

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030122\
 Data File : BF127120.D
 Acq On : 01 Mar 2022 17:07
 Operator : CG\JU
 Sample : N1689-07
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-43

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-BF021622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127120.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.110	477	480	484	rVB	83620	78145	2.40%	0.474%
2	5.510	545	548	557	rVB	517487	449275	13.82%	2.727%
3	6.510	715	718	723	rBV	415063	376182	11.57%	2.284%
4	6.886	779	782	786	rVB	672705	567801	17.46%	3.447%
5	7.451	873	878	881	rBV	1813887	1865005	57.35%	11.322%
6	7.622	903	907	911	rBV	55243	45944	1.41%	0.279%
7	8.069	979	983	993	rBV	150788	159046	4.89%	0.966%
8	8.175	996	1001	1003	rVV	846854	781128	24.02%	4.742%
9	8.192	1003	1004	1007	rVB	90971	57232	1.76%	0.347%
10	9.251	1178	1184	1187	rBV	3682331	3252061	100.00%	19.742%
11	9.322	1192	1196	1198	rVB	43800	36806	1.13%	0.223%
12	9.733	1262	1266	1274	rBV2	70636	122194	3.76%	0.742%
13	9.822	1278	1281	1284	rBV	47755	41448	1.27%	0.252%
14	9.933	1296	1300	1303	rVB	1031502	833061	25.62%	5.057%
15	10.251	1348	1354	1361	rBV2	44895	57988	1.78%	0.352%
16	10.327	1364	1367	1369	rVV	112817	104725	3.22%	0.636%
17	10.345	1369	1370	1374	rVB2	69449	49077	1.51%	0.298%
18	10.480	1388	1393	1396	rVB3	21403	35278	1.08%	0.214%
19	10.722	1430	1434	1437	rBV	1071798	872708	26.84%	5.298%
20	10.827	1450	1452	1457	rVB4	41093	42057	1.29%	0.255%
21	10.927	1466	1469	1474	rBV3	36798	40484	1.24%	0.246%
22	11.116	1498	1501	1504	rVB3	41895	38434	1.18%	0.233%
23	11.274	1524	1528	1530	rBV2	43681	46044	1.42%	0.280%
24	11.304	1530	1533	1538	rVB4	40747	51332	1.58%	0.312%
25	11.369	1541	1544	1547	rVB	163195	131281	4.04%	0.797%
26	11.421	1550	1553	1556	rBV	1036898	854787	26.28%	5.189%
27	11.545	1571	1574	1576	rVB	41219	36844	1.13%	0.224%
28	11.580	1577	1580	1587	rBV	139727	159272	4.90%	0.967%
29	11.657	1587	1593	1596	rBV6	38574	60043	1.85%	0.364%
30	11.804	1616	1618	1620	rVB	72434	49745	1.53%	0.302%
31	11.939	1638	1641	1644	rBV	77033	72932	2.24%	0.443%
32	11.974	1644	1647	1650	rVB	158255	137763	4.24%	0.836%
33	12.192	1681	1684	1687	rVB2	63758	51799	1.59%	0.314%
34	12.392	1715	1718	1720	rBV	42279	43375	1.33%	0.263%
35	12.445	1724	1727	1729	rBV	53022	46357	1.43%	0.281%
36	12.598	1751	1753	1756	rVB4	43804	38305	1.18%	0.233%

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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-BF021622.M
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37	12.639	1757	1760	1766	rVB3	52055	62746	1.93%	0.381%
38	12.792	1781	1786	1788	rVB2	44738	63879	1.96%	0.388%
39	13.015	1819	1824	1827	rBV	3232755	3128545	96.20%	18.992%
40	13.610	1923	1925	1929	rVB	38258	36883	1.13%	0.224%
41	13.645	1929	1931	1934	rVB	48329	38249	1.18%	0.232%
42	13.910	1970	1976	1983	rBV3	174418	418125	12.86%	2.538%
43	14.068	1999	2003	2007	rBV	692654	560846	17.25%	3.405%
44	15.562	2252	2257	2262	rBV	382124	477544	14.68%	2.899%

