

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111720\
 Data File : BF122358.D
 Acq On : 17 Nov 2020 21:29
 Operator : JU/CG
 Sample : L4771-01
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CD-BH-01-0-1

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-BF110920.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122358.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.151	6	11	22	rVB	901804	1174127	22.48%	2.679%
2	5.075	503	508	514	rBV	87075	107765	2.06%	0.246%
3	5.475	571	576	579	rBV	4792130	4396060	84.17%	10.030%
4	6.481	742	747	750	rBV	4441615	4561258	87.33%	10.407%
5	6.863	809	812	816	rBV	1909885	1496863	28.66%	3.415%
6	7.422	903	907	911	rBV	3128318	3070966	58.80%	7.007%
7	8.151	1027	1031	1034	rBV	2347158	1955197	37.44%	4.461%
8	9.228	1209	1214	1217	rBV	6131449	5222790	100.00%	11.917%
9	9.345	1227	1234	1241	rVB2	287368	310826	5.95%	0.709%
10	9.616	1277	1280	1290	rVB	363782	326685	6.25%	0.745%
11	9.904	1325	1329	1333	rBV	2680684	2283479	43.72%	5.210%
12	10.486	1424	1428	1436	rBV	298537	268431	5.14%	0.612%
13	10.692	1458	1463	1466	rBV	3671961	3395589	65.01%	7.748%
14	10.963	1506	1509	1513	rVB	68254	60536	1.16%	0.138%
15	11.392	1578	1582	1584	rBV	2414336	2218551	42.48%	5.062%
16	11.410	1584	1585	1588	rVB	131563	88991	1.70%	0.203%
17	11.574	1609	1613	1617	rBV	121356	116211	2.23%	0.265%
18	11.916	1668	1671	1676	rBV2	402944	388239	7.43%	0.886%
19	12.216	1718	1722	1725	rVB	68852	74128	1.42%	0.169%
20	12.374	1745	1749	1752	rBV	539214	456816	8.75%	1.042%
21	12.433	1756	1759	1763	rVV	244140	290030	5.55%	0.662%
22	12.468	1763	1765	1772	rVB3	57749	89408	1.71%	0.204%
23	12.598	1784	1787	1790	rBV	168673	171936	3.29%	0.392%
24	12.639	1791	1794	1797	rVB	112594	105415	2.02%	0.241%
25	12.704	1802	1805	1810	rBV	137148	173827	3.33%	0.397%
26	12.827	1820	1826	1829	rVB	152942	174126	3.33%	0.397%
27	12.974	1847	1851	1855	rBV	5285992	4844255	92.75%	11.053%
28	13.186	1884	1887	1890	rBV	106913	128065	2.45%	0.292%
29	13.874	2001	2004	2015	rBV	548735	686411	13.14%	1.566%
30	14.027	2024	2030	2033	rBV	2105735	2135880	40.90%	4.873%
31	14.510	2109	2112	2118	rVB2	88473	105182	2.01%	0.240%
32	14.962	2185	2189	2197	rBV	125708	165623	3.17%	0.378%
33	15.062	2204	2206	2215	rVB	58118	120932	2.32%	0.276%
34	15.157	2219	2222	2224	rBV	74970	88272	1.69%	0.201%
35	15.186	2224	2227	2234	rVB2	192818	288947	5.53%	0.659%
36	15.498	2275	2280	2285	rBV	1506031	1837264	35.18%	4.192%

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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-BF110920.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.980	2358	2362	2367	rBV	81514	120748	2.31%	0.276%
38	16.039	2367	2372	2380	rBV5	72226	184521	3.53%	0.421%
39	17.574	2630	2633	2645	rVB5	58588	143362	2.74%	0.327%

