

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051521\
 Data File : BF123952.D
 Acq On : 15 May 2021 18:55
 Operator : JU/CG
 Sample : M2392-23 2X
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-08-COMP

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-BF051421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123952.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	8	13	19	rVB	261266	315575	58.20%	5.772%
2	2.269	27	31	36	rVB	18255	22630	4.17%	0.414%
3	5.510	578	582	585	rBV	619304	520472	95.99%	9.519%
4	6.516	748	753	756	rBV	638977	531671	98.06%	9.724%
5	6.722	786	788	794	rBV	16696	12725	2.35%	0.233%
6	6.904	815	819	822	rBV	371822	293837	54.19%	5.374%
7	7.457	909	913	917	rVB	382719	337726	62.29%	6.177%
8	8.186	1033	1037	1040	rBV	496380	364263	67.18%	6.662%
9	9.263	1216	1220	1223	rBV	652216	542212	100.00%	9.916%
10	9.651	1283	1286	1290	rVB	74761	51293	9.46%	0.938%
11	9.939	1332	1335	1339	rVB	414943	358271	66.08%	6.552%
12	10.727	1465	1469	1472	rBV	341327	289506	53.39%	5.295%
13	10.851	1486	1490	1491	rBV2	4900	6283	1.16%	0.115%
14	11.427	1585	1588	1591	rBV	408062	323003	59.57%	5.907%
15	11.451	1591	1592	1595	rVV	24952	14180	2.62%	0.259%
16	11.498	1598	1600	1605	rVB2	7093	6410	1.18%	0.117%
17	11.886	1663	1666	1669	rBV4	4517	6962	1.28%	0.127%
18	11.927	1671	1673	1675	rVV3	5885	6675	1.23%	0.122%
19	11.951	1675	1677	1681	rVB2	34244	30567	5.64%	0.559%
20	12.045	1688	1693	1695	rBV4	9849	11394	2.10%	0.208%
21	12.639	1791	1794	1798	rVB	56724	48446	8.93%	0.886%
22	12.821	1823	1825	1826	rBV2	7834	7363	1.36%	0.135%
23	12.868	1830	1833	1836	rVB	55819	47448	8.75%	0.868%
24	13.016	1854	1858	1861	rBV	533100	480709	88.66%	8.792%
25	13.074	1866	1868	1873	rBV5	10441	18561	3.42%	0.339%
26	13.174	1882	1885	1886	rBV3	7443	6261	1.15%	0.115%
27	13.198	1887	1889	1891	rVV3	13913	11678	2.15%	0.214%
28	13.221	1891	1893	1896	rVB4	11668	11556	2.13%	0.211%
29	13.268	1896	1901	1902	rBV5	13421	18548	3.42%	0.339%
30	13.710	1973	1976	1978	rBV4	13386	16672	3.07%	0.305%
31	13.821	1993	1995	1998	rBV3	9180	9068	1.67%	0.166%
32	13.910	2007	2010	2014	rBV3	90559	82902	15.29%	1.516%
33	14.068	2033	2037	2040	rBV	330200	333444	61.50%	6.098%
34	14.357	2082	2086	2089	rBV6	18518	34211	6.31%	0.626%
35	14.421	2095	2097	2098	rBV2	14724	8147	1.50%	0.149%
36	14.545	2116	2118	2122	rVB5	26839	27964	5.16%	0.511%

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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	14.592	2124	2126	2127	rBV2	15571	10323	1.90%	0.189%
38	15.562	2287	2291	2295	rVB	155179	181864	33.54%	3.326%
39	15.715	2315	2317	2318	rBV2	15433	11038	2.04%	0.202%
40	16.127	2385	2387	2389	rVB3	14465	9274	1.71%	0.170%
41	16.621	2469	2471	2472	rBV2	11522	7010	1.29%	0.128%
42	17.286	2582	2584	2587	rVB4	12212	9987	1.84%	0.183%
43	17.803	2671	2672	2674	rBV2	12037	10999	2.03%	0.201%
44	18.292	2753	2755	2758	rBV4	7959	9388	1.73%	0.172%
45	18.468	2783	2785	2789	rBV6	9407	9284	1.71%	0.170%