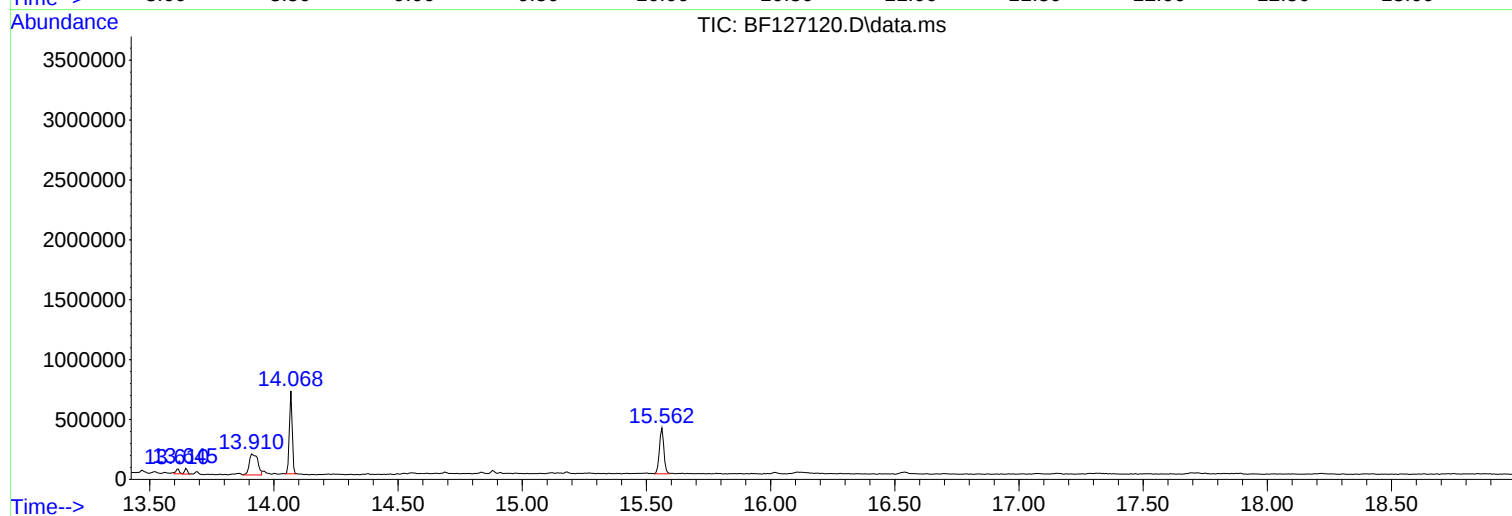
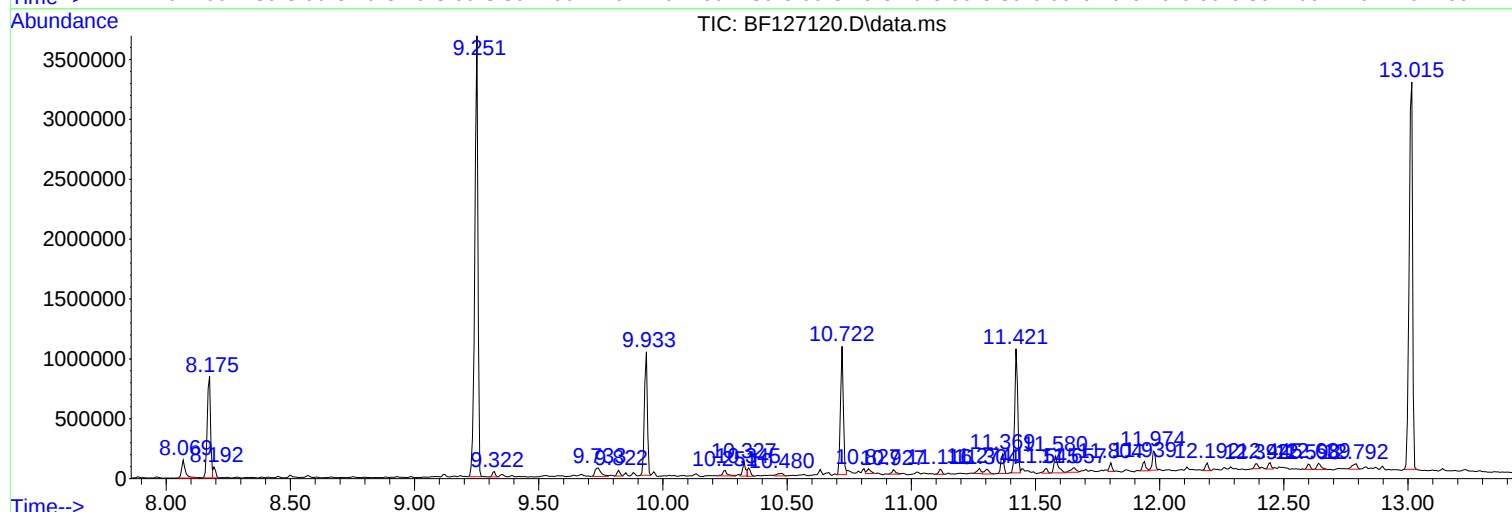
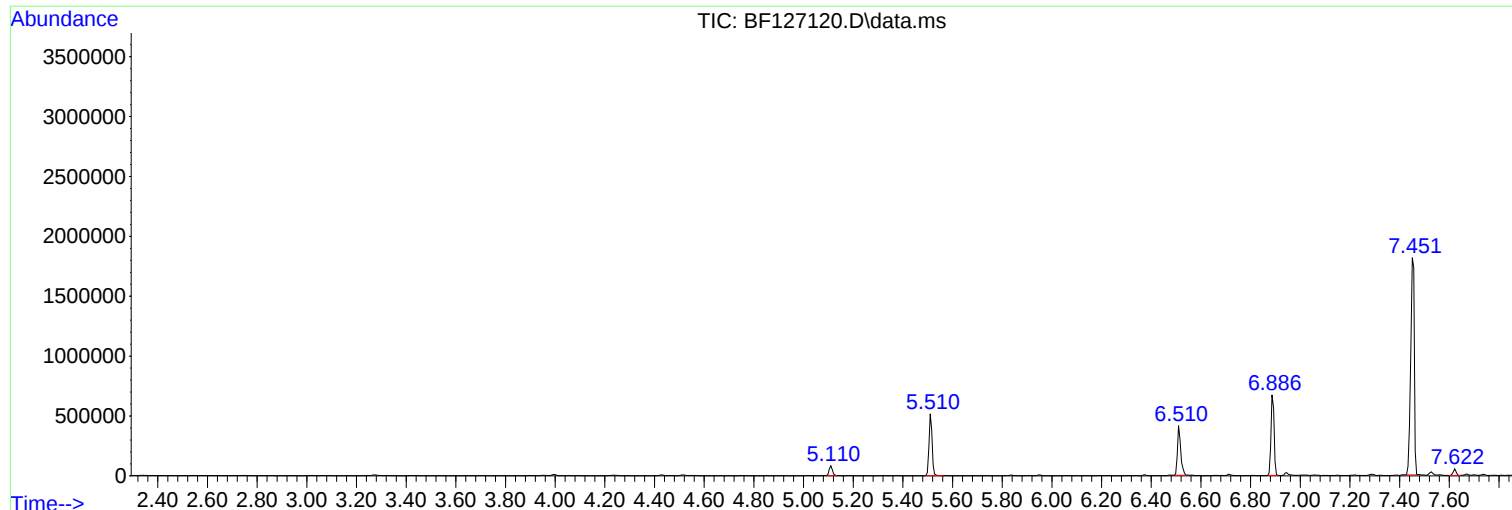
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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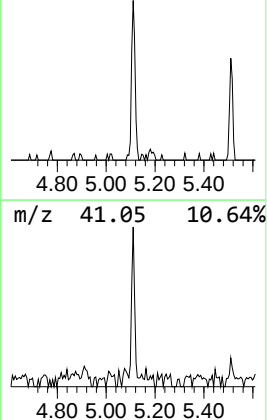
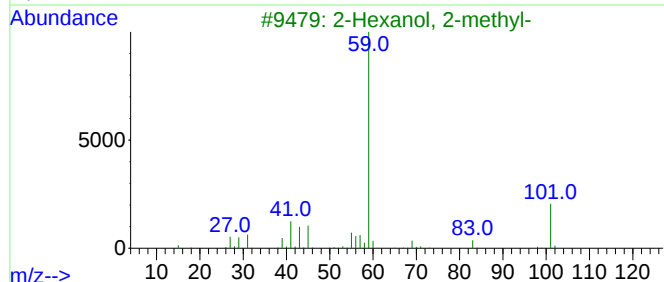
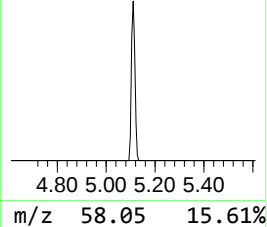
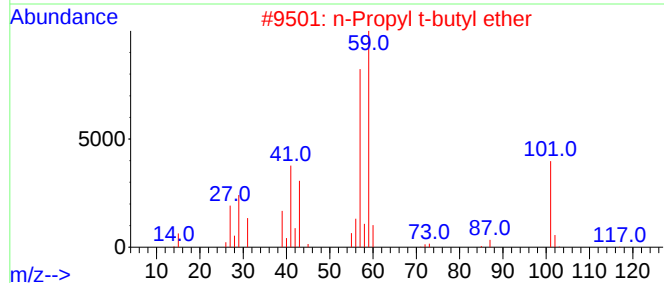
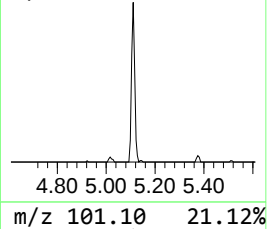
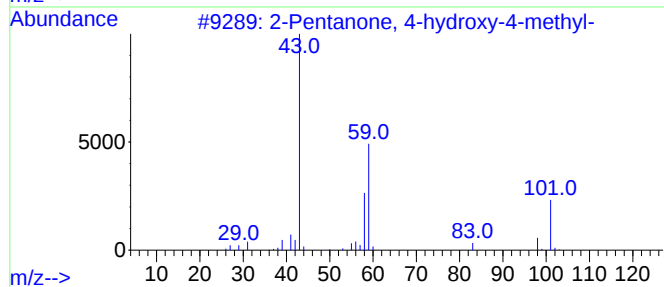
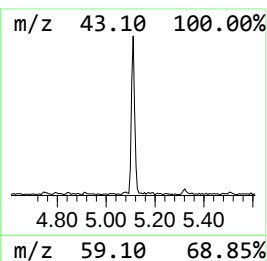
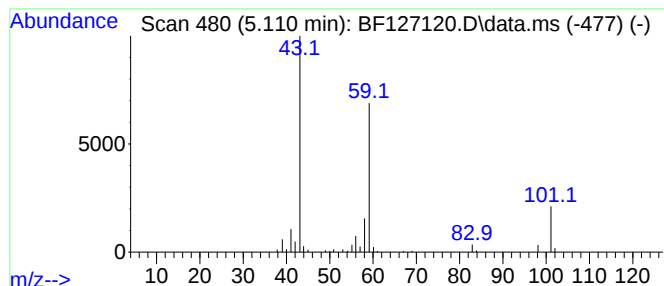
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	2.75 ng	78145	1,4-Dichlorobenzene-d4	6.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		