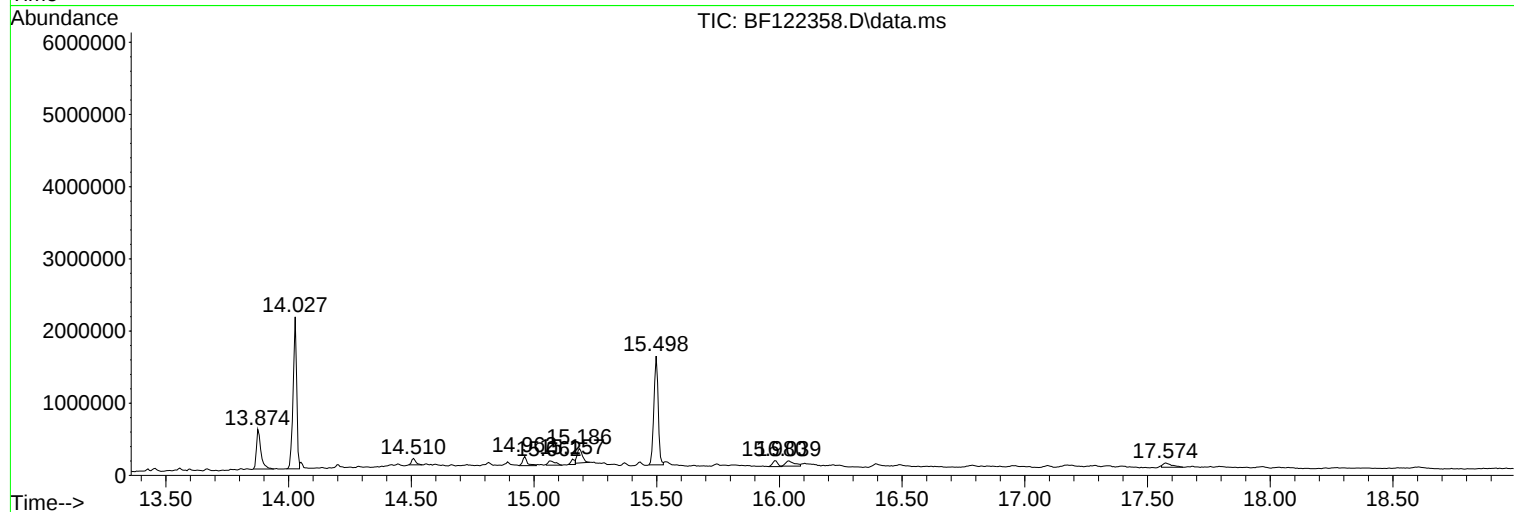
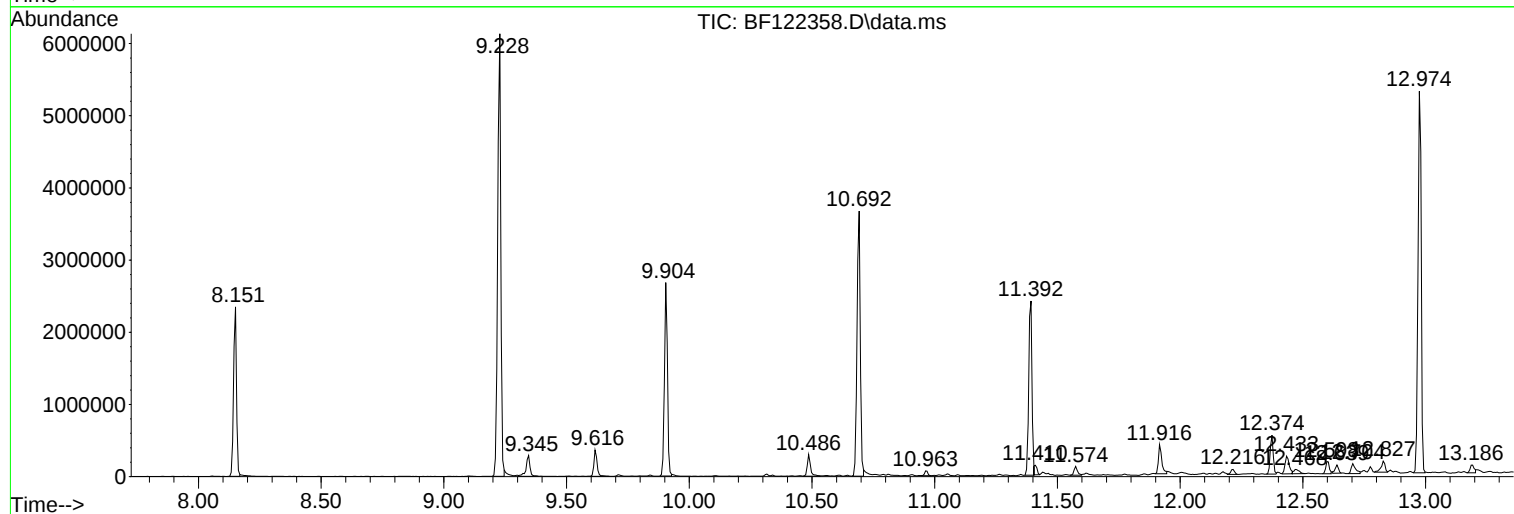
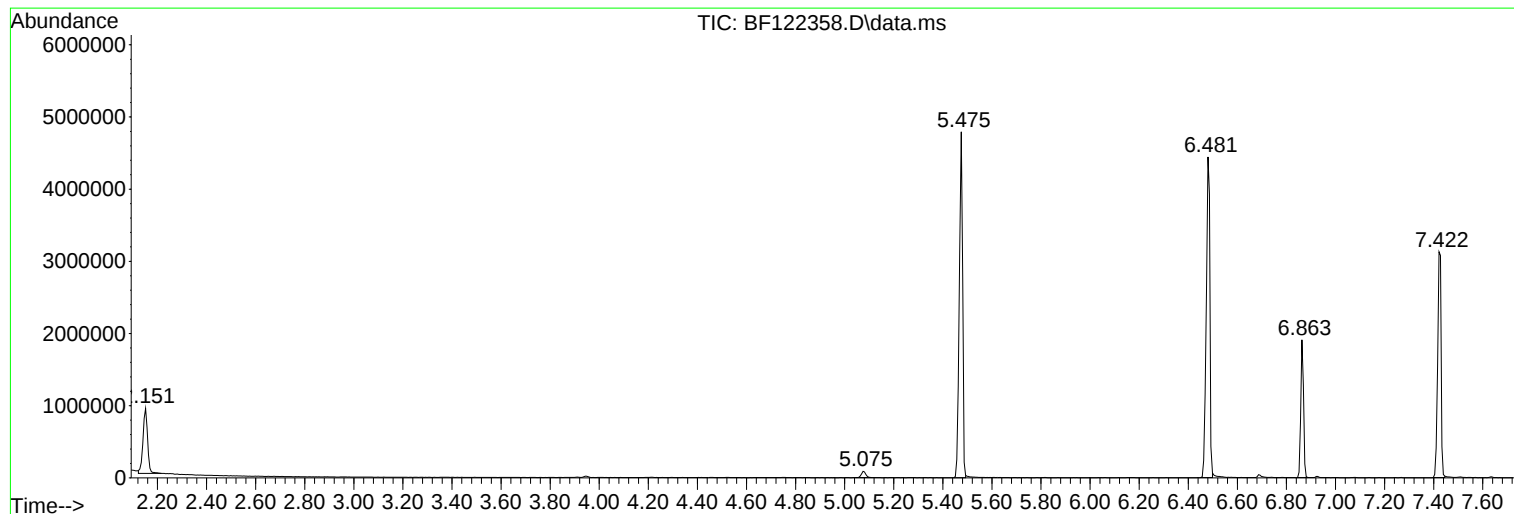
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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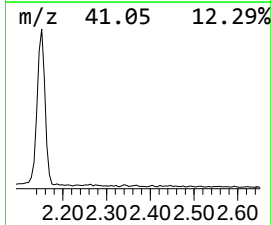
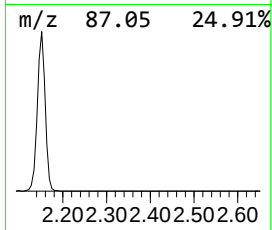
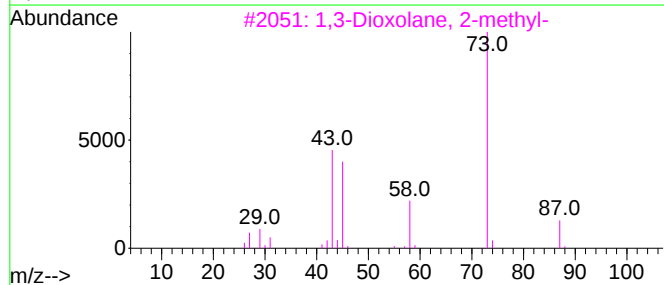
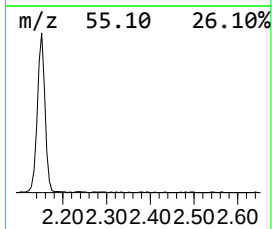
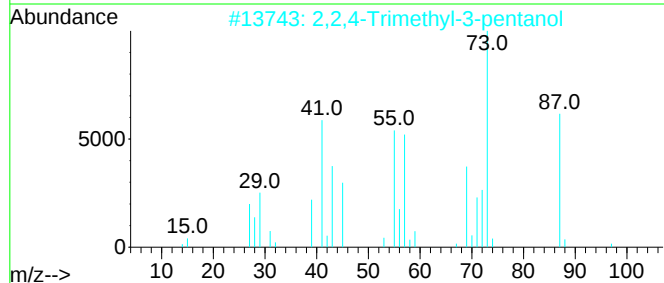
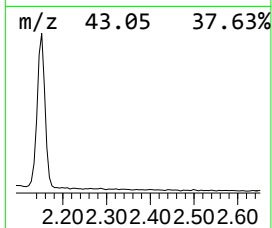
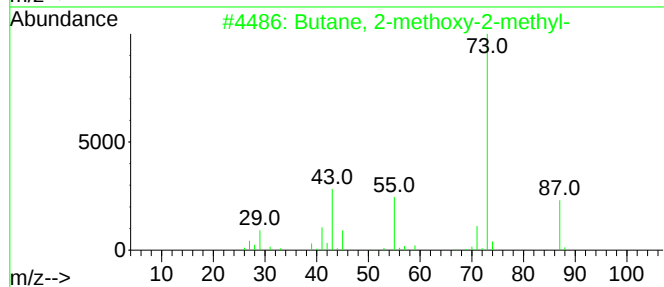
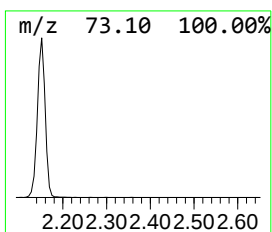
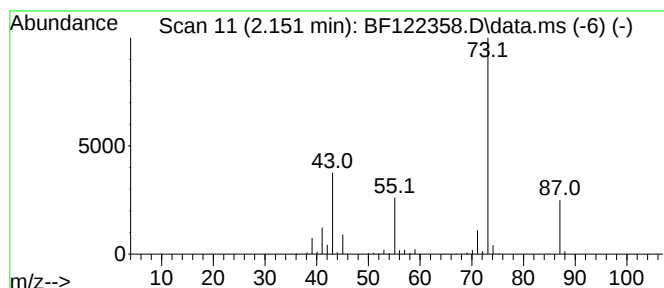
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.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.
2.151	15.69 ng	1174130	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12



