

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012721\
 Data File : BM028571.D
 Acq On : 27 Jan 2021 16:07
 Operator : CG/JU
 Sample : M1236-08
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PS1419LN

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: BM028571.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	305	312	321	rVB	27950	39311	4.85%	0.656%
2	5.528	392	398	411	rVB	323322	471689	58.19%	7.874%
3	7.175	671	678	690	rBV	300628	499075	61.57%	8.331%
4	7.969	807	813	821	rVB	94281	144855	17.87%	2.418%
5	9.145	1005	1013	1024	rBV	188012	312706	38.57%	5.220%
6	10.780	1282	1291	1299	rBV	120839	199109	24.56%	3.324%
7	13.239	1702	1709	1718	rVB	436377	629476	77.65%	10.508%
8	14.615	1937	1943	1949	rVB	169276	242345	29.90%	4.045%
9	16.104	2190	2196	2206	rBV	334847	470737	58.07%	7.858%
10	16.745	2299	2305	2313	rBV	16927	21793	2.69%	0.364%
11	17.345	2401	2407	2413	rBV	200500	266501	32.88%	4.449%
12	17.503	2431	2434	2439	rBV	10750	13623	1.68%	0.227%
13	18.098	2530	2535	2542	rBV4	18243	29209	3.60%	0.488%
14	18.227	2551	2557	2566	rBV	158427	216643	26.72%	3.616%
15	18.715	2636	2640	2645	rBV2	7836	12606	1.56%	0.210%
16	18.974	2680	2684	2689	rBV	49131	57801	7.13%	0.965%
17	19.062	2695	2699	2705	rVB	14269	17410	2.15%	0.291%
18	19.127	2706	2710	2717	rBV2	5270	8599	1.06%	0.144%
19	19.368	2744	2751	2758	rBV7	17361	37171	4.59%	0.620%
20	19.492	2767	2772	2782	rBV	46458	70276	8.67%	1.173%
21	19.603	2788	2791	2795	rVB	13037	14502	1.79%	0.242%
22	19.945	2843	2849	2854	rBV	632062	810647	100.00%	13.532%
23	20.133	2877	2881	2886	rBV	7486	9856	1.22%	0.165%
24	20.609	2958	2962	2968	rBV	13155	19642	2.42%	0.328%
25	20.815	2993	2997	3001	rBV	46684	55222	6.81%	0.922%
26	20.856	3001	3004	3008	rVV2	12050	13164	1.62%	0.220%
27	21.180	3056	3059	3066	rBV	95798	116841	14.41%	1.950%
28	21.486	3106	3111	3117	rBV	246466	315919	38.97%	5.274%
29	22.650	3304	3309	3316	rVB	415830	542016	66.86%	9.048%
30	23.750	3490	3496	3507	rVB2	172838	331921	40.95%	5.541%

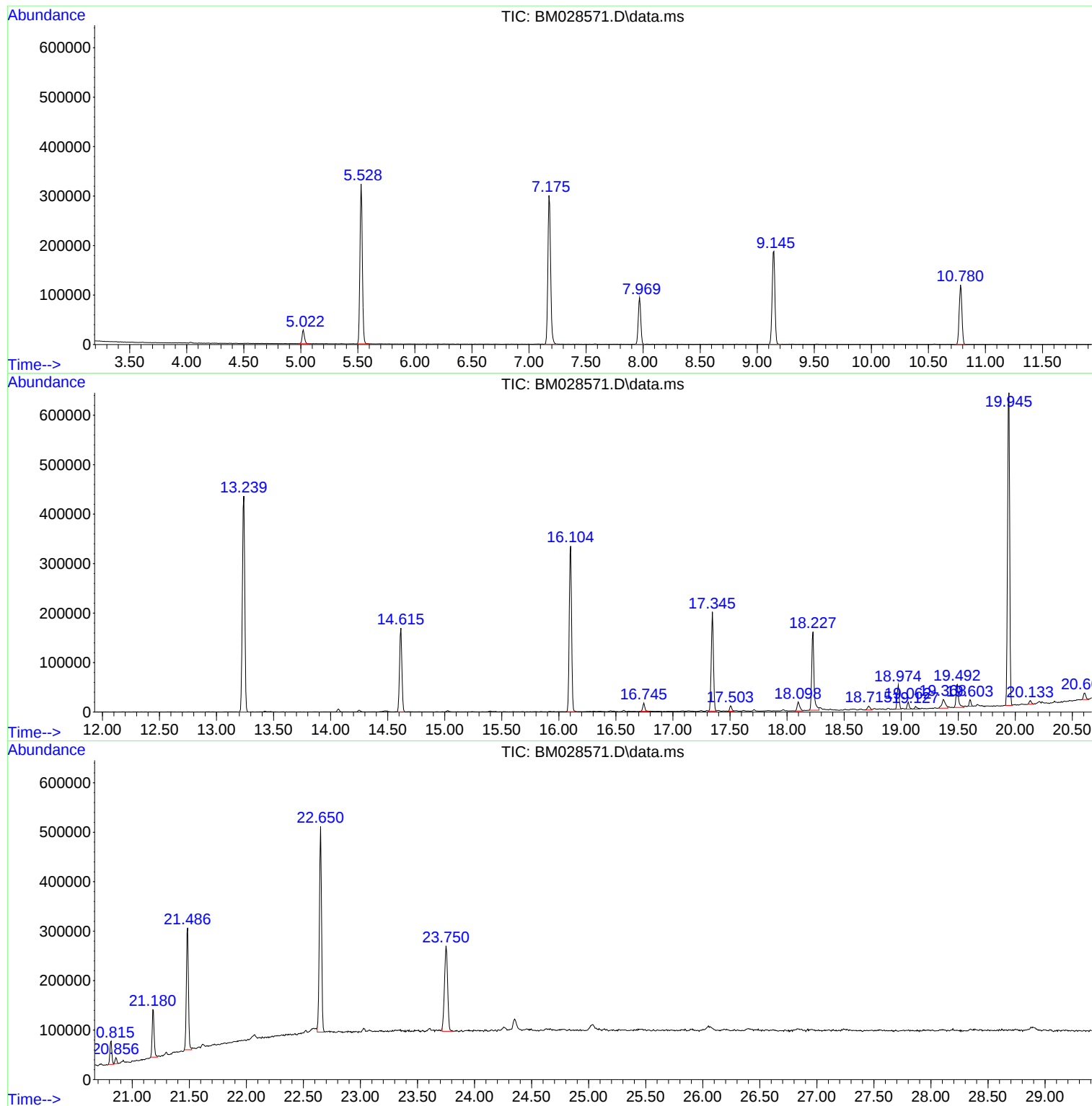
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Instrument :
BNA_M
ClientSampleId :
PS1419LN

