

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012721\
 Data File : BM028576.D
 Acq On : 27 Jan 2021 19:09
 Operator : CG/JU
 Sample : M1242-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 0014-048-COMP-G

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: BM028576.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.522	390	397	407	rBB	360680	517891	36.36%	8.835%
2	7.169	670	677	688	rBV	340861	551802	38.74%	9.414%
3	7.969	806	813	820	rBB	92249	143690	10.09%	2.451%
4	9.140	1005	1012	1021	rBV	200717	322882	22.67%	5.509%
5	10.781	1284	1291	1297	rBV	123742	198155	13.91%	3.381%
6	13.233	1702	1708	1715	rVB	357465	524012	36.78%	8.940%
7	14.616	1936	1943	1951	rBV	169649	244525	17.17%	4.172%
8	16.098	2190	2195	2205	rBV	368052	501917	35.23%	8.563%
9	17.345	2401	2407	2411	rBV	195469	267559	18.78%	4.565%
10	17.386	2411	2414	2419	rVB	20394	27015	1.90%	0.461%
11	18.221	2551	2556	2562	rBV	71238	110840	7.78%	1.891%
12	18.974	2677	2684	2688	rBV	48349	69551	4.88%	1.187%
13	19.062	2695	2699	2701	rBV	15426	23442	1.65%	0.400%
14	20.409	2903	2928	2948	rBV3	208972	1424538	100.00%	24.303%
15	20.809	2994	2996	3001	rVB	54133	57986	4.07%	0.989%
16	21.180	3056	3059	3071	rVB3	90396	154414	10.84%	2.634%
17	21.480	3105	3110	3115	rVB	245230	340622	23.91%	5.811%
18	23.750	3490	3496	3512	rVB2	181771	380677	26.72%	6.495%

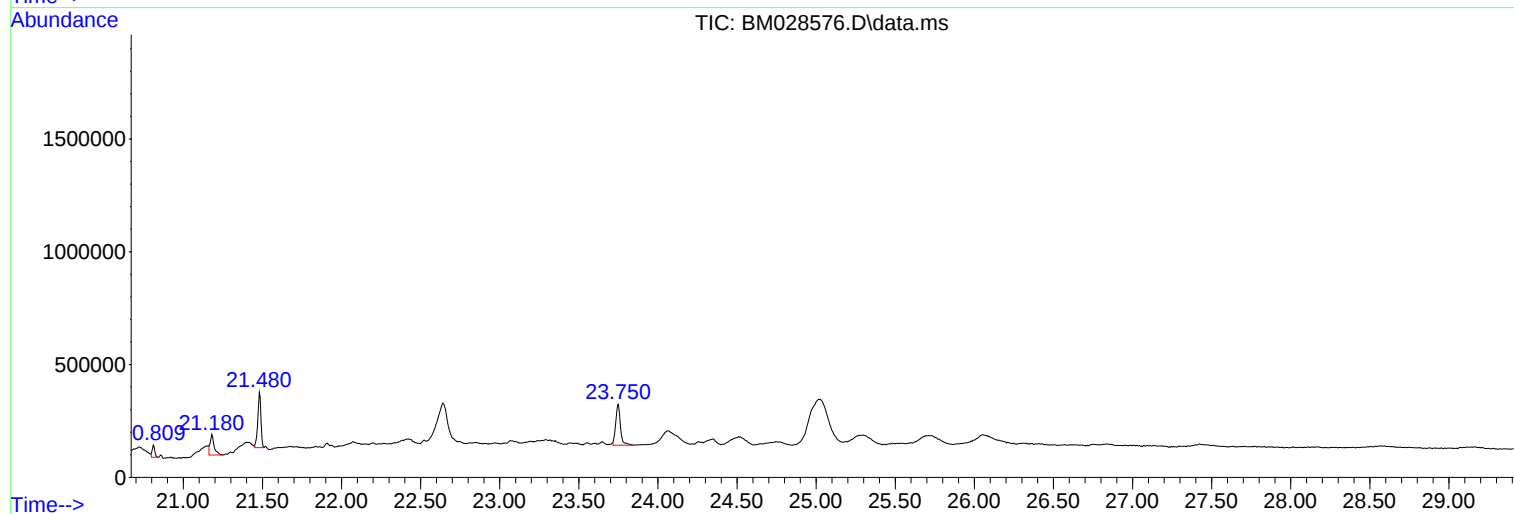
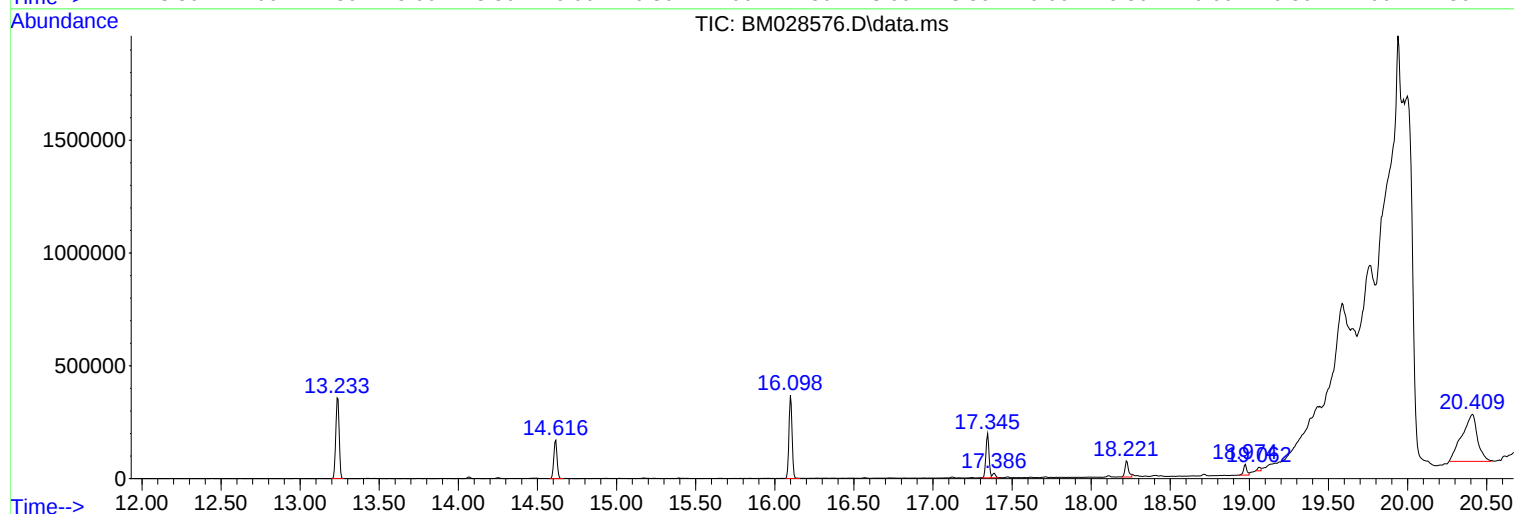
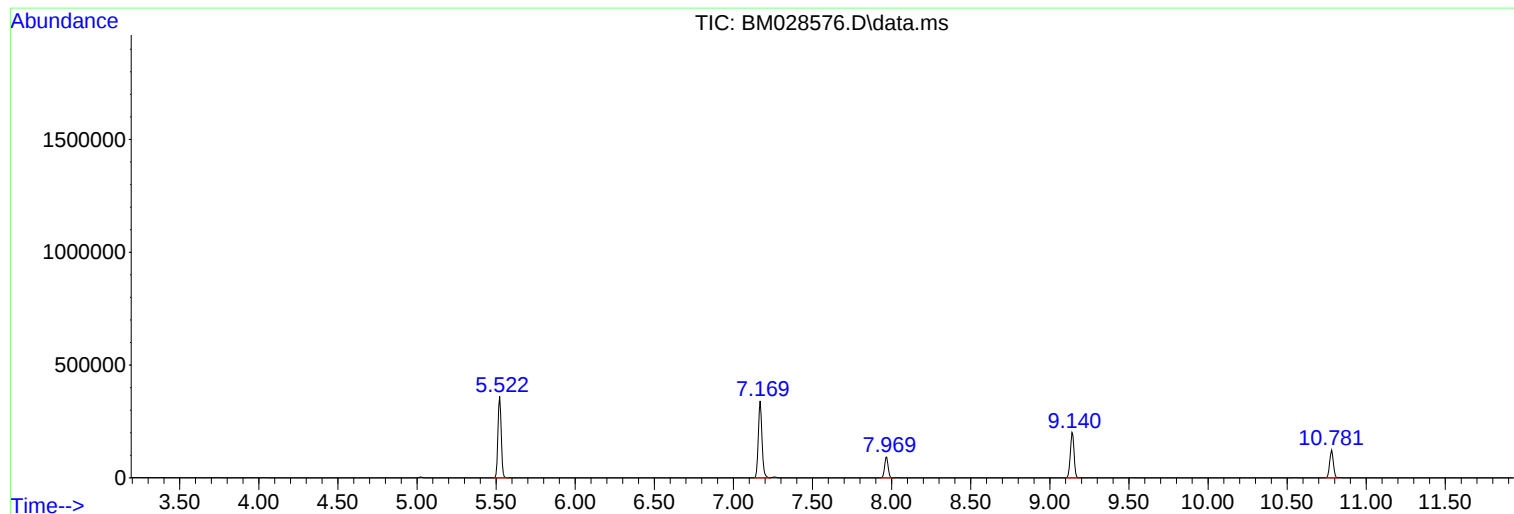
