

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042421\
 Data File : BF123718.D
 Acq On : 24 Apr 2021 15:45
 Operator : JU/CG
 Sample : M2107-03
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-29-9.5-10.0

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: BF123718.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.022	493	499	507	rBV	282304	342988	6.37%	0.848%
2	5.440	566	570	573	rBV	5657877	5096515	94.70%	12.596%
3	6.451	738	742	757	rVB	5279033	5381707	100.00%	13.301%
4	6.822	801	805	808	rBV	1563705	1373153	25.52%	3.394%
5	7.381	895	900	903	rBV	3900800	3469016	64.46%	8.574%
6	8.104	1019	1023	1026	rBV	2295092	1758399	32.67%	4.346%
7	9.181	1202	1206	1209	rBV	6617457	5290172	98.30%	13.075%
8	9.298	1222	1226	1230	rBV	493491	408943	7.60%	1.011%
9	9.569	1268	1272	1275	rBV	158372	135912	2.53%	0.336%
10	9.857	1317	1321	1325	rBV	2410872	1870129	34.75%	4.622%
11	10.445	1418	1421	1428	rBV4	43728	69038	1.28%	0.171%
12	10.645	1451	1455	1458	rBV	4150065	3570780	66.35%	8.825%
13	11.345	1570	1574	1577	rBV	2344870	1965898	36.53%	4.859%
14	12.933	1840	1844	1847	rBV	5838455	5302506	98.53%	13.105%
15	13.133	1870	1878	1879	rBV8	35408	68147	1.27%	0.168%
16	13.474	1932	1936	1940	rBV2	90857	88866	1.65%	0.220%
17	13.845	1995	1999	2019	rBV2	277293	777696	14.45%	1.922%
18	13.986	2019	2023	2026	rBV	2005469	1651513	30.69%	4.082%
19	14.463	2099	2104	2107	rBV	65919	70474	1.31%	0.174%
20	14.768	2153	2156	2159	rBV	68493	64618	1.20%	0.160%
21	15.104	2209	2213	2217	rBV	68217	92151	1.71%	0.228%
22	15.445	2266	2271	2275	rBV	993995	1253096	23.28%	3.097%
23	15.480	2275	2277	2285	rVB2	68009	101761	1.89%	0.252%
24	15.915	2347	2351	2360	rVB	62579	106830	1.99%	0.264%
25	16.421	2432	2437	2441	rBV3	45304	84627	1.57%	0.209%
26	17.704	2650	2655	2662	rVB9	29933	66672	1.24%	0.165%

Sum of corrected areas: 40461607

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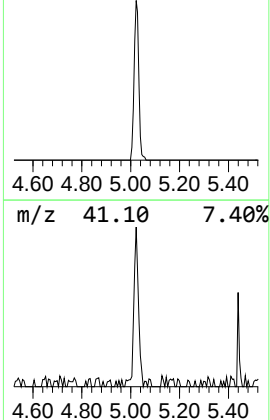
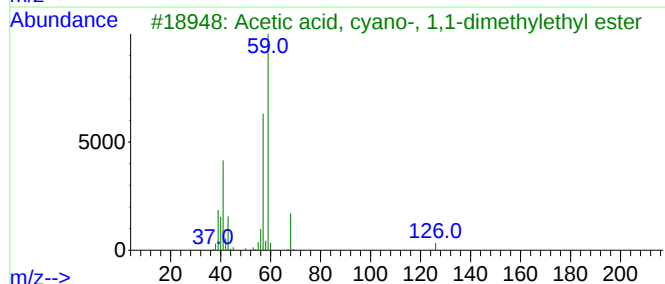
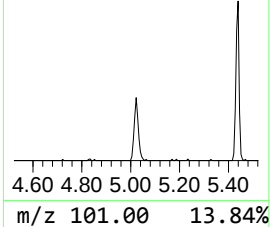
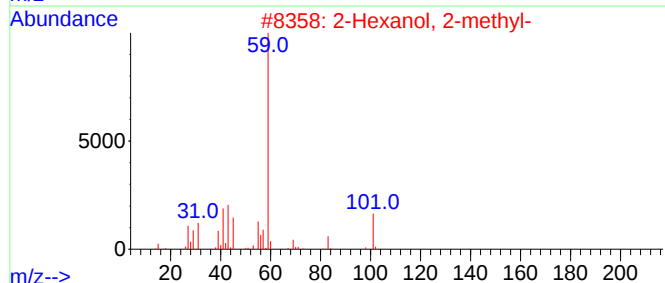
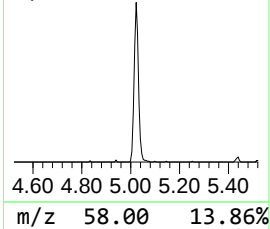
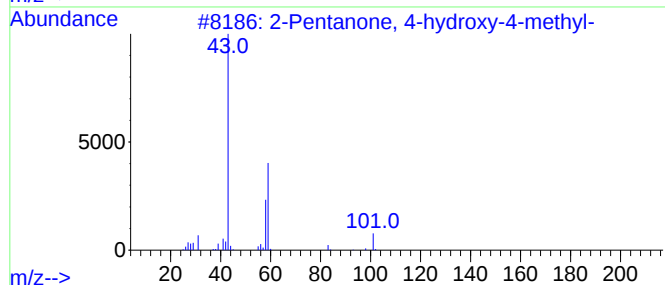
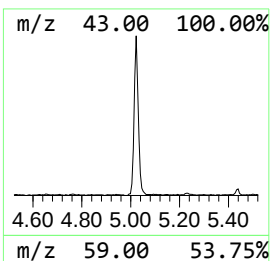
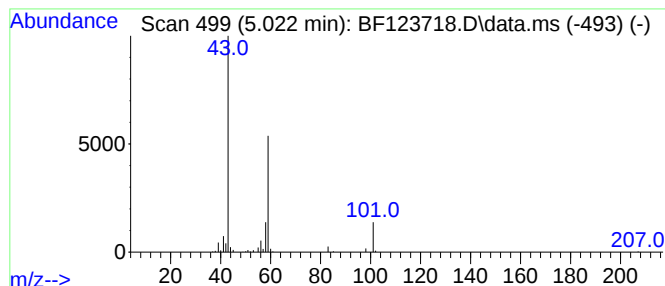
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	5.00 ng	342988	1,4-Dichlorobenzene-d4	6.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
5			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9