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



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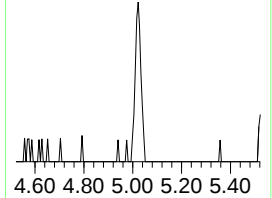
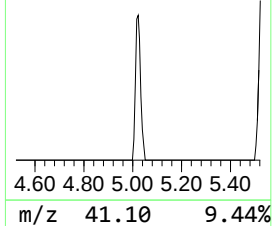
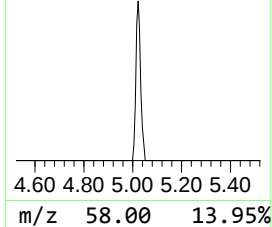
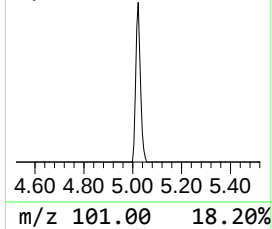
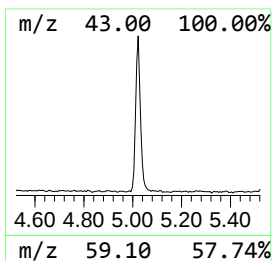
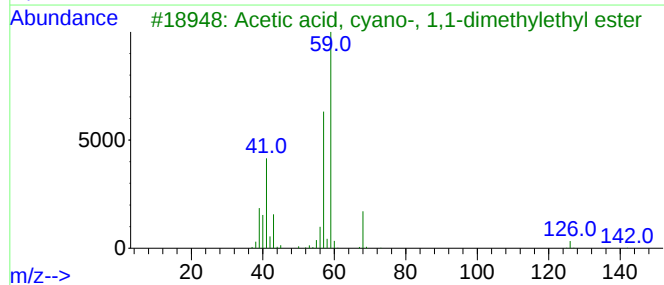
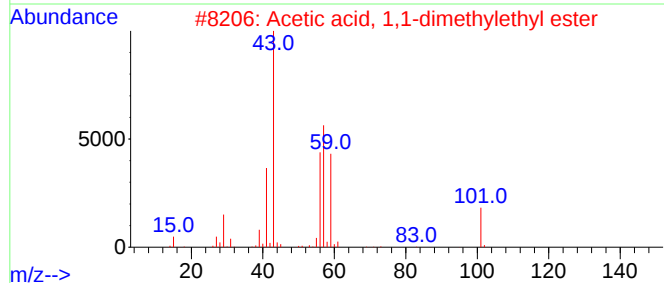
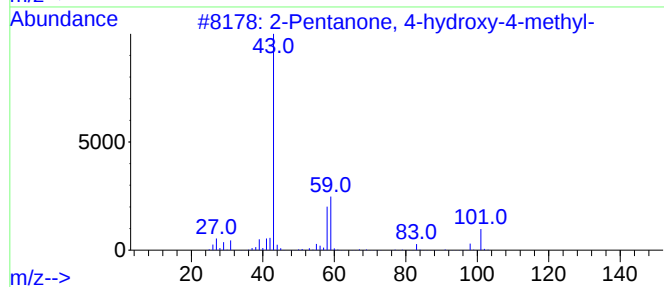
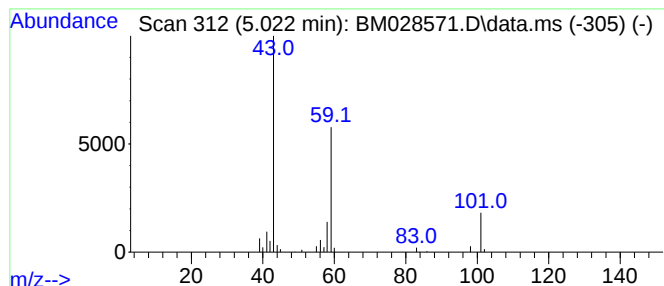
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	5.43 ng	39311	1,4-Dichlorobenzene-d4	7.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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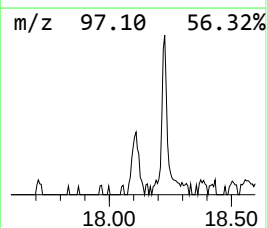
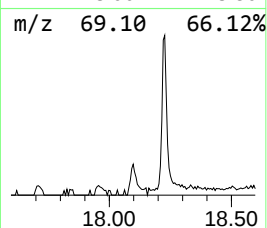
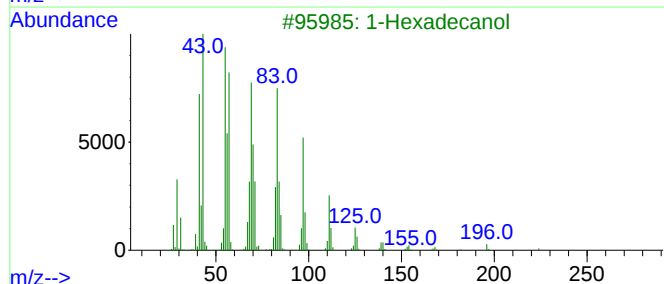
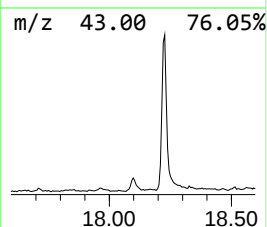
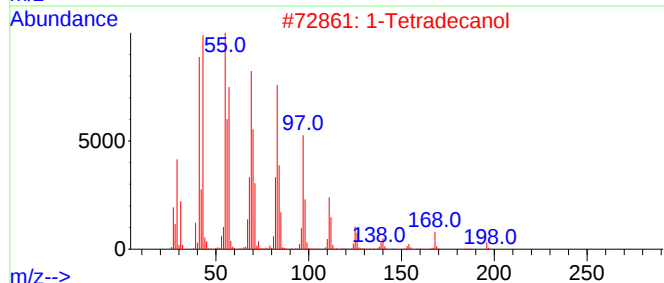
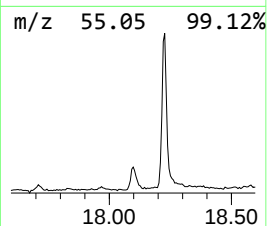
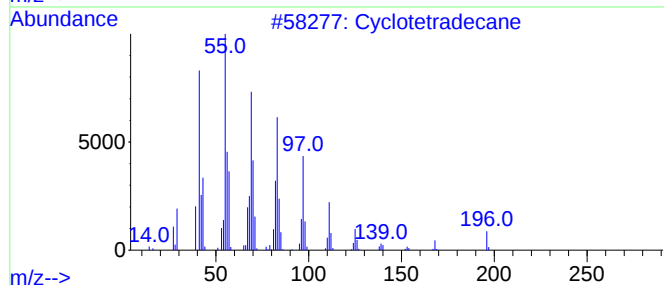
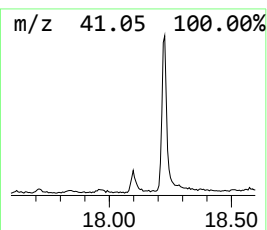
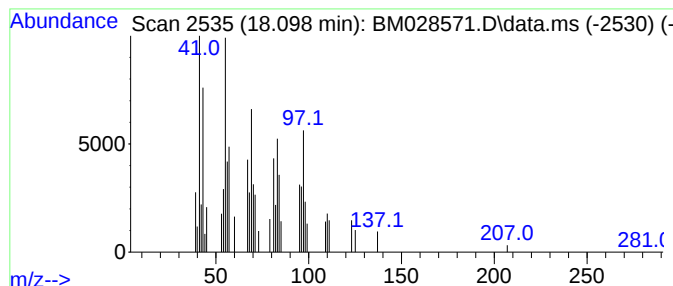
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Peak Number 2 unknown18.09 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.098	2.19 ng	29209	Phenanthrene-d10	17.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetradecane	196	C14H28	000295-17-0	46
2			1-Tetradecanol	214	C14H30O	000112-72-1	46
3			1-Hexadecanol	242	C16H34O	036653-82-4	43
4			2H-Cyclopentacycloocten-2-one, d...	180	C12H20O	055103-65-6	43
5			5-Octadecene, (E)-	252	C18H36	007206-21-5	43