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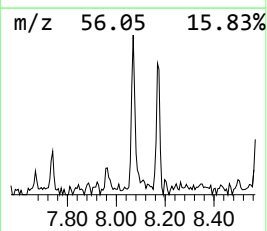
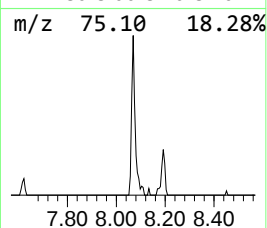
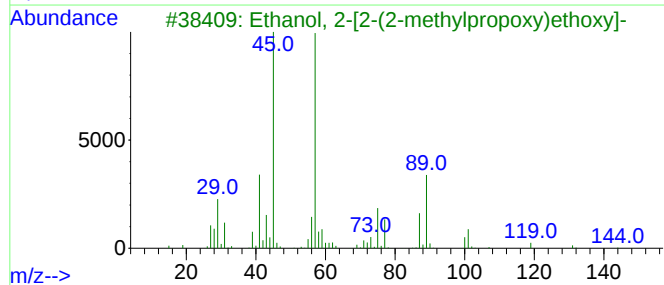
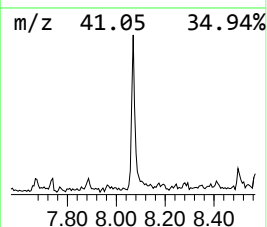
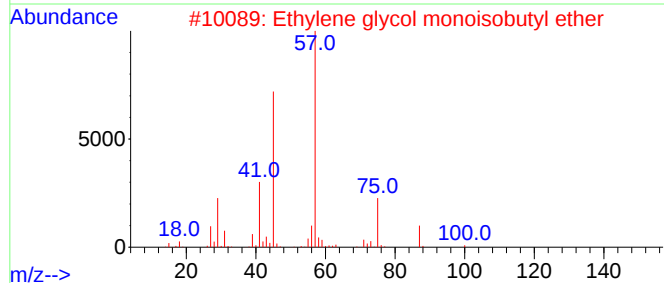
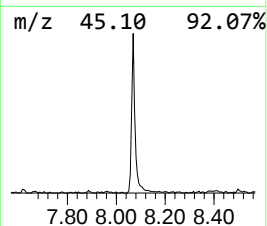
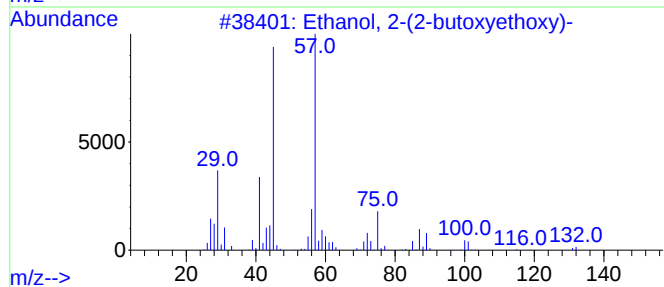
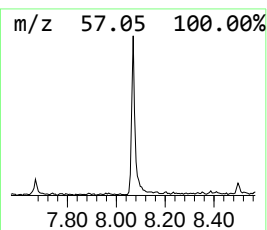
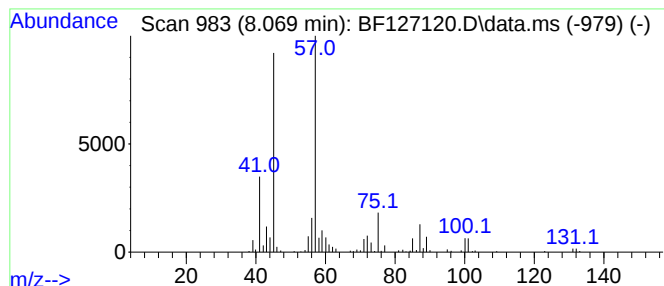
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.069	4.07 ng	159046	Naphthalene-d8	8.175