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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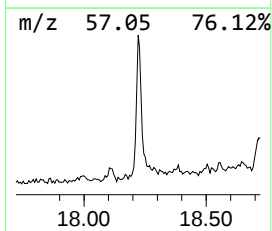
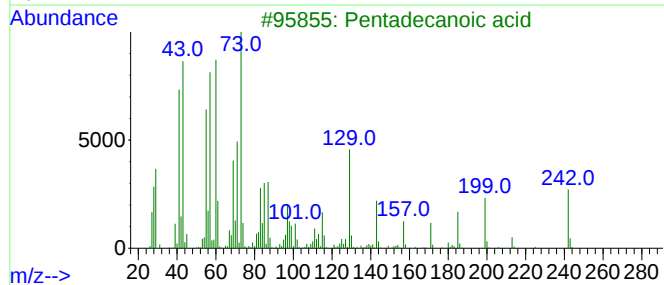
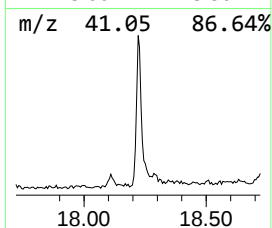
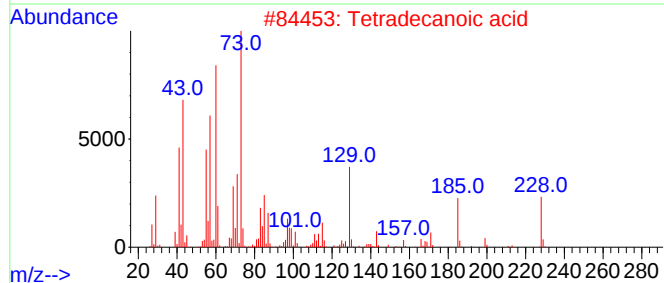
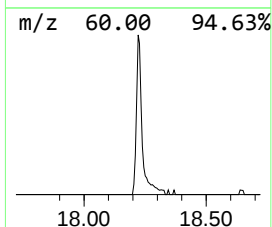
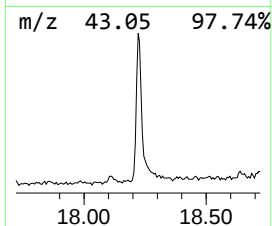
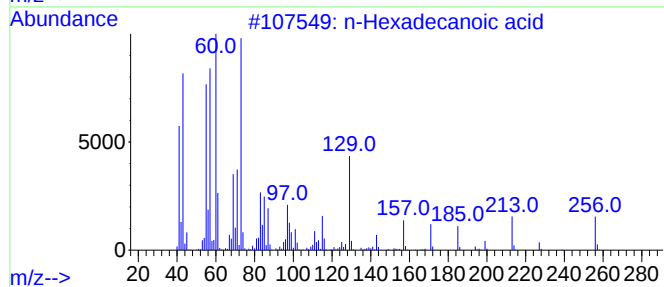
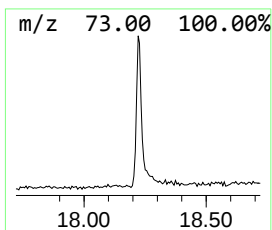
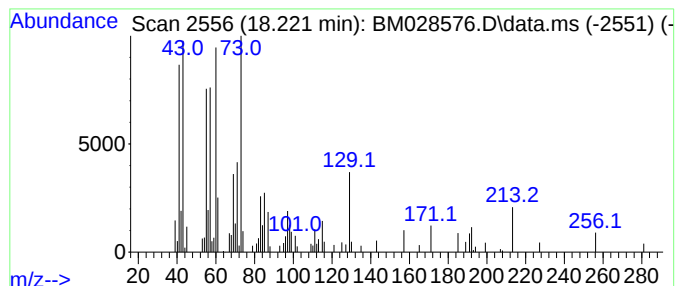
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.221	8.29 ng	110840	Phenanthrene-d10	17.345

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	83
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4			Tridecanoic acid	214	C13H26O2	000638-53-9	72
5			Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	18



