

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042221\
 Data File : BM029597.D
 Acq On : 22 Apr 2021 17:05
 Operator : CG/JU
 Sample : M2106-06
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SB-23-14.5-15.0

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: BM029597.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	392	398	409	rBV	717931	1056993	36.09%	5.919%
2	6.810	659	667	682	rBV	709478	1133968	38.72%	6.350%
3	7.634	801	807	816	rBV	229394	368886	12.60%	2.066%
4	8.787	996	1003	1019	rBV	415622	712388	24.33%	3.989%
5	10.410	1272	1279	1292	rBV	277544	474027	16.19%	2.654%
6	12.892	1694	1701	1716	rBV	1248406	1816203	62.02%	10.170%
7	13.739	1838	1845	1853	rBV	41476	64722	2.21%	0.362%
8	14.275	1930	1936	1949	rVB2	457958	675231	23.06%	3.781%
9	14.827	2023	2030	2041	rBV	55404	171123	5.84%	0.958%
10	15.769	2184	2190	2199	rBV	1032127	1460093	49.86%	8.176%
11	16.439	2297	2304	2310	rBV9	24656	49606	1.69%	0.278%
12	17.021	2397	2403	2410	rBV	580050	829111	28.31%	4.643%
13	17.804	2532	2536	2540	rBV7	15668	30128	1.03%	0.169%
14	17.933	2552	2558	2578	rBV	755120	1172535	40.04%	6.565%
15	19.215	2771	2776	2791	rVB	393707	613053	20.93%	3.433%
16	19.468	2814	2819	2826	rBV	158746	230155	7.86%	1.289%
17	19.651	2845	2850	2862	rBV	2351037	2928573	100.00%	16.398%
18	19.945	2897	2900	2903	rBV4	21384	31389	1.07%	0.176%
19	20.004	2904	2910	2921	rVB2	74753	199131	6.80%	1.115%
20	20.457	2985	2987	2994	rVB5	21997	34571	1.18%	0.194%
21	20.927	3061	3067	3074	rVB	308989	457958	15.64%	2.564%