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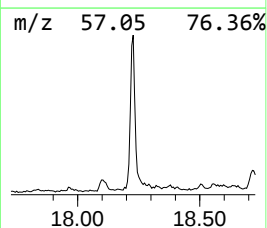
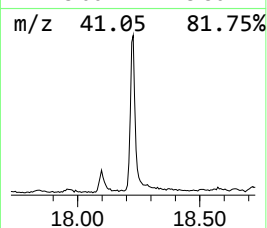
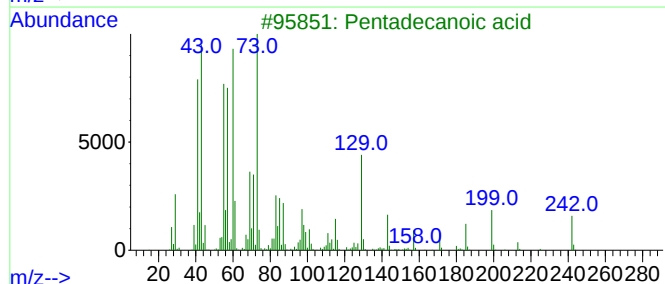
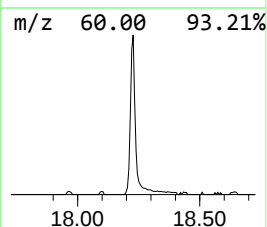
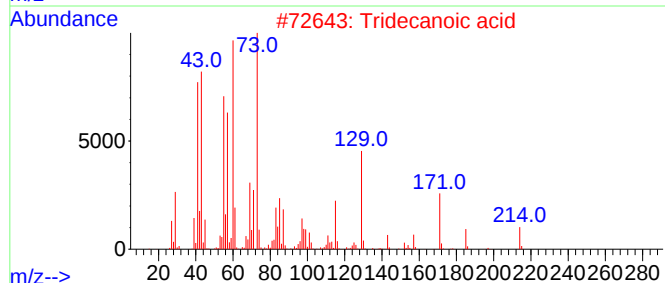
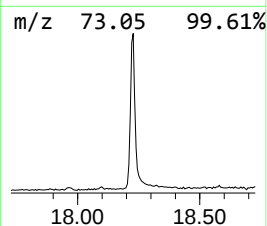
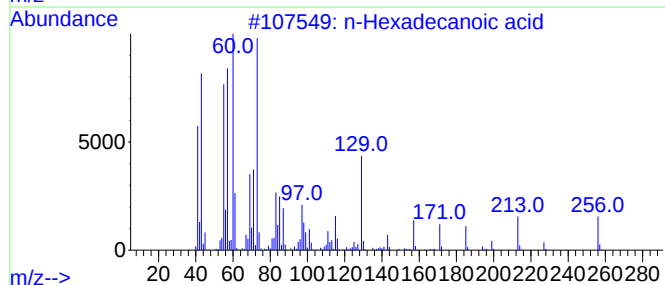
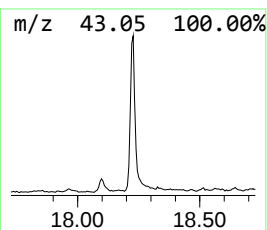
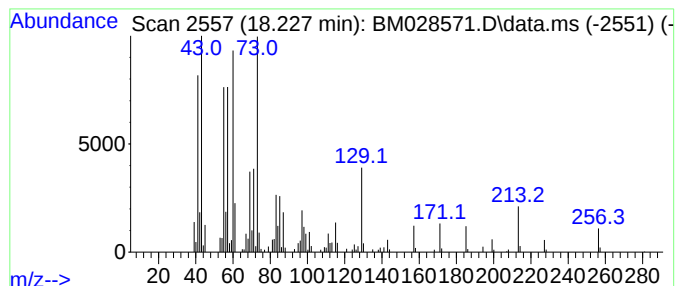
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.227	16.26 ng	216643	Phenanthrene-d10	17.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			n-Decanoic acid	172	C10H20O2	000334-48-5	86
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	83



