

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042321\
 Data File : BM029620.D
 Acq On : 23 Apr 2021 19:31
 Operator : CG/JU
 Sample : M2089-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 FK-GF-02-072-A

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-BM042121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029620.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.228	391	398	419	rBV	1098202	1557138	35.32%	5.526%
2	6.811	659	667	682	rBV	1024050	1650333	37.44%	5.856%
3	7.628	800	806	816	rBV	287877	453285	10.28%	1.609%
4	8.781	994	1002	1013	rBV	604694	1032757	23.43%	3.665%
5	10.404	1271	1278	1284	rBV	341300	595806	13.52%	2.114%
6	10.457	1284	1287	1293	rVB	29959	49023	1.11%	0.174%
7	12.893	1693	1701	1714	rBV	1698782	2486519	56.41%	8.824%
8	13.181	1743	1750	1757	rBV	82123	136722	3.10%	0.485%
9	13.734	1839	1844	1854	rVB	33253	56263	1.28%	0.200%
10	14.275	1929	1936	1942	rBV	583306	850508	19.29%	3.018%
11	14.334	1942	1946	1956	rVB	61313	95960	2.18%	0.341%
12	14.675	1999	2004	2013	rBV	34745	58711	1.33%	0.208%
13	15.322	2109	2114	2119	rBV	51930	73395	1.66%	0.260%
14	15.410	2125	2129	2139	rBV	62454	105078	2.38%	0.373%
15	15.763	2183	2189	2199	rBV	1490035	2133755	48.41%	7.572%
16	16.839	2368	2372	2378	rVB2	28301	45446	1.03%	0.161%