22	21.204	3109	3114	3122	rBV	822079	1078457	36.83%	6.039%
23	23.392	3480	3486	3494	rVB	608259	1145520	39.12%	6.414%
24	25.803	3889	3896	3908	rVB3	426925	1125223	38.42%	6.301%

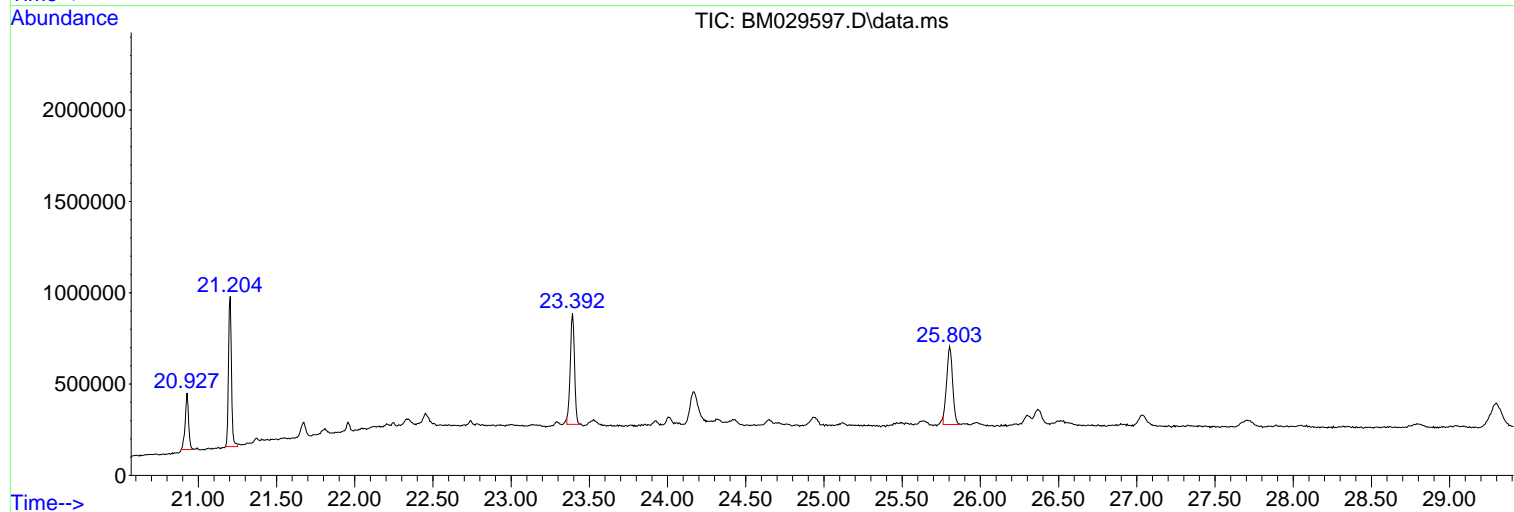
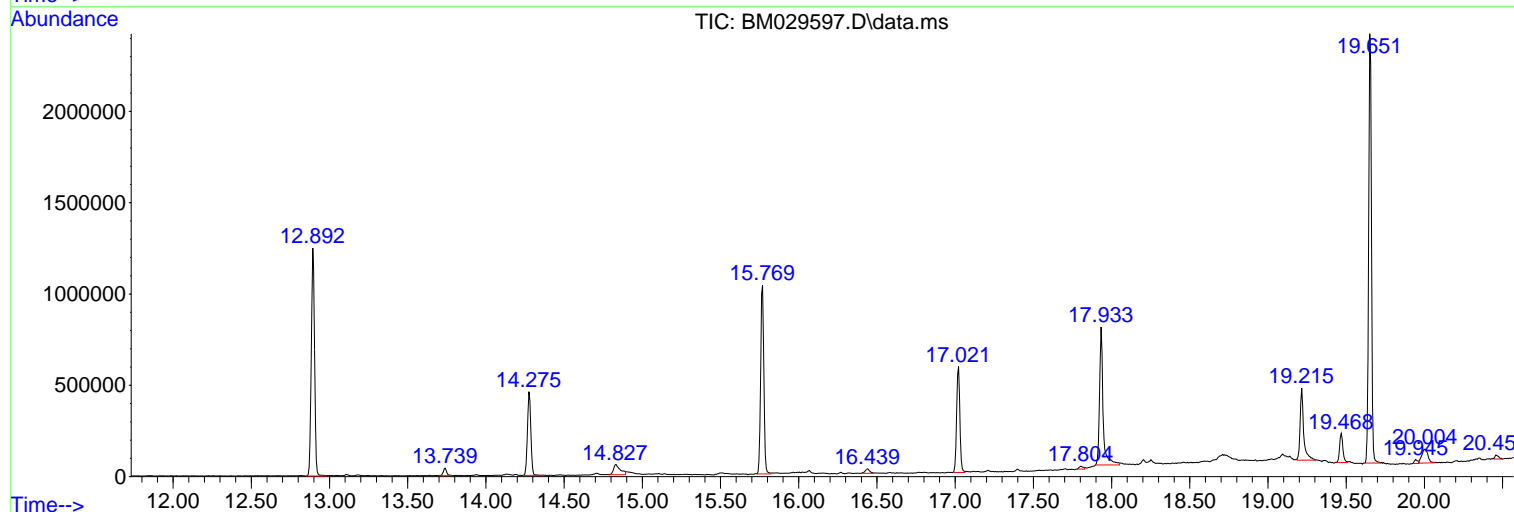
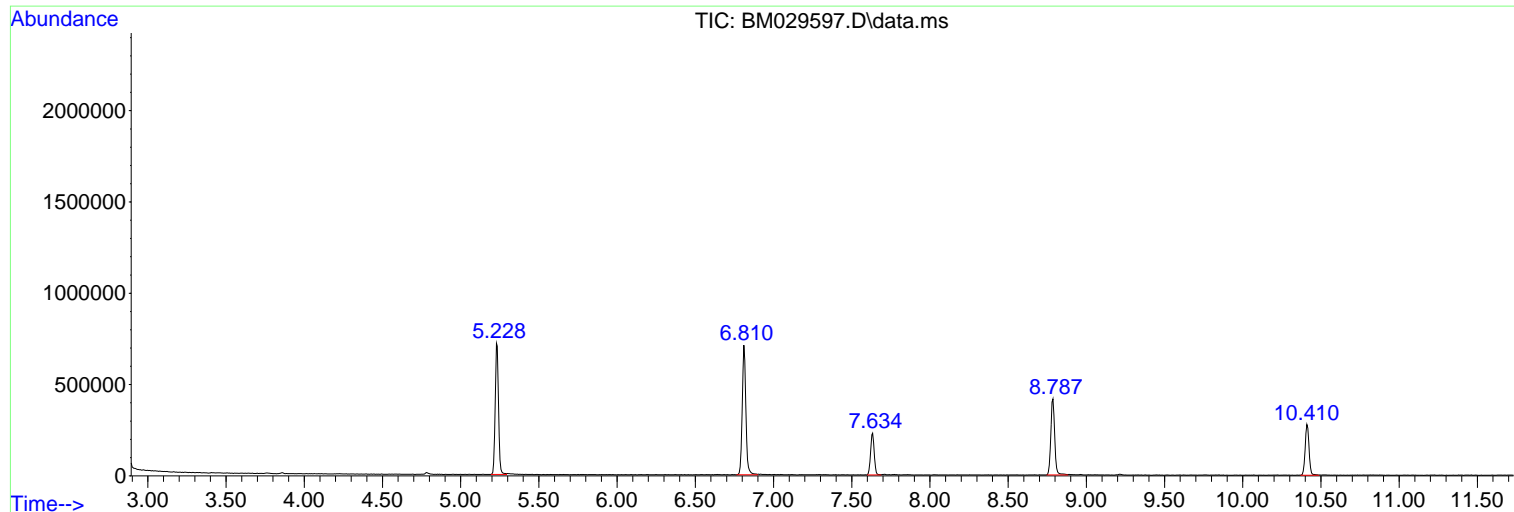
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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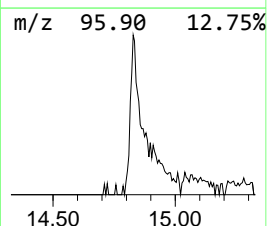
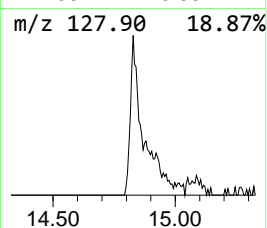
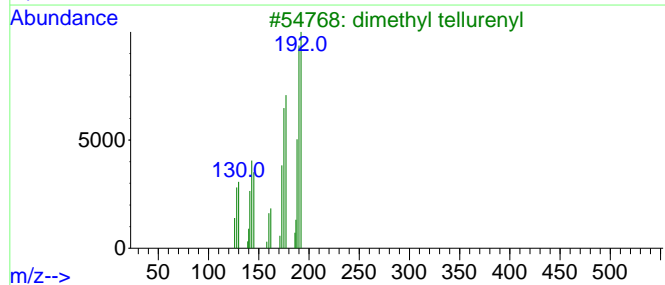
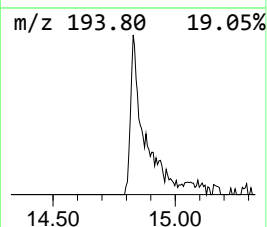
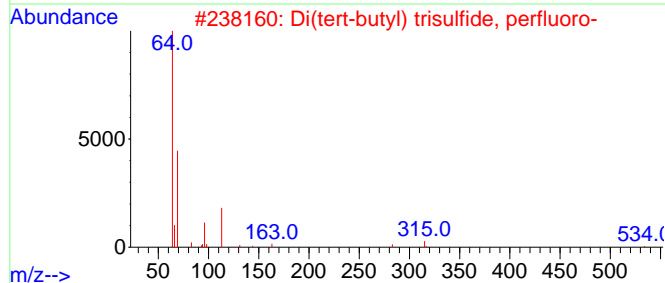
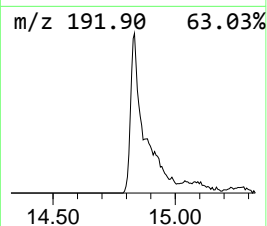
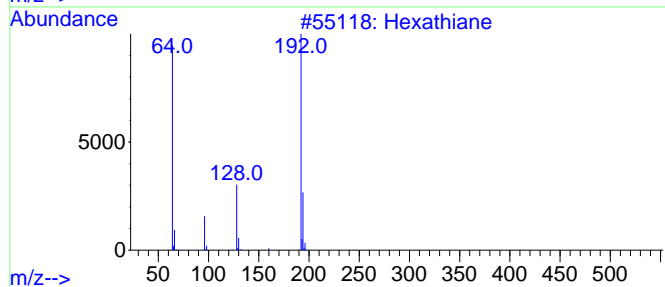
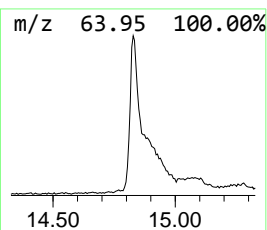
