

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM043021\
 Data File : BM029732.D
 Acq On : 30 Apr 2021 16:47
 Operator : CG/JU
 Sample : M2077-05
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SB-20-14.5-15.0-DUP

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-BM043021.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029732.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.193	386	392	402	rBV	728325	1021914	17.99%	3.873%
2	6.775	652	661	679	rBV	650498	1065615	18.76%	4.039%
3	7.593	792	800	809	rBV	223933	355748	6.26%	1.348%
4	7.957	856	862	869	rVB	90758	143888	2.53%	0.545%
5	8.745	989	996	1014	rVB	413962	705988	12.43%	2.676%
6	10.369	1265	1272	1276	rBV	271978	448677	7.90%	1.701%
7	10.416	1276	1280	1288	rVB	126452	215037	3.79%	0.815%
8	12.039	1549	1556	1563	rBV	149161	242709	4.27%	0.920%
9	12.263	1584	1594	1603	rVB	100892	171158	3.01%	0.649%
10	12.851	1687	1694	1710	rBV	1245858	1875958	33.02%	7.110%
11	13.145	1737	1744	1751	rBV	338610	532221	9.37%	2.017%
12	13.698	1834	1838	1848	rVV	64455	99691	1.75%	0.378%
13	14.239	1919	1930	1936	rBV2	495839	747238	13.15%	2.832%
14	14.298	1936	1940	1949	rVB	134250	207416	3.65%	0.786%
15	14.639	1992	1998	2007	rVB	112579	164551	2.90%	0.624%
16	14.798	2017	2025	2028	rBV2	25188	59694	1.05%	0.226%
17	15.286	2101	2108	2118	rBV	164697	248424	4.37%	0.942%
18	15.374	2118	2123	2132	rVV	264946	436422	7.68%	1.654%
19	15.733	2177	2184	2193	rBV	1186883	1723386	30.34%	6.532%
20	16.804	2360	2366	2374	rVB2	45118	84331	1.48%	0.320%
21	16.980	2390	2396	2400	rBV	595358	874885	15.40%	3.316%
22	17.021	2400	2403	2410	rVV	484331	709677	12.49%	2.690%
23	17.115	2411	2419	2425	rVB	71934	134520	2.37%	0.510%
24	17.304	2446	2451	2456	rBV3	53024	85594	1.51%	0.324%
25	17.892	2547	2551	2559	rVB2	149976	244183	4.30%	0.925%
26	18.051	2573	2578	2582	rBV2	74663	121410	2.14%	0.460%
27	19.045	2742	2747	2751	rBV	325264	443980	7.82%	1.683%
28	19.080	2751	2753	2755	rVV	80371	89626	1.58%	0.340%
29	19.104	2755	2757	2762	rVB	89381	100025	1.76%	0.379%
30	19.404	2800	2808	2813	rBV2	213001	367019	6.46%	1.391%
31	19.615	2839	2844	2857	rVB	2438457	2924068	51.47%	11.083%
32	19.909	2890	2894	2897	rBV	52843	65502	1.15%	0.248%
33	20.898	3058	3062	3067	rBV3	168626	236642	4.17%	0.897%
34	21.168	3102	3108	3112	rBV	887291	1197035	21.07%	4.537%
35	23.339	3471	3477	3489	rVB	667578	1207361	21.25%	4.576%
36	27.874	4241	4248	4258	rVB	402328	1351782	23.79%	5.123%

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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 28.503 4337 4355 4370 rVB5 1028104 5681060 100.00% 21.532%