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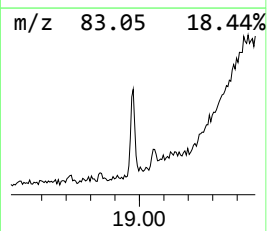
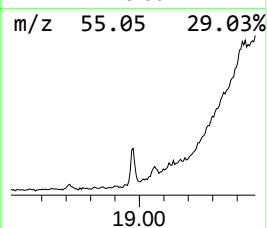
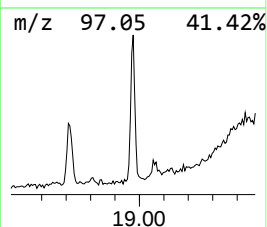
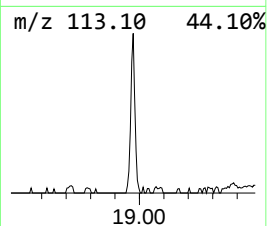
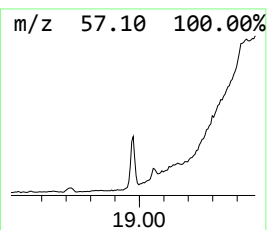
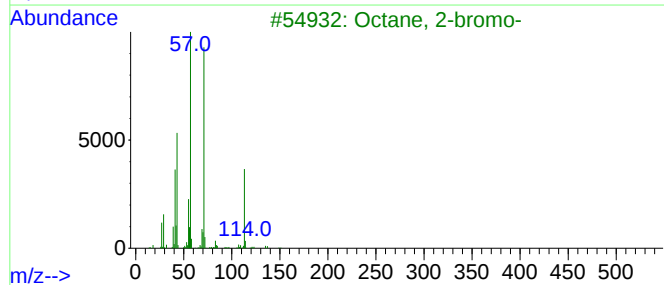
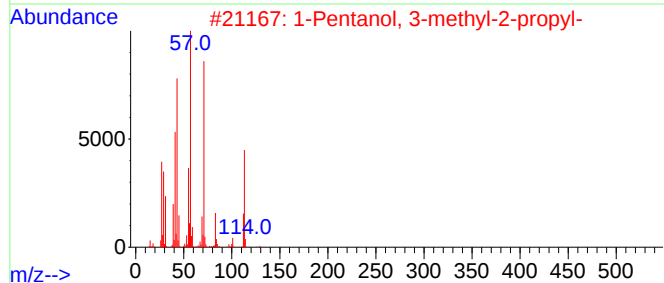
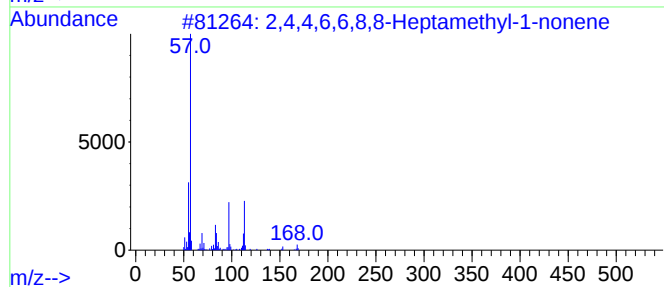
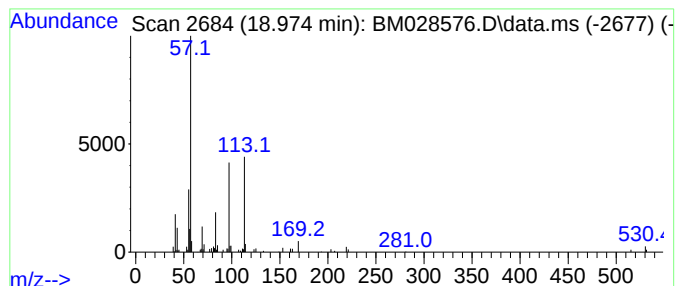
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown18.974 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.974	5.20 ng	69551	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	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	38		
3	Octane, 2-bromo-	192	C8H17Br	000557-35-7	32		
4	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	32		