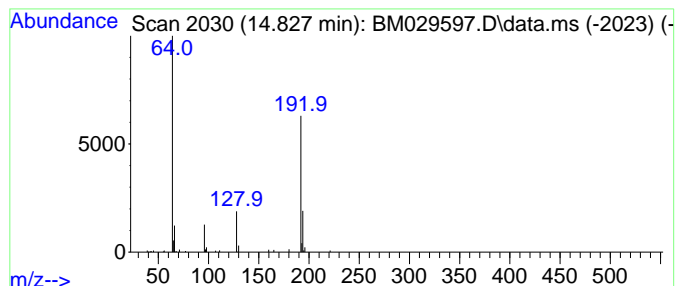
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 1 Hexathiane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.828	5.07 ng	171123	Acenaphthene-d10	14.275

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexathiane	192	S6	013798-23-7	91
2		Di(tert-butyl) trisulfide, perfl...	534	C8F18S3	016005-64-4	9
3		dimethyl tellurenyl	192	C2H6STe	1000374-19-6	5
4		Sulfur dioxide	64	O2S	007446-09-5	4
5		Ethyl Chloride	64	C2H5Cl	000075-00-3	4



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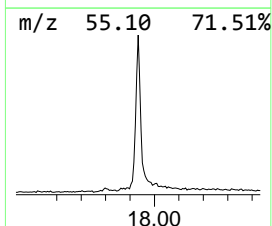
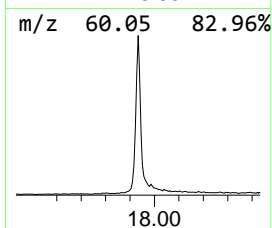
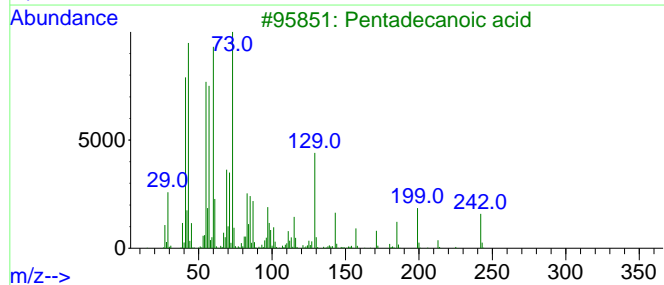
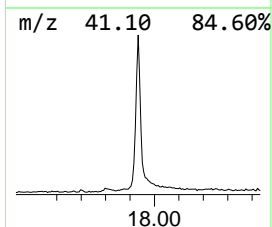
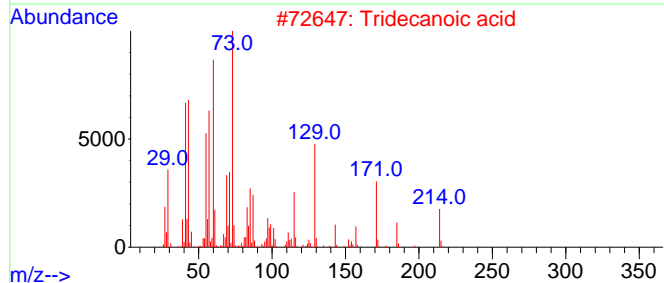