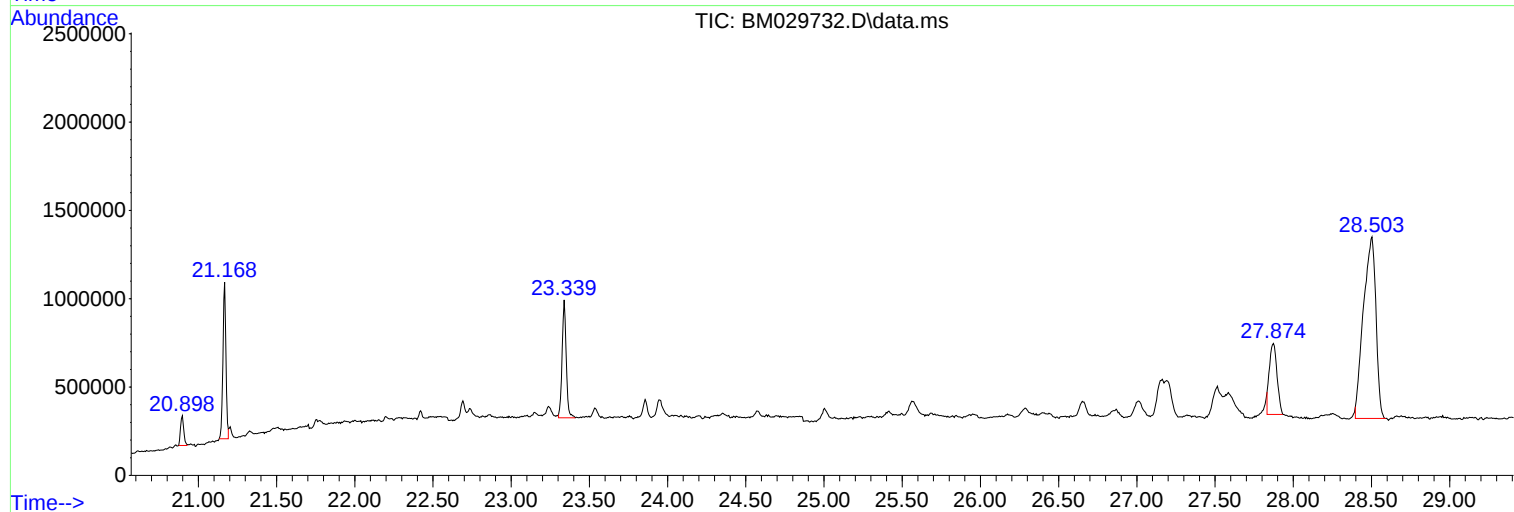
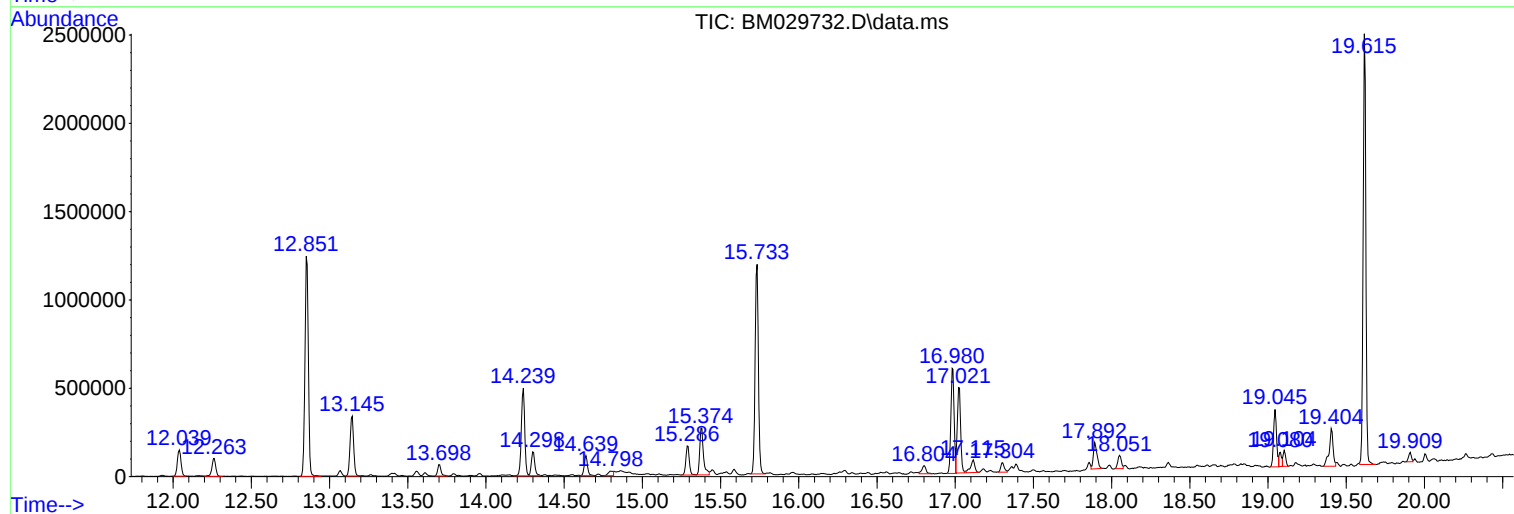
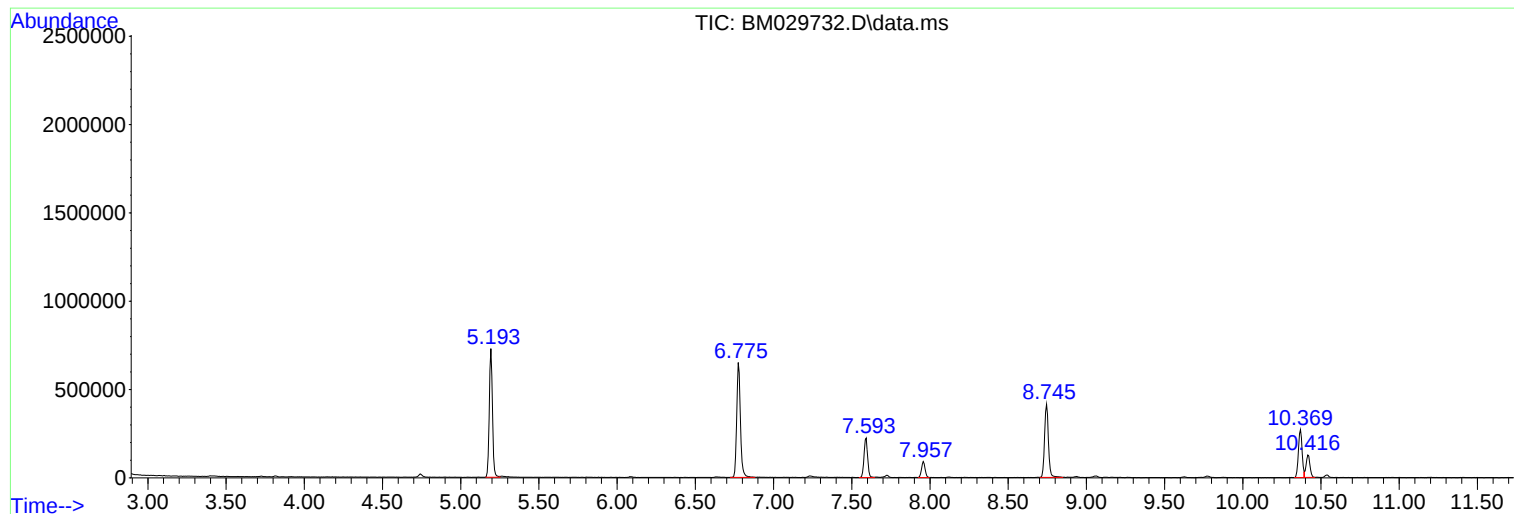
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM043021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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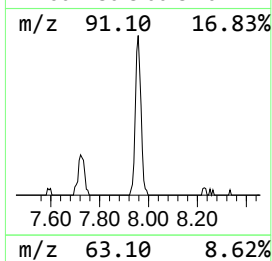
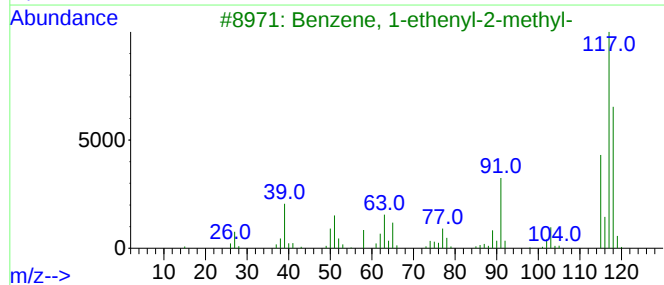
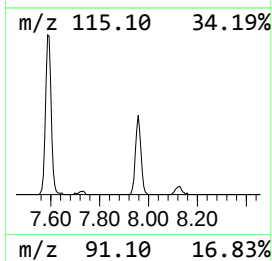