17	17.016	2396	2402	2406	rBV	704708	1028377	23.33%	3.649%
18	17.057	2406	2409	2415	rVB	439087	595155	13.50%	2.112%
19	17.145	2420	2424	2431	rVB	103575	164117	3.72%	0.582%
20	17.422	2464	2471	2481	rBV	48636	91114	2.07%	0.323%
21	17.892	2547	2551	2553	rBV	40672	63205	1.43%	0.224%
22	17.927	2553	2557	2566	rVV2	450359	681203	15.45%	2.417%
23	18.086	2579	2584	2588	rBV2	65278	111297	2.52%	0.395%
24	19.016	2739	2742	2746	rVB2	35854	44506	1.01%	0.158%
25	19.074	2747	2752	2757	rBV	574252	837016	18.99%	2.970%
26	19.222	2771	2777	2791	rBV	1455561	2362149	53.59%	8.382%
27	19.439	2806	2814	2824	rVB	514301	857785	19.46%	3.044%
28	19.651	2845	2850	2862	rVB	3674186	4408126	100.00%	15.643%
29	19.939	2896	2899	2902	rVB	70000	78551	1.78%	0.279%
30	19.974	2903	2905	2909	rVB2	56146	56035	1.27%	0.199%
31	20.039	2913	2916	2920	rVB2	59589	65757	1.49%	0.233%
32	20.927	3063	3067	3074	rBV3	484963	681451	15.46%	2.418%
33	21.198	3107	3113	3117	rBV2	1097808	1683760	38.20%	5.975%
34	21.233	3117	3119	3126	rVB	233553	305483	6.93%	1.084%
35	21.792	3211	3214	3222	rBV2	99121	180704	4.10%	0.641%
36	22.368	3308	3312	3318	rVB	200083	282715	6.41%	1.003%

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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