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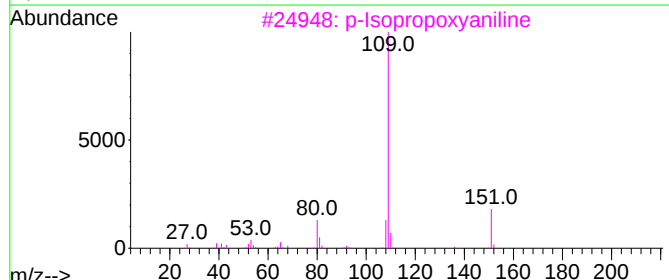
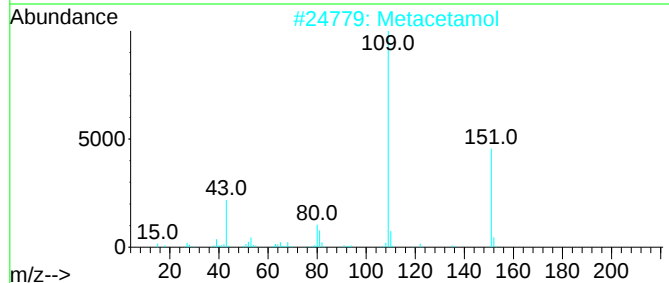
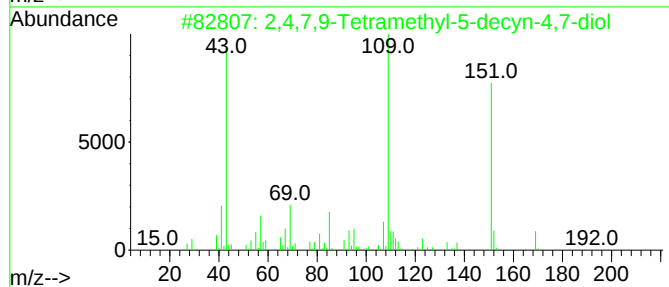
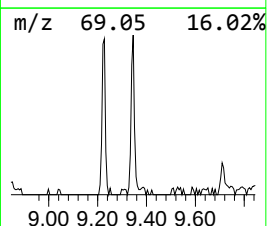
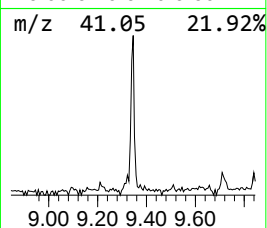
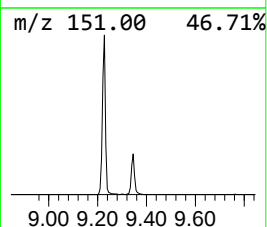
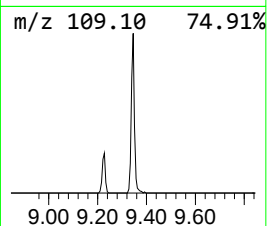
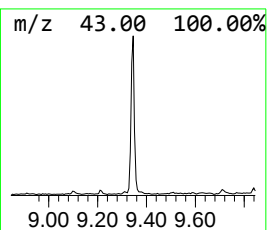
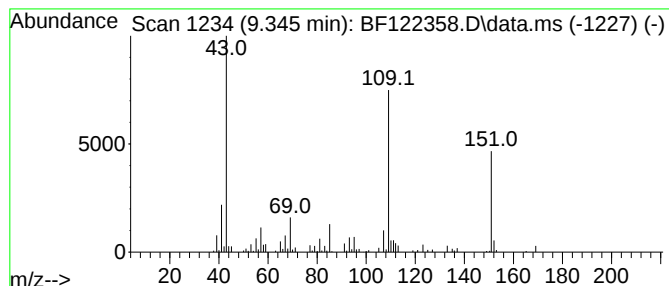
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Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.345	2.72 ng	310826	Acenaphthene-d10	9.904