5	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	27		



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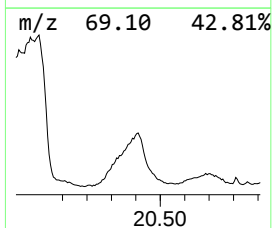
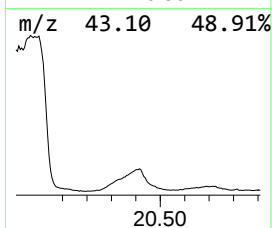
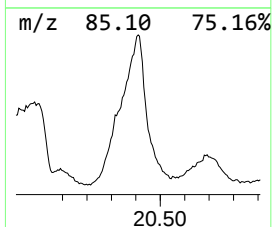
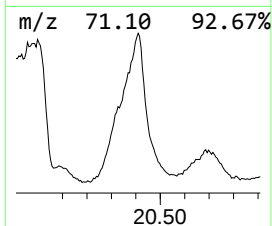
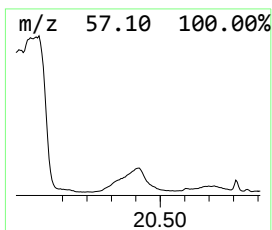
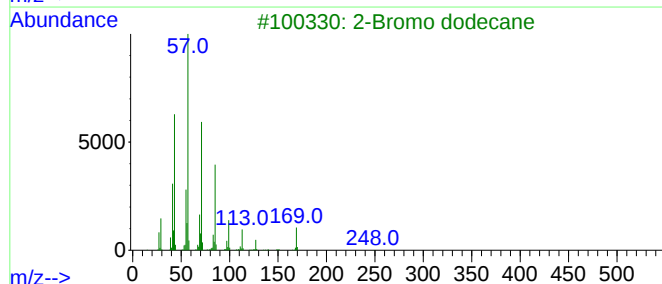
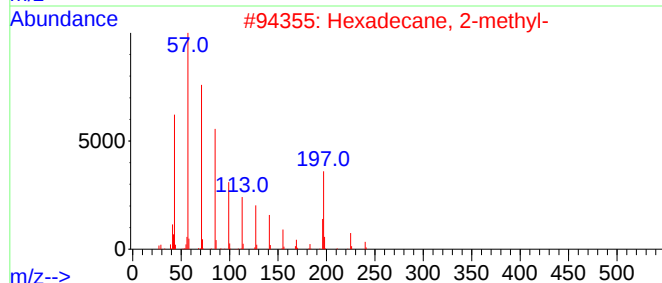
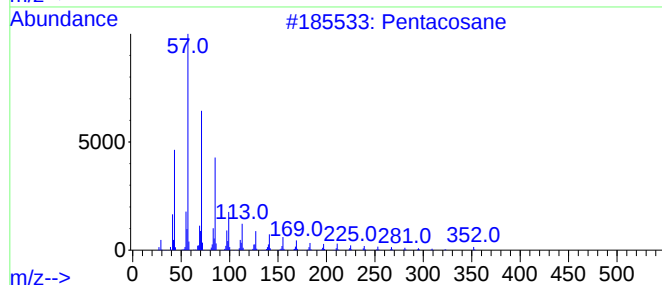
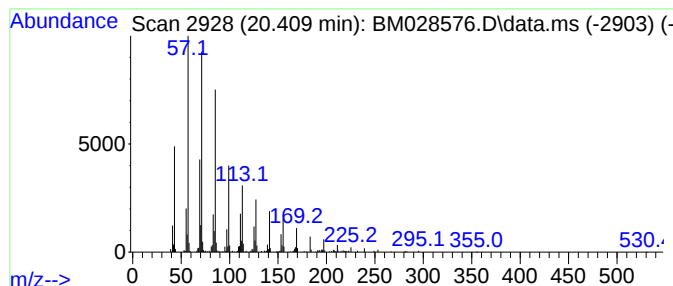
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Pentacosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.409	83.64 ng	1424540	Chrysene-d12	21.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	90
2			Hexadecane, 2-methyl-	240	C17H36	001560-92-5	90
3			2-Bromo dodecane	248	C12H25Br	013187-99-0	53