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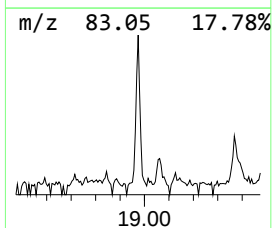
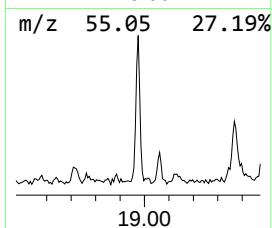
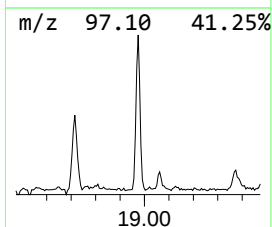
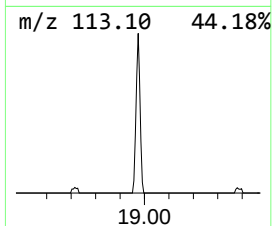
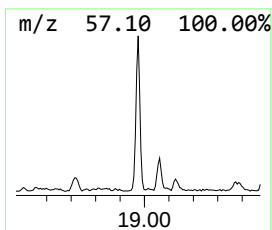
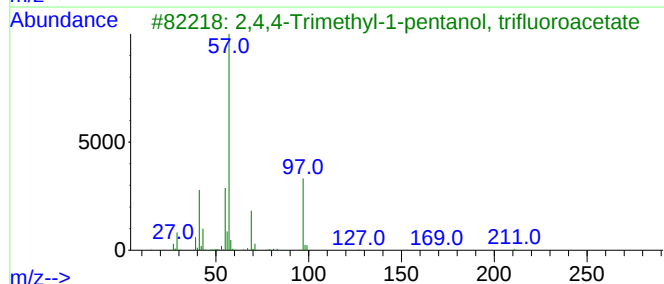
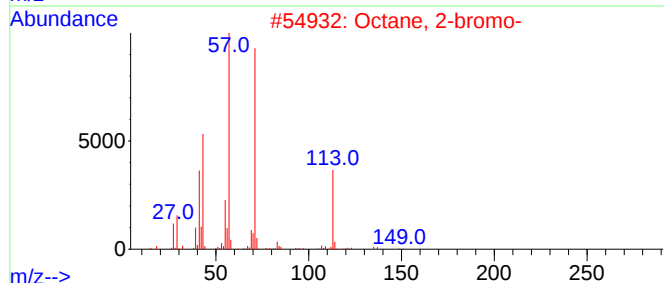
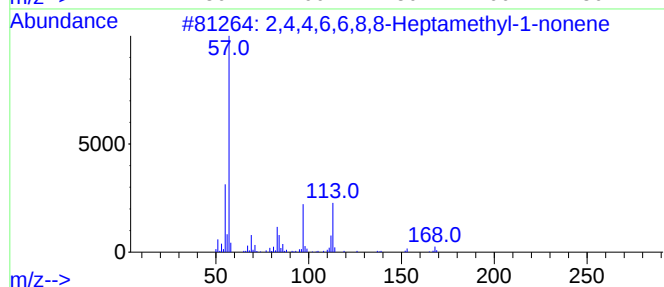
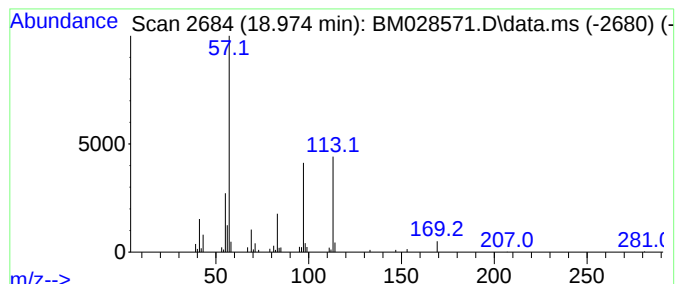
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Peak Number 4 unknown18.97 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.974	4.34 ng	57801	Phenanthrene-d10	17.345