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91	
2	Metacetamol	151	C8H9NO2	000621-42-1	59	
3	p-Isopropoxyaniline	151	C9H13NO	007664-66-6	59	
4	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	59	
5	(-)-10-Camphorsulfonyl chloride	250	C10H15ClO3S	039262-22-1	56	



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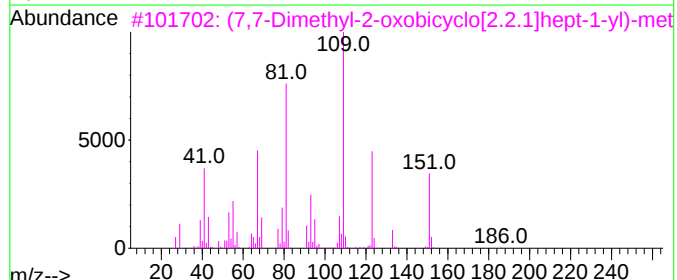
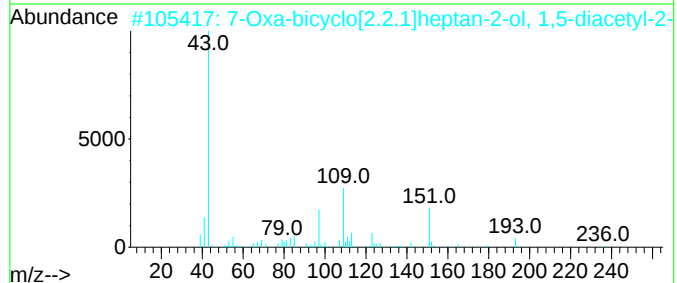
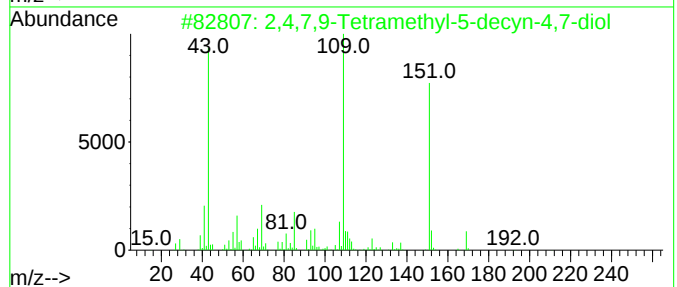
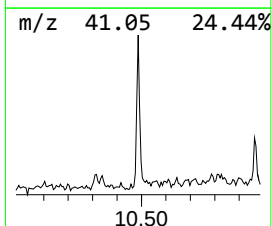
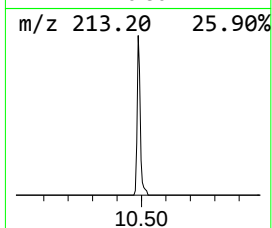
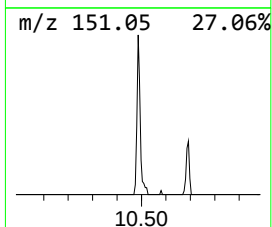
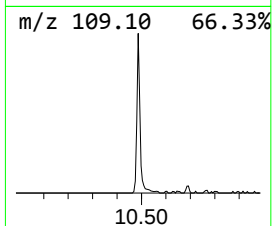
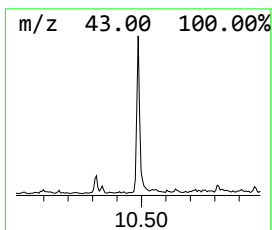
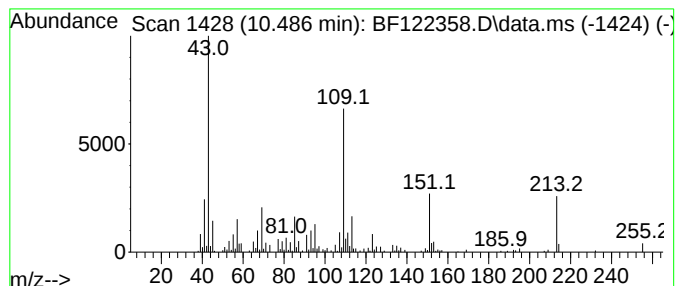
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown10.486 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.486	2.35 ng	268431	Acenaphthene-d10	9.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	43		
2	7-Oxa-bicyclo[2.2.1]heptan-2-ol,...	254	C14H22O4	329362-13-2	35		
3	(7,7-Dimethyl-2-oxobicyclo[2.2.1...	250	C10H15ClO3S	1000194-76-1	32		
4	Acetaminophen	151	C8H9NO2	000103-90-2	30		
5	Diacetamate	193	C10H11NO3	002623-33-8	27		