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	22.739	3370	3375	3379	rBV	300666	534237	12.12%	1.896%
38	23.292	3465	3469	3476	rVB2	257367	466663	10.59%	1.656%
39	23.392	3480	3486	3491	rVV2	694940	1220093	27.68%	4.330%

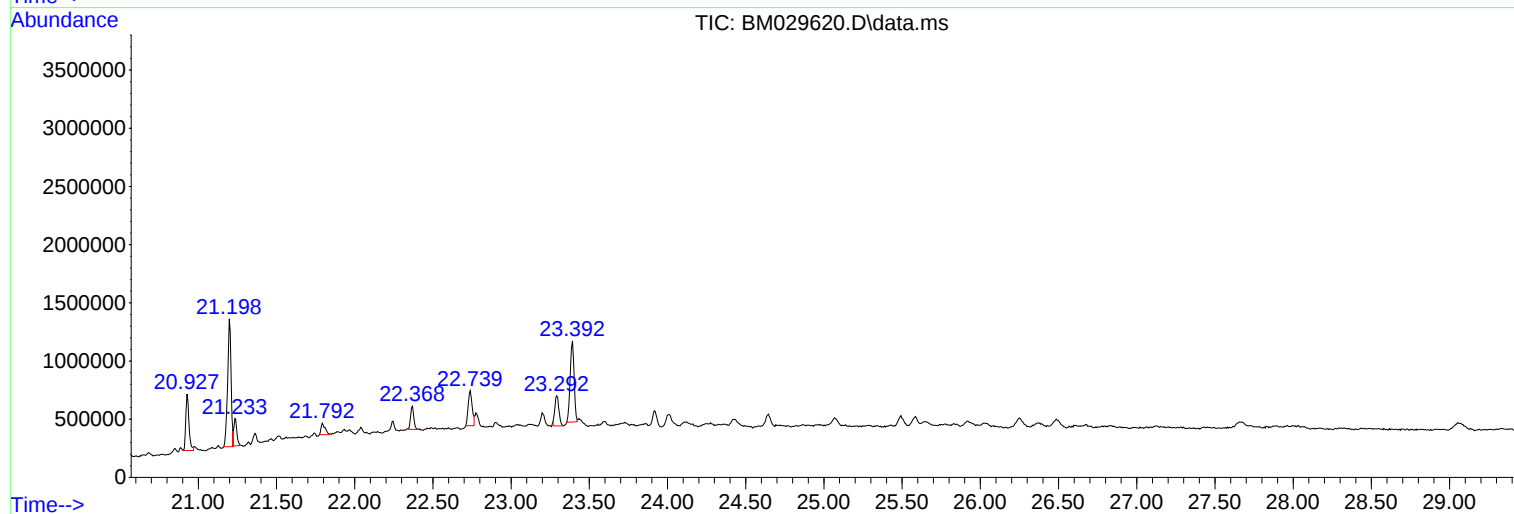
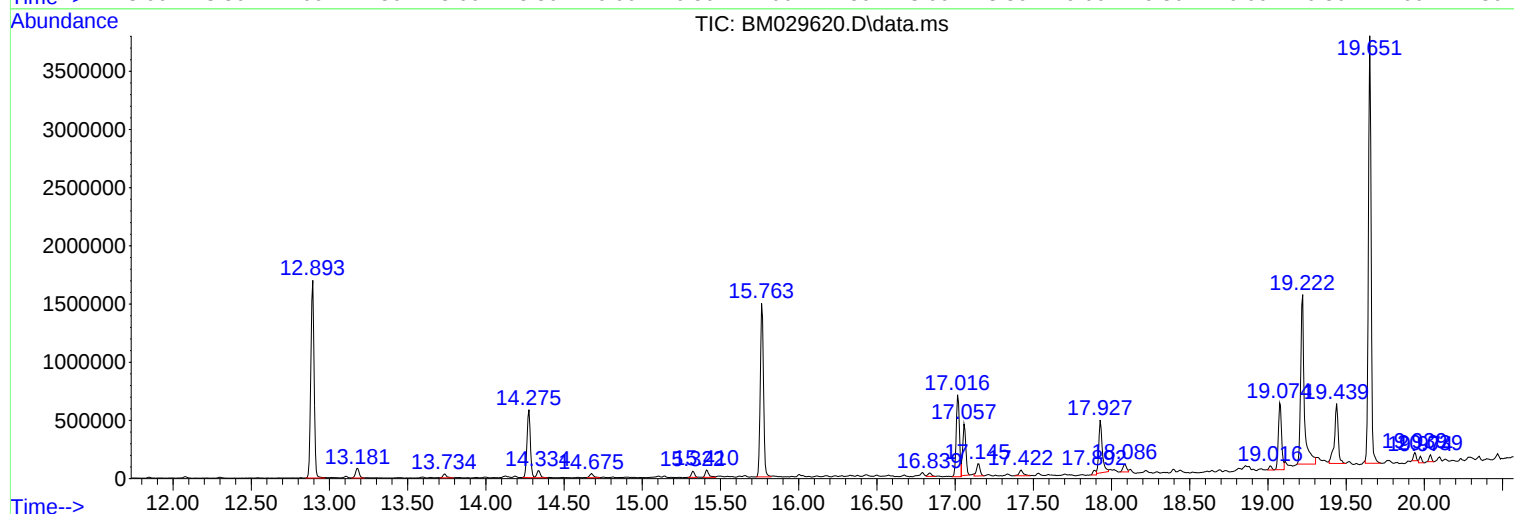
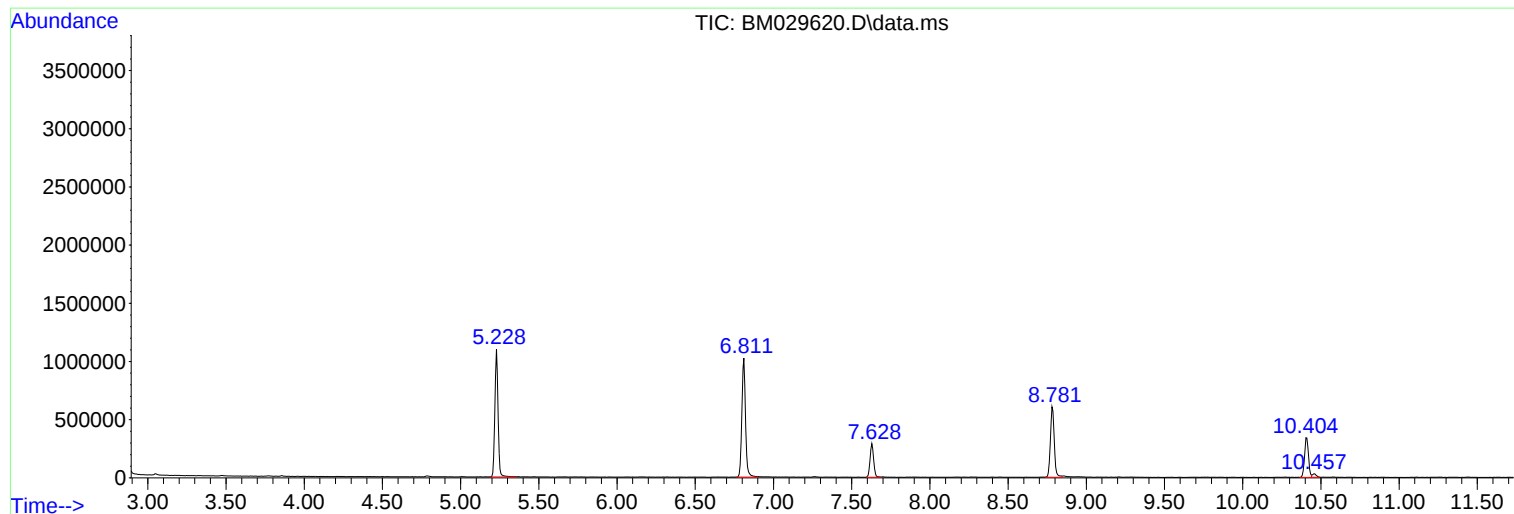
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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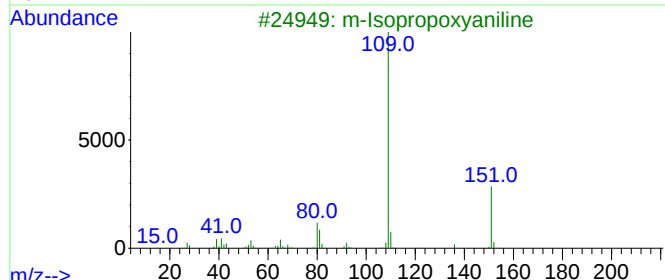
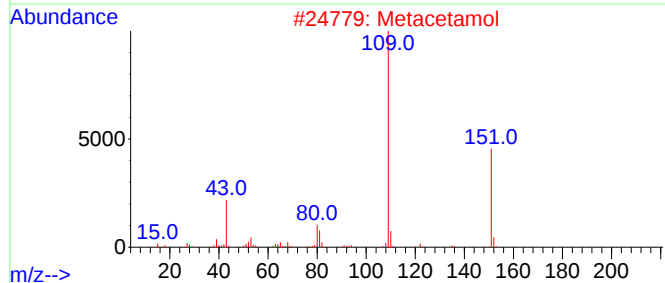
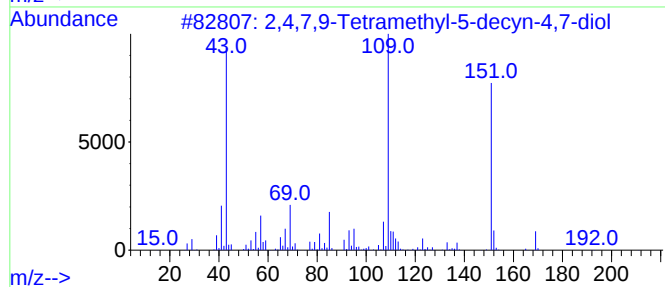
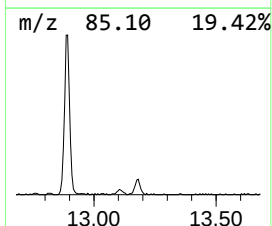
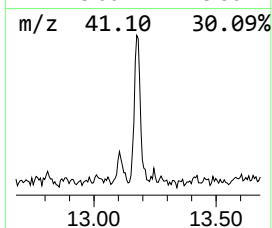
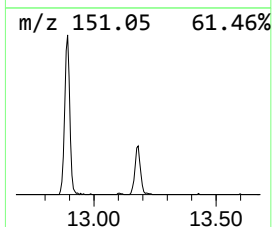
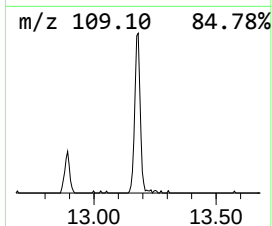
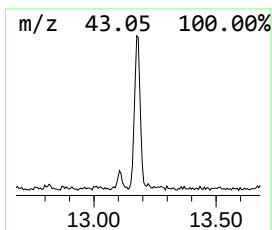
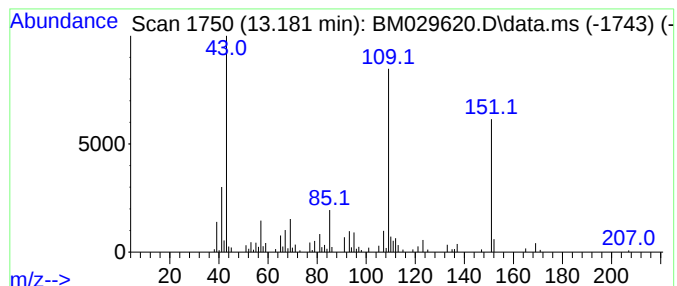
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.181	3.22 ng	136722	Acenaphthene-d10	14.275

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	90	
2	Metacetamol	151	C8H9NO2	000621-42-1	52	
3	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	52	
4	Butanamide, N-acetyl-N-(4-hydrox...	221	C12H15NO3	1000107-08-7	50	
5	p-Isopropoxyaniline	151	C9H13NO	007664-66-6	50	



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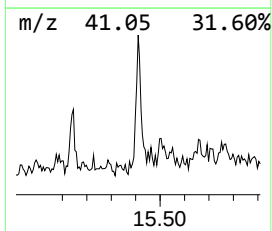
