

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012821\
 Data File : BM028590.D
 Acq On : 28 Jan 2021 16:44
 Operator : CG/JU
 Sample : M1251-07
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 400024

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_M\Methods\8270-BM012021.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM028590.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.516	389	396	405	rVB	441813	654028	72.74%	9.682%
2	7.157	668	675	688	rBV	432114	678989	75.52%	10.052%
3	7.963	805	812	819	rBV	121444	190291	21.16%	2.817%
4	9.139	1004	1012	1020	rBV	267287	430395	47.87%	6.372%
5	10.781	1280	1291	1297	rBV	163280	265568	29.54%	3.931%
6	13.233	1702	1708	1719	rBV	542137	773486	86.03%	11.451%
7	14.063	1844	1849	1855	rVB	14203	19933	2.22%	0.295%
8	14.610	1936	1942	1949	rVB	211319	311689	34.67%	4.614%
9	16.098	2189	2195	2204	rBV	447084	607491	67.56%	8.993%
10	16.998	2344	2348	2354	rBV	26800	34264	3.81%	0.507%
11	17.345	2401	2407	2411	rBV	233599	329680	36.67%	4.881%
12	17.386	2411	2414	2421	rVB	21157	27918	3.11%	0.413%
13	18.221	2550	2556	2561	rBV	113840	154195	17.15%	2.283%
14	18.404	2581	2587	2591	rBV4	5818	10674	1.19%	0.158%
15	18.974	2677	2684	2687	rBV	16677	23032	2.56%	0.341%
16	19.062	2692	2699	2704	rVB4	5581	10814	1.20%	0.160%
17	19.127	2706	2710	2714	rVV4	8336	11281	1.25%	0.167%
18	19.386	2749	2754	2758	rVB	52130	73177	8.14%	1.083%
19	19.486	2767	2771	2777	rBV	54088	70701	7.86%	1.047%
20	19.709	2805	2809	2811	rBV3	9063	11283	1.25%	0.167%
21	19.745	2811	2815	2820	rVB	49639	64911	7.22%	0.961%
22	19.939	2843	2848	2853	rBV	718014	899123	100.00%	13.311%
23	20.062	2865	2869	2875	rBV7	3766	9062	1.01%	0.134%
24	20.233	2896	2898	2902	rVB2	10786	11931	1.33%	0.177%
25	20.333	2912	2915	2921	rBV4	6276	11590	1.29%	0.172%
26	20.392	2921	2925	2928	rVV	9225	12929	1.44%	0.191%
27	20.603	2958	2961	2966	rVB	11271	16202	1.80%	0.240%
28	20.809	2992	2996	3001	rBV	42625	53950	6.00%	0.799%
29	20.856	3001	3004	3008	rVB2	11534	13998	1.56%	0.207%
30	21.180	3055	3059	3071	rBV2	115609	150825	16.77%	2.233%
31	21.480	3104	3110	3114	rBV	300610	422988	47.04%	6.262%
32	21.515	3114	3116	3122	rVB	34269	44880	4.99%	0.664%
