

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100820\
 Data File : BF121898.D
 Acq On : 8 Oct 2020 19:53
 Operator : JU/CG
 Sample : L4309-02
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OWLS-HEAD-BH-02-B

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

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-BF091020.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.957	484	488	503	rBV	96899	134057	5.60%	0.741%
2	5.381	556	560	579	rBV	1660913	1803528	75.35%	9.971%
3	6.398	729	733	763	rBV	1792820	1887715	78.87%	10.437%
4	6.757	790	794	803	rBV	761679	602629	25.18%	3.332%
5	7.322	886	890	903	rBV	1406082	1308432	54.66%	7.234%
6	8.039	1008	1012	1028	rBV	799398	802260	33.52%	4.436%
7	9.116	1191	1195	1207	rBV	2745850	2383241	99.57%	13.177%
8	9.510	1259	1262	1272	rBV	184377	194740	8.14%	1.077%
9	9.792	1307	1310	1322	rVB	1036451	912921	38.14%	5.047%
10	10.586	1441	1445	1461	rBV	1331003	1319761	55.14%	7.297%
11	11.280	1559	1563	1570	rBV	978147	934216	39.03%	5.165%
12	12.863	1828	1832	1836	rBV	2639335	2393557	100.00%	13.234%
13	13.092	1868	1871	1880	rBV3	18590	29983	1.25%	0.166%
14	13.774	1982	1987	2002	rBV2	203460	525010	21.93%	2.903%
15	13.916	2007	2011	2022	rVB	703315	728120	30.42%	4.026%
16	14.380	2086	2090	2093	rBV2	43523	38592	1.61%	0.213%
17	14.421	2093	2097	2106	rVV4	28586	67663	2.83%	0.374%
18	14.680	2137	2141	2145	rBV	35278	34996	1.46%	0.193%
19	14.751	2149	2153	2158	rVB	30660	36257	1.51%	0.200%
20	14.821	2162	2165	2170	rVB	52119	50403	2.11%	0.279%
21	15.004	2193	2196	2201	rVB	65663	69961	2.92%	0.387%
22	15.080	2201	2209	2217	rBV4	40780	114660	4.79%	0.634%
23	15.357	2251	2256	2268	rBV	594694	785929	32.84%	4.345%
24	15.562	2287	2291	2295	rVB3	36435	45467	1.90%	0.251%
25	15.780	2324	2328	2334	rVB	78366	112012	4.68%	0.619%
26	15.886	2339	2346	2358	rBV4	54030	194566	8.13%	1.076%
27	16.262	2407	2410	2416	rVB3	19770	28616	1.20%	0.158%
28	16.539	2451	2457	2465	rVB2	84417	156775	6.55%	0.867%
29	16.815	2500	2504	2514	rVB	39683	82646	3.45%	0.457%
30	16.992	2525	2534	2536	rBV7	37953	99161	4.14%	0.548%
31	17.345	2588	2594	2608	rVB7	22027	82173	3.43%	0.454%
32	17.892	2681	2687	2695	rVB5	27679	70038	2.93%	0.387%
33	18.274	2747	2752	2762	rVB10	22070	56843	2.37%	0.314%

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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-BF091020.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