4			Borane, diethyl(decyloxy)-	226	C14H31BO	1000152-34-3	38
5			Decane, 3-bromo-	220	C10H21Br	030571-71-2	35



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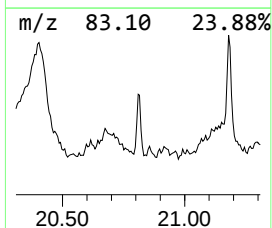
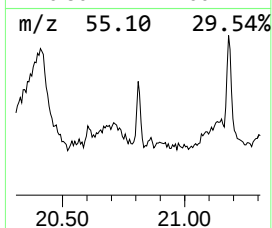
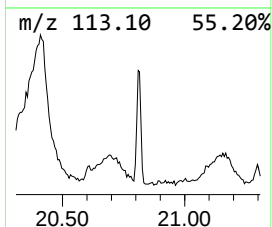
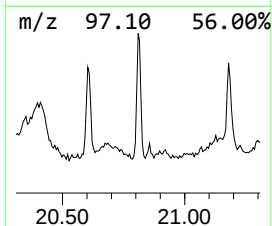
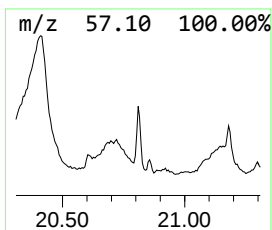
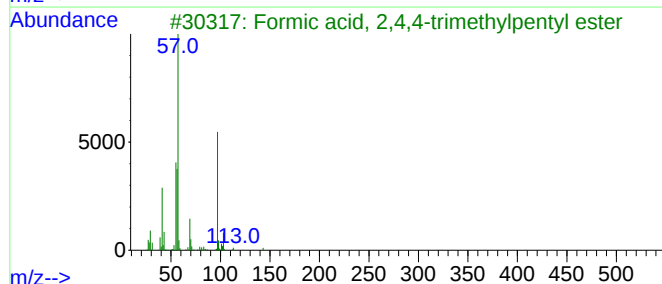
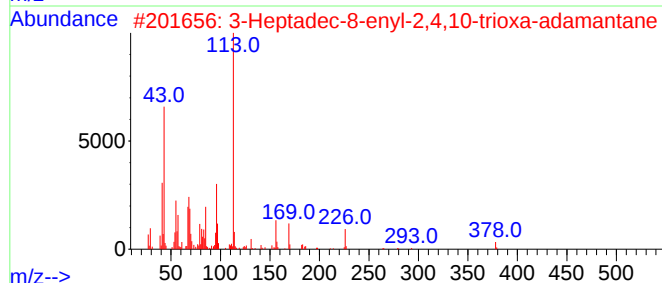
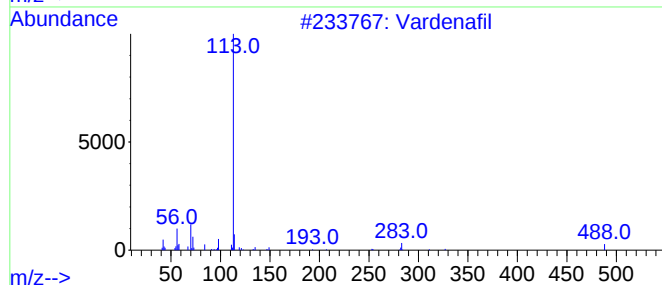
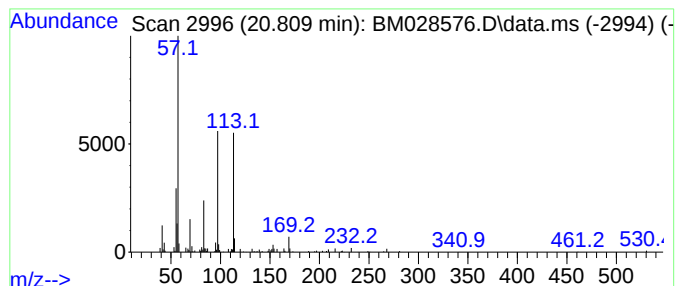
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Peak Number 4 unknown20.809 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.809	3.40 ng	57986	Chrysene-d12	21.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Vardenafil	488	C23H32N6O4S	224785-90-4	22