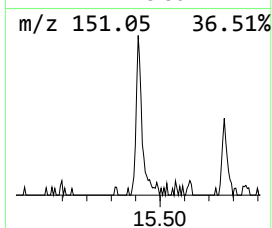
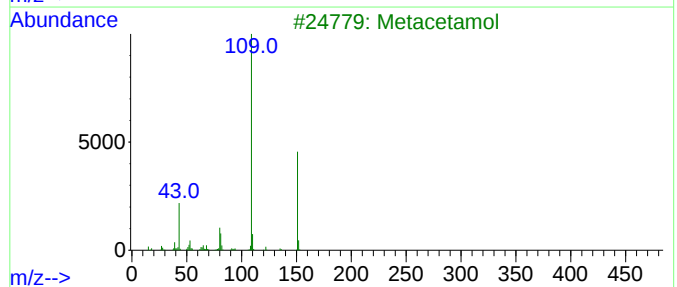
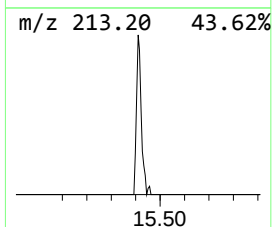
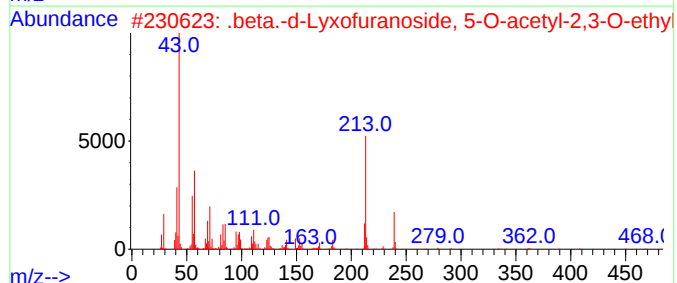
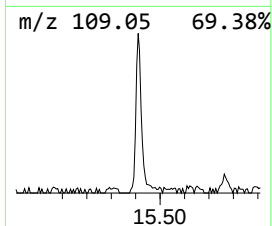
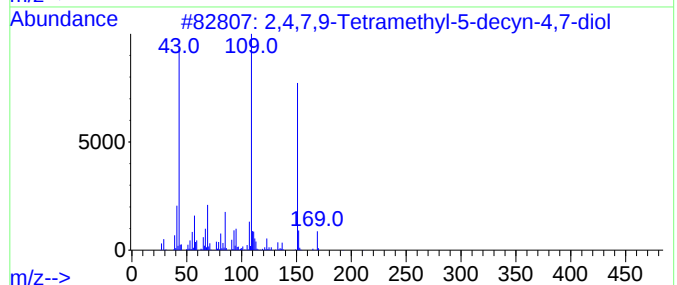
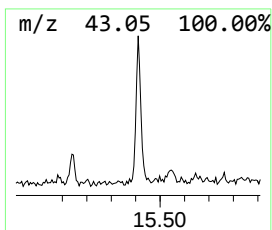
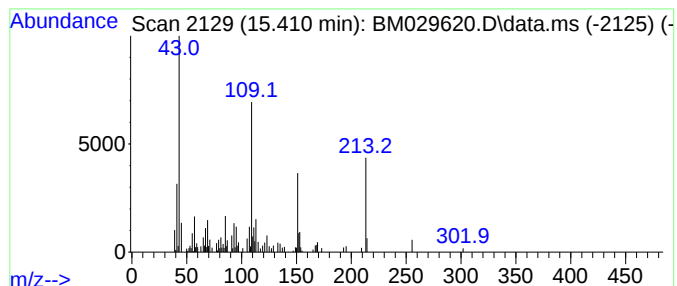
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown15.410 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.410	2.47 ng	105078	Acenaphthene-d10	14.275

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	43		
2	.beta.-d-Lyxofuranoside, 5-O-ace...	468	C25H45BO7	1000152-90-9	35		
3	Metacetamol	151	C8H9NO2	000621-42-1	25		
4	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	25		
5	E-8-Methyl-9-tetradecen-1-ol ace...	268	C17H32O2	1000130-81-4	22		



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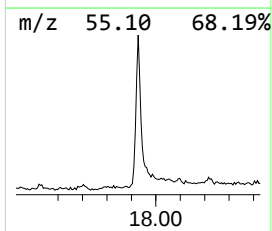
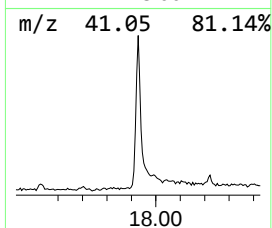
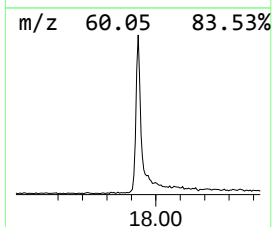
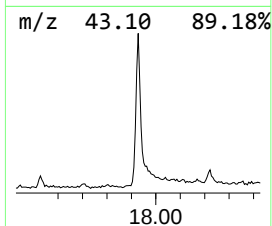
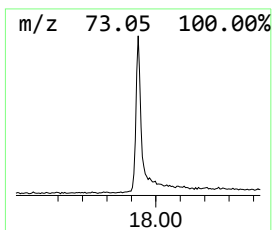
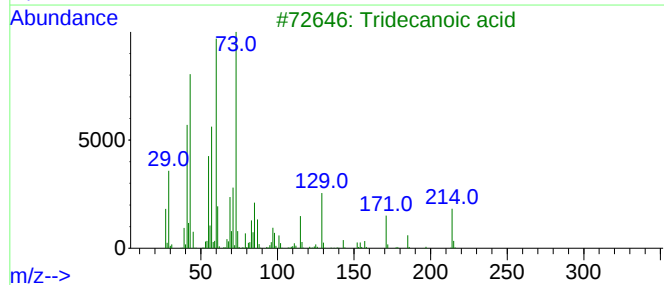
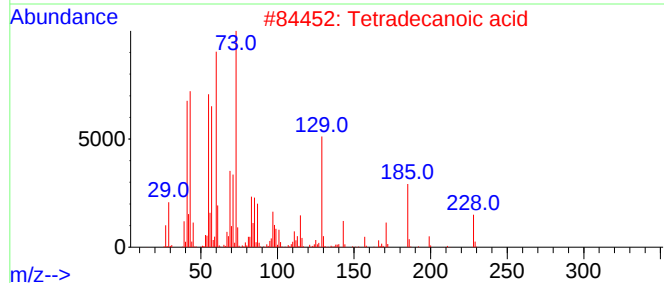
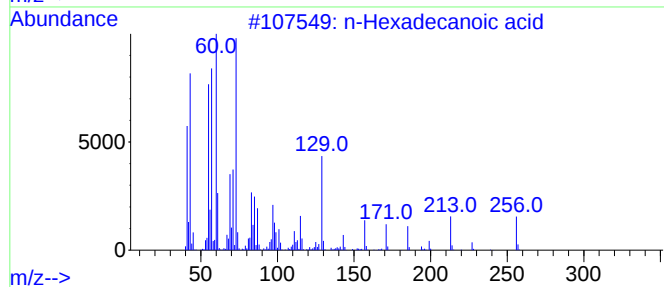
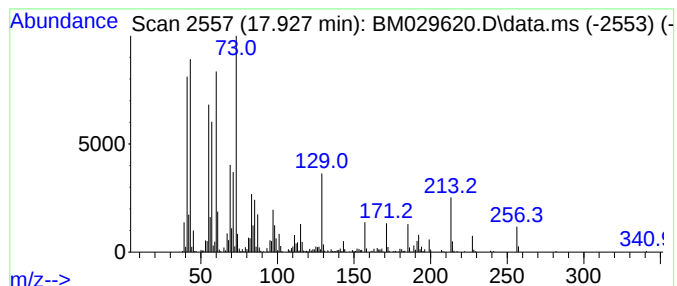