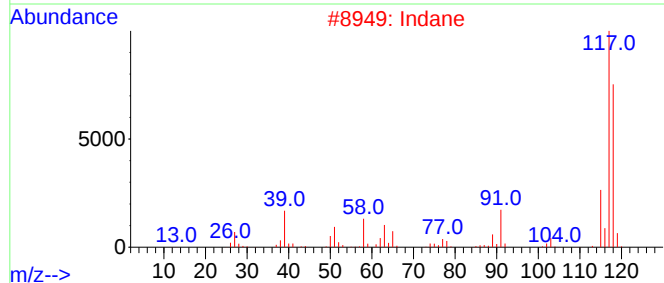
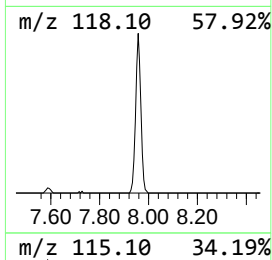
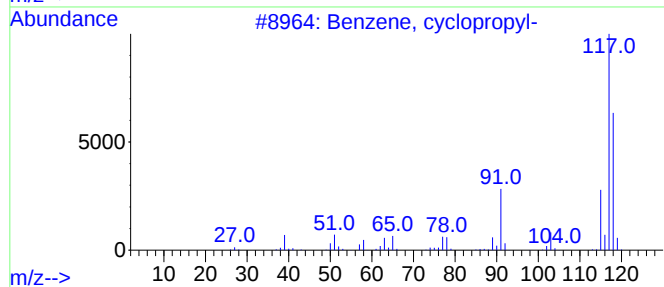
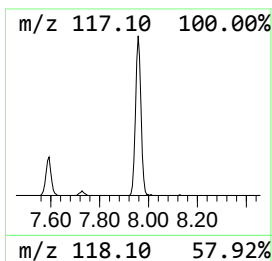
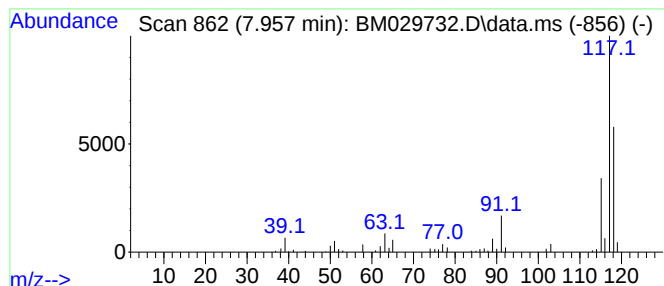
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Peak Number 1 Benzene, cyclopropyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.957	8.09 ng	143888	1,4-Dichlorobenzene-d4	7.593