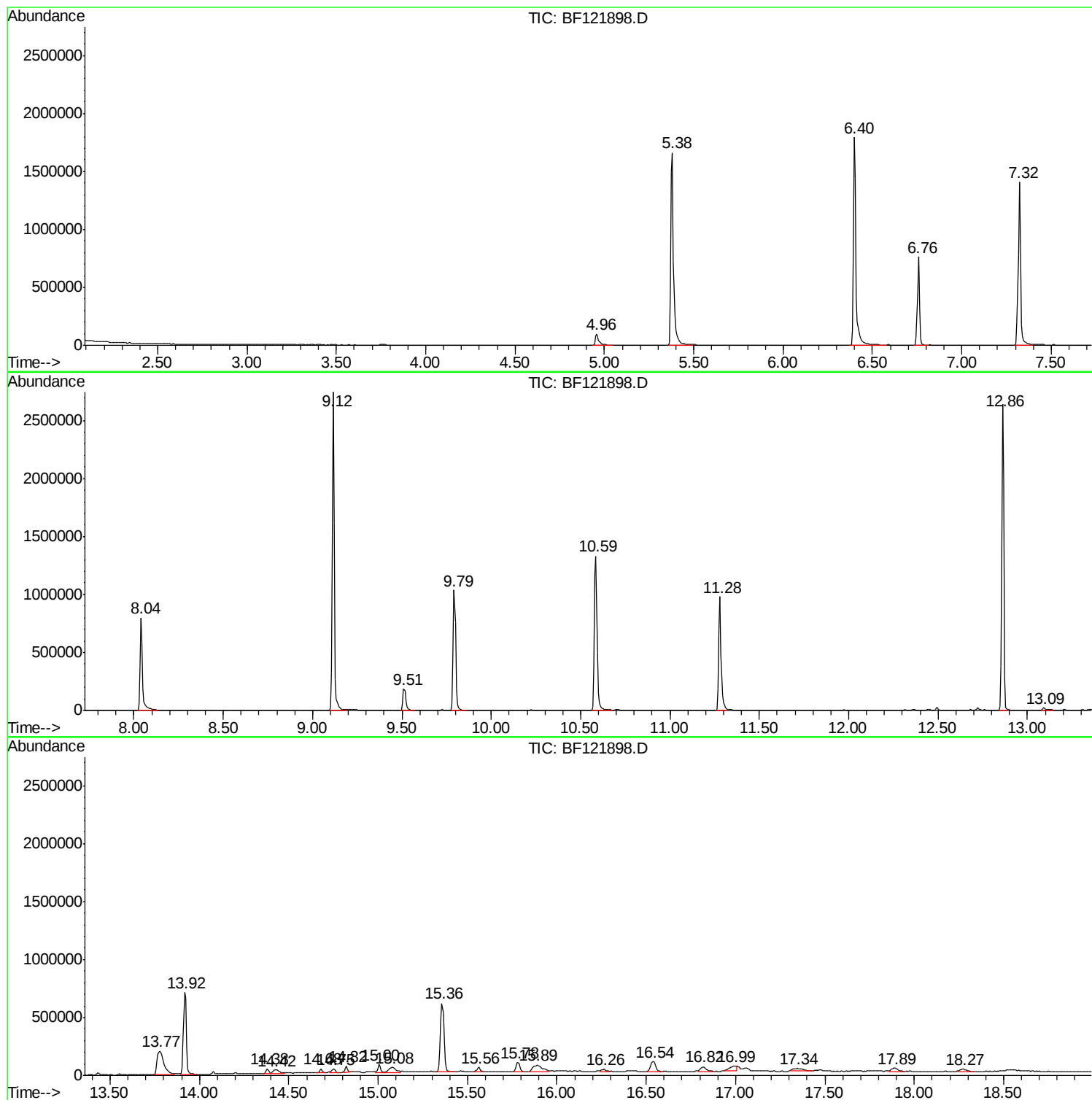
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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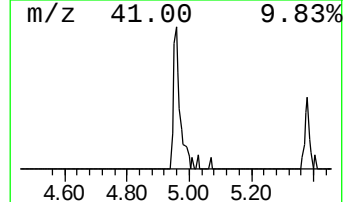
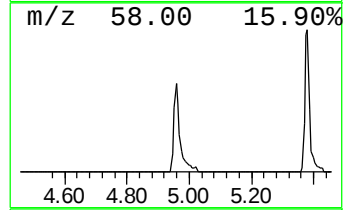
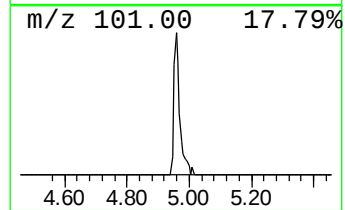
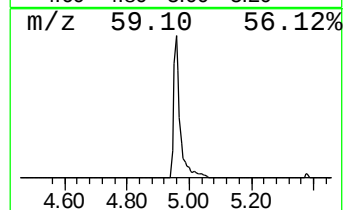
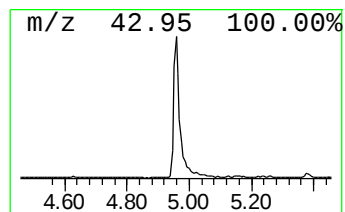
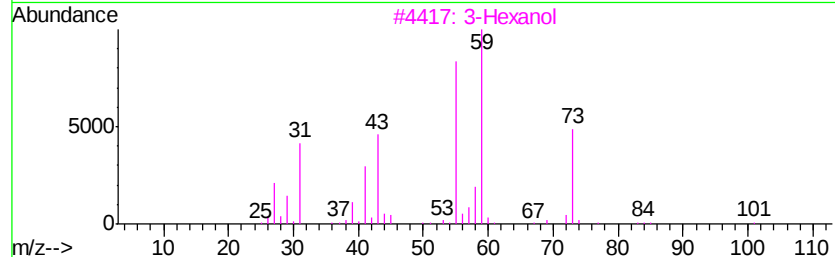
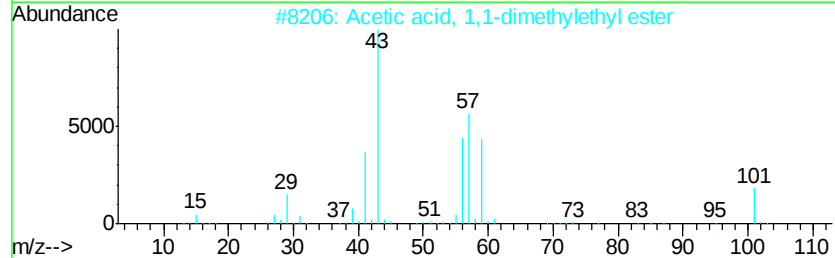
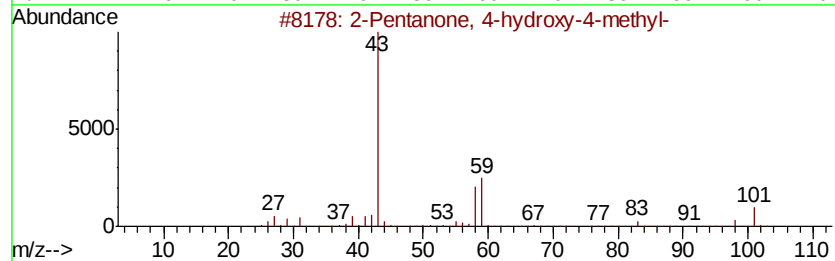
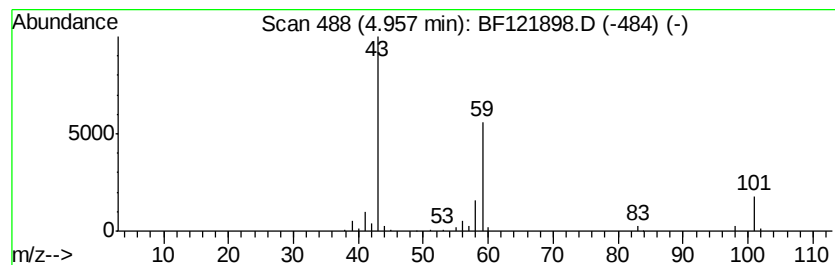
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	4.45 ng	134057	1,4-Dichlorobenzene-d4	6.76

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			3-Hexanol	102	C6H14O	000623-37-0	33
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32



