H26O	010486-19-8	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081922\
Data File : BF129909.D
Acq On : 19 Aug 2022 13:34
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Sample : N4227-21
Misc :
ALS Vial : 10 Sample Multiplier: 1

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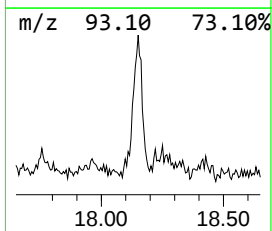
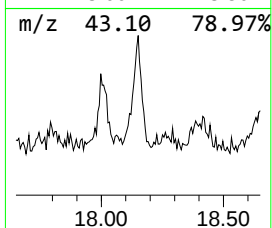
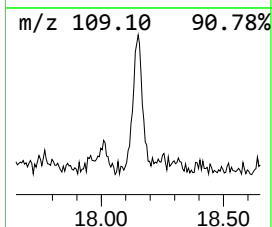
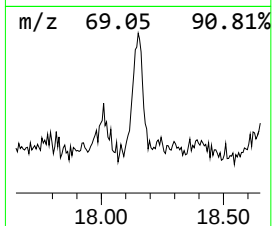
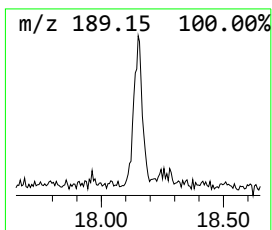
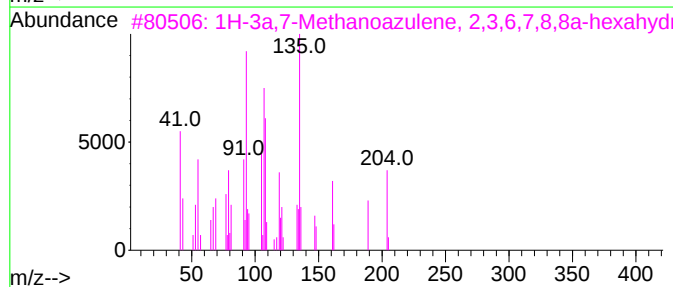
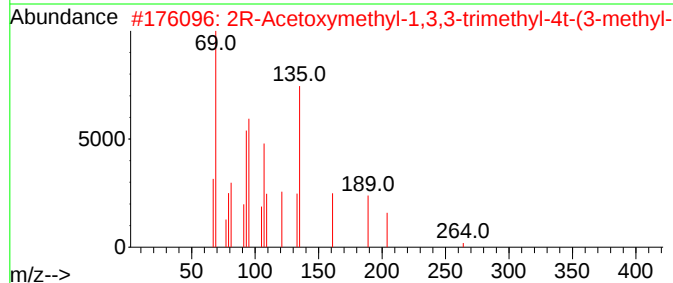
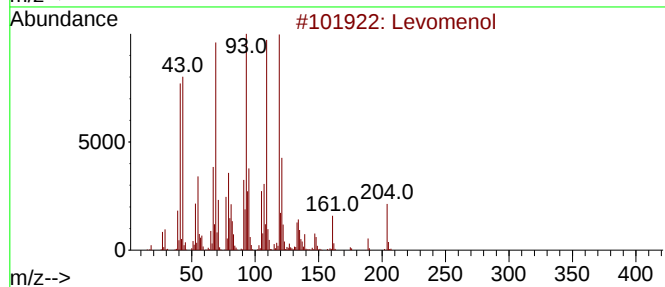
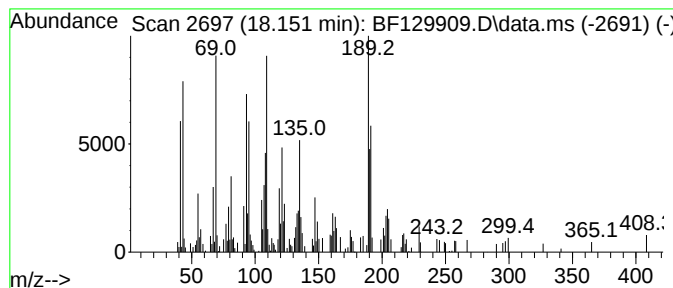
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown18.151 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.151	6.07 ng	218027	Perylene-d12	15.439

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Levomenol	222	C15H26O	023089-26-1	38
2		2R-Acetoxyethyl-1,3,3-trimethyl...	282	C17H30O3	1000144-12-4	27
3		1H-3a,7-Methanoazulene, 2,3,6,7,...	204	C15H24	000560-32-7	25
4		Benzene, 1,3,5-tris(1-methylethyl)-	204	C15H24	000717-74-8	11
5		Modephene	204	C15H24	068269-87-4	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081922\
Data File : BF129909.D
Acq On : 19 Aug 2022 13:34
Operator : CG\JU
Sample : N4227-21
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.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-...	5.004	5.7	ng	186699	1	6.792	657339	20.0
Behenic alcohol	13.804	8.9	ng	264086	5	13.974	590590	20.0
Triphenylphosph...	14.063	6.4	ng	188727	5	13.974	590590	20.0
1-Hexadecanol	14.445	2.6	ng	78091	5	13.974	590590	20.0
Eicosane, 1-iodo-	15.045	2.1	ng	74572	6	15.439	718297	20.0
Heptadecane, 2,...	15.833	4.3	ng	153914	6	15.439	718297	20.0
Tridecane	16.904	2.5	ng	88535	6	15.439	718297	20.0
(S,E)-8,12,15,1...	16.998	41.5	ng	1489360	6	15.439	718297	20.0
unknown17.998	17.998	2.5	ng	91734	6	15.439	718297	20.0
unknown18.151	18.151	6.1	ng	218027	6	15.439	718297	20.0