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, cyclopropyl-	118	C9H10	000873-49-4	87
2		Indane	118	C9H10	000496-11-7	87
3		Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	59
4		Δtacyclene	118	C9H10	007785-10-6	50
5		Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	49



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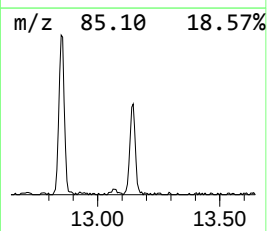
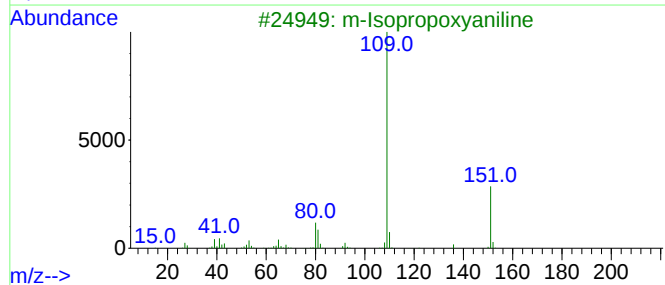
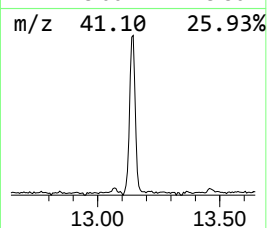
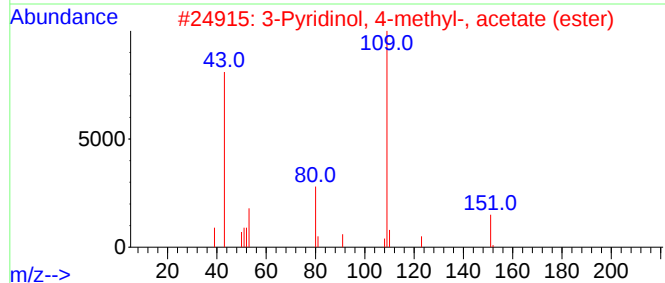
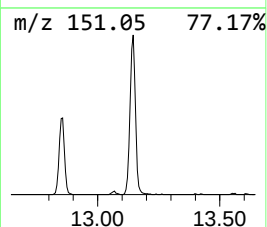
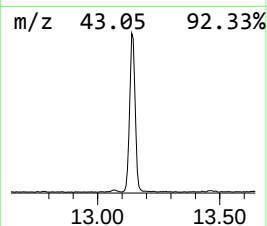
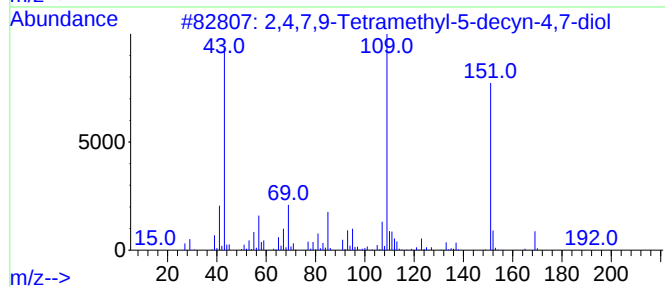
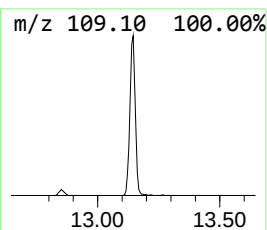
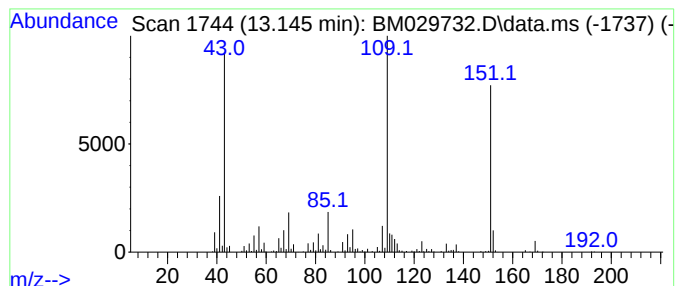
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Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.145	14.24 ng	532221	Acenaphthene-d10	14.239

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91	
2	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	59	
3	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	59	
4	Acetamide, N-(2-hydroxyphenyl)-	151	C8H9NO2	000614-80-2	59	
5	2-Propenal, 3-(2,2,6-trimethyl-7...	194	C12H18O2	055759-91-6	40	



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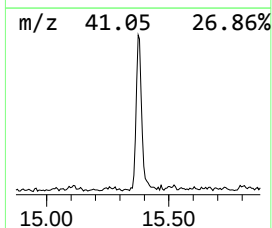
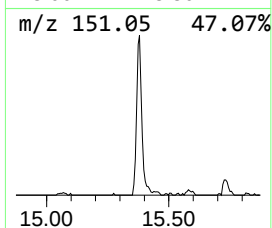
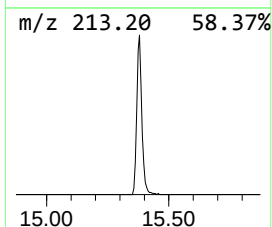
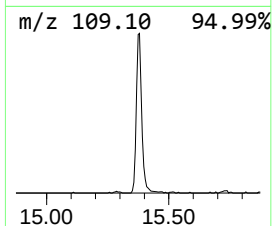
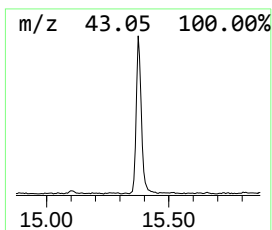
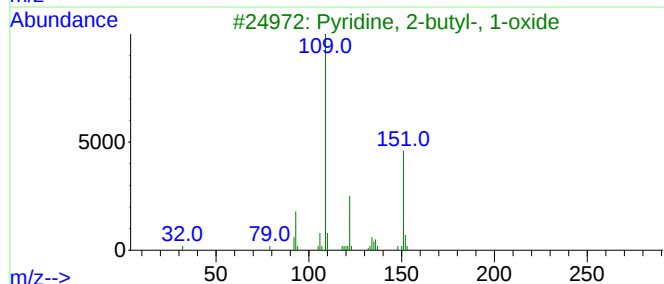
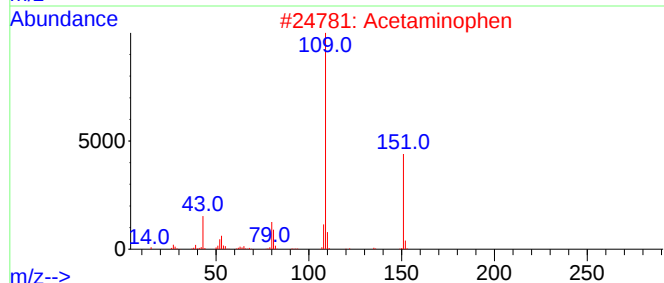
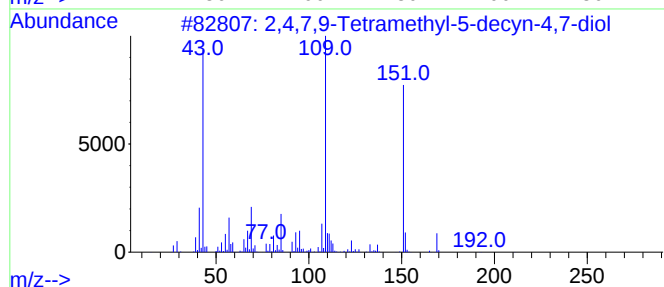
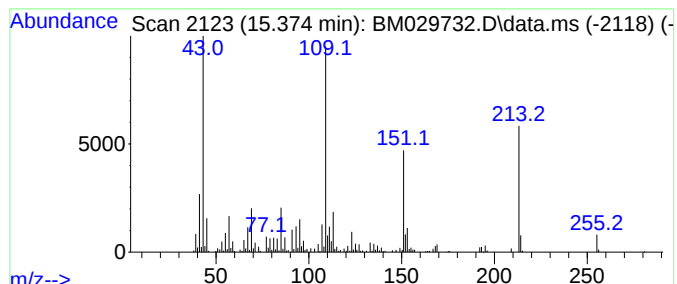
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 unknown15.37 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.374	11.68 ng	436422	Acenaphthene-d10	14.239