33	23.750	3490	3496	3502	rVB2	198644	353644	39.33%	5.235%

Sum of corrected areas: 6754922

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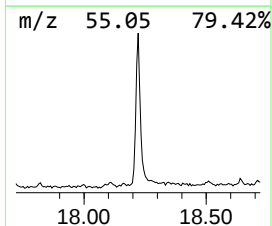
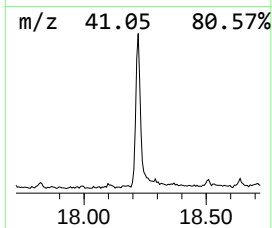
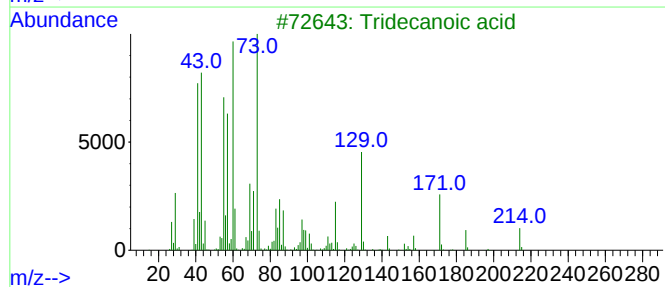
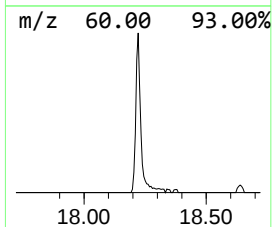
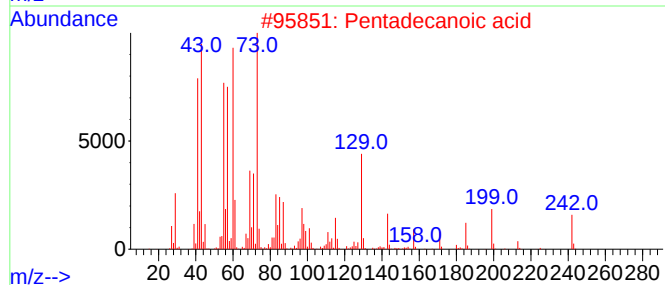
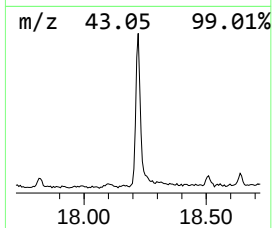
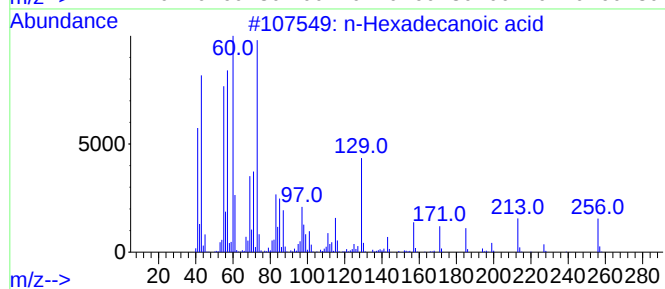
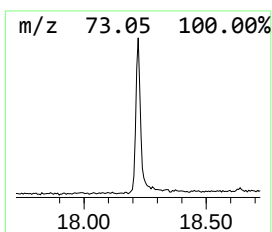
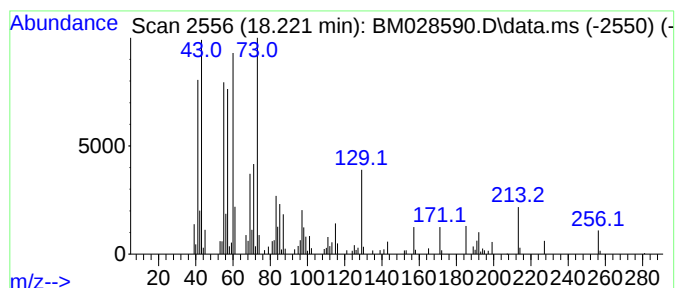
Instrument :
BNA_M
ClientSampleId :
400024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.221	9.35 ng	154195	Phenanthrene-d10	17.345	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70



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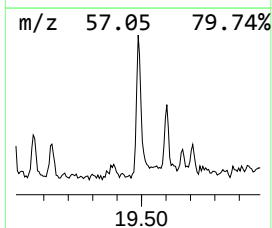
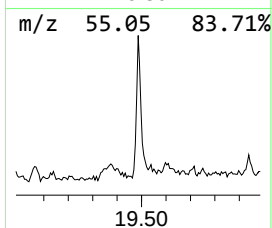
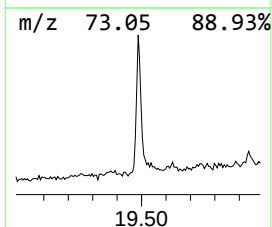
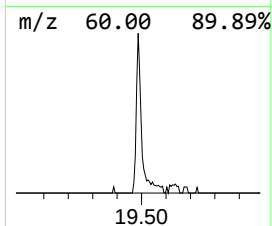
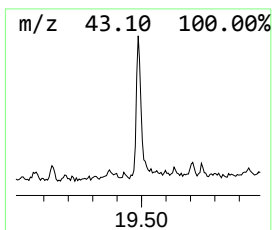
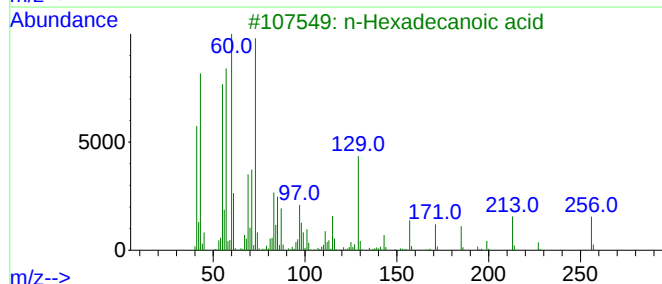
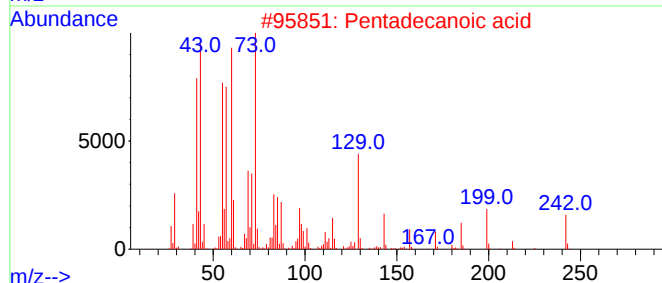
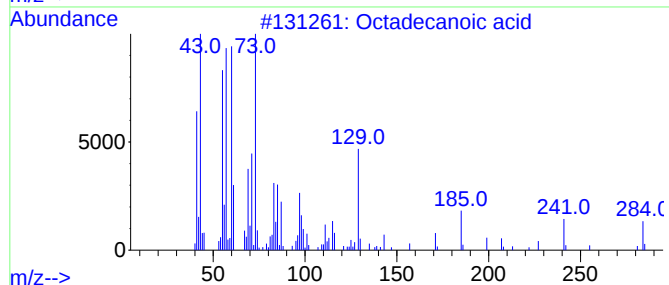
