

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042021\
 Data File : BF123651.D
 Acq On : 20 Apr 2021 19:42
 Operator : JU/CG
 Sample : M2076-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-13-0-2.0

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-BF041521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123651.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.063	501	506	512	rVB	63375	78940	1.24%	0.153%
2	5.469	571	575	579	rBV	6625624	5895650	92.28%	11.450%
3	6.481	743	747	764	rVB	6013639	6380513	99.86%	12.391%
4	6.845	806	809	813	rBV	1788053	1502756	23.52%	2.918%
5	7.410	900	905	908	rBV	4555292	4103600	64.23%	7.969%
6	8.133	1024	1028	1031	rBV	2528933	1973960	30.90%	3.833%
7	9.210	1207	1211	1215	rBV	6787515	6389214	100.00%	12.408%
8	9.327	1227	1231	1235	rBV	505294	453705	7.10%	0.881%
9	9.604	1275	1278	1281	rBV	160825	125250	1.96%	0.243%
10	9.892	1323	1327	1330	rBV	2654769	2113508	33.08%	4.104%
11	10.474	1423	1426	1437	rBV	261699	394379	6.17%	0.766%
12	10.680	1457	1461	1464	rBV	5027589	4522724	70.79%	8.783%
13	11.233	1550	1555	1560	rBV5	44589	82098	1.28%	0.159%
14	11.380	1576	1580	1582	rBV	2746698	2251146	35.23%	4.372%
15	11.404	1582	1584	1587	rVV	278192	213275	3.34%	0.414%
16	11.451	1587	1592	1596	rVB3	92994	108152	1.69%	0.210%
17	11.569	1609	1612	1618	rBV3	52537	79203	1.24%	0.154%
18	11.910	1667	1670	1674	rBV	450822	363133	5.68%	0.705%
19	11.992	1681	1684	1686	rBV	70098	70100	1.10%	0.136%
20	12.592	1780	1786	1789	rBV	782144	692594	10.84%	1.345%
21	12.633	1789	1793	1796	rVB	178671	172972	2.71%	0.336%
22	12.821	1816	1825	1828	rBV	682191	708589	11.09%	1.376%
23	12.868	1831	1833	1839	rVB3	52749	66285	1.04%	0.129%
24	12.974	1846	1851	1854	rVB	6795920	6290392	98.45%	12.216%
25	13.151	1879	1881	1884	rVB2	76565	71784	1.12%	0.139%
26	13.204	1885	1890	1892	rBV	91704	115187	1.80%	0.224%
27	13.774	1981	1987	1990	rBV4	39972	76663	1.20%	0.149%
28	13.880	2000	2005	2022	rBV3	432240	1000437	15.66%	1.943%