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	46
2		Acetaminophen	151	C8H9NO2	000103-90-2	43
3		Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	38
4		m-Isopropoxyaniline	151	C9H13NO	041406-00-2	38
5		Metacetamol	151	C8H9NO2	000621-42-1	38



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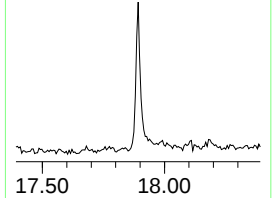
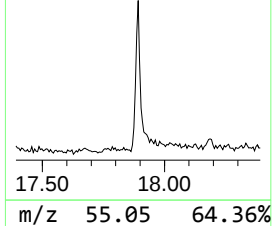
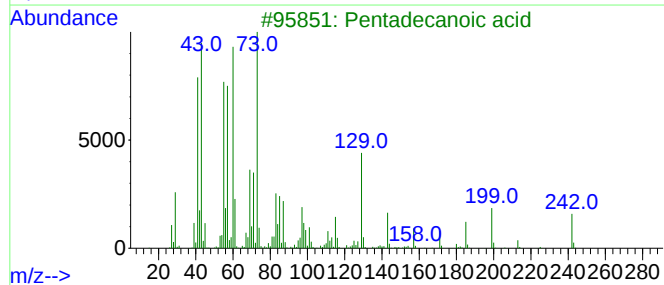
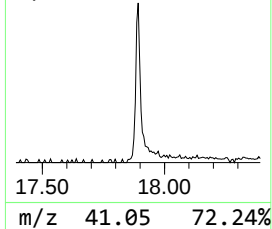
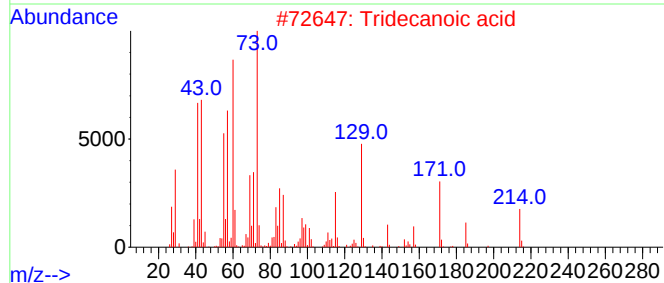
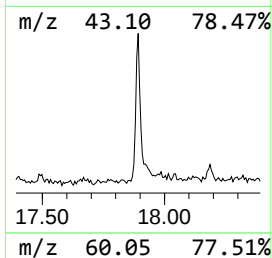
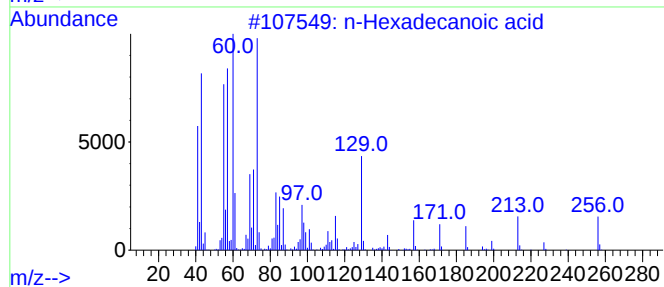
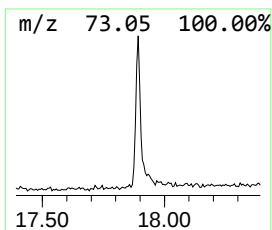
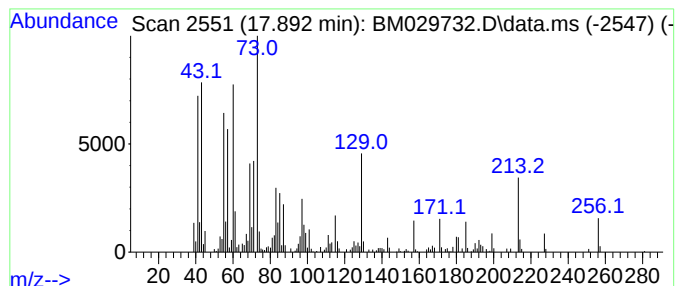
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.892	5.58 ng	244183	Phenanthrene-d10	16.986

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	86
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			n-Decanoic acid	172	C10H20O2	000334-48-5	76
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	70