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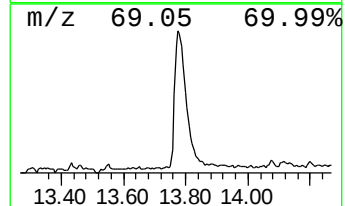
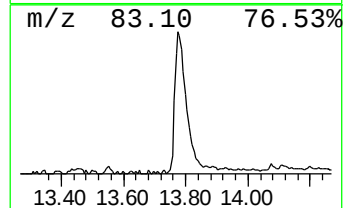
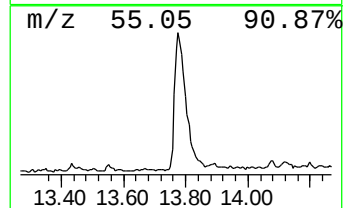
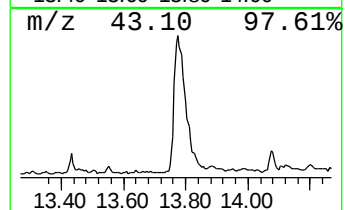
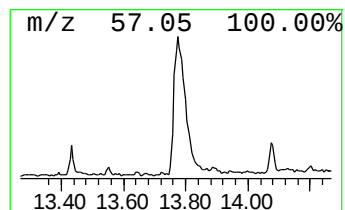
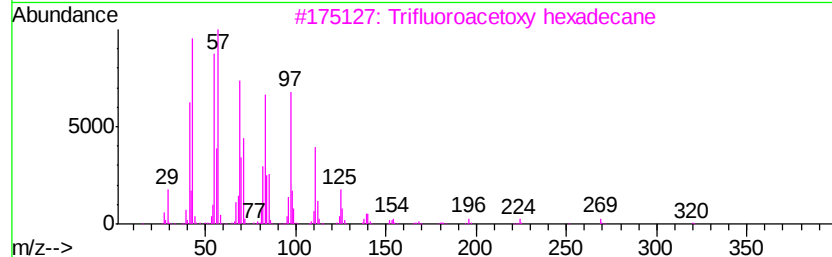
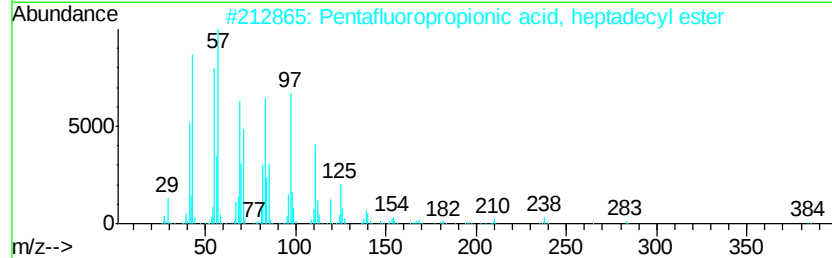
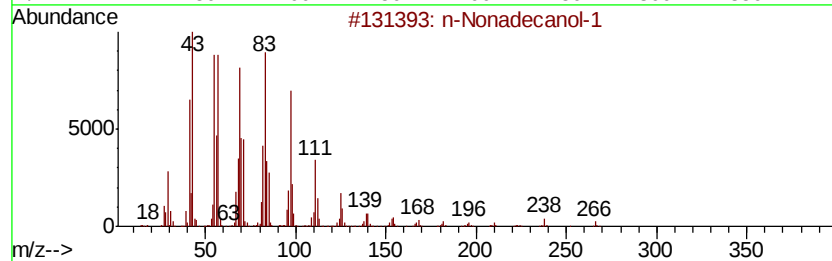
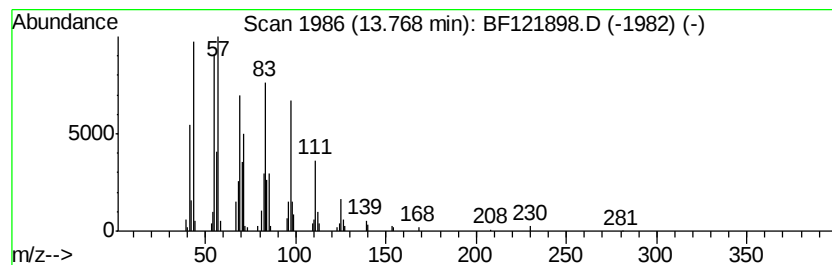
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Nonadecanol-1 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	14.42 ng	525010	Chrysene-d12	13.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
2		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	94
3		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
5		1-Heneicosanol	312	C21H44O	015594-90-8	93



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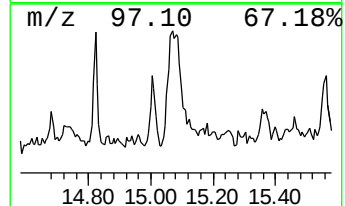
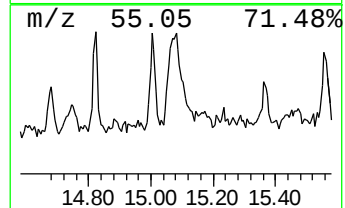
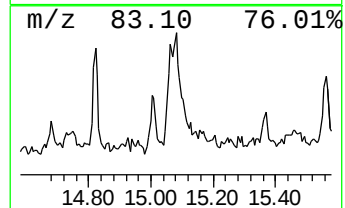
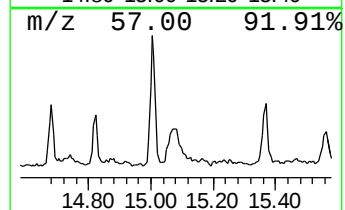
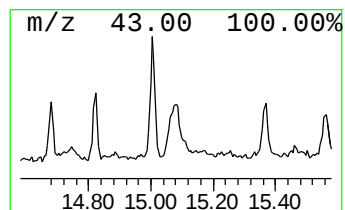
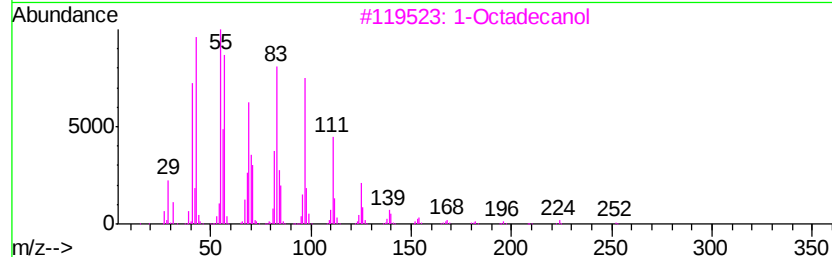
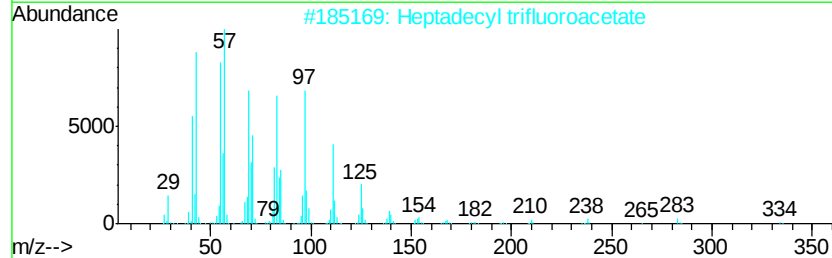
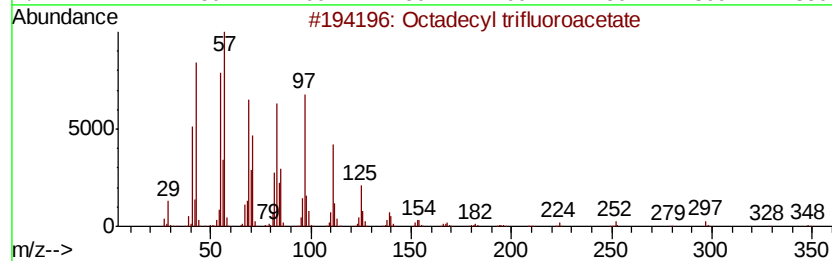
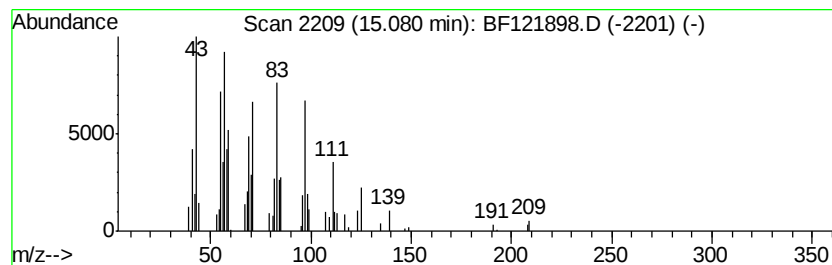
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octadecyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.08	2.92 ng	114660	Perylene-d12		15.36
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	76
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	70
3	1-Octadecanol	270	C18H38O	000112-92-5	64
4	Octacosanol	410	C28H58O	000557-61-9	64
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	64