29	14.027	2024	2030	2032	rVV2	1944083	1978629	30.97%	3.843%
30	14.051	2032	2034	2040	rVB	237628	214999	3.37%	0.418%
31	14.504	2107	2111	2114	rBV2	91683	115213	1.80%	0.224%
32	15.068	2203	2207	2210	rBV	188364	281589	4.41%	0.547%
33	15.157	2218	2222	2224	rBV	112863	126454	1.98%	0.246%
34	15.374	2255	2259	2264	rBV	111525	138420	2.17%	0.269%
35	15.433	2266	2269	2275	rVB	164890	208913	3.27%	0.406%
36	15.504	2275	2281	2285	rBV	1170659	1456486	22.80%	2.829%

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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

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37	15.539	2285	2287	2292	rVB3	108823	133845	2.09%	0.260%
38	15.986	2358	2363	2368	rBV	116513	171111	2.68%	0.332%
39	16.503	2446	2451	2454	rBV3	54038	87522	1.37%	0.170%
40	16.974	2526	2531	2539	rVB2	89099	162173	2.54%	0.315%
41	17.415	2601	2606	2614	rVB2	60484	121035	1.89%	0.235%

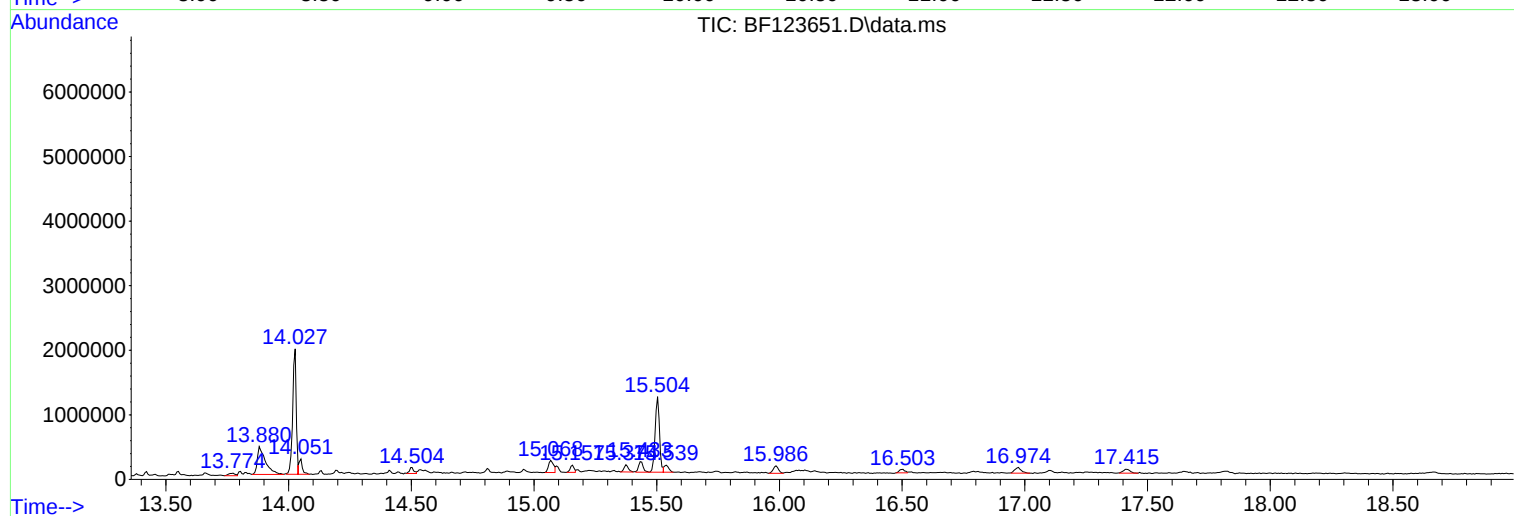
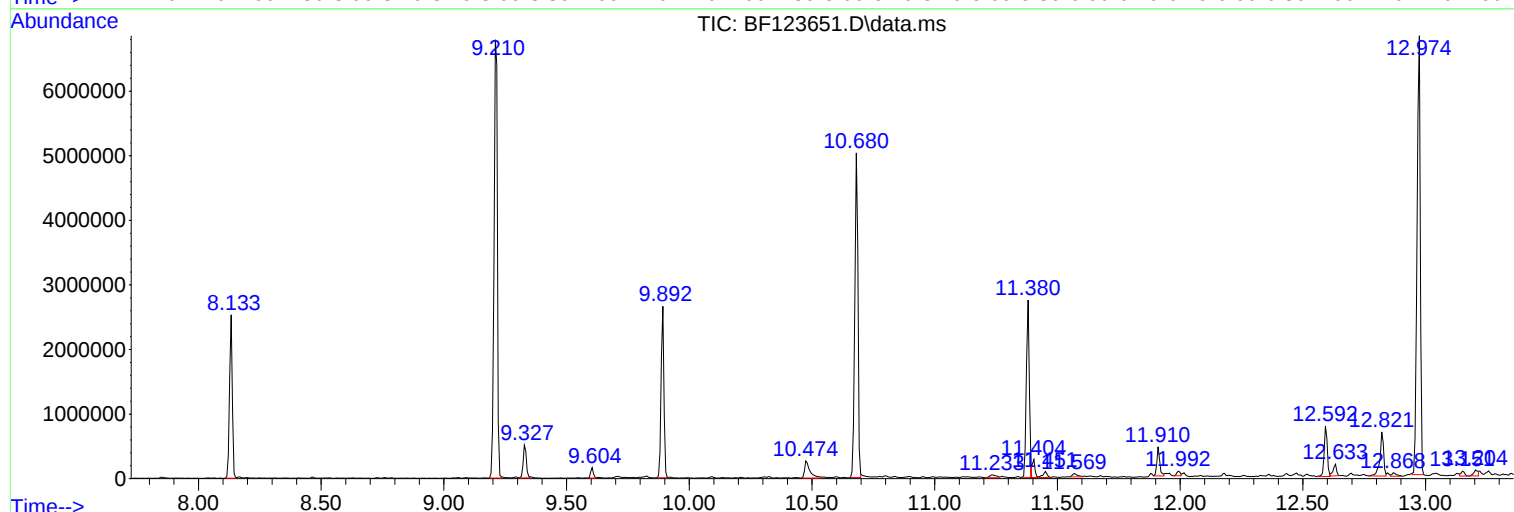