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.927	13.25 ng	681203	Phenanthrene-d10	17.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	89
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5			Octadecanoic acid	284	C18H36O2	000057-11-4	76



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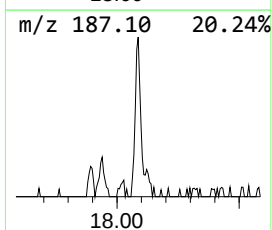
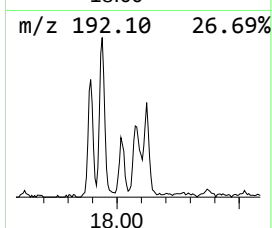
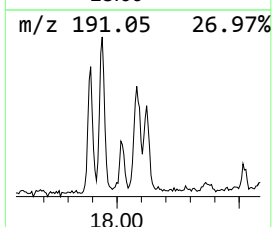
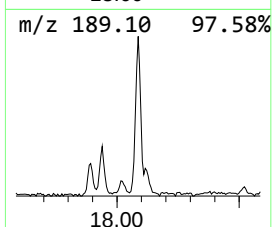
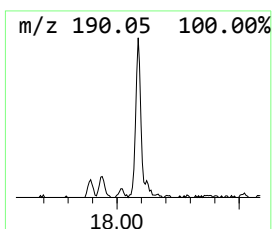
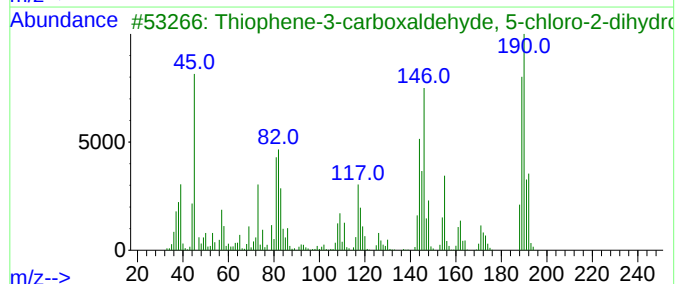
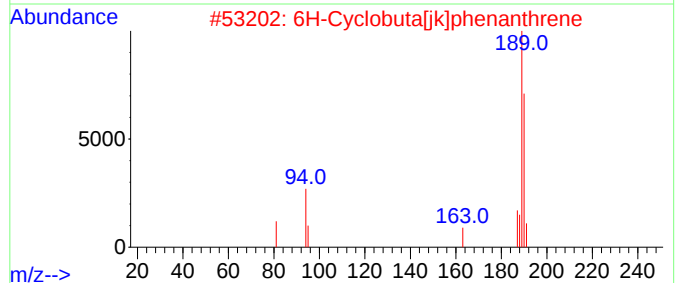
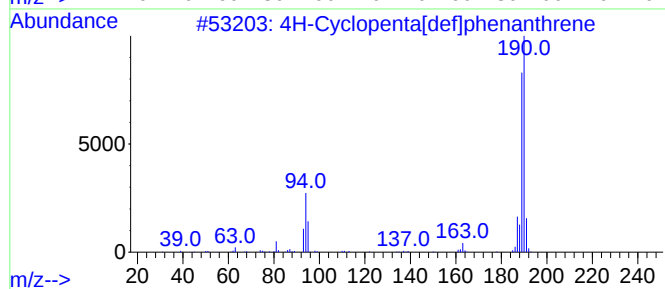
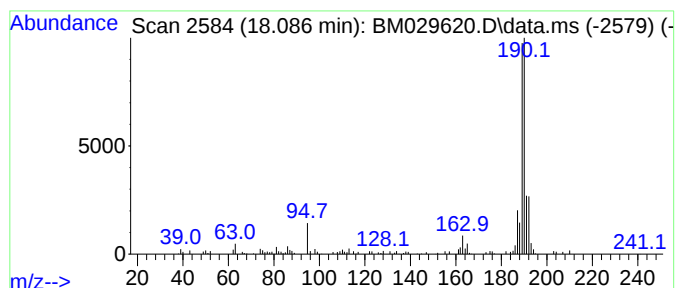
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.086	2.16 ng	111297	Phenanthrene-d10	17.016	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
3	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	50
4	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	36
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	36



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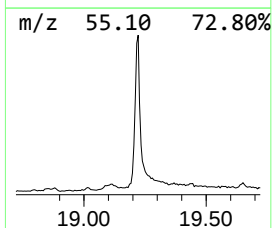
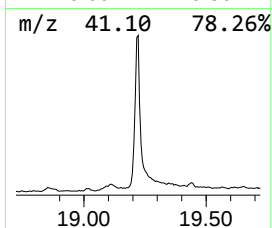
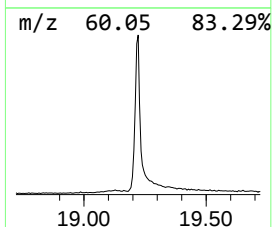
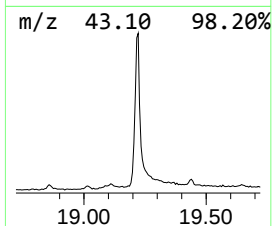
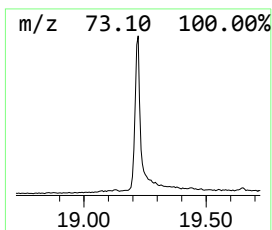
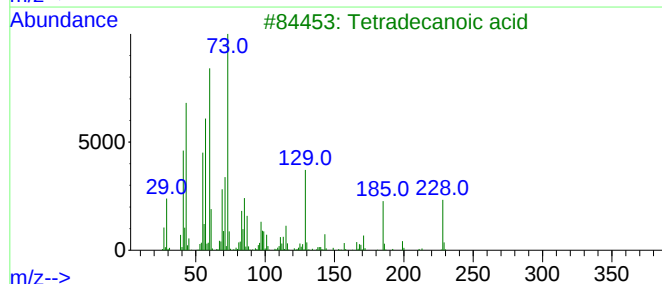
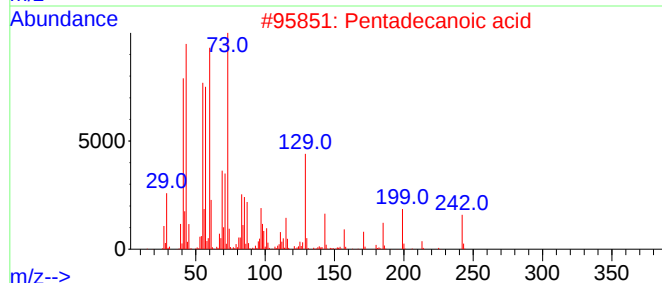