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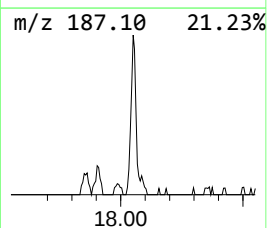
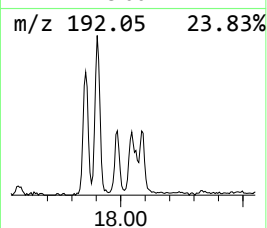
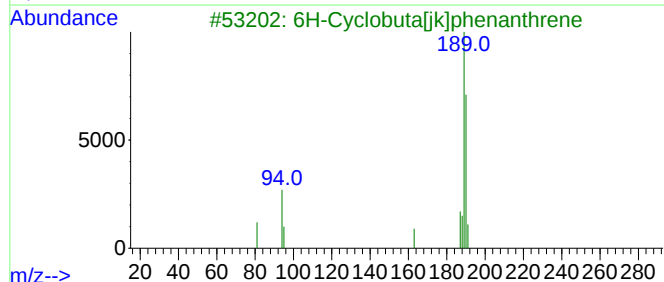
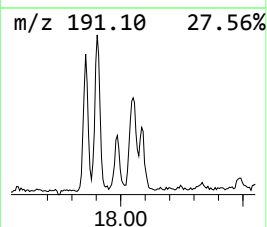
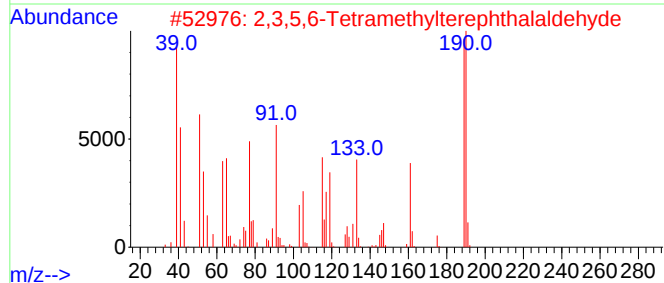
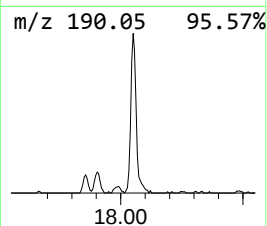
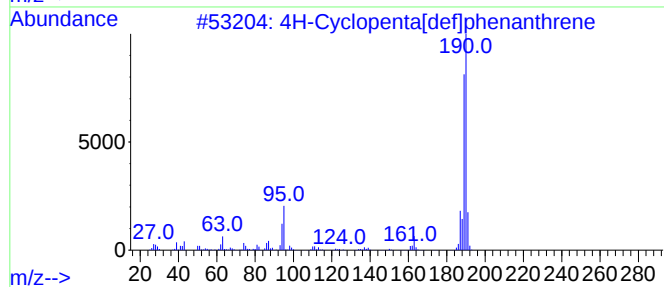
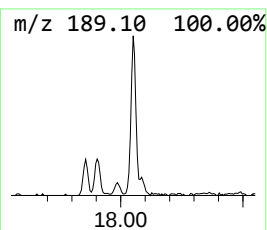
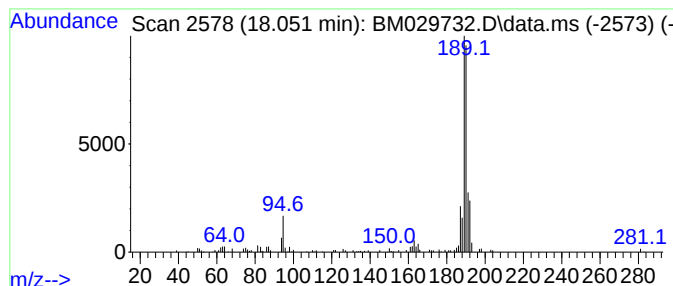
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.051	2.78 ng	121410	Phenanthrene-d10	16.986

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2			2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	50
3			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
4			2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	33
5			Pyrimidine, 2-chloro-5-phenyl-	190	C10H7ClN2	022536-62-5	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM043021\
Data File : BM029732.D
Acq On : 30 Apr 2021 16:47
Operator : CG/JU
Sample : M2077-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-20-14.5-15.0-DUP

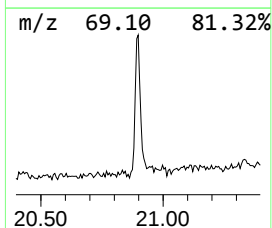
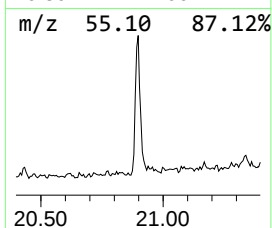
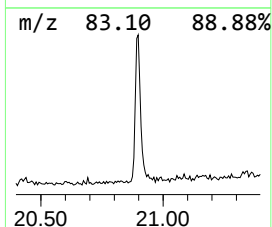
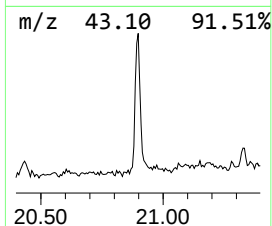
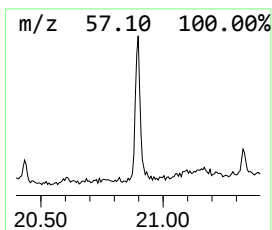
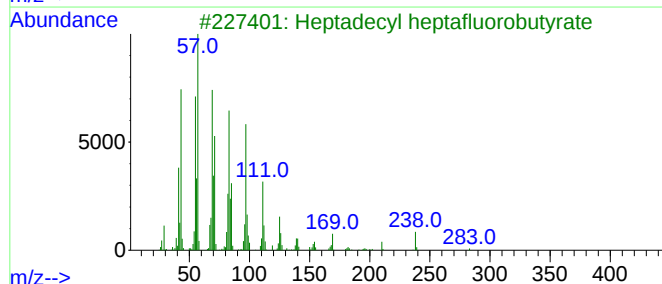
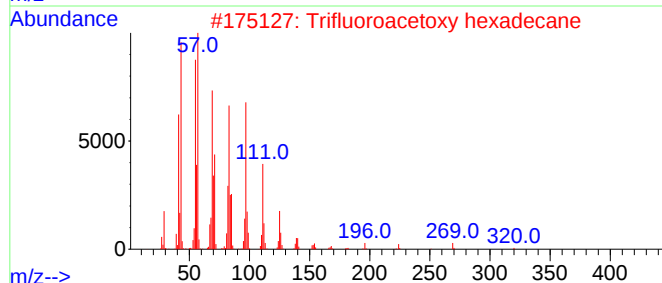
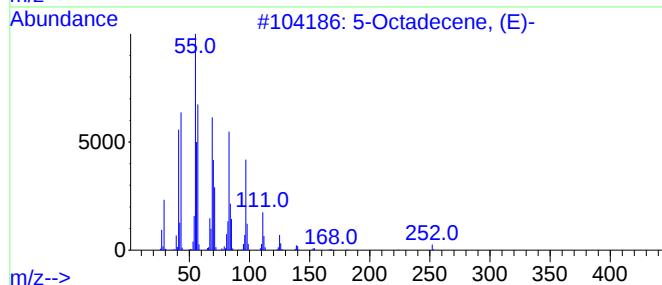
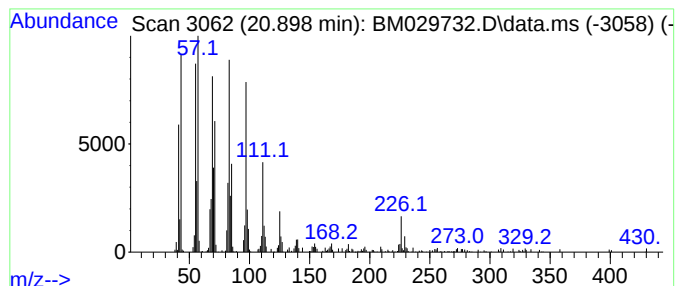
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 5-Octadecene, (E)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.898	3.95 ng	236642	Chrysene-d12	21.168