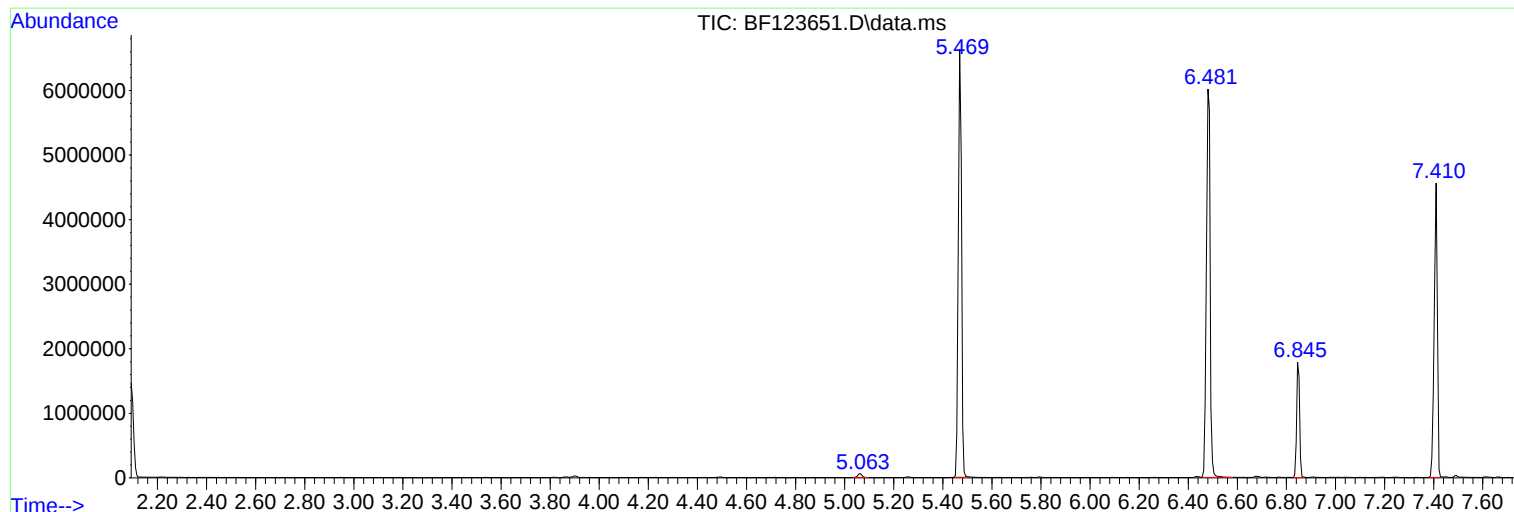
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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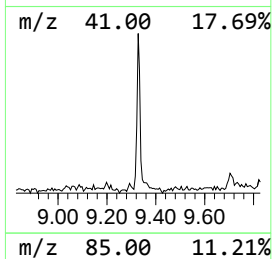
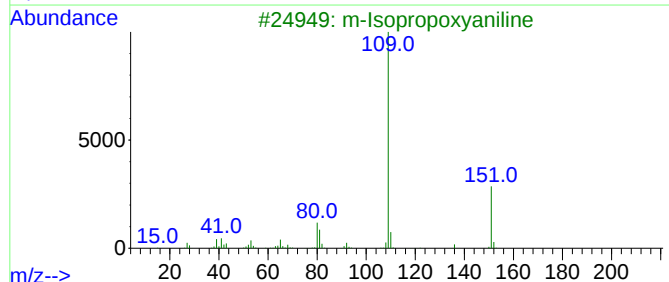
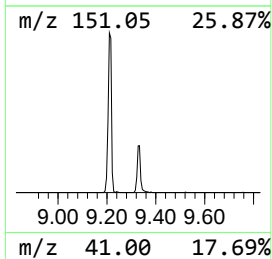
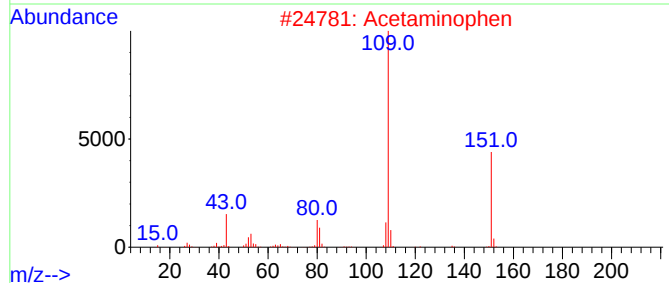
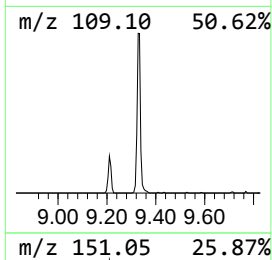
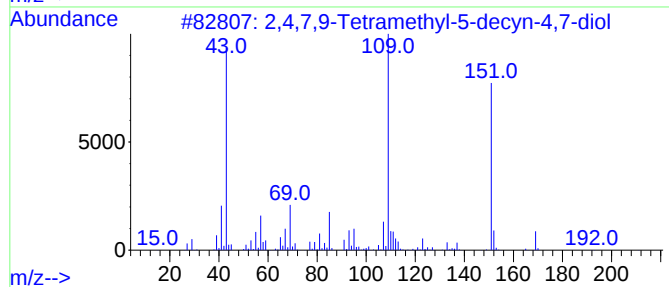
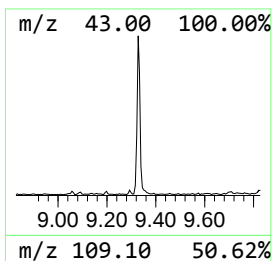
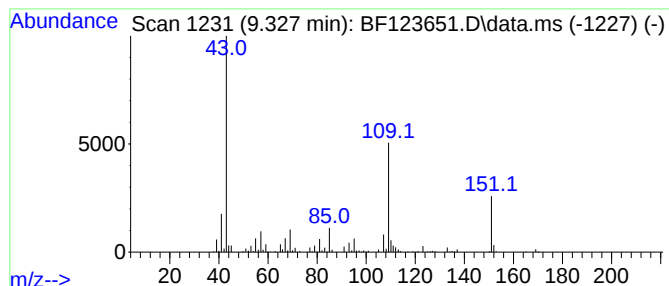
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown9.327 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.327	4.29 ng	453705	Acenaphthene-d10	9.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	38		
2	Acetaminophen	151	C8H9NO2	000103-90-2	38		
3	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	38		
4	Metacetamol	151	C8H9NO2	000621-42-1	38		
5	Cyclohexanol, 3,3,5-trimethyl-, ...	142	C9H18O	000767-54-4	37		



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ClientSampleId :