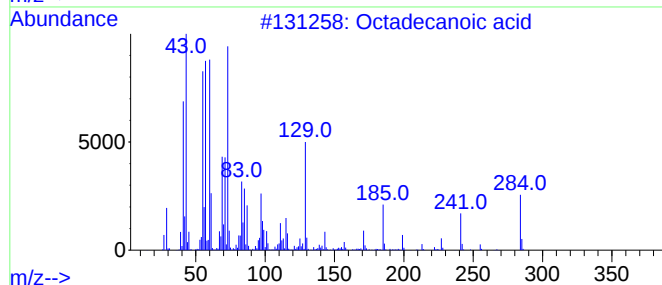
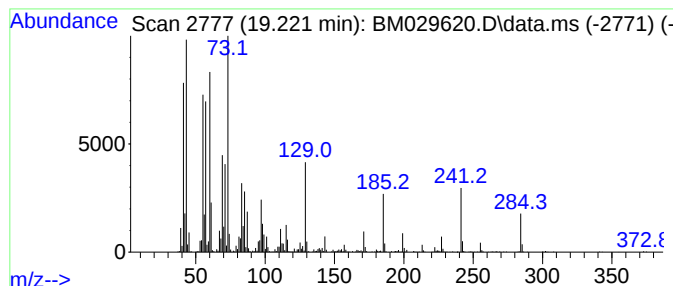
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.221	28.06 ng	2362150	Chrysene-d12	21.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
5			Tridecanoic acid	214	C13H26O2	000638-53-9	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042321\
Data File : BM029620.D
Acq On : 23 Apr 2021 19:31
Operator : CG/JU
Sample : M2089-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FK-GF-02-072-A

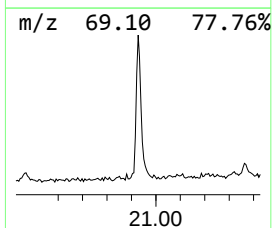
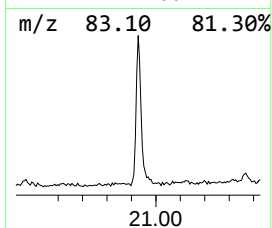
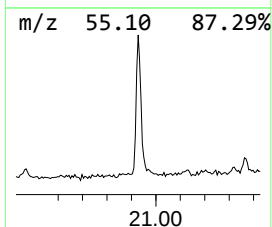
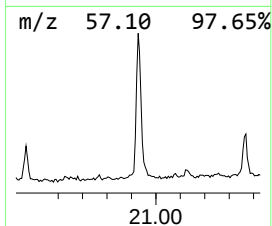
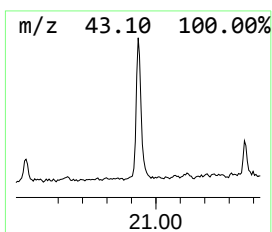
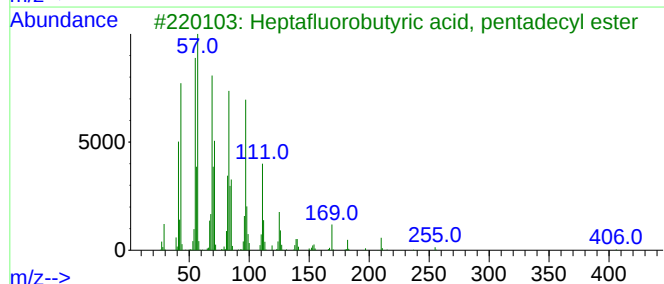
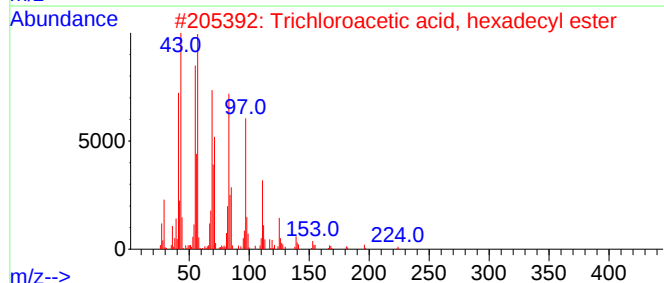
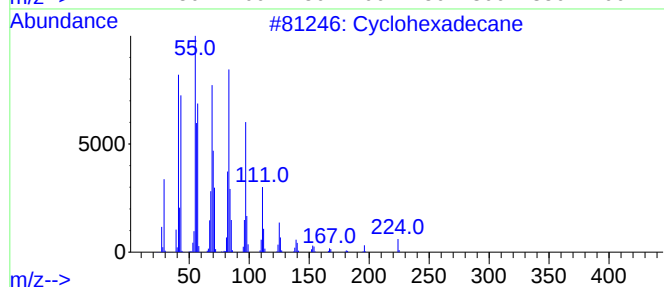
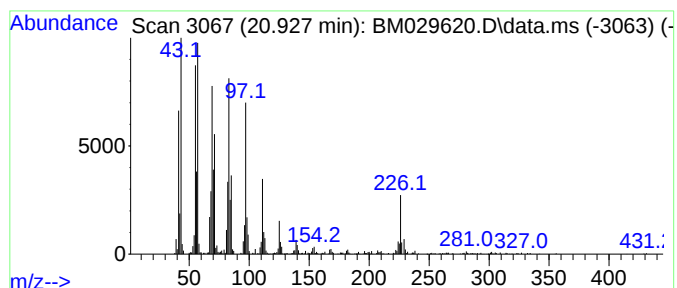
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclohexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.927	8.09 ng	681451	Chrysene-d12	21.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	95
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5			E-14-Hexadecenal	238	C16H30O	330207-53-9	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042321\
Data File : BM029620.D
Acq On : 23 Apr 2021 19:31