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3			Ethanol, 2-[2-(2-methylpropoxy)ethoxy]-	162	C8H18O3	018912-80-6	56
4			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
5			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53



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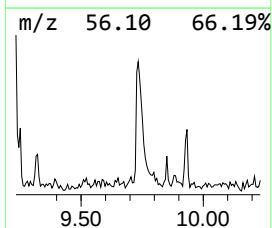
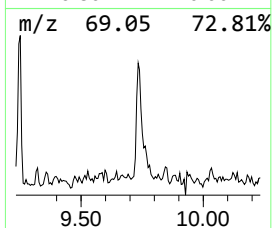
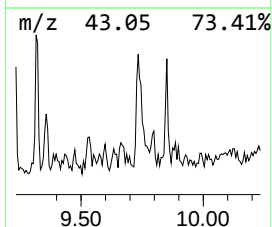
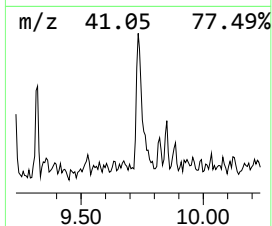
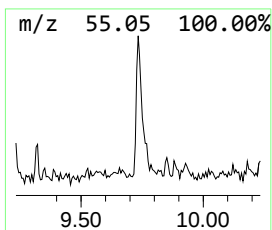
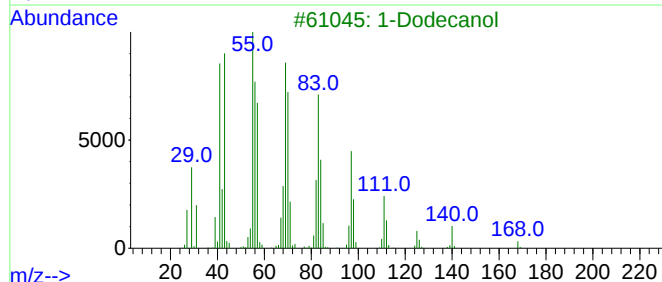
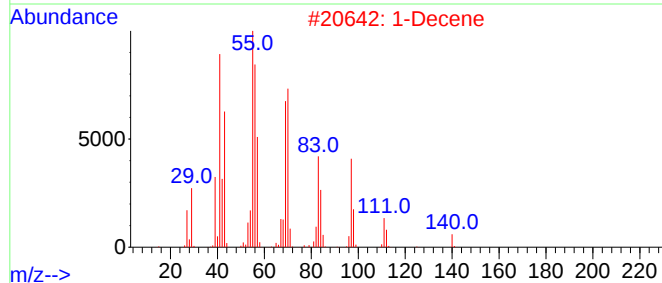
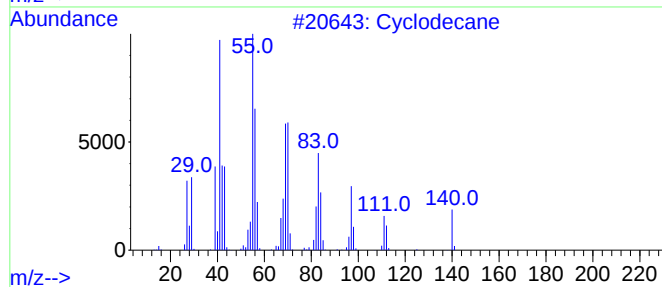
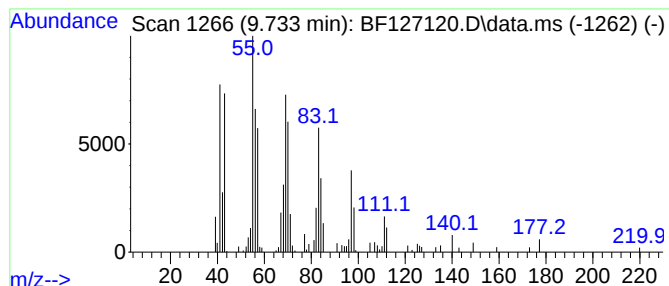
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Cyclodecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.733	2.93 ng	122194	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclodecane	140	C10H20	000293-96-9	95
2			1-Decene	140	C10H20	000872-05-9	94
3			1-Dodecanol	186	C12H26O	000112-53-8	91
4			1-Tridecene	182	C13H26	002437-56-1	90
5			2-Butenedioic acid (Z)-, monodod...	284	C16H28O4	002424-61-5	90