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	Octane, 2-bromo-	192	C8H17Br	000557-35-7	38	
3	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	38	
4	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	37	
5	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	35	



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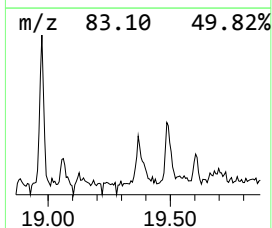
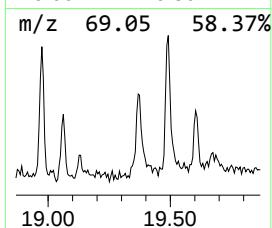
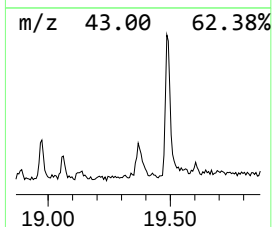
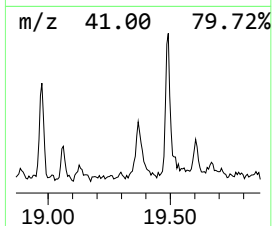
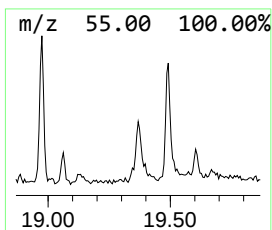
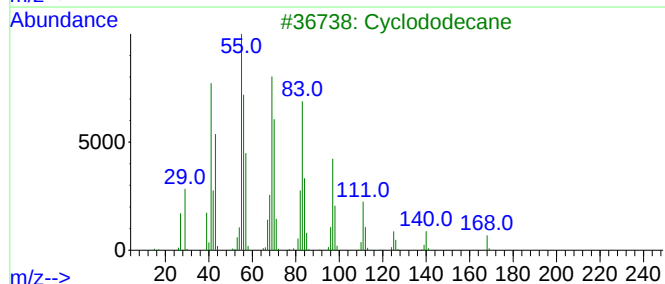
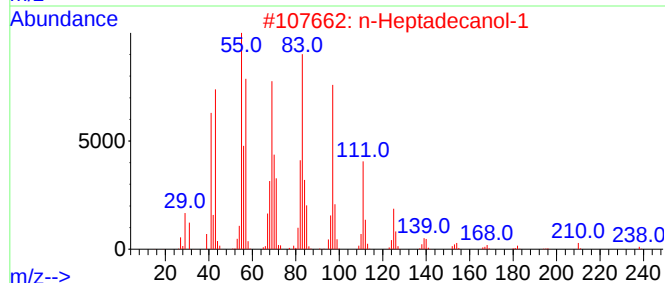
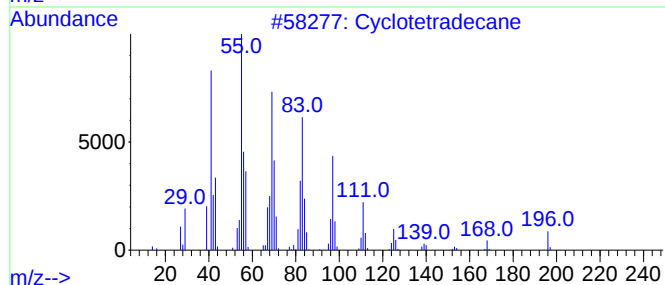
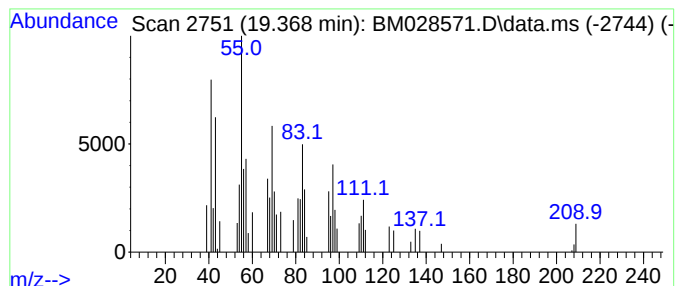
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Peak Number 5 Cyclotetradecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.368	2.79 ng	37171	Phenanthrene-d10	17.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetradecane	196	C14H28	000295-17-0	58
2			n-Heptadecanol-1	256	C17H36O	001454-85-9	53
3			Cyclododecane	168	C12H24	000294-62-2	49
4			Cycloheptane, methyl-	112	C8H16	004126-78-7	46
5			1-Tetradecanol	214	C14H30O	000112-72-1	43