Operator : CG/JU
Sample : M2089-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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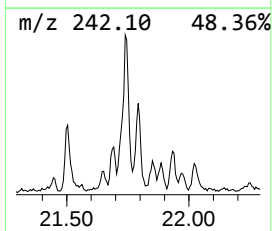
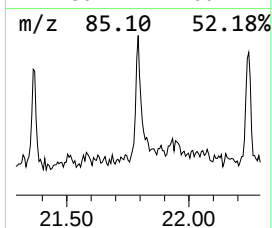
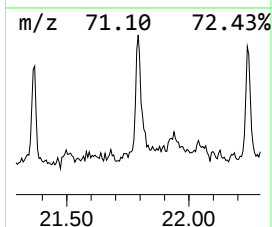
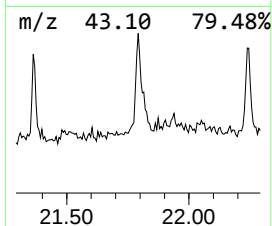
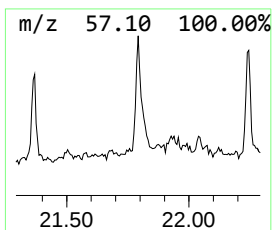
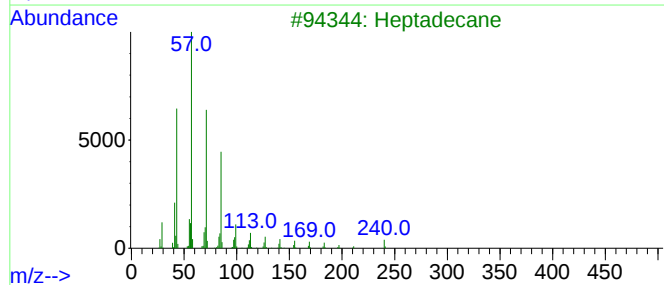
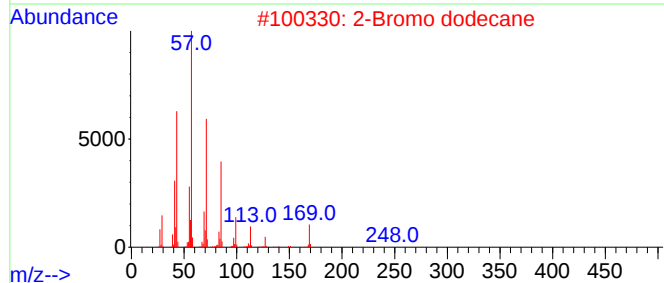
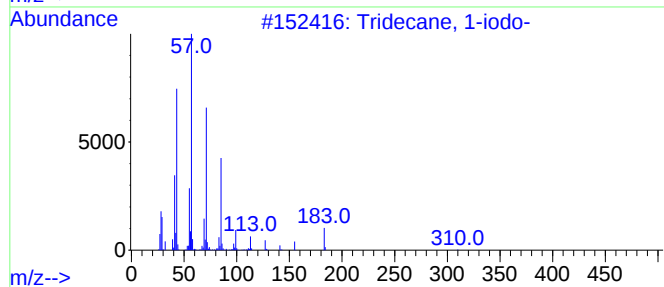
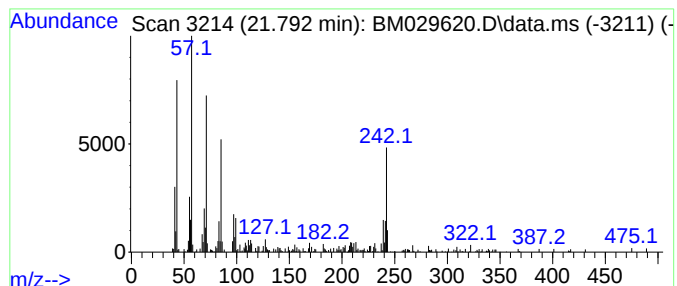
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tridecane, 1-iodo- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.792	2.15 ng	180704	Chrysene-d12	21.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	90
2			2-Bromo dodecane	248	C12H25Br	013187-99-0	89
3			Heptadecane	240	C17H36	000629-78-7	64
4			Hexadecane	226	C16H34	000544-76-3	50
5			Octacosane	394	C28H58	000630-02-4	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042321\
Data File : BM029620.D
Acq On : 23 Apr 2021 19:31
Operator : CG/JU
Sample : M2089-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FK-GF-02-072-A

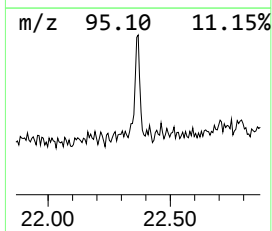
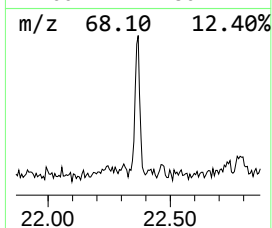
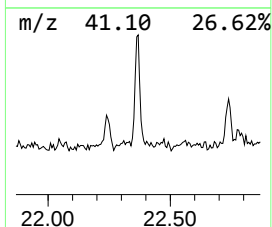
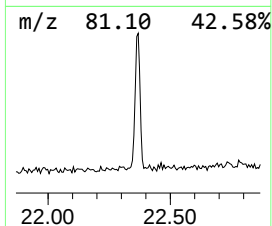