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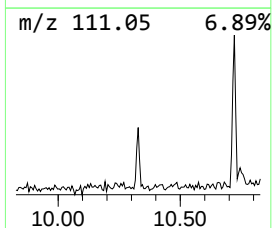
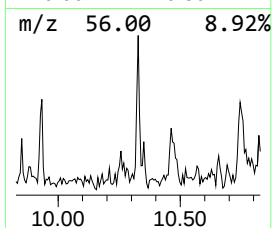
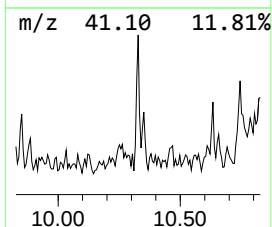
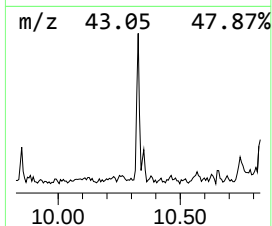
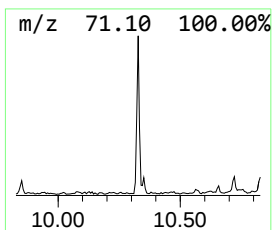
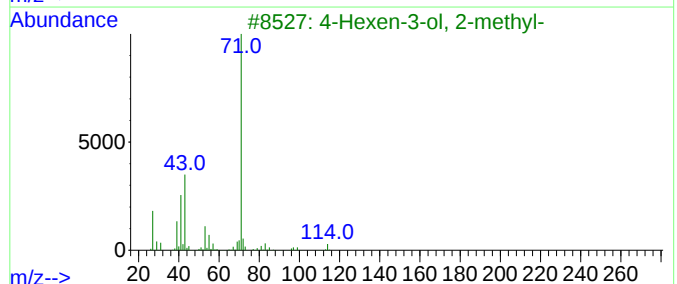
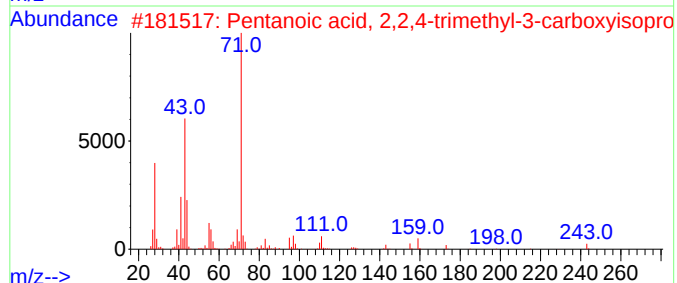
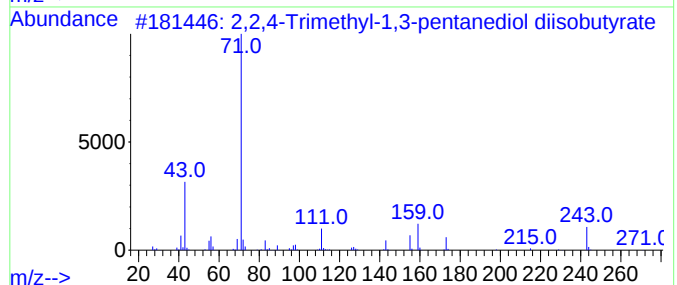
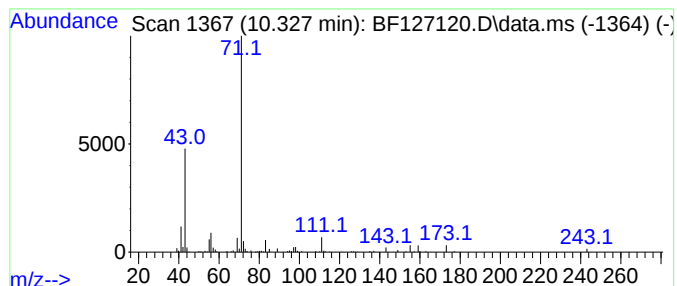
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.327	2.51 ng	104725	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	83		
2	Pentanoic acid, 2,2,4-trimethyl-...	286	C16H30O4	1000140-77-5	64		
3	4-Hexen-3-ol, 2-methyl-	114	C7H14O	004798-60-1	64		
4	2,2'-Bifuran, octahydro-	142	C8H14O2	001592-33-2	50		
5	Butanoic acid, 2-butoxy-1-methyl...	216	C11H20O4	007492-70-8	50		