Sum of corrected areas: 5467800

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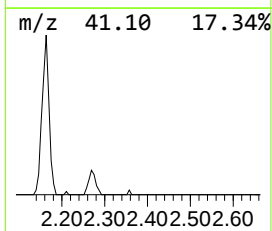
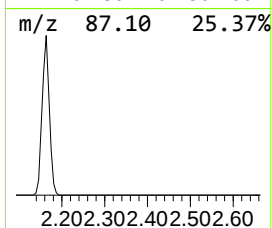
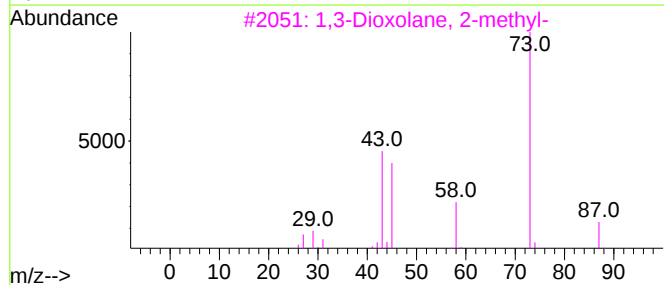
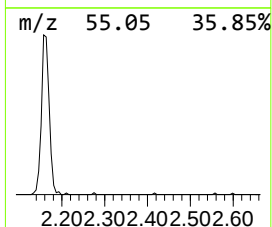
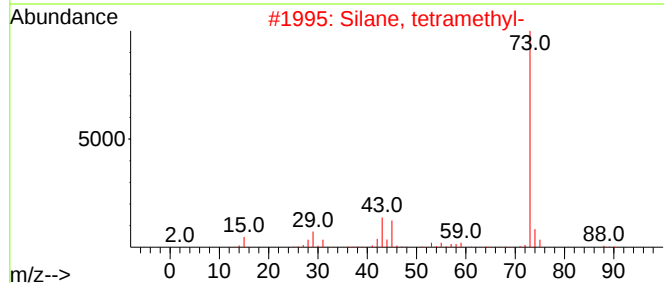
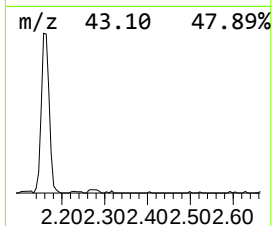
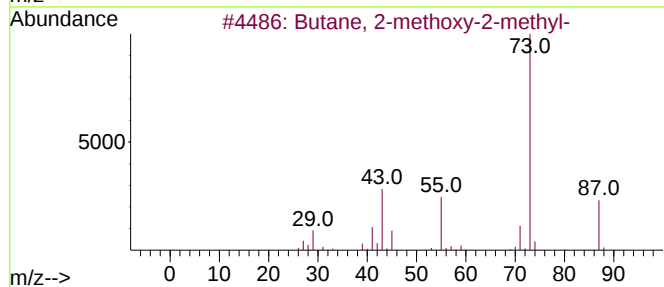
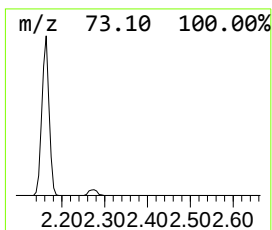
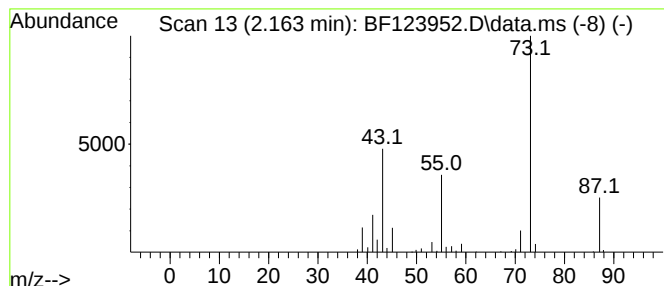
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.163	21.48 ng	315575	1,4-Dichlorobenzene-d4	6.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
4			3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	9
5			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	9