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Octadecene, (E)-	252	C18H36	007206-21-5	93
2			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
4			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5			17-Pentatriacontene	491	C35H70	006971-40-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM043021\
Data File : BM029732.D
Acq On : 30 Apr 2021 16:47
Operator : CG/JU
Sample : M2077-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-20-14.5-15.0-DUP

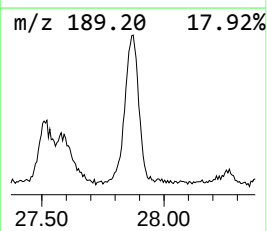
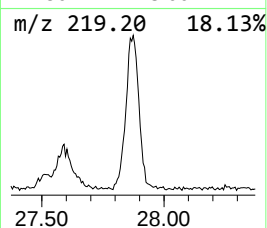
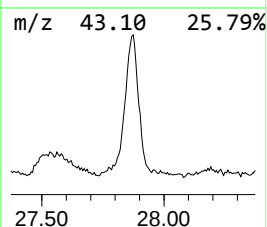
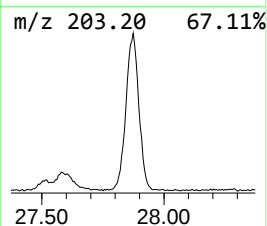
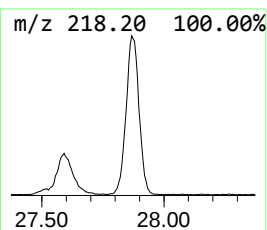
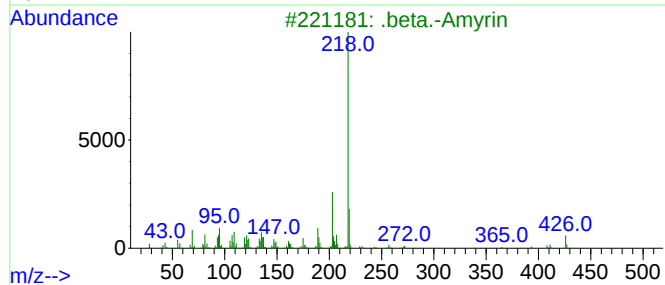
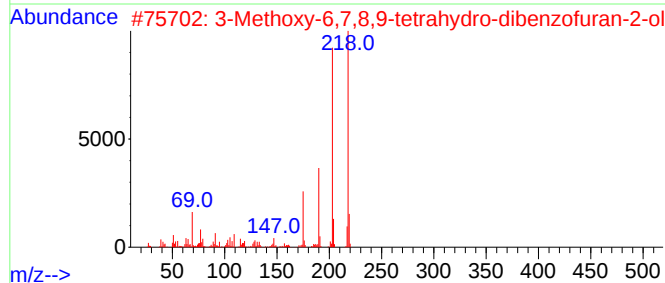
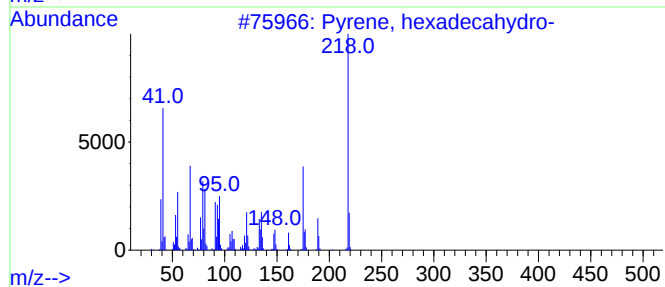
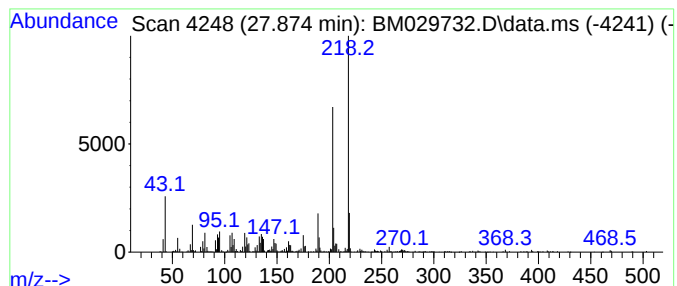
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pyrene, hexadecahydro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.874	22.39 ng	1351780	Perylene-d12	23.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrene, hexadecahydro-	218	C16H26	002435-85-0	78
2			3-Methoxy-6,7,8,9-tetrahydro-dib...	218	C13H14O3	1000186-57-9	74
3			.beta.-Amyrin	426	C30H50O	000559-70-6	72
4			2H-1-Benzopyran-2-one, 6-acetyl-...	260	C14H12O5	129812-31-3	64
5			8-Amino-6,7-dimethoxy-4-methylqu...	218	C12H14N2O2	1000213-07-2	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM043021\
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Sample : M2077-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-20-14.5-15.0-DUP