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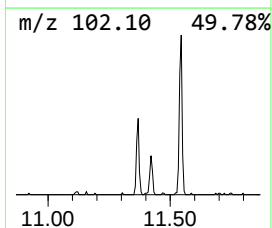
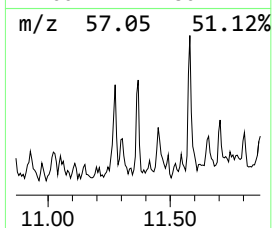
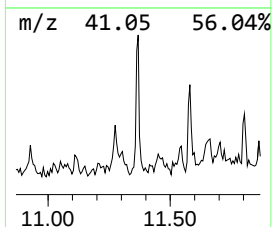
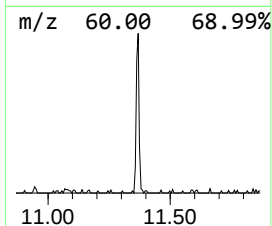
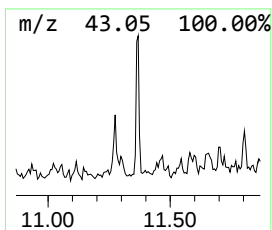
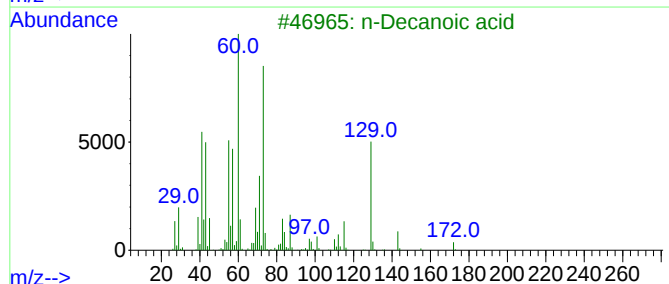
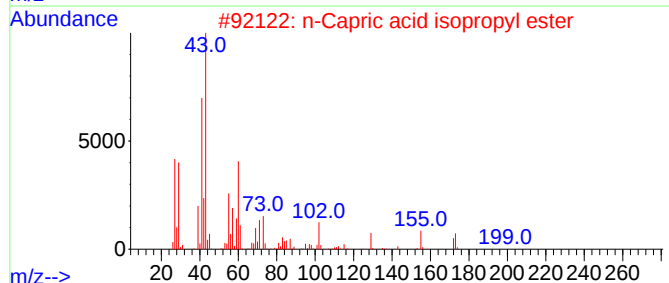
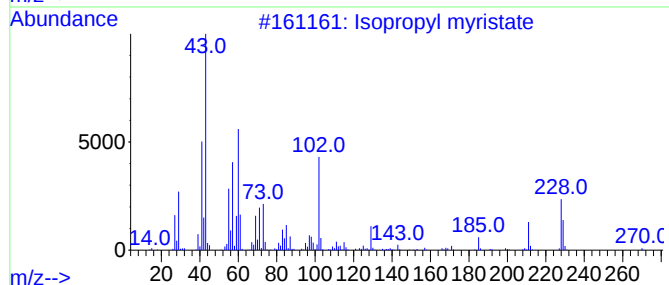
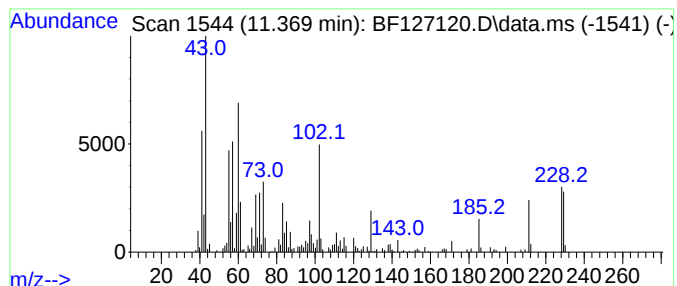
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Isopropyl myristate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.368	3.07 ng	131281	Phenanthrene-d10	11.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl myristate	270	C17H34O2	000110-27-0	91
2			n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	35
3			n-Decanoic acid	172	C10H20O2	000334-48-5	27
4			Heptanoic acid	130	C7H14O2	000111-14-8	14
5			Cyclooctylamine, N-trimethylacetyl-	211	C13H25NO	540795-02-6	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030122\
Data File : BF127120.D
Acq On : 01 Mar 2022 17:07
Operator : CG\JU
Sample : N1689-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-43

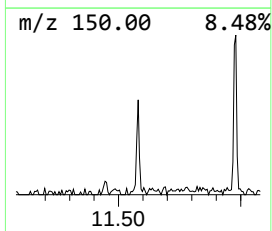
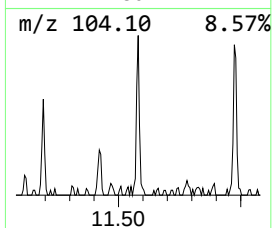
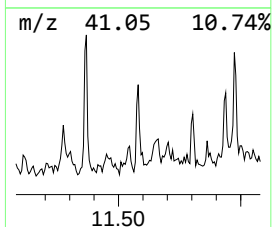
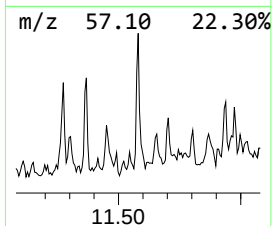
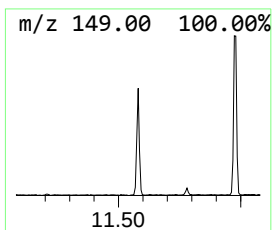
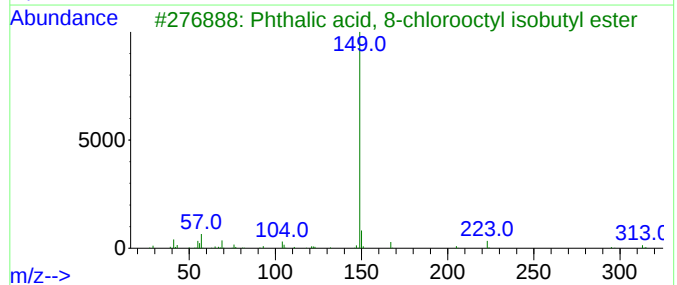
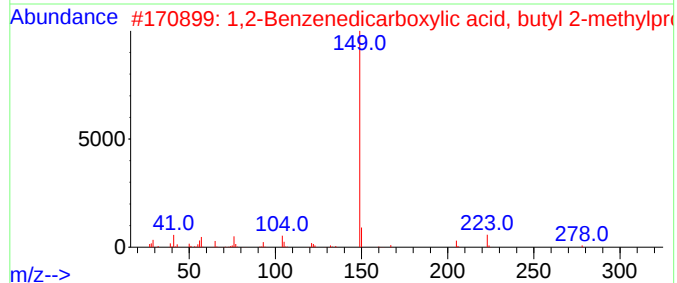
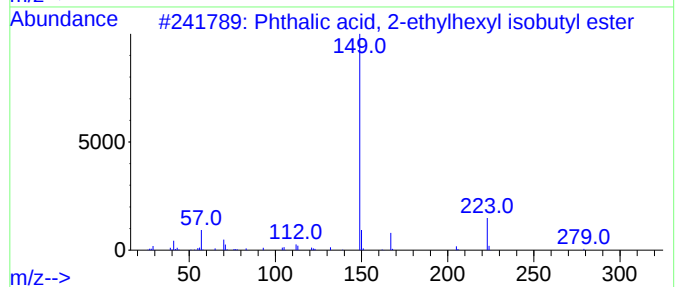
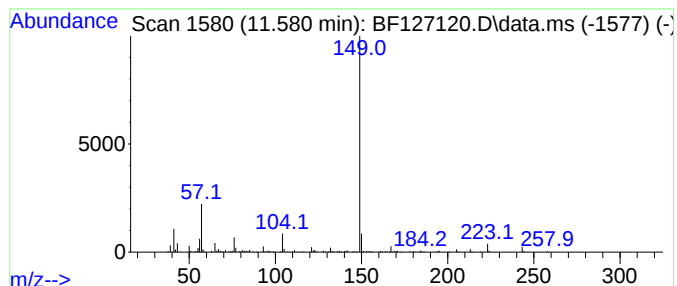
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Phthalic acid, 2-ethylhexyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.580	3.73 ng	159272	Phenanthrene-d10	11.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic acid, 2-ethylhexyl isob...	334	C20H30O4	1000308-98-0	72
2			1,2-Benzenedicarboxylic acid, bu...	278	C16H22O4	017851-53-5	72
3			Phthalic acid, 8-chlorooctyl iso...	368	C20H29ClO4	1000356-85-8	72
4			1,2-Benzenedicarboxylic acid, di...	250	C14H18O4	000131-16-8	72
5			Phthalic acid, ethyl 2-methylall...	248	C14H16O4	1000315-19-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030122\
Data File : BF127120.D
Acq On : 01 Mar 2022 17:07
Operator : CG\JU
Sample : N1689-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-43