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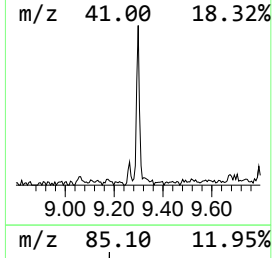
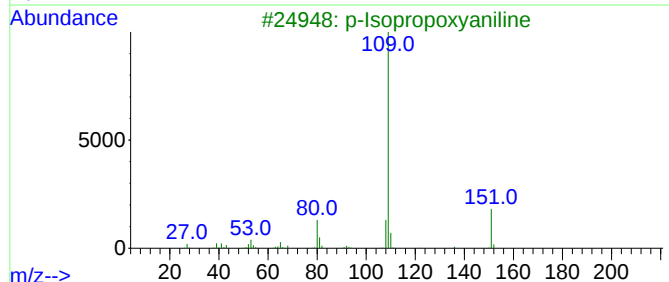
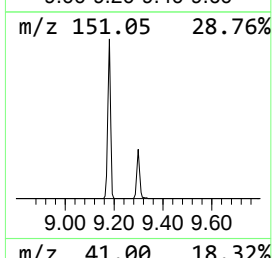
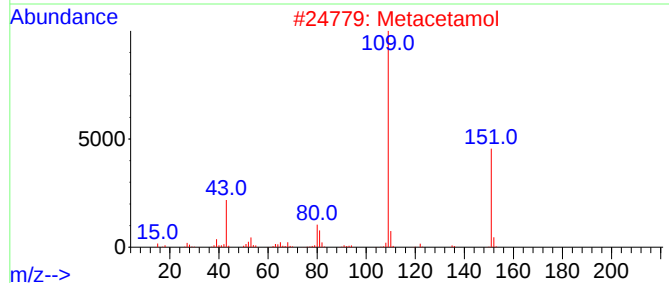
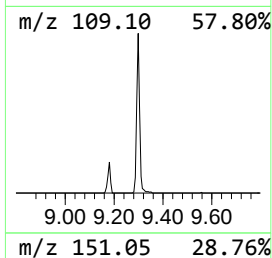
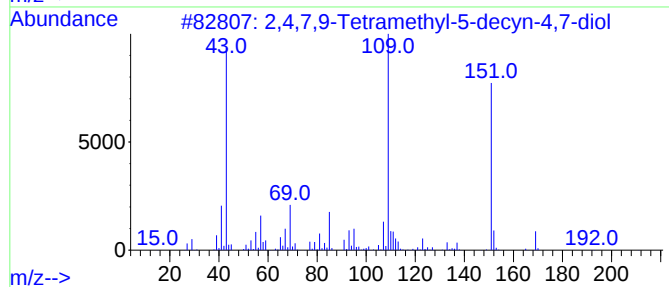
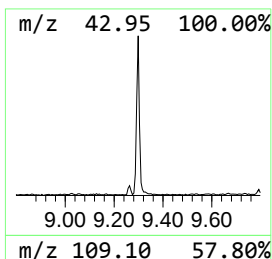
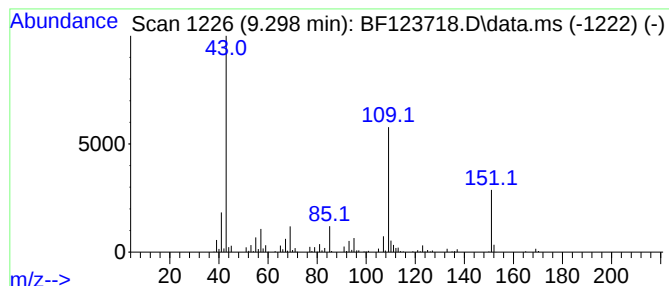
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Peak Number 2 unknown9.298 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.298	4.37 ng	408943	Acenaphthene-d10	9.857