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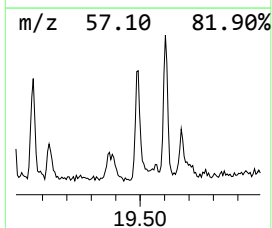
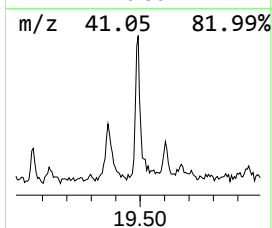
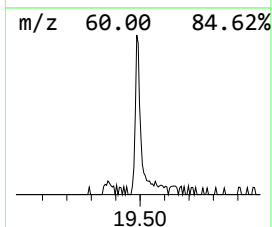
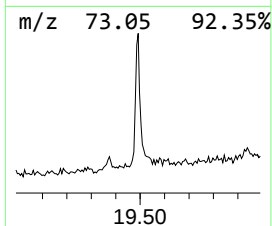
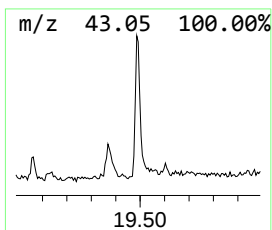
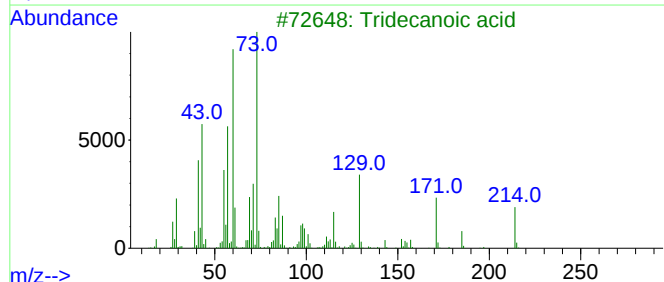
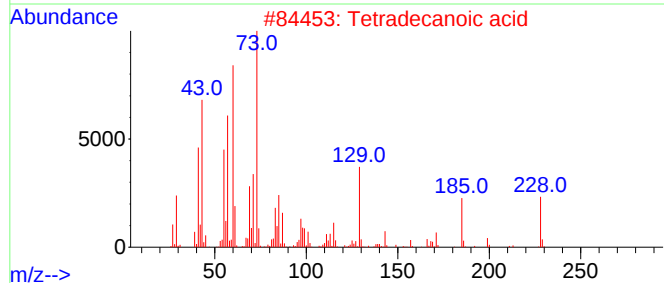
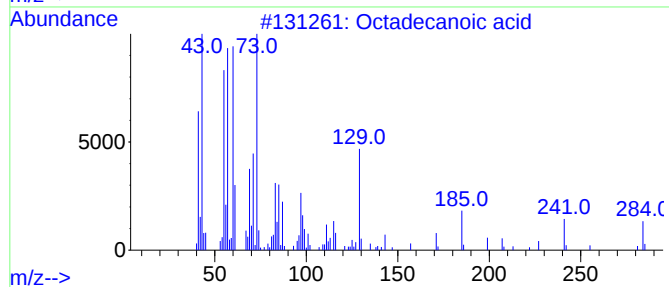
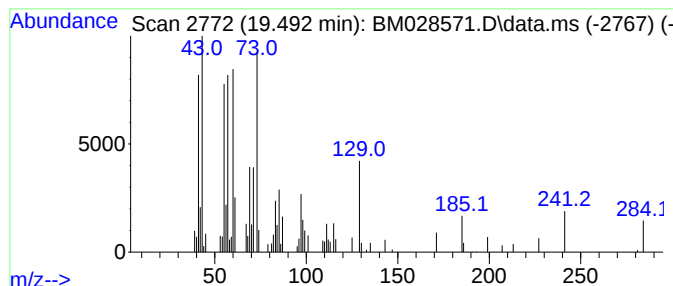
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.492	4.45 ng	70276	Chrysene-d12	21.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	97
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3			Tridecanoic acid	214	C13H26O2	000638-53-9	80
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012721\
Data File : BM028571.D
Acq On : 27 Jan 2021 16:07
Operator : CG/JU
Sample : M1236-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PS1419LN

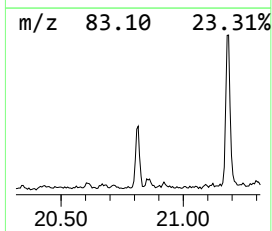
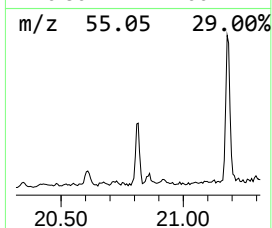
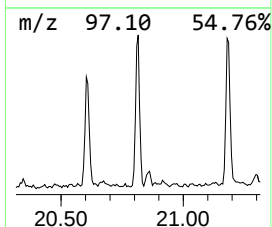
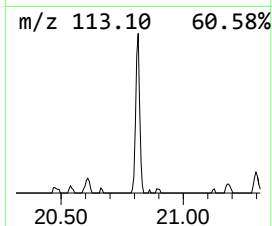
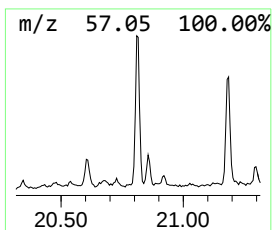
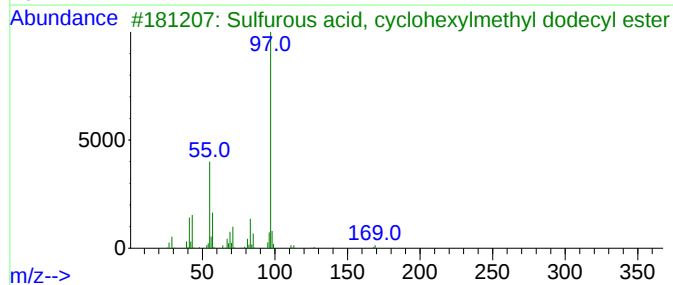
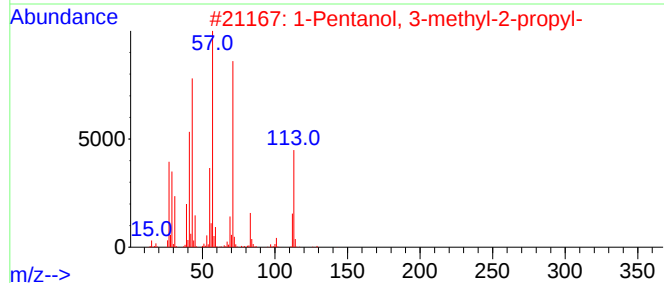
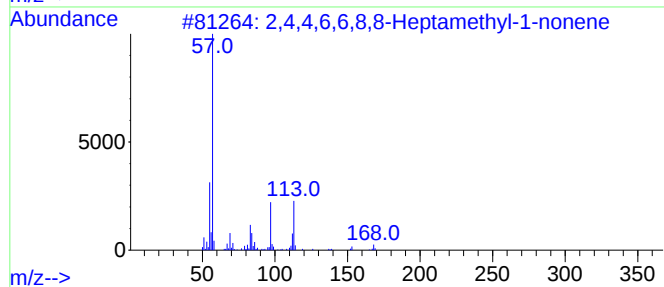
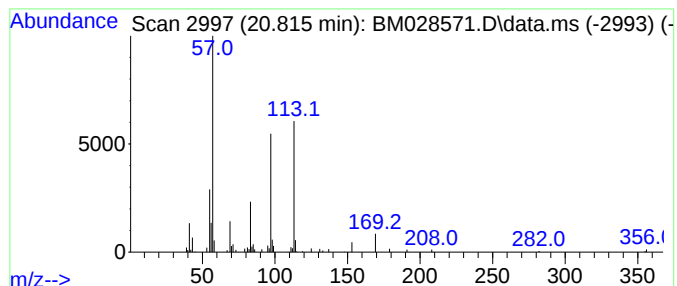
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.815	3.50 ng	55222	Chrysene-d12	21.486