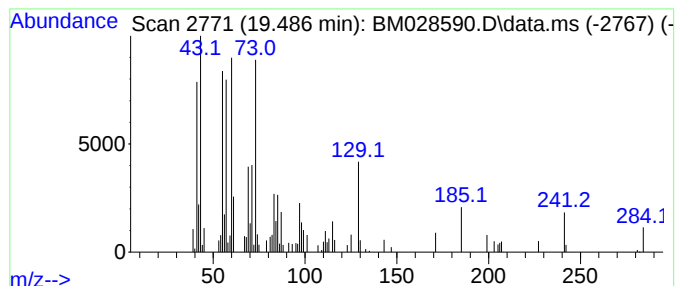
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.486	3.34 ng	70701	Chrysene-d12	21.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	97
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



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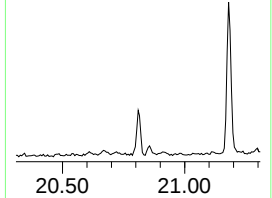
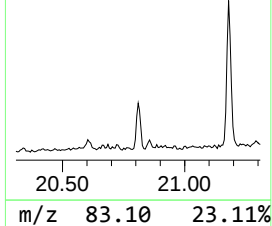
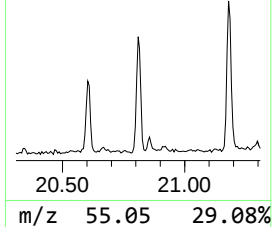
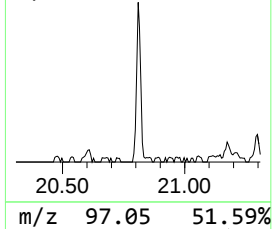
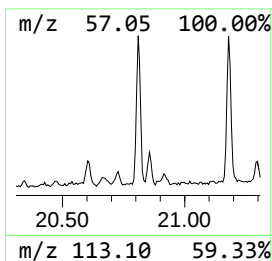
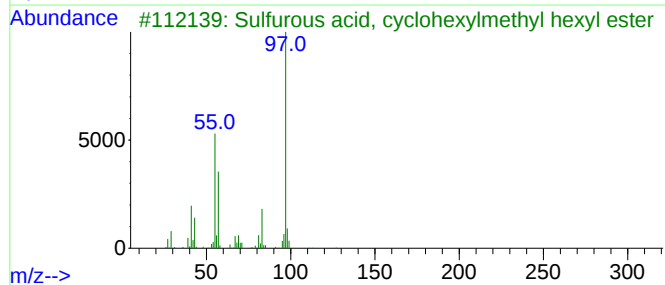
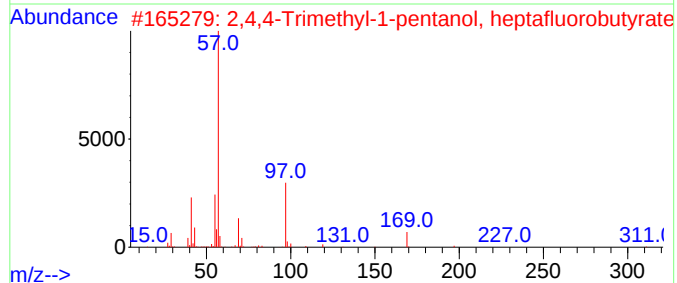
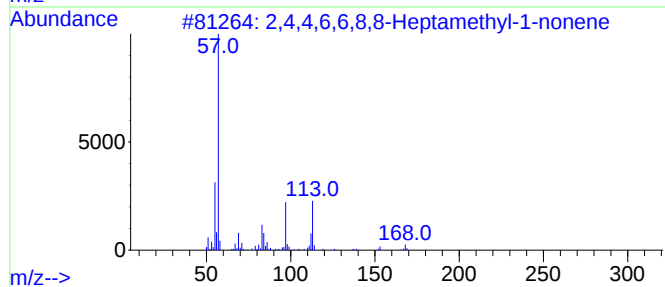
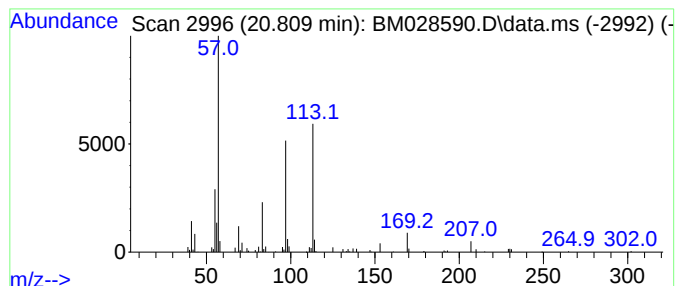
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 unknown20.80 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.809	2.55 ng	53950	Chrysene-d12	21.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	47		
2	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	35		
3	Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1000309-21-6	32		
4	Sulfurous acid, cyclohexylmethyl...	276	C14H28O3S	1000309-21-7	32		