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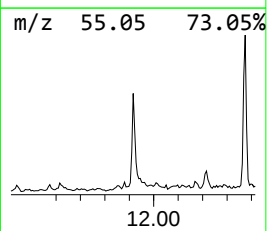
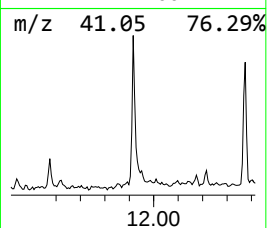
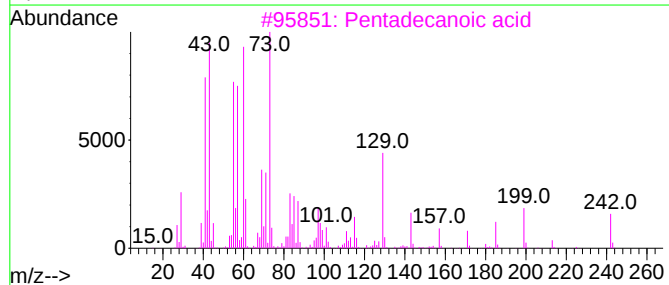
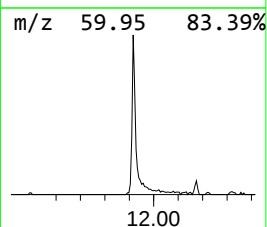
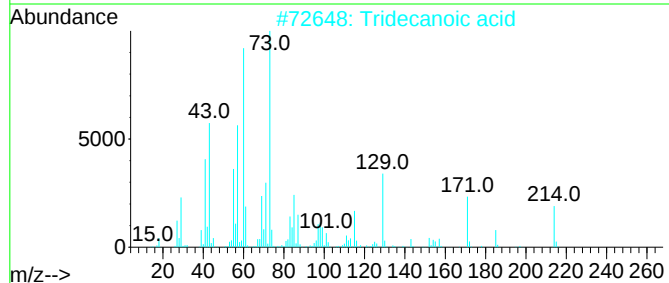
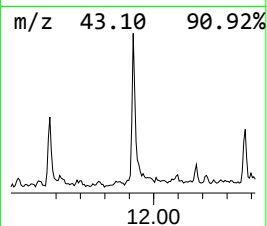
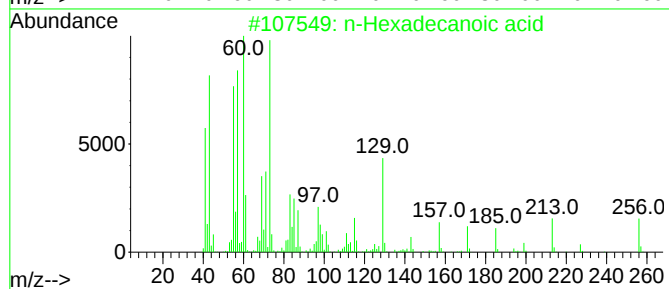
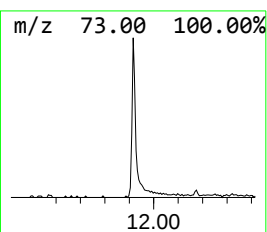
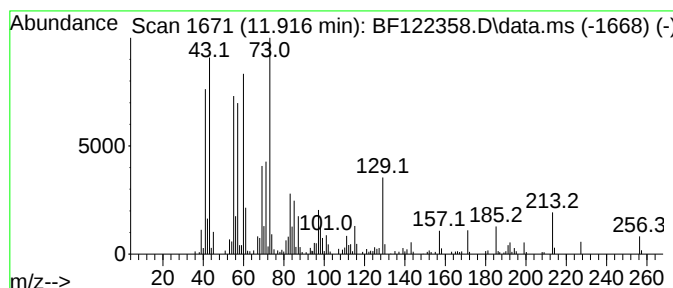
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	3.50 ng	388239	Phenanthrene-d10	11.392

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	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	25



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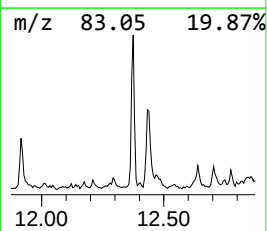
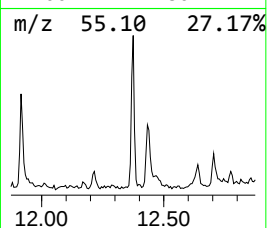
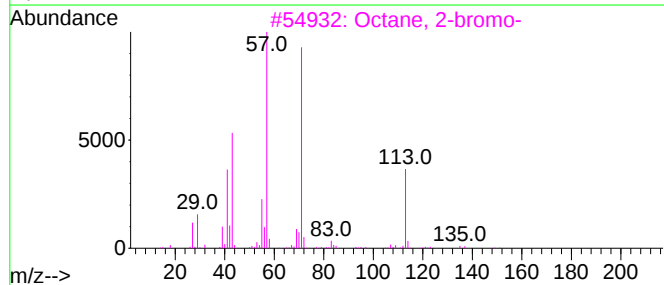
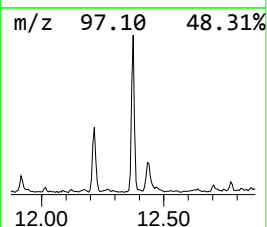
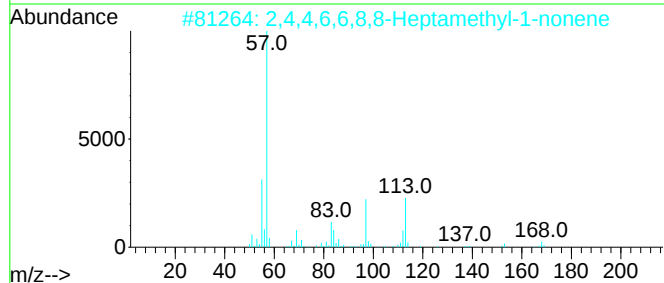
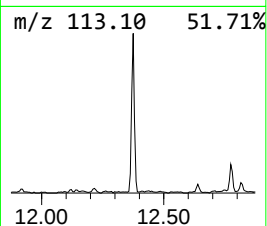
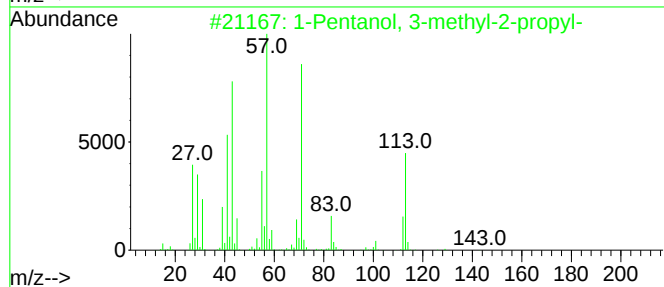
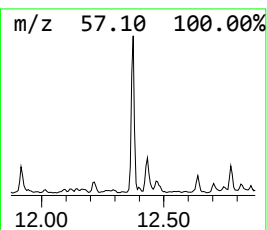
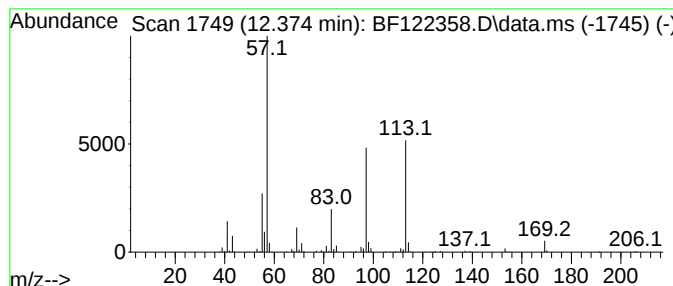
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown12.374 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.374	4.12 ng	456816	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	40
2			2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	38
3			Octane, 2-bromo-	192	C8H17Br	000557-35-7	32
4			2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	32
5			Vardenafil	488	C23H32N6O4S	224785-90-4	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111720\
Data File : BF122358.D
Acq On : 17 Nov 2020 21:29
Operator : JU/CG
Sample : L4771-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CD-BH-01-0-1