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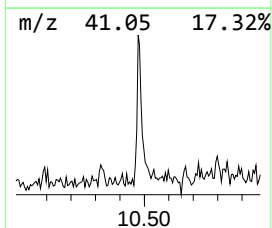
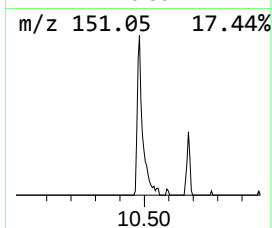
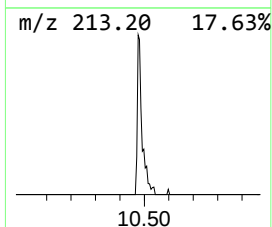
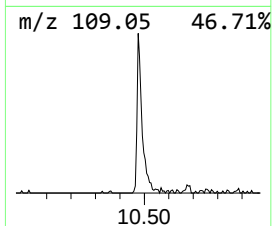
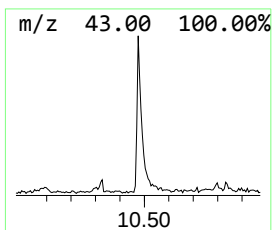
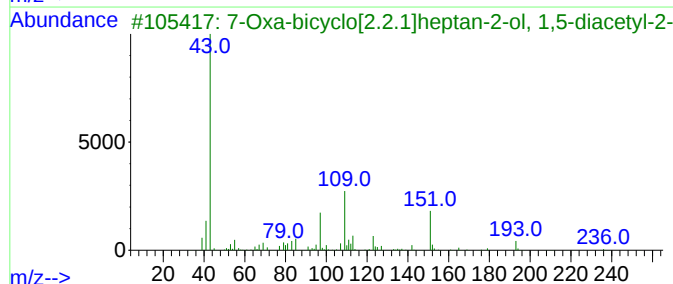
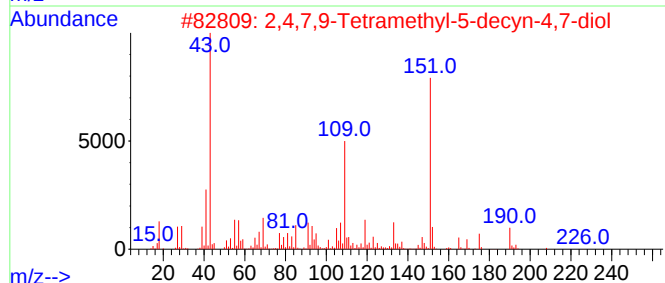
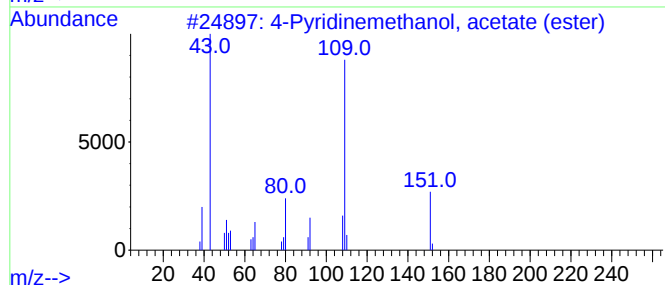
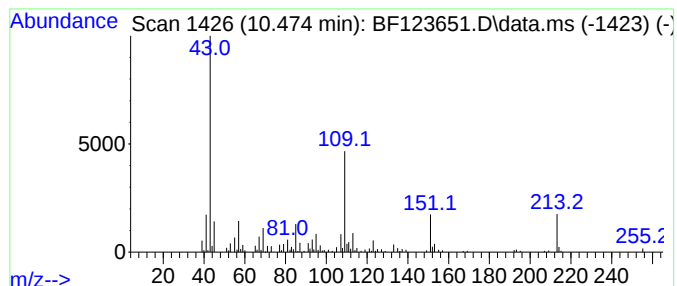
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown10.475 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.475	3.73 ng	394379	Acenaphthene-d10	9.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Pyridinemethanol, acetate (ester)	151	C8H9NO2	001007-48-3	38
2			2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	38
3			7-Oxa-bicyclo[2.2.1]heptan-2-ol,...	254	C14H22O4	329362-13-2	32
4			4-(1,5-Dihydroxy-2,6,6-trimethyl...	224	C13H20O3	1000191-85-2	25
5			3,6-Dimethyl-6-hepten-4-yn-3-ol	138	C9H14O	003601-67-0	16