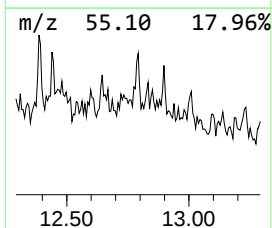
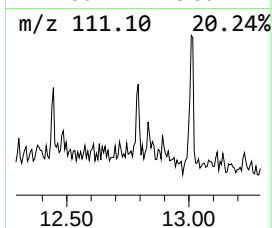
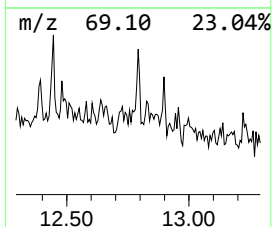
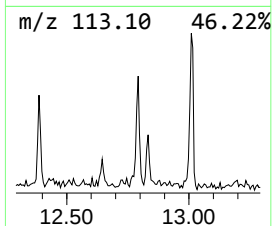
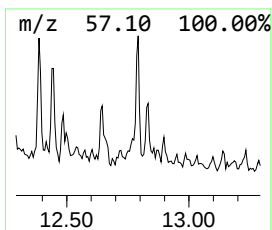
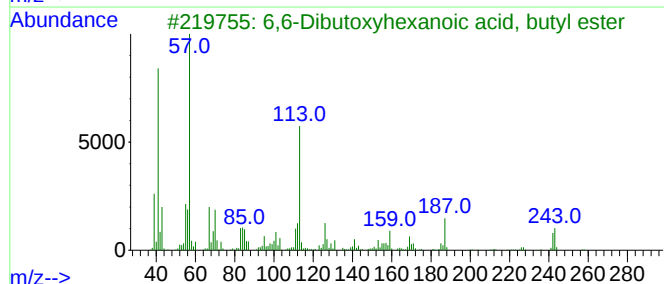
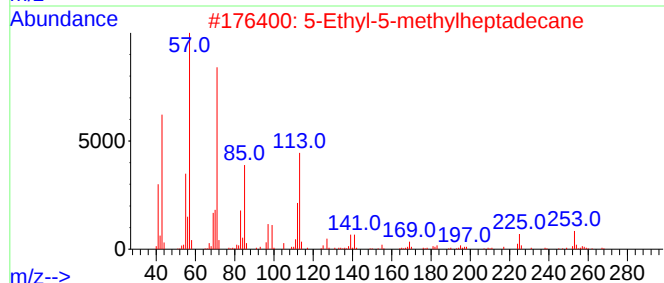
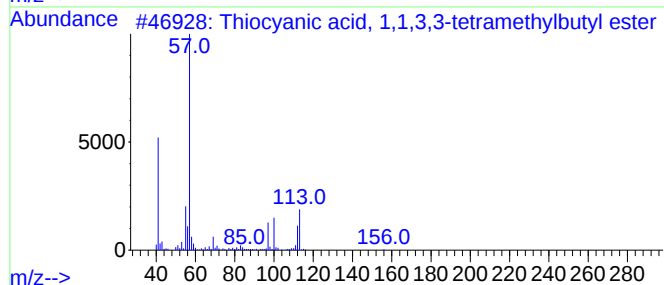
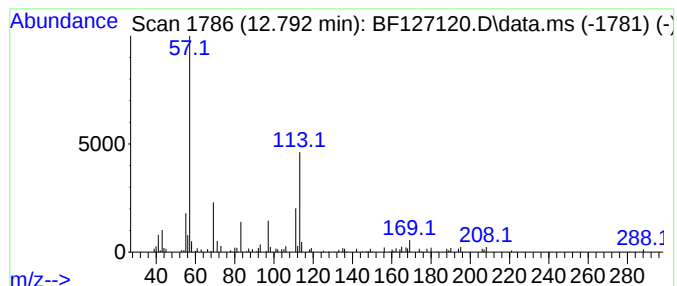
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown12.792 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.792	2.28 ng	63879	Chrysene-d12	14.068