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ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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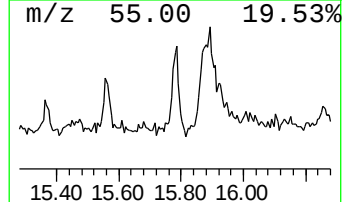
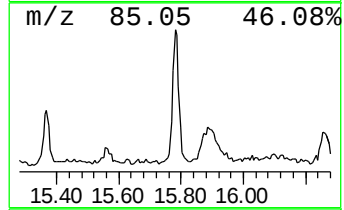
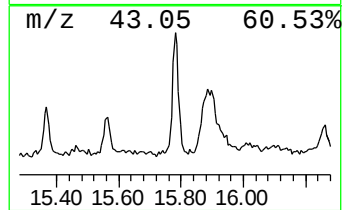
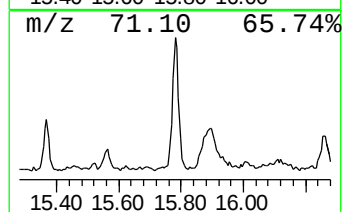
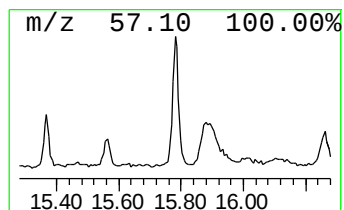
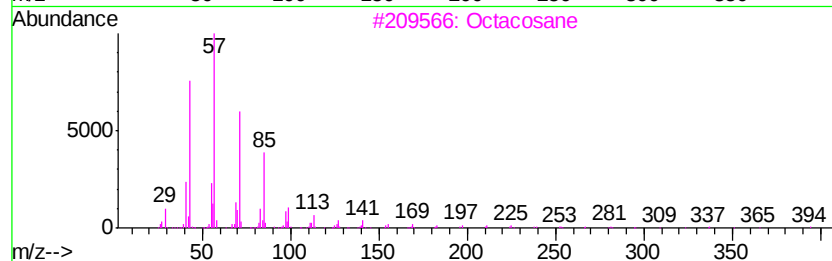
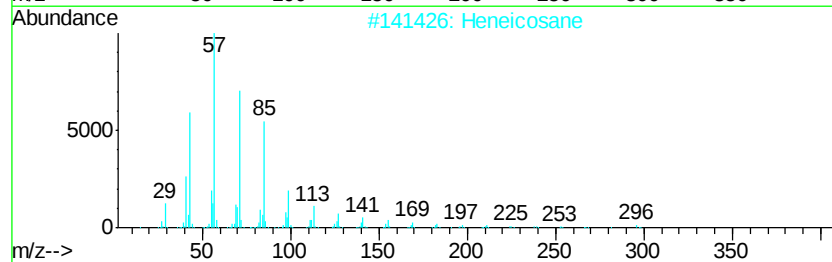
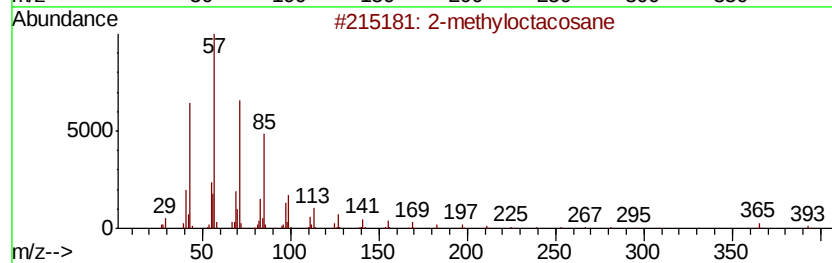
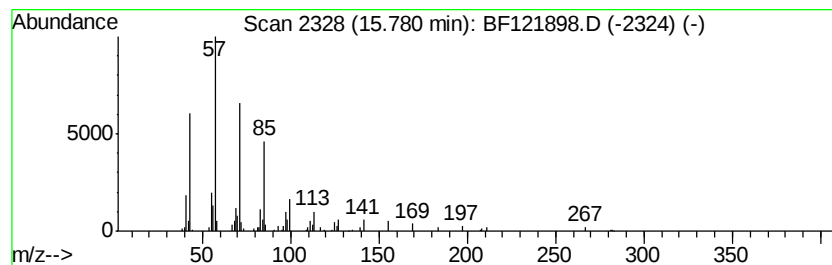
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 2-methyloctacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.78	2.85 ng	112012	Perylene-d12	15.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5		triacontane	422	C30H62	000638-68-6	91