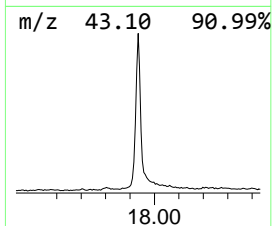
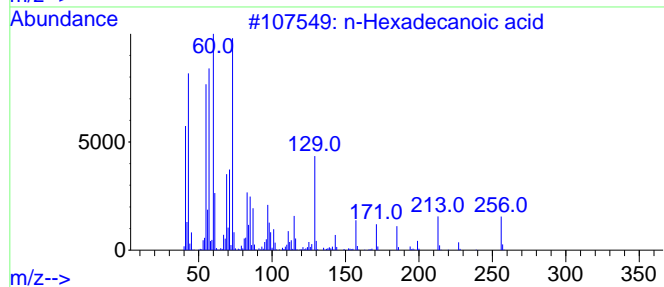
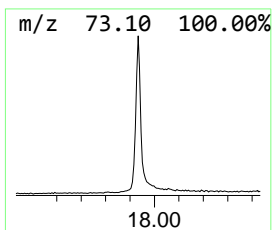
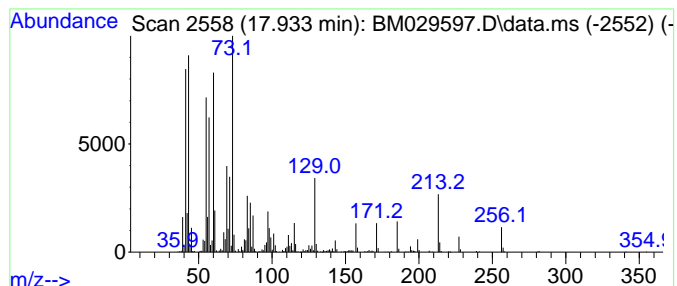
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 Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.933	28.28 ng	1172540	Phenanthrene-d10	17.021

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	94
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4		Octadecanoic acid	284	C18H36O2	000057-11-4	76
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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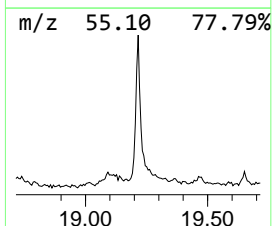
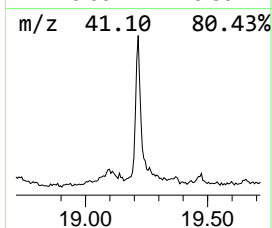
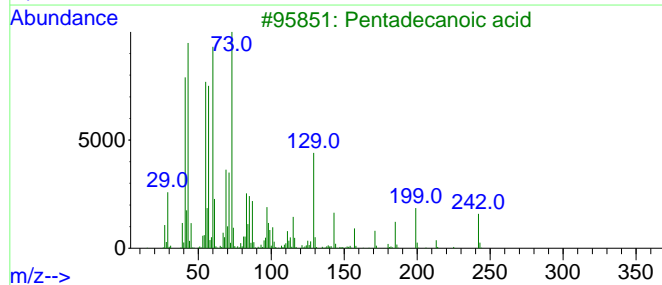
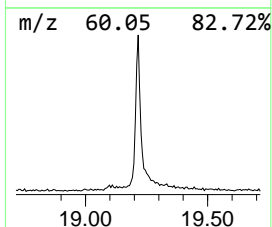