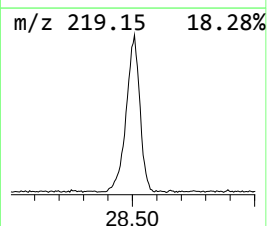
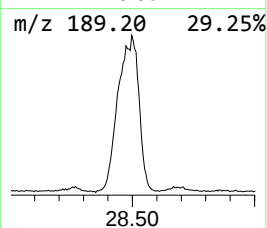
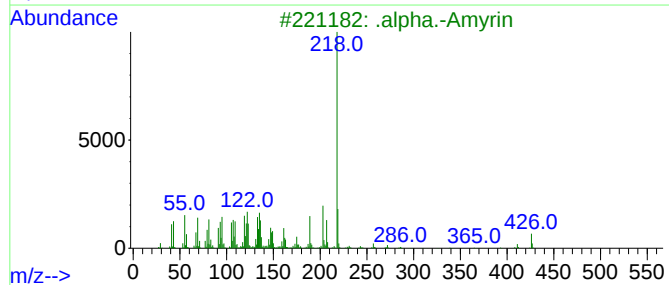
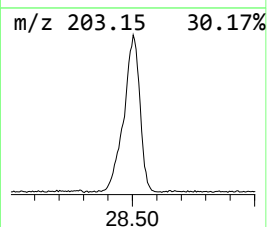
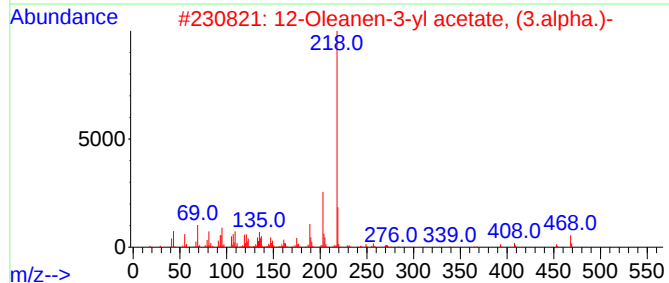
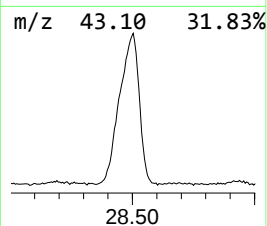
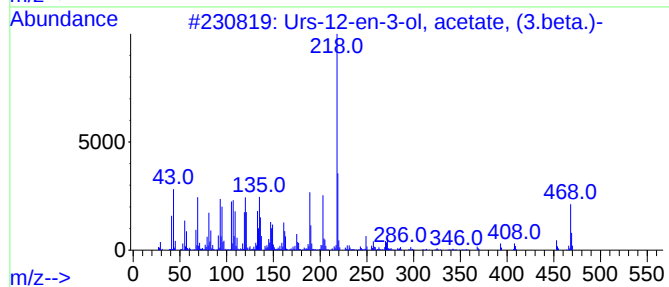
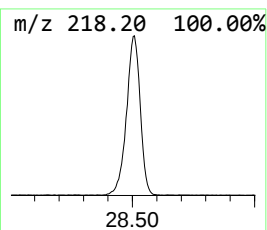
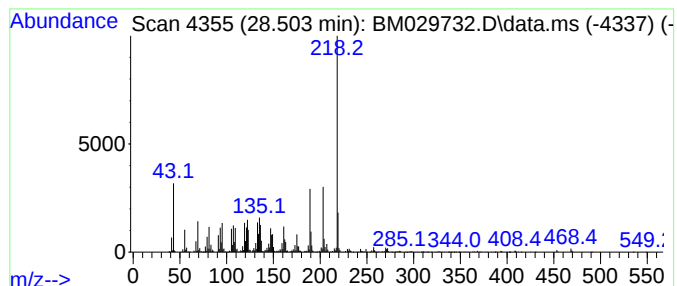
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM043021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Urs-12-en-3-ol, acetate, (3... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.503	94.11 ng	5681060	Perylene-d12	23.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Urs-12-en-3-ol, acetate, (3.beta.)-	468	C32H52O2	000863-76-3	94
2			12-Oleanen-3-yl acetate, (3.alph...	468	C32H52O2	033055-28-6	94
3			.alpha.-Amyrin	426	C30H50O	000638-95-9	81
4			.alpha.-Amyrin, trimethylsilyl e...	498	C33H58OSi	1000374-76-6	74
5			5(1H)-Azulenone, 2,4,6,7,8,8a-he...	218	C15H22O	006754-66-1	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM043021\
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Acq On : 30 Apr 2021 16:47
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Sample : M2077-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-20-14.5-15.0-DUP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM043021.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
Benzene, cyclop...	7.957	8.1	ng	143888	1	7.593	355748	20.0
2,4,7,9-Tetrame...	13.145	14.2	ng	532221	3	14.239	747238	20.0
unknown15.37	15.374	11.7	ng	436422	3	14.239	747238	20.0
n-Hexadecanoic ...	17.892	5.6	ng	244183	4	16.986	874885	20.0
4H-Cyclopenta[d...	18.051	2.8	ng	121410	4	16.986	874885	20.0
5-Octadecene, (E)-	20.898	4.0	ng	236642	5	21.168	1197040	20.0
Pyrene, hexadec...	27.874	22.4	ng	1351780	6	23.339	1207360	20.0
Urs-12-en-3-ol,...	28.503	94.1	ng	5681060	6	23.339	1207360	20.0