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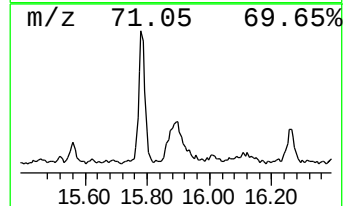
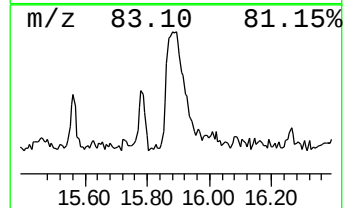
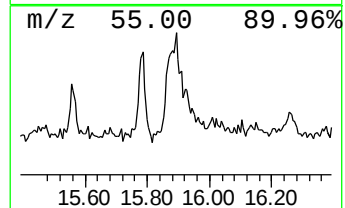
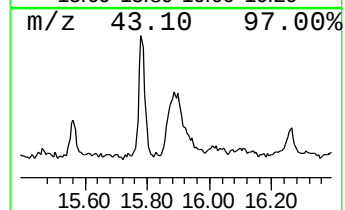
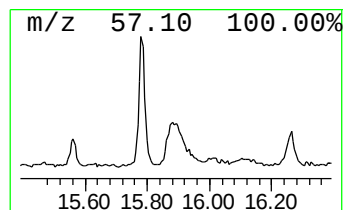
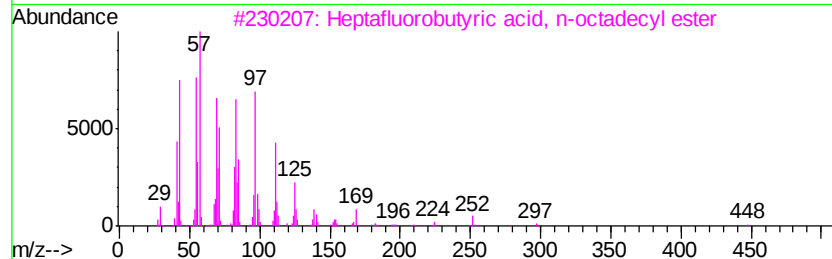
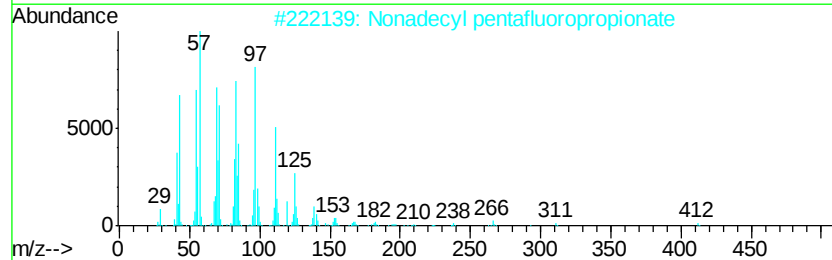
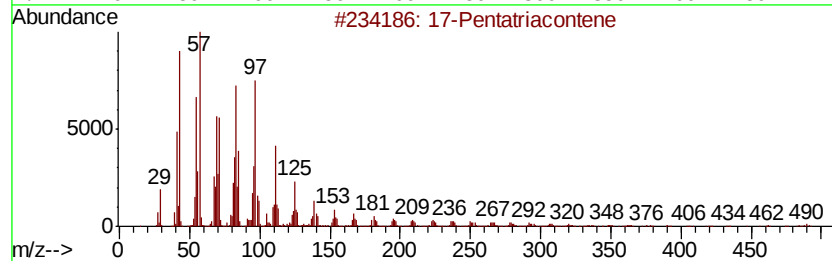
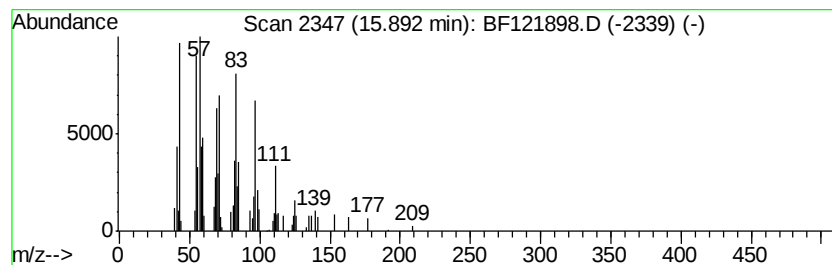
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 17-Pentatriacontene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.89	4.95 ng	194566	Perylene-d12	15.36

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		17-Pentatriacontene	491	C35H70	006971-40-0	90
2		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	87
3		Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	87
4		Pentafluoropropionic acid, heptafluorobutyl ester	402	C20H35F5O2	959218-78-1	87
5		Pentafluoropropionic acid, octadecyl ester	416	C21H37F5O2	959261-25-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100820\
Data File : BF121898.D
Acq On : 8 Oct 2020 19:53
Operator : JU/CG
Sample : L4309-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