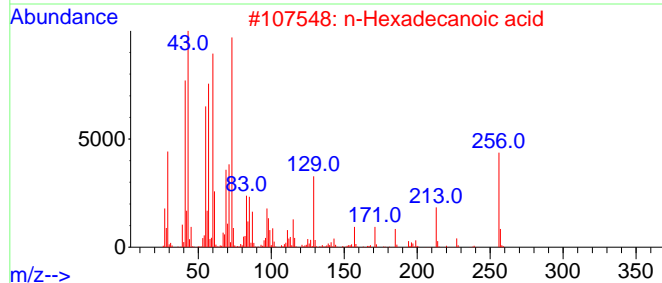
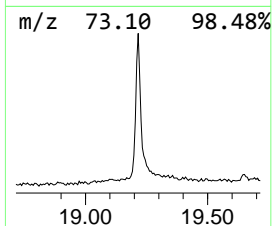
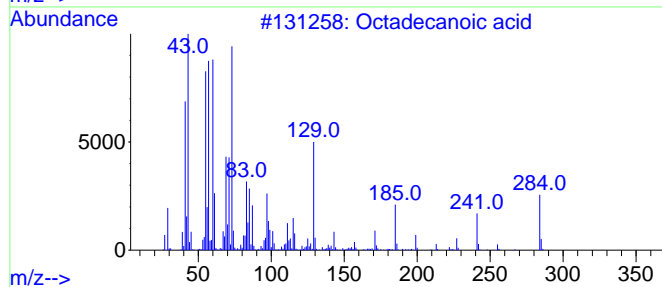
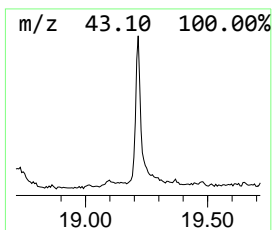
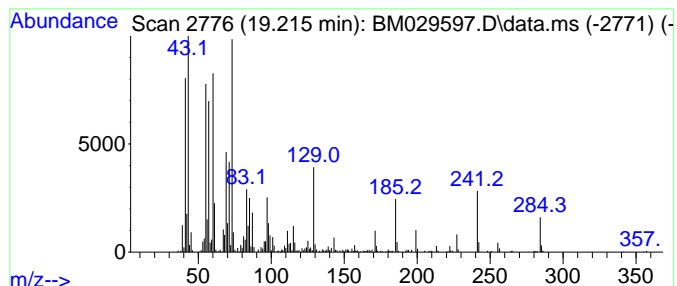
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 Peak Number 3 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.215	11.37 ng	613053	Chrysene-d12	21.203

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80



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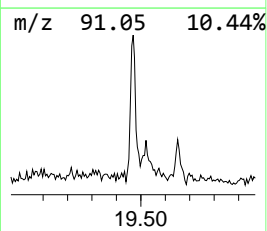
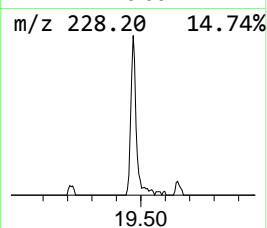
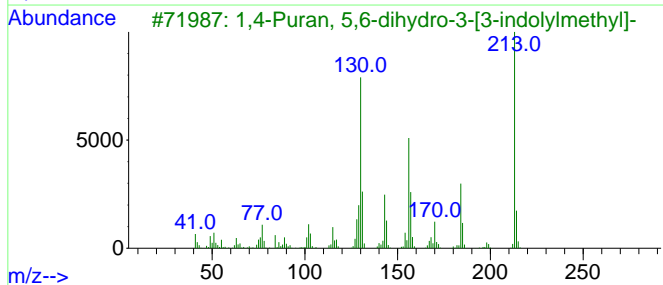
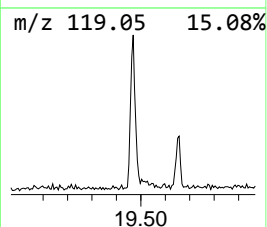
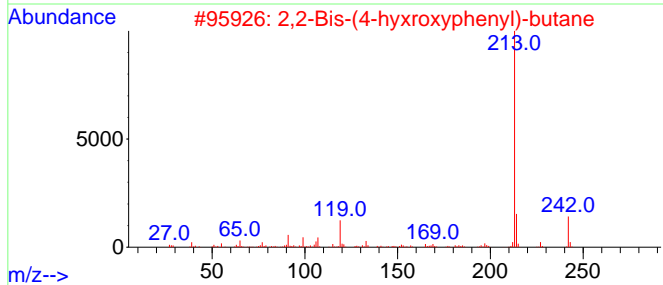
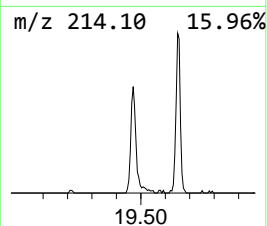
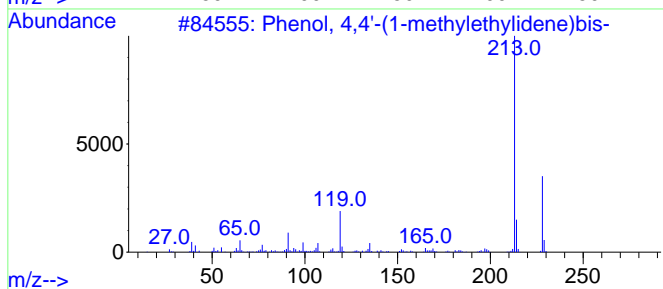