2			3-Heptadec-8-enyl-2,4,10-trioxa-...	378	C24H42O3	1000189-57-5	17
3			Formic acid, 2,4,4-trimethylpent...	158	C9H18O2	1000368-95-2	16
4			2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	16
5			Oxazole, 2,4-dimethyl-	97	C5H7NO	007208-05-1	14



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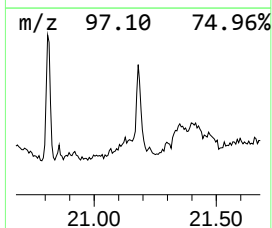
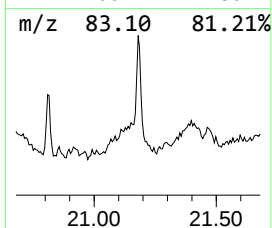
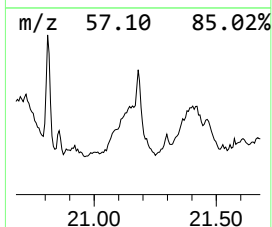
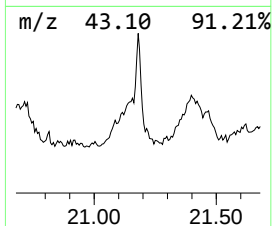
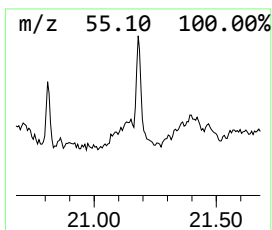
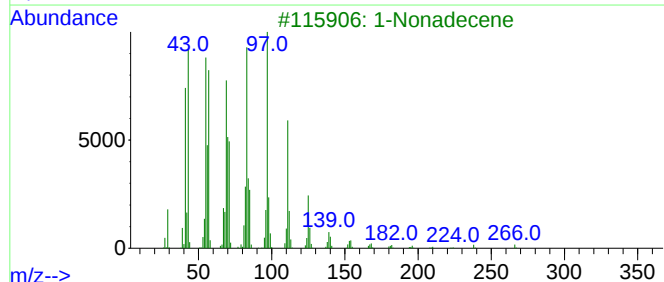
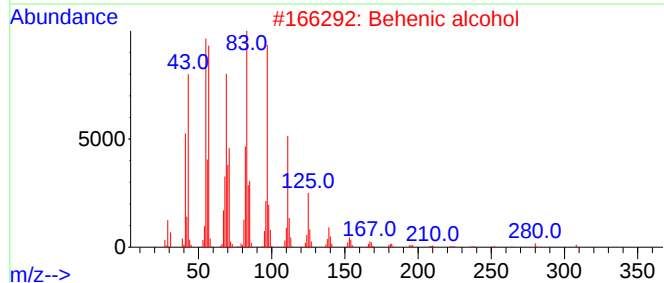
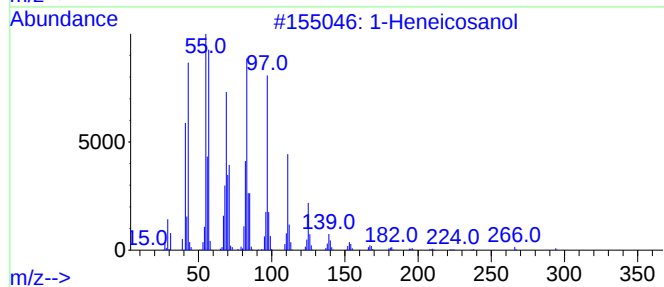
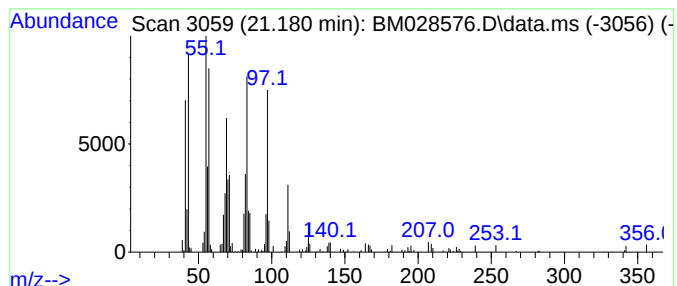
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Heneicosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.180	9.07 ng	154414	Chrysene-d12	21.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	94
2			Behenic alcohol	326	C22H46O	000661-19-8	91
3			1-Nonadecene	266	C19H38	018435-45-5	91
4			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
5			1-Docosene	308	C22H44	001599-67-3	87



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TIC Library : C:\DATABASE\NIST11.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	18.221	8.3	ng	110840	4	17.345	267559	20.0
unknown18.974	18.974	5.2	ng	69551	4	17.345	267559	20.0
Pentacosane	20.409	83.6	ng	1424540	5	21.480	340622	20.0
unknown20.809	20.809	3.4	ng	57986	5	21.480	340622	20.0
1-Heneicosanol	21.180	9.1	ng	154414	5	21.480	340622	20.0