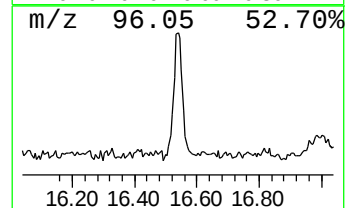
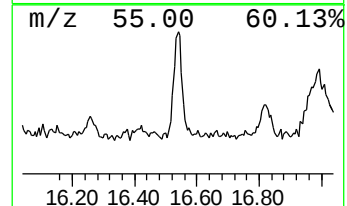
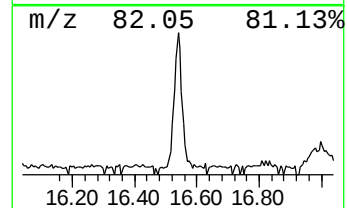
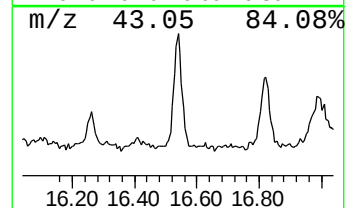
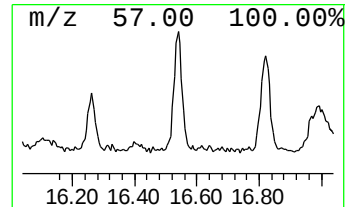
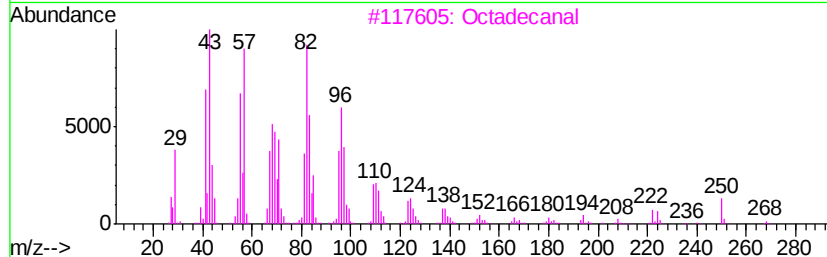
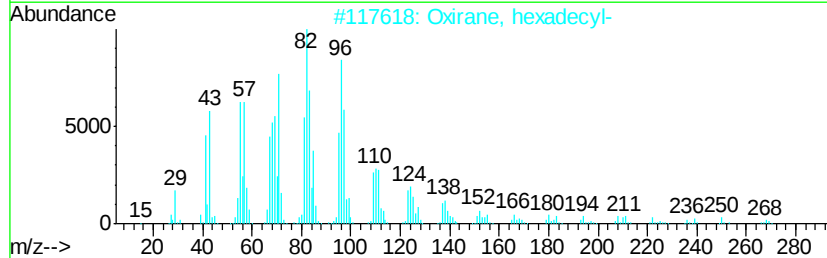
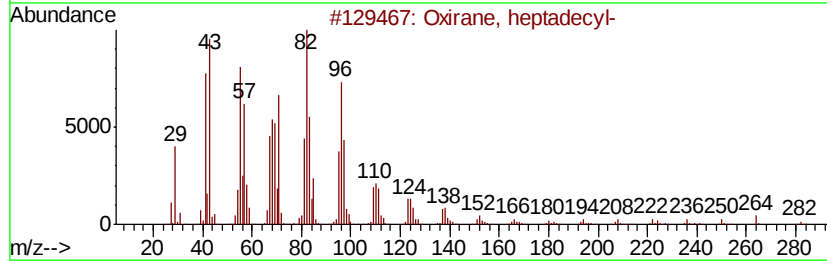
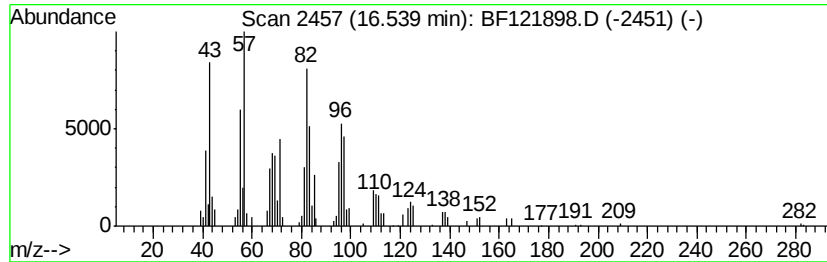
Instrument :
BNA_F
ClientSampleId :
OWLS-HEAD-BH-02-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Oxirane, heptadecyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.54	3.99 ng	156775	Perylene-d12	15.36
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Oxirane, heptadecyl-	282 C19H38O	067860-04-2	95
2	Oxirane, hexadecyl-	268 C18H36O	007390-81-0	94
3	Octadecanal	268 C18H36O	000638-66-4	90
4	Hexadecanal	240 C16H32O	000629-80-1	74
5	1,19-Eicosadiene	278 C20H38	014811-95-1	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100820\
Data File : BF121898.D
Acq On : 8 Oct 2020 19:53
Operator : JU/CG
Sample : L4309-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OWLS-HEAD-BH-02-B

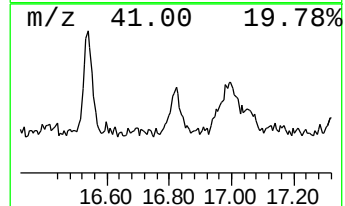
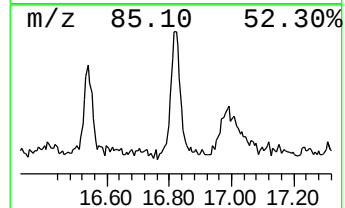
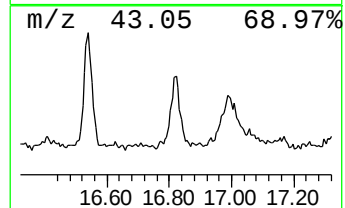
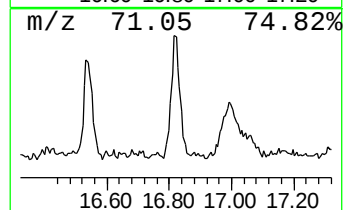
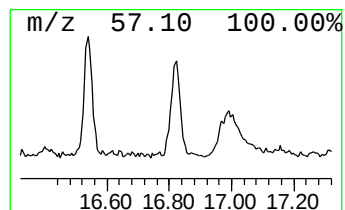
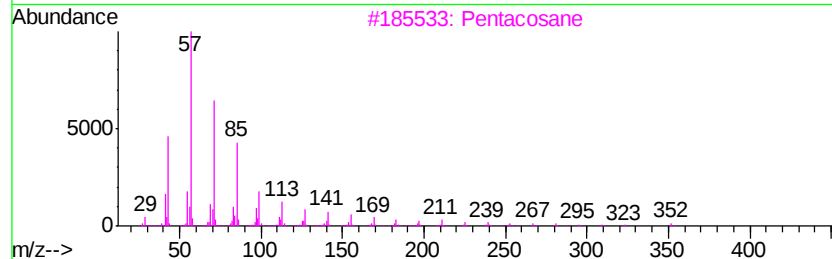
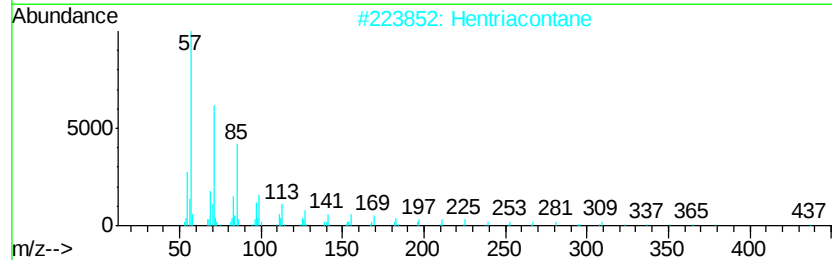
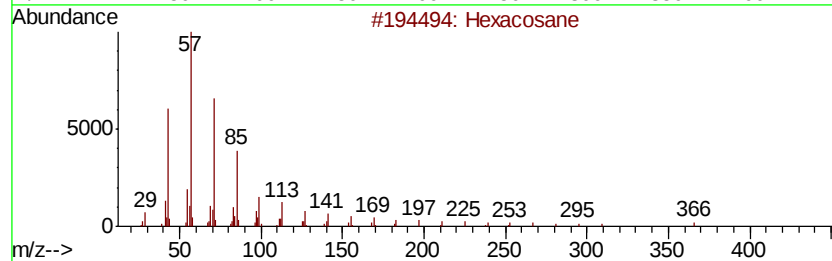
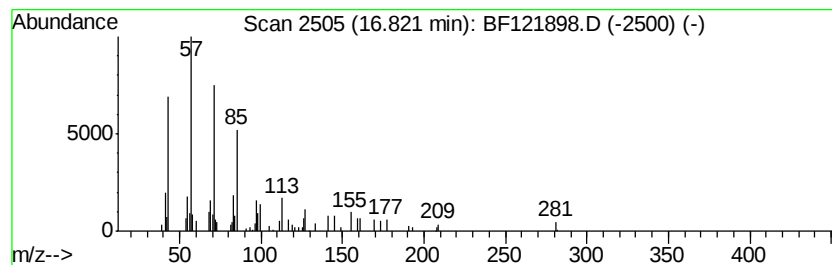
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.82	2.10 ng	82646	Perylene-d12	15.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	90
2		Hentriacontane	437	C31H64	000630-04-6	87
3		Pentacosane	352	C25H52	000629-99-2	87
4		Octadecane, 3-ethyl-5-(2-ethylbu...	366	C26H54	055282-12-7	86
5		Heptacosane	380	C27H56	000593-49-7	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100820\
 Data File : BF121898.D
 Acq On : 8 Oct 2020 19:53
 Operator : JU/CG
 Sample : L4309-02
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