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	64		
2	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	37		
3	Sulfurous acid, cyclohexylmethyl...	346	C19H38O3S	1000309-22-0	27		
4	Octane, 2-bromo-	192	C8H17Br	000557-35-7	25		
5	Pyrazole, 3-nitro-	113	C3H3N3O2	026621-44-3	25		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012721\
Data File : BM028571.D
Acq On : 27 Jan 2021 16:07
Operator : CG/JU
Sample : M1236-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PS1419LN

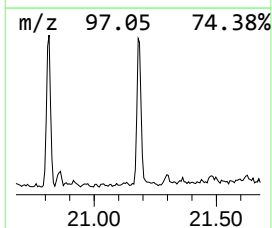
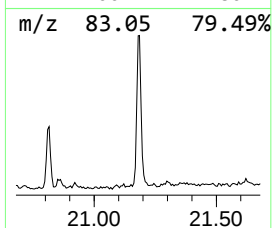
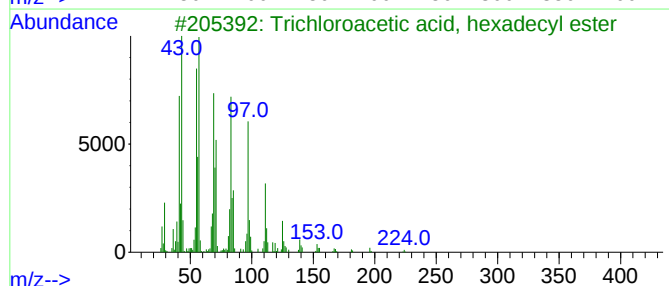
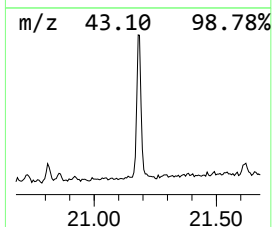
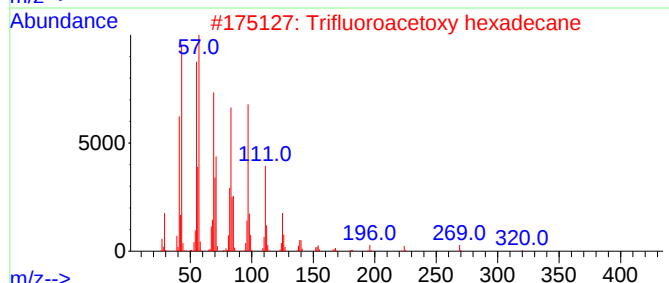
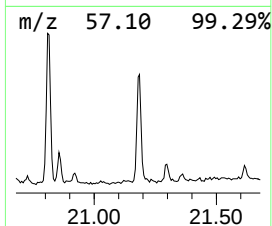
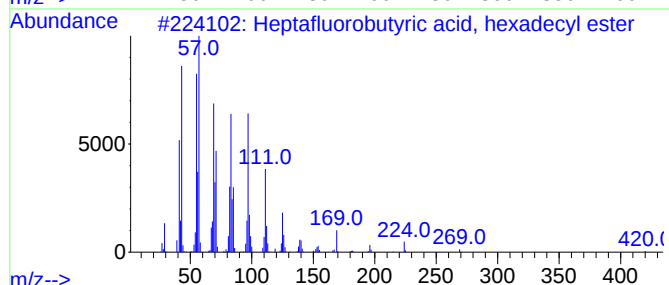
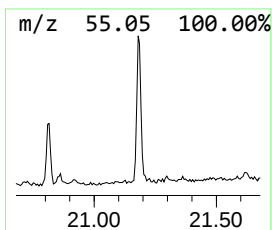
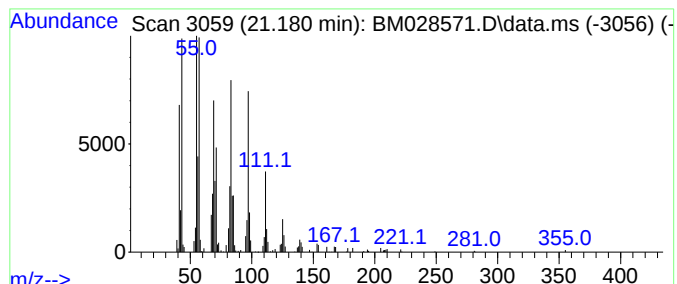
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptafluorobutyric acid, he... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.180	7.40 ng	116841	Chrysene-d12	21.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	95
2			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
4			1-Docosene	308	C22H44	001599-67-3	94
5			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012721\
Data File : BM028571.D
Acq On : 27 Jan 2021 16:07
Operator : CG/JU
Sample : M1236-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PS1419LN