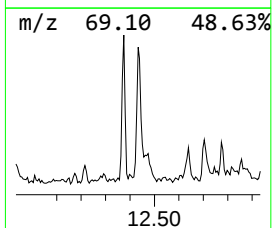
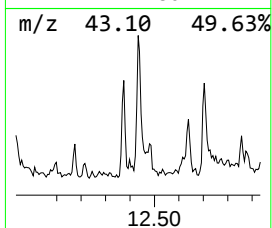
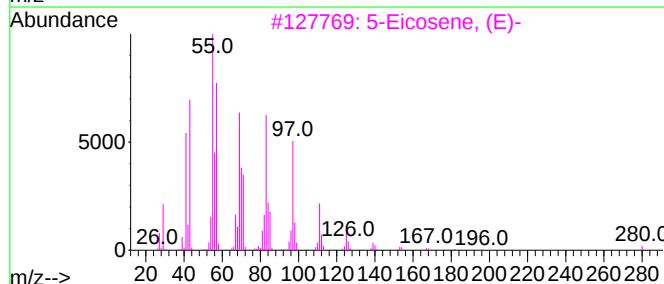
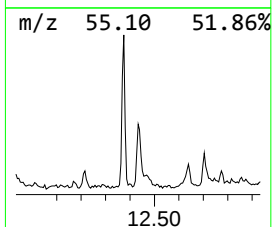
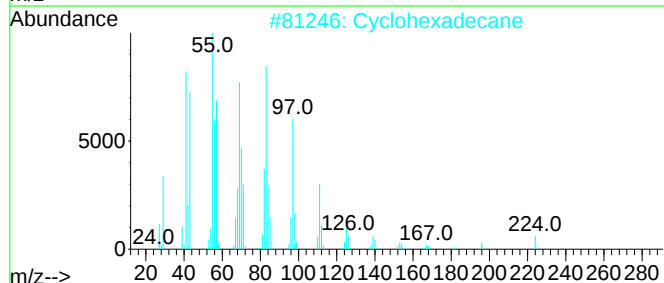
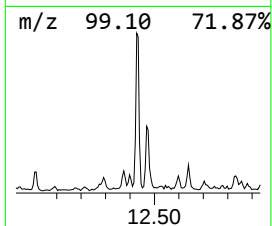
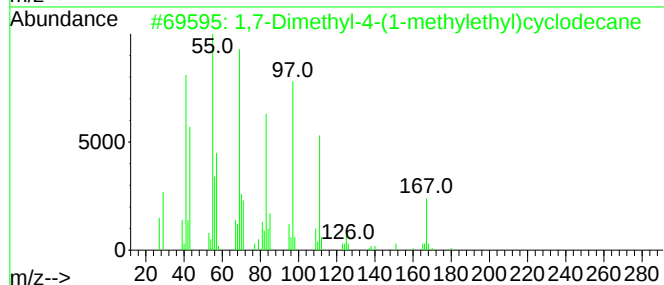
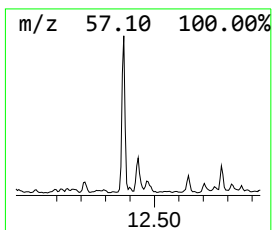
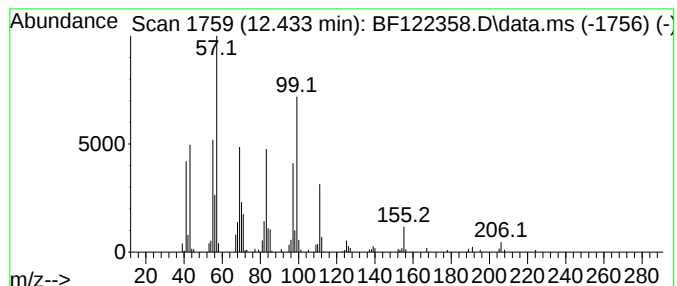
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown12.433 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.433	2.61 ng	290030	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,7-Dimethyl-4-(1-methylethyl)cy...	210	C15H30	000645-10-3	49
2			Cyclohexadecane	224	C16H32	000295-65-8	46
3			5-Eicosene, (E)-	280	C20H40	074685-30-6	45
4			5-Octadecene, (E)-	252	C18H36	007206-21-5	38
5			1-Hexadecanol	242	C16H34O	036653-82-4	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111720\
Data File : BF122358.D
Acq On : 17 Nov 2020 21:29
Operator : JU/CG
Sample : L4771-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CD-BH-01-0-1