5	5,11-Diethyl-8-methyl-7,9-dioxap...	286	C18H38O2	1000334-83-1	32		



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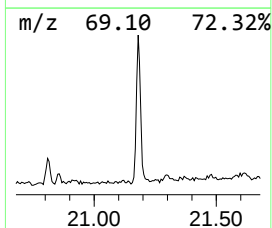
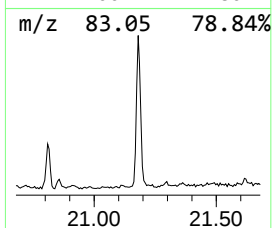
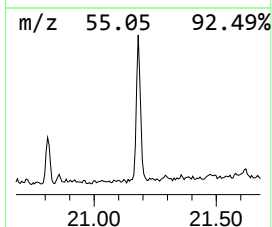
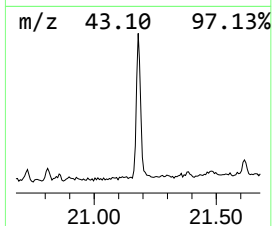
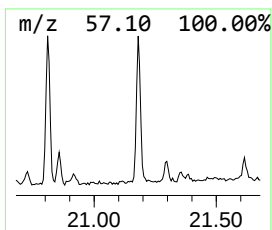
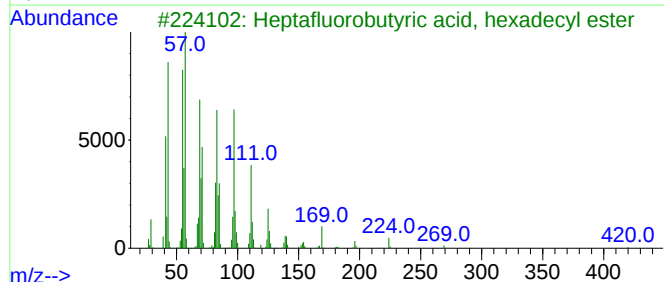
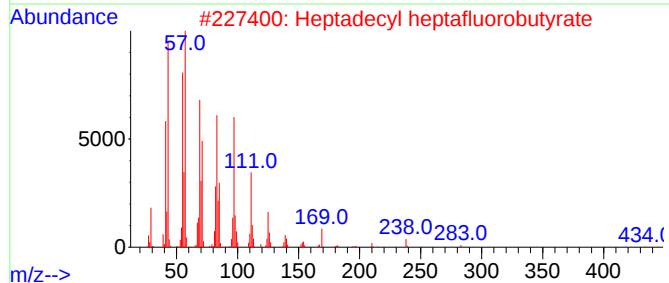
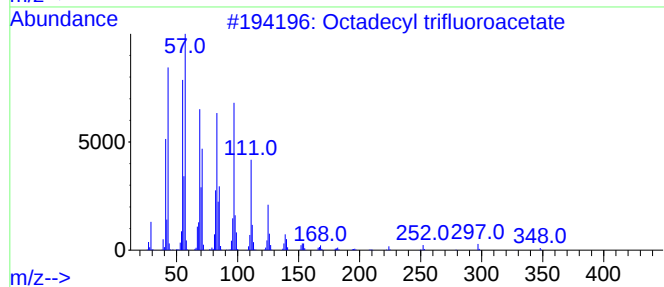
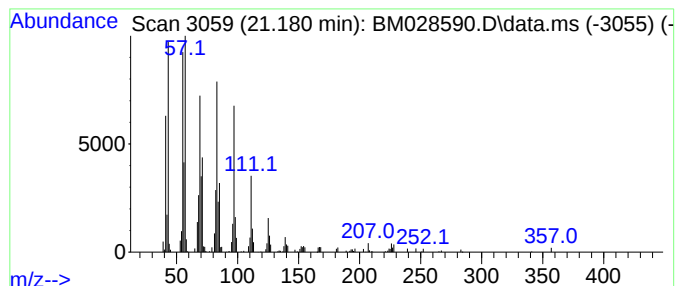
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Peak Number 4 Octadecyl trifluoroacetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.180	7.13 ng	150825	Chrysene-d12	21.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
4			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	94
5			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	18.221	9.3	ng	154195	4	17.345	329680	20.0
Octadecanoic acid	19.486	3.3	ng	70701	5	21.480	422988	20.0
unknown20.80	20.809	2.5	ng	53950	5	21.480	422988	20.0
Octadecyl trifl...	21.180	7.1	ng	150825	5	21.480	422988	20.0