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	49
2		Metacetamol	151	C8H9NO2	000621-42-1	38
3		p-Isopropoxyaniline	151	C9H13NO	007664-66-6	38
4		Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	38
5		Cyclohexanol, 3,3,5-trimethyl-	142	C9H18O	000116-02-9	32



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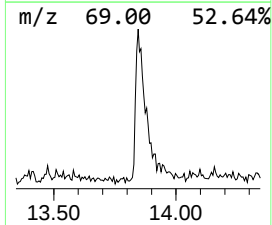
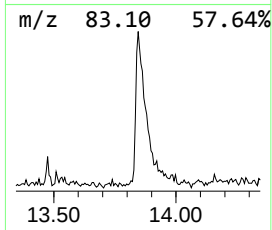
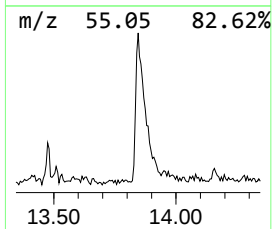
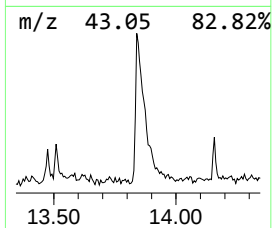
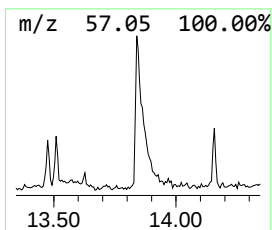
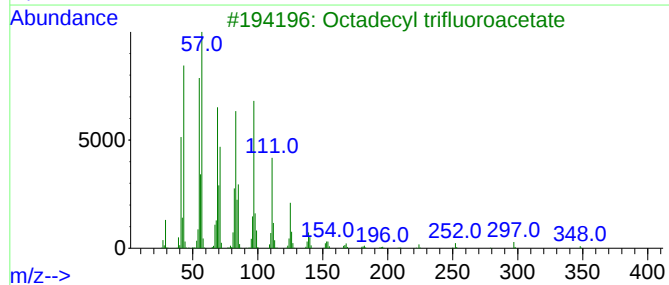
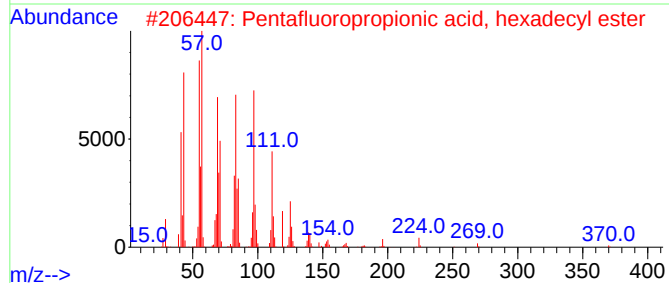
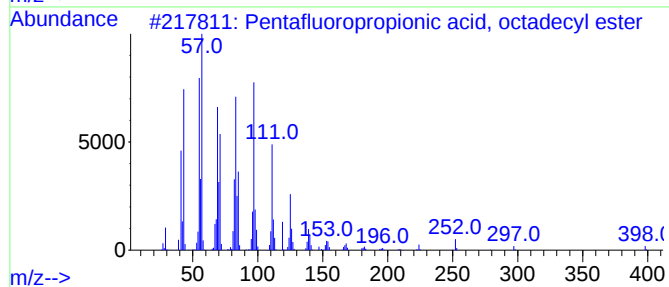
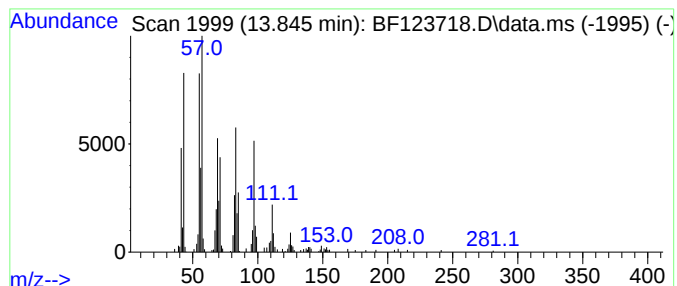
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Peak Number 3 Pentafluoropropionic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.845	9.42 ng	777696	Chrysene-d12	13.986

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
2			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
3			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
4			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
5			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91



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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-...	5.022	5.0	ng	342988	1	6.822	1373150	20.0
unknown9.298	9.298	4.4	ng	408943	3	9.857	1870130	20.0
Pentafluoroprop...	13.845	9.4	ng	777696	5	13.986	1651510	20.0