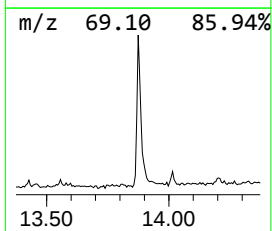
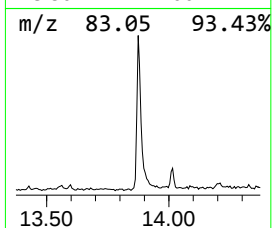
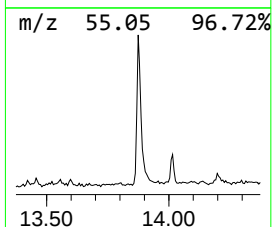
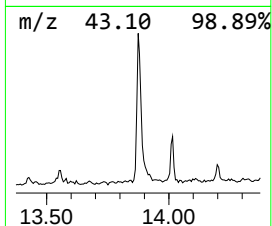
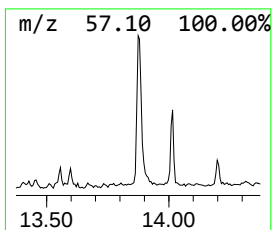
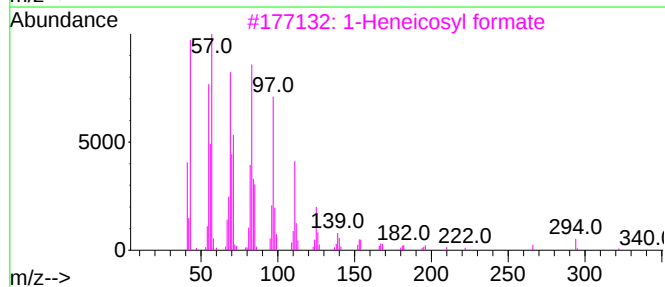
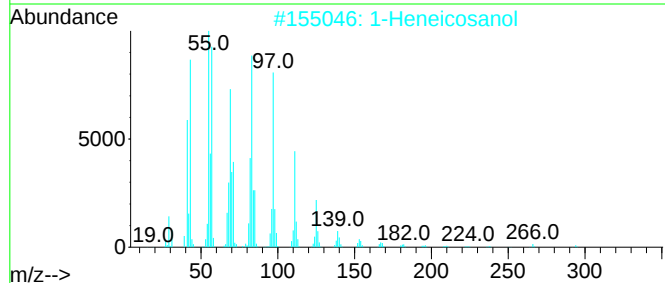
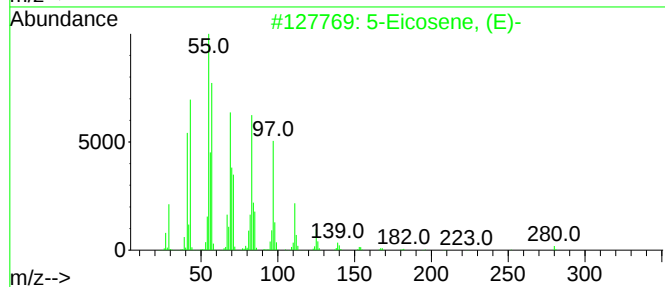
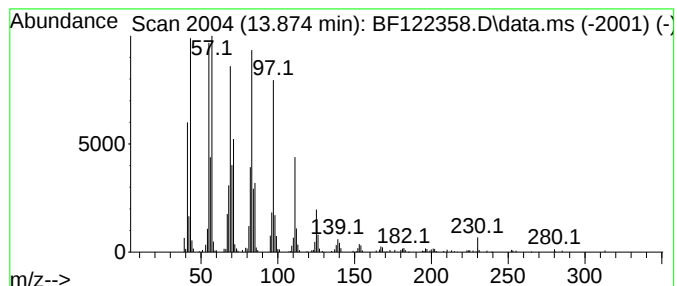
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 5-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	6.43 ng	686411	Chrysene-d12	14.027

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2		1-Heneicosanol	312	C21H44O	015594-90-8	95
3		1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
4		Cyclopentadecane	210	C15H30	000295-48-7	94
5		Behenic alcohol	326	C22H46O	000661-19-8	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111720\
Data File : BF122358.D
Acq On : 17 Nov 2020 21:29
Operator : JU/CG
Sample : L4771-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CD-BH-01-0-1

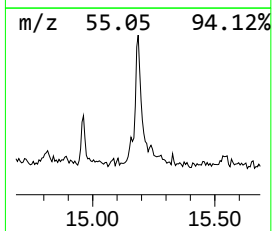
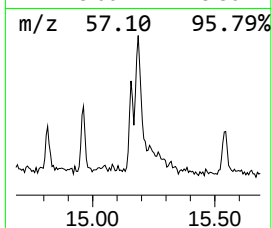
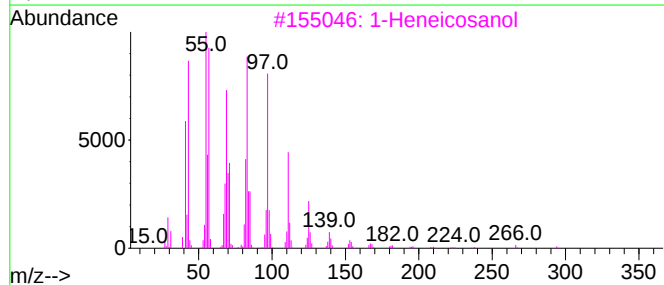
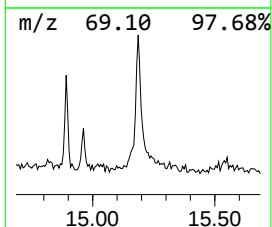
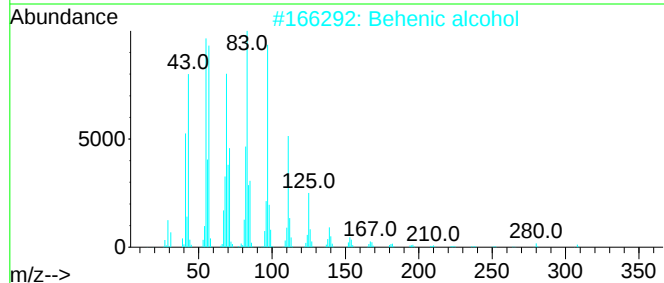
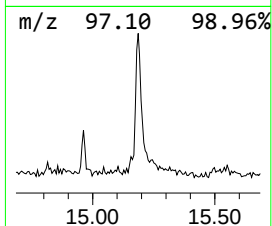
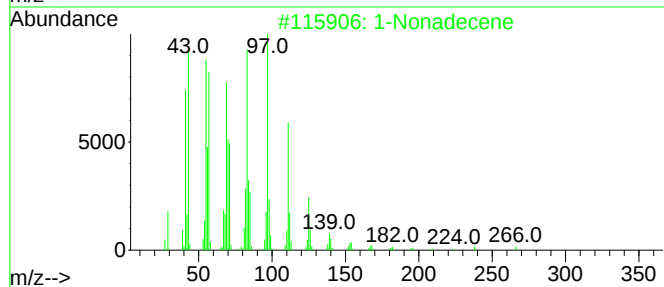
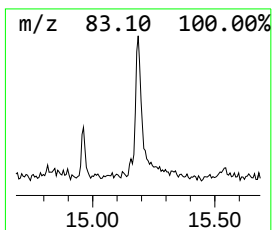
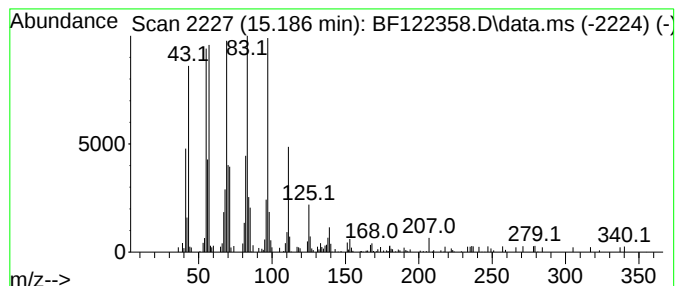
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Nonadecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.186	3.15 ng	288947	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene			266	C19H38	018435-45-5	94
2	Behenic alcohol			326	C22H46O	000661-19-8	91
3	1-Heneicosanol			312	C21H44O	015594-90-8	91
4	1-Octadecanol			270	C18H38O	000112-92-5	87
5	n-Nonadecanol-1			284	C19H40O	001454-84-8	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111720\
Data File : BF122358.D
Acq On : 17 Nov 2020 21:29
Operator : JU/CG
Sample : L4771-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