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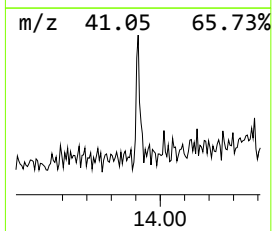
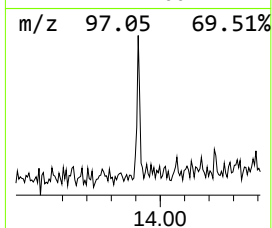
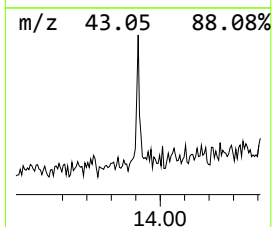
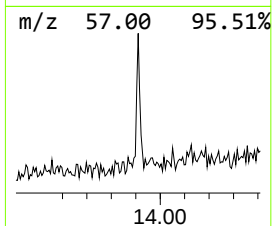
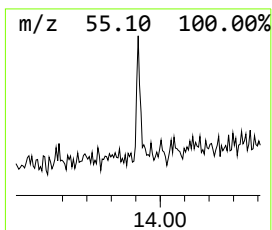
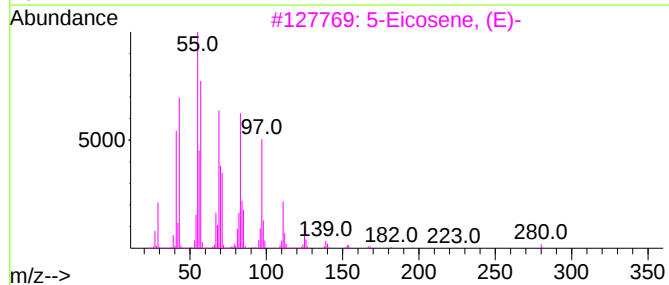
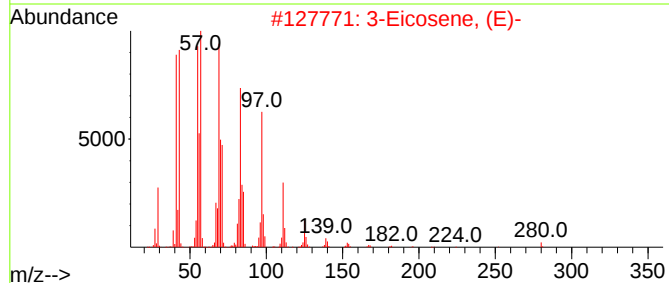
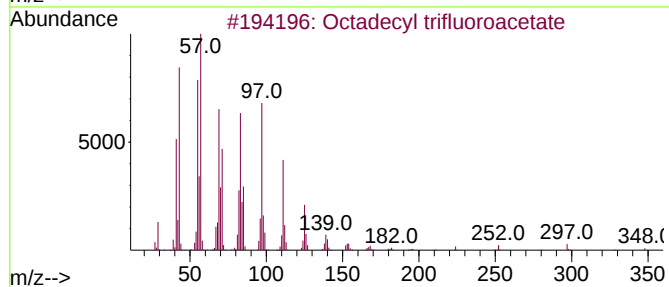
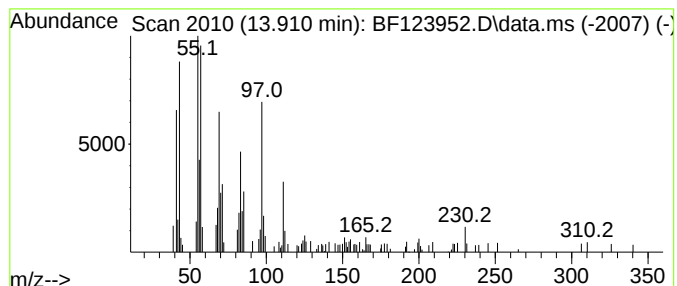
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Octadecyl trifluoroacetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	4.97 ng	82902	Chrysene-d12	14.068

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	64
2		3-Eicosene, (E)-	280	C20H40	074685-33-9	64
3		5-Eicosene, (E)-	280	C20H40	074685-30-6	58
4		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	58
5		9-Eicosene, (E)-	280	C20H40	074685-29-3	58