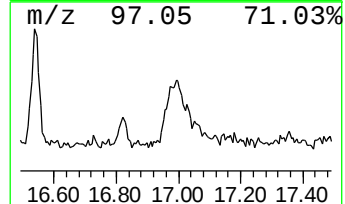
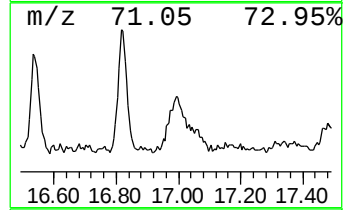
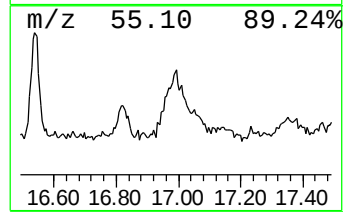
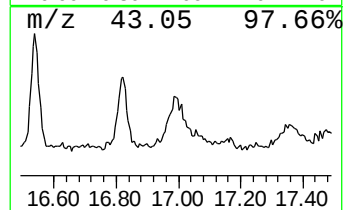
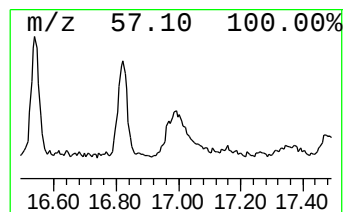
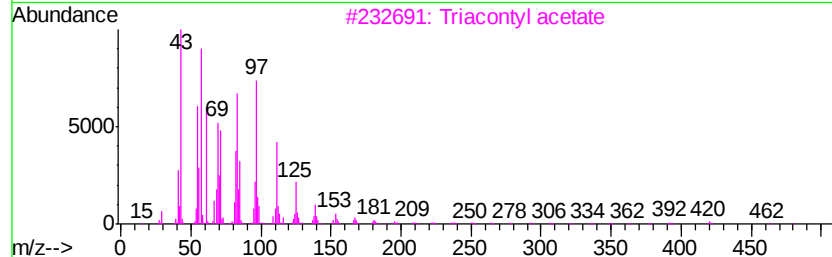
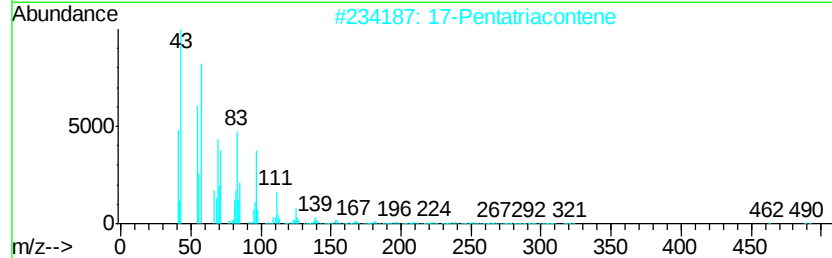
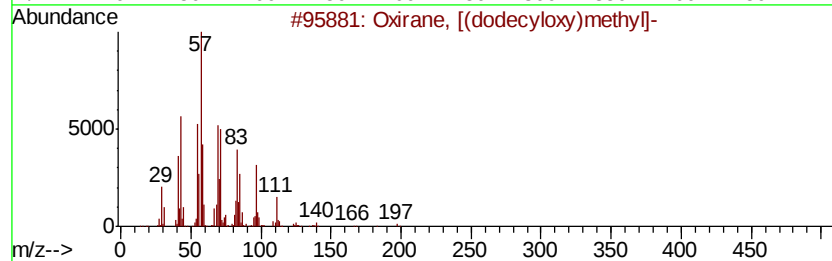
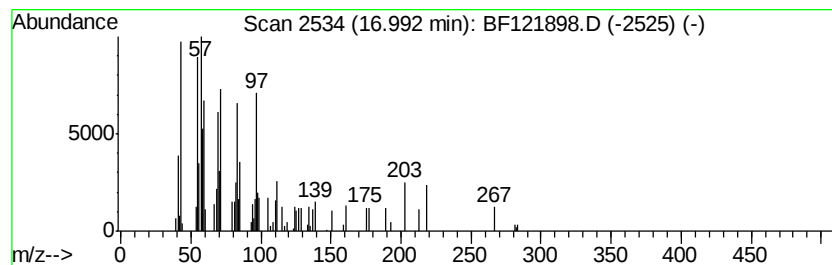
Instrument :
 BNA_F
 ClientSampleId :
 OWLS-HEAD-BH-02-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091020.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 8 Oxirane, [(dodecyloxy)methyl]- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.99	2.52 ng	99161	Perylene-d12	15.36	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	52
2	17-Pentatriacontene	491	C35H70	006971-40-0	49
3	Triacetyl acetate	480	C32H64O2	041755-58-2	43
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	43
5	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100820\
Data File : BF121898.D
Acq On : 8 Oct 2020 19:53
Operator : JU/CG
Sample : L4309-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OWLS-HEAD-BH-02-B