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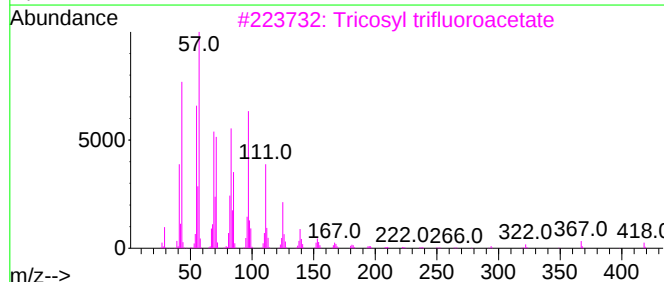
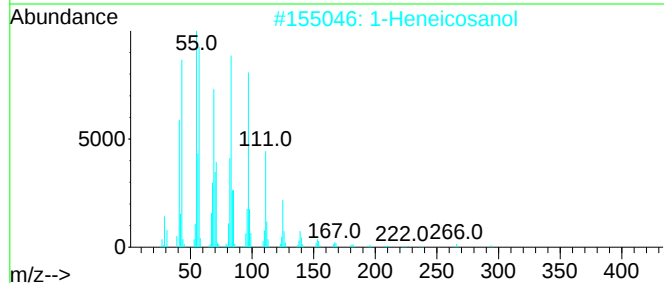
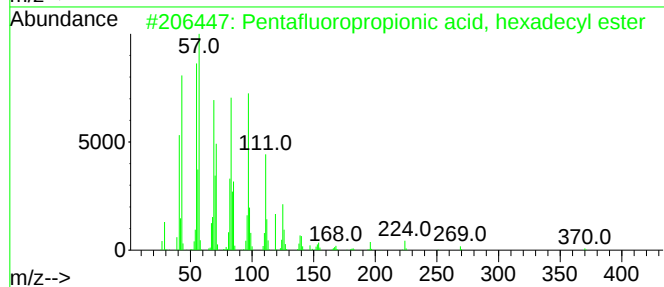
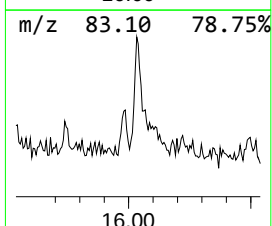
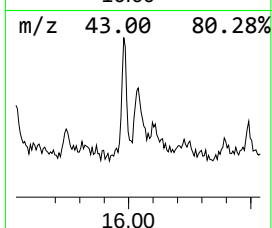
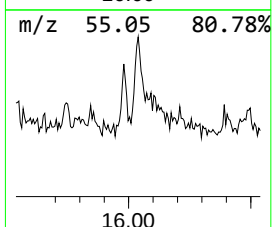
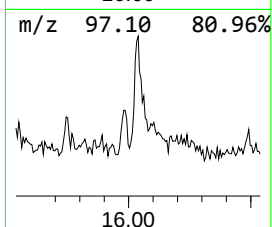
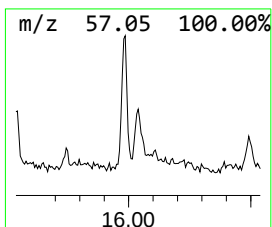
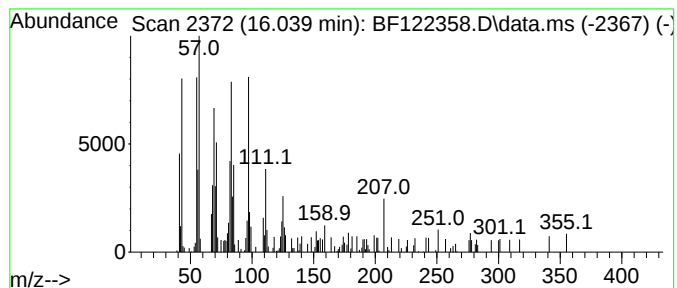
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentafluoropropionic acid, ... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.039	2.01 ng	184521	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	93
2			1-Heneicosanol	312	C21H44O	015594-90-8	90
3			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	87
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87
5			Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111720\
Data File : BF122358.D
Acq On : 17 Nov 2020 21:29
Operator : JU/CG
Sample : L4771-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CD-BH-01-0-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.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
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2,4,7,9-Tetrame...	9.345	2.7	ng	310826	3	9.904	2283480	20.0
unknown10.486	10.486	2.4	ng	268431	3	9.904	2283480	20.0
n-Hexadecanoic ...	11.916	3.5	ng	388239	4	11.392	2218550	20.0
unknown12.374	12.374	4.1	ng	456816	4	11.392	2218550	20.0
unknown12.433	12.433	2.6	ng	290030	4	11.392	2218550	20.0
5-Eicosene, (E)-	13.874	6.4	ng	686411	5	14.027	2135880	20.0
1-Nonadecene	15.186	3.1	ng	288947	6	15.498	1837260	20.0
Pentafluoroprop...	16.039	2.0	ng	184521	6	15.498	1837260	20.0