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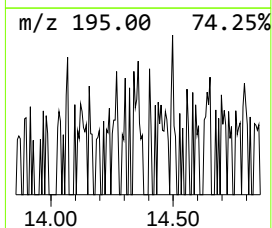
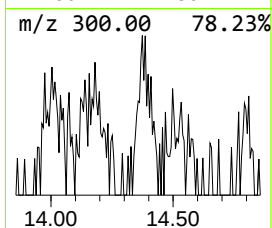
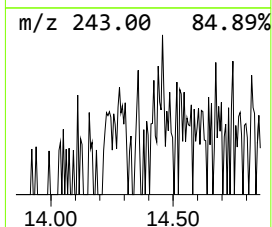
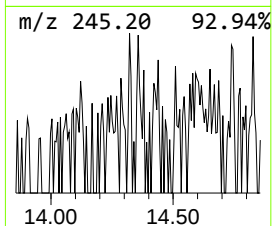
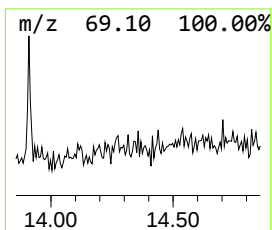
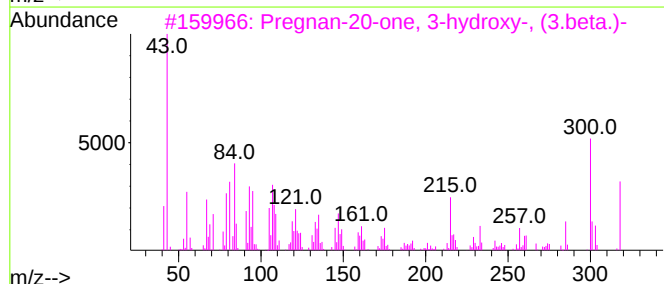
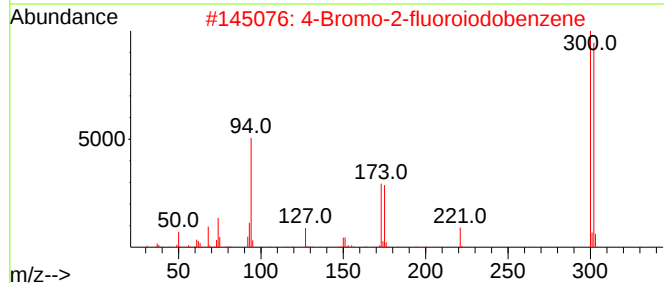
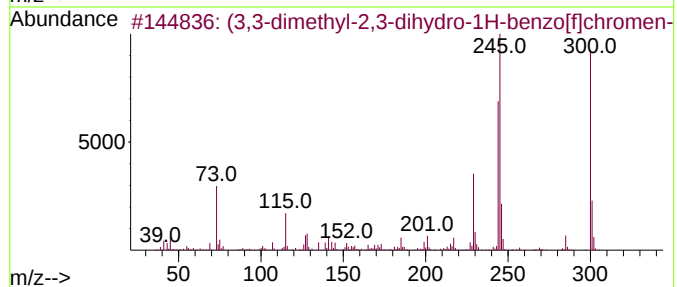
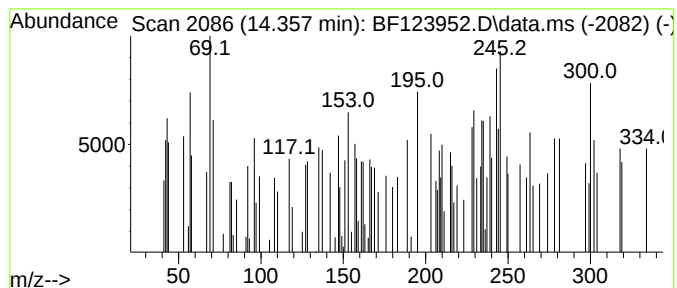
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown14.357 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.357	2.05 ng	34211	Chrysene-d12	14.068

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(3,3-dimethyl-2,3-dihydro-1H-ben...	300	C18H24O2Si	1000372-24-0	12
2			4-Bromo-2-fluoriodobenzene	300	C6H3BrFI	105931-73-5	10
3			Pregnan-20-one, 3-hydroxy-, (3.b...	318	C21H34O2	004406-37-5	10
4			4'-Bromo-flavone	300	C15H9BrO2	020525-20-6	9
5			(4-Chloro-benzo[1,2,5]thiadiazol...	300	C12H13ClN2O3S	313267-93-5	9



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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
Butane, 2-metho...	2.163	21.5	ng	315575	1	6.904	293837	20.0
Octadecyl trifl...	13.910	5.0	ng	82902	5	14.068	333444	20.0
unknown14.357	14.357	2.0	ng	34211	5	14.068	333444	20.0