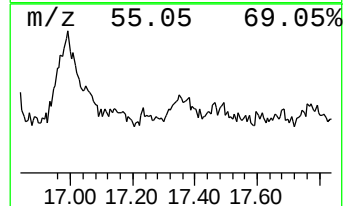
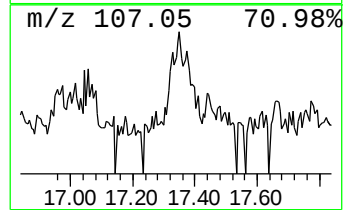
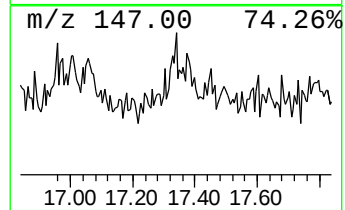
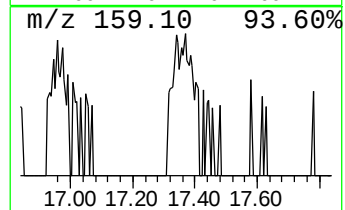
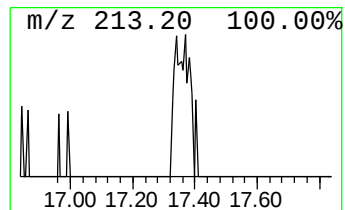
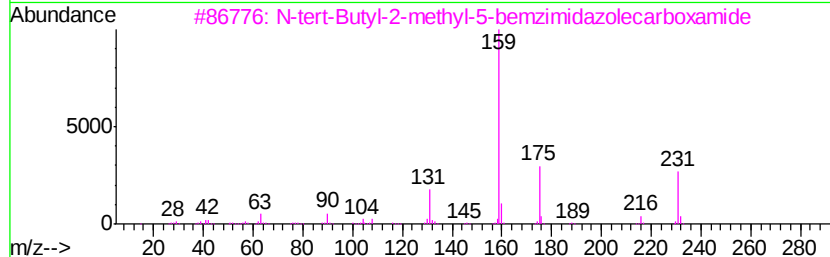
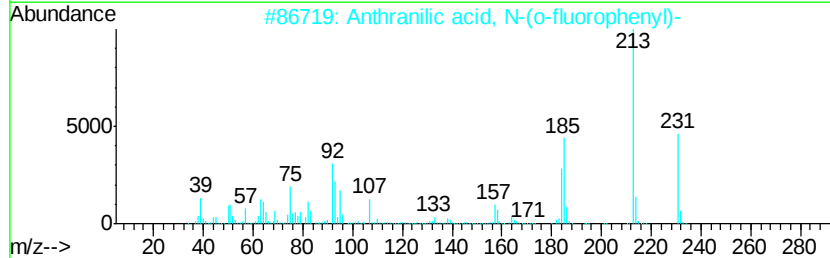
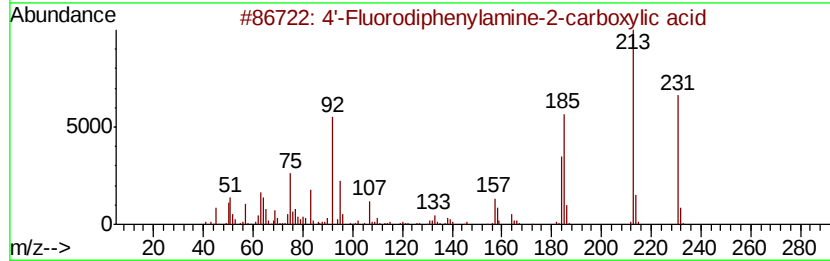
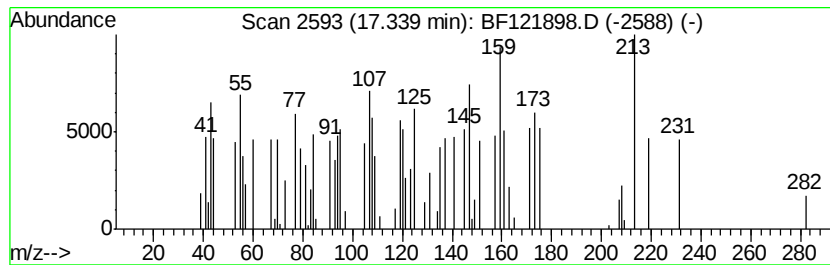
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown17.34 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.34	2.09 ng	82173	Perylene-d12	15.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4'-Fluorodiphenylamine-2-carboxy...	231	C13H10FN02	000054-60-4	11
2		Anthranilic acid, N-(o-fluorophe...	231	C13H10FN02	000054-58-0	10
3		N-tert-Butyl-2-methyl-5-benzimid...	231	C13H17N3O	096749-58-5	9
4		N-Isobutyl-2-methyl-5-benzimidaz...	231	C13H17N3O	096713-60-9	9
5		6-Methyl(pentamethylene)silyloxy...	326	C20H42OSi	1000278-79-4	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100820\
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Sample : L4309-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
OWLS-HEAD-BH-02-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.96	4.5	ng	134057	1	6.76	602629	20.0
n-Nonadecanol-1	13.77	14.4	ng	525010	5	13.92	728120	20.0
Octadecyl trifluo...	15.08	2.9	ng	114660	6	15.36	785929	20.0
2-methyloctacosane	15.78	2.9	ng	112012	6	15.36	785929	20.0
17-Pentatriacontene	15.89	5.0	ng	194566	6	15.36	785929	20.0
Oxirane, heptadecyl-	16.54	4.0	ng	156775	6	15.36	785929	20.0
Hexacosane	16.82	2.1	ng	82646	6	15.36	785929	20.0
Oxirane, [(dodecy...	16.99	2.5	ng	99161	6	15.36	785929	20.0
unknown17.34	17.34	2.1	ng	82173	6	15.36	785929	20.0