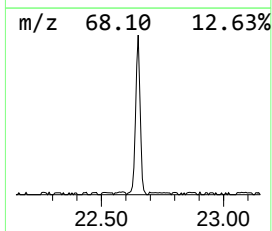
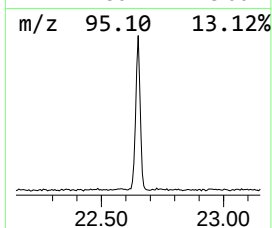
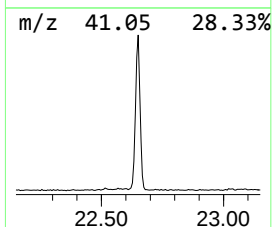
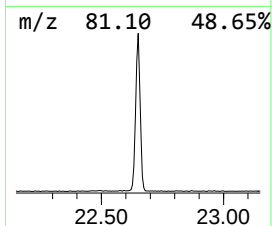
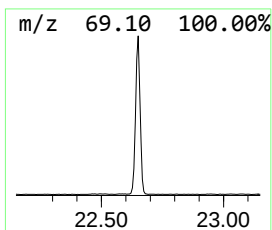
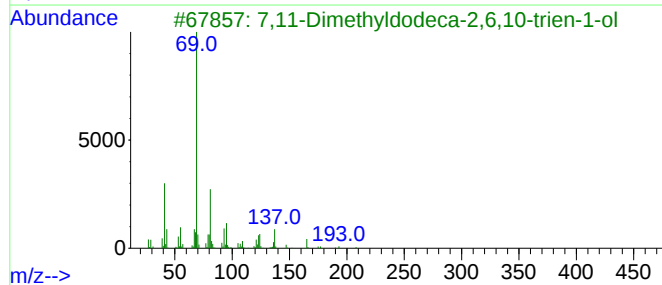
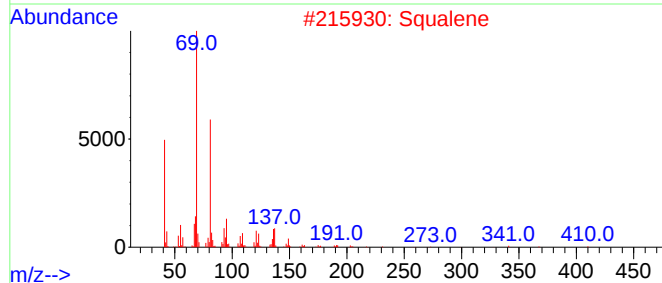
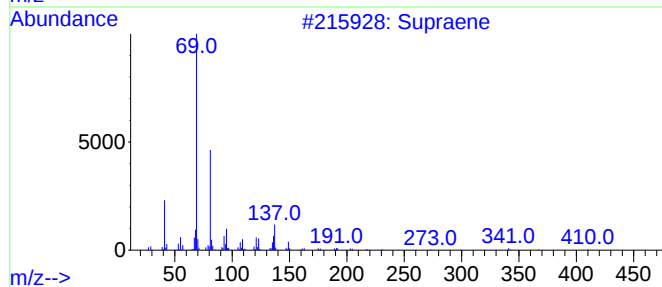
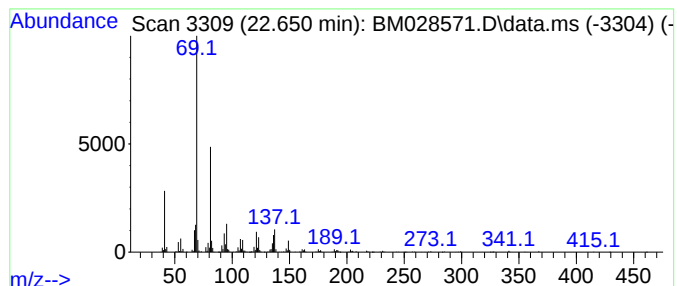
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Supraene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.650	32.66 ng	542016	Perylene-d12	23.750

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			Squalene	410	C30H50	000111-02-4	91
3			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4			(.+/-)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	72
5			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012721\
Data File : BM028571.D
Acq On : 27 Jan 2021 16:07
Operator : CG/JU
Sample : M1236-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.022	5.4	ng	39311	1	7.969	144855	20.0
unknown18.09	18.098	2.2	ng	29209	4	17.345	266501	20.0
n-Hexadecanoic ...	18.227	16.3	ng	216643	4	17.345	266501	20.0
unknown18.97	18.974	4.3	ng	57801	4	17.345	266501	20.0
Cyclotetradecane	19.368	2.8	ng	37171	4	17.345	266501	20.0
Octadecanoic acid	19.492	4.5	ng	70276	5	21.486	315919	20.0
2,4,4,6,6,8,8-H...	20.815	3.5	ng	55222	5	21.486	315919	20.0
Heptafluorobuty...	21.180	7.4	ng	116841	5	21.486	315919	20.0
Supraene	22.650	32.7	ng	542016	6	23.750	331921	20.0