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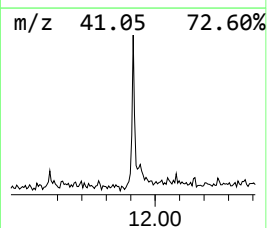
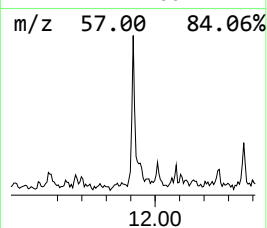
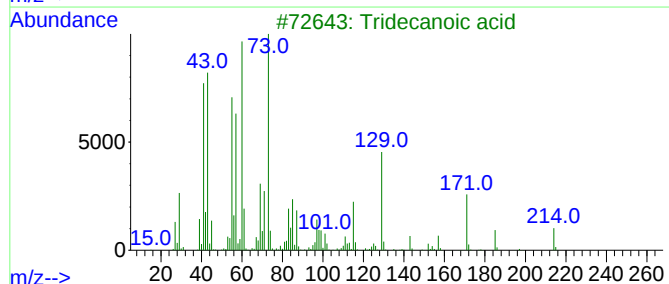
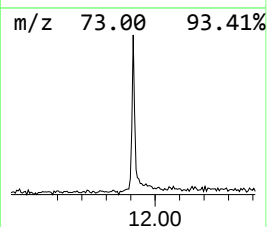
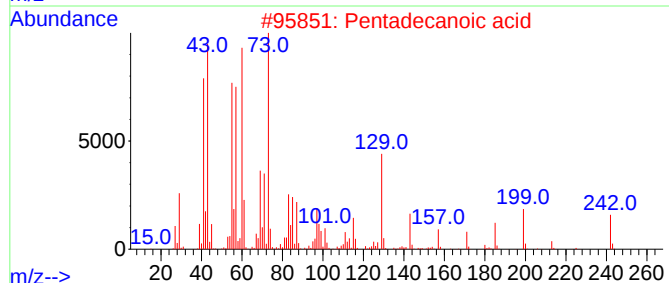
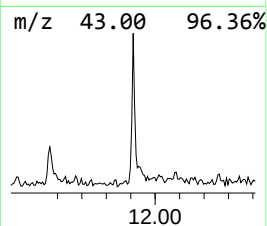
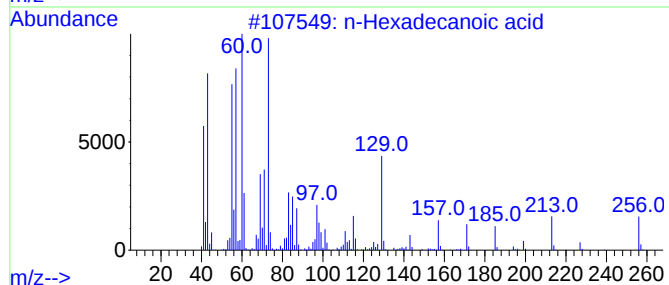
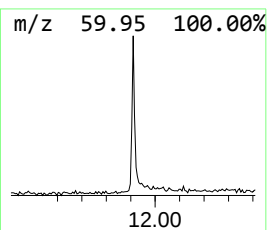
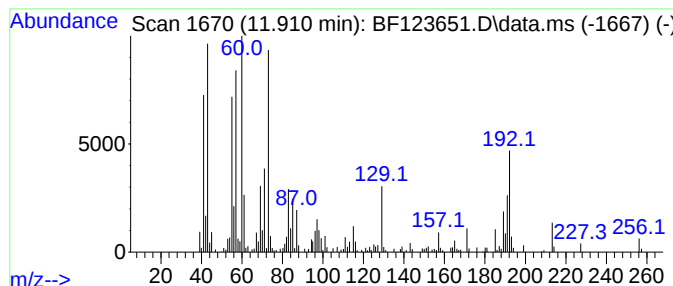
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	3.23 ng	363133	Phenanthrene-d10	11.380

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
3			Tridecanoic acid	214	C13H26O2	000638-53-9	64
4			n-Decanoic acid	172	C10H20O2	000334-48-5	64
5			Undecanoic acid	186	C11H22O2	000112-37-8	58



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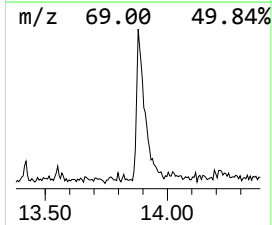
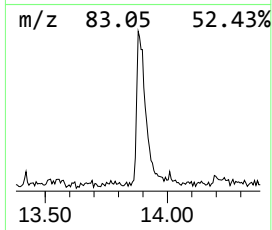
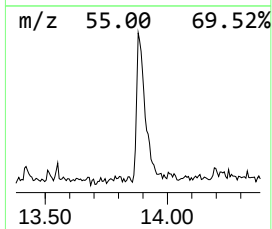
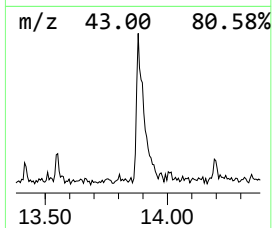
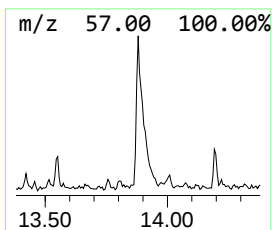
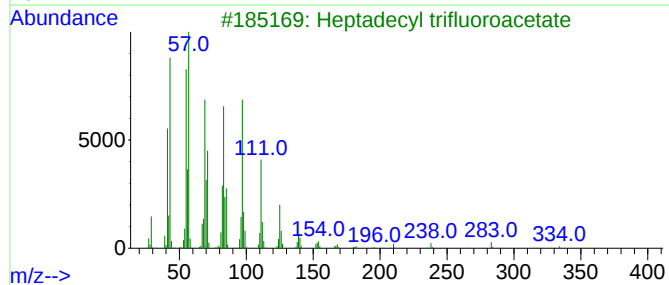