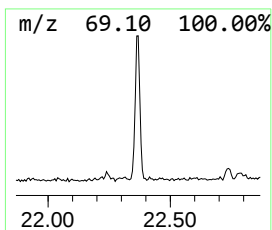
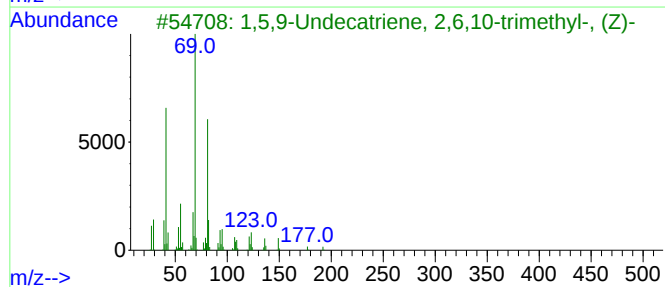
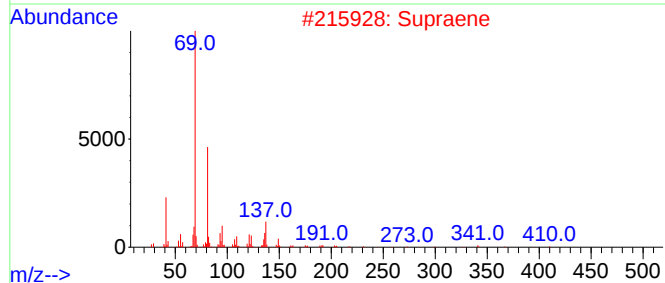
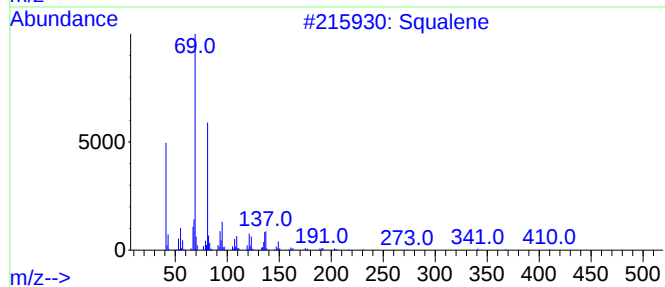
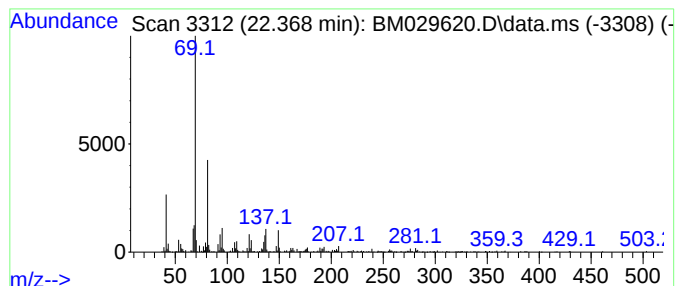
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.368	4.63 ng	282715	Perylene-d12	23.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	74
2			Supraene	410	C30H50	007683-64-9	74
3			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	72
4			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
5			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042321\
Data File : BM029620.D
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Operator : CG/JU
Sample : M2089-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042121.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
2,4,7,9-Tetrame...	13.181	3.2	ng	136722	3	14.275	850508	20.0
unknown15.410	15.410	2.5	ng	105078	3	14.275	850508	20.0
n-Hexadecanoic ...	17.927	13.3	ng	681203	4	17.016	1028380	20.0
4H-Cyclopenta[d...	18.086	2.2	ng	111297	4	17.016	1028380	20.0
Octadecanoic acid	19.221	28.1	ng	2362150	5	21.198	1683760	20.0
Cyclohexadecane	20.927	8.1	ng	681451	5	21.198	1683760	20.0
Tridecane, 1-iodo-	21.792	2.1	ng	180704	5	21.198	1683760	20.0
Squalene	22.368	4.6	ng	282715	6	23.392	1220090	20.0