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiocyanic acid, 1,1,3,3-tetrame...	171	C9H17NS	089601-36-5	42
2			5-Ethyl-5-methylheptadecane	282	C20H42	1000360-42-5	38
3			6,6-Dibutoxyhexanoic acid, butyl...	316	C18H36O4	1000280-29-0	33
4			Sulfurous acid, 2-ethylhexyl pen...	404	C23H48O3S	1000309-19-8	17
5			Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030122\
Data File : BF127120.D
Acq On : 01 Mar 2022 17:07
Operator : CG\JU
Sample : N1689-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-43

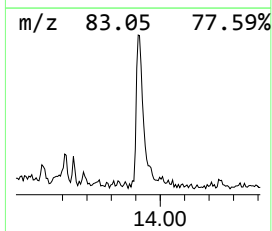
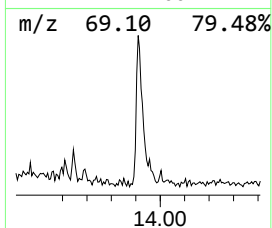
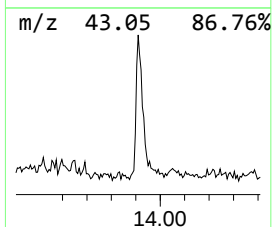
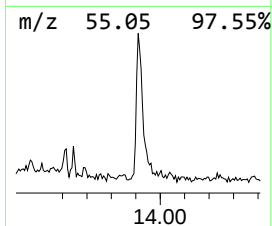
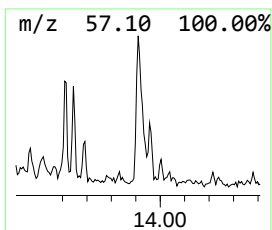
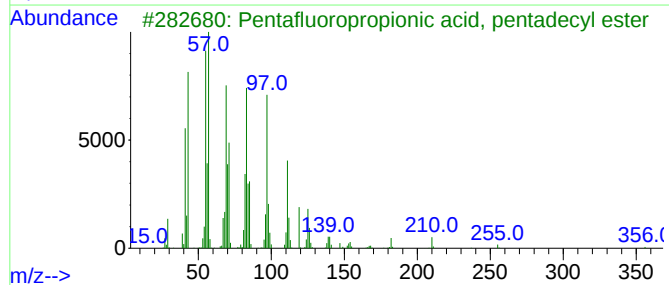
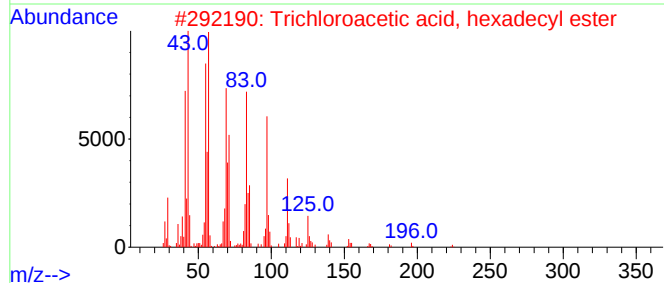
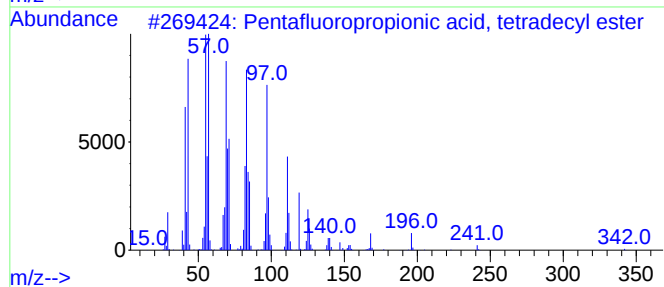
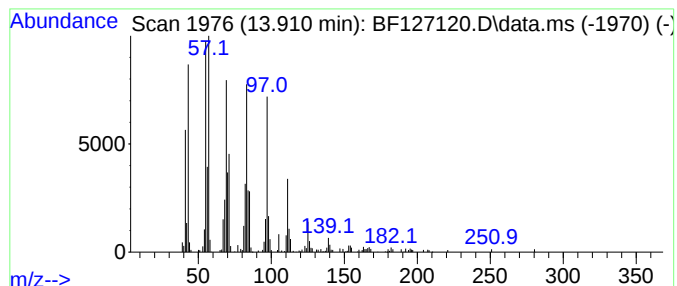
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentafluoropropionic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	14.91 ng	418125	Chrysene-d12	14.068

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	94
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4			1-Heneicosanol	312	C21H44O	015594-90-8	94
5			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030122\
Data File : BF127120.D
Acq On : 01 Mar 2022 17:07
Operator : CG\JU
Sample : N1689-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-43

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.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-...	5.110	2.8	ng	78145	1	6.886	567801	20.0
Ethanol, 2-(2-b...	8.069	4.1	ng	159046	2	8.175	781128	20.0
Cyclodecane	9.733	2.9	ng	122194	3	9.933	833061	20.0
2,2,4-Trimethyl...	10.327	2.5	ng	104725	3	9.933	833061	20.0
Isopropyl myris...	11.368	3.1	ng	131281	4	11.422	854787	20.0
Phthalic acid, ...	11.580	3.7	ng	159272	4	11.422	854787	20.0
unknown12.792	12.792	2.3	ng	63879	5	14.068	560846	20.0
Pentafluoroprop...	13.910	14.9	ng	418125	5	14.068	560846	20.0