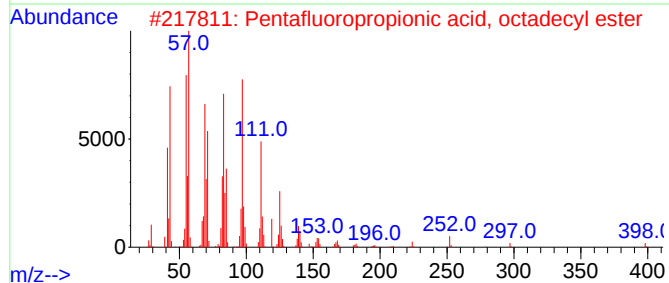
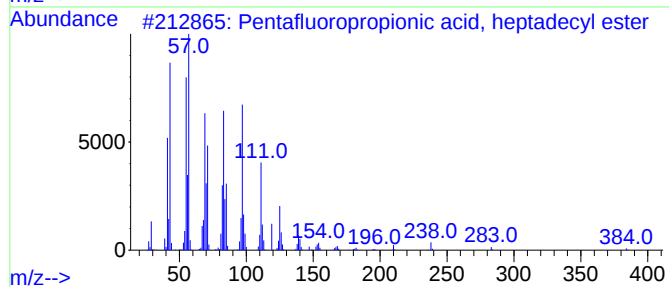
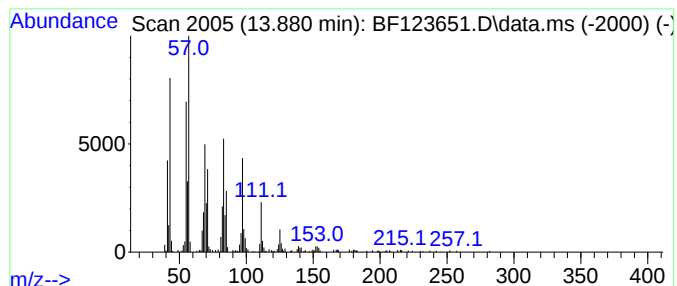
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Peak Number 4 Pentafluoropropionic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	10.11 ng	1000440	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
2			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
3			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
5			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91



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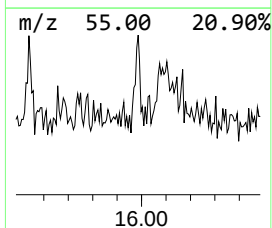
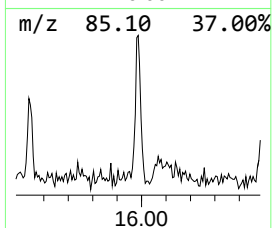
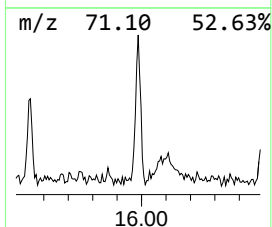
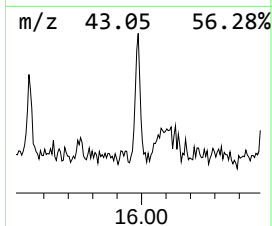
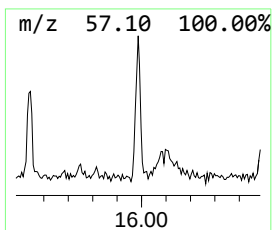
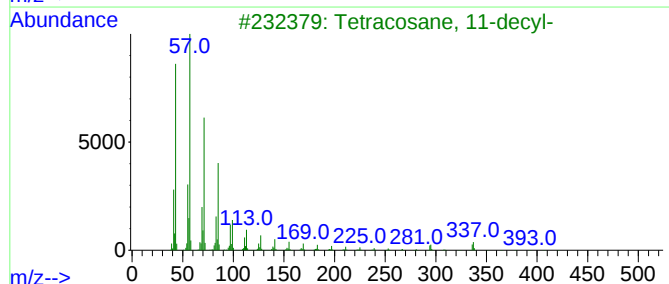
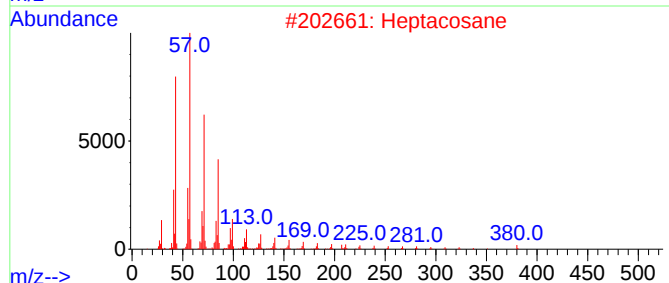
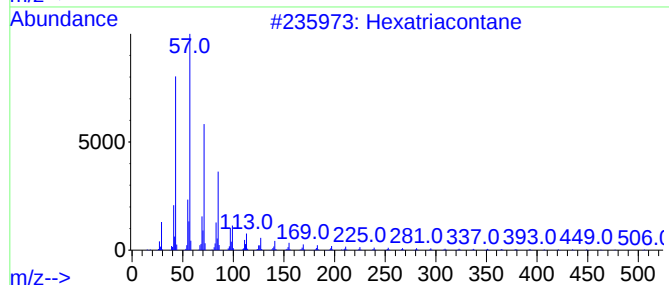
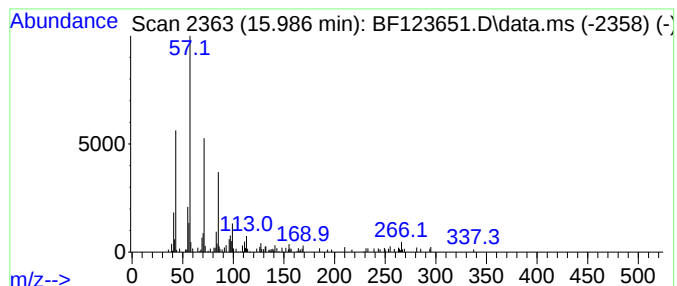
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Hexatriacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.986	2.35 ng	171111	Perylene-d12	15.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexatriacontane	507	C36H74	000630-06-8	81
2			Heptacosane	380	C27H56	000593-49-7	76
3			Tetracosane, 11-decyl-	479	C34H70	055429-84-0	74
4			Octacosane	394	C28H58	000630-02-4	74
5			Eicosane	282	C20H42	000112-95-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042021\
Data File : BF123651.D
Acq On : 20 Apr 2021 19:42
Operator : JU/CG
Sample : M2076-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-13-0-2.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.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
unknown9.327	9.327	4.3	ng	453705	3	9.892	2113510	20.0
unknown10.475	10.475	3.7	ng	394379	3	9.892	2113510	20.0
n-Hexadecanoic ...	11.910	3.2	ng	363133	4	11.380	2251150	20.0
Pentafluoroprop...	13.880	10.1	ng	1000440	5	14.027	1978630	20.0
Hexatriacontane	15.986	2.4	ng	171111	6	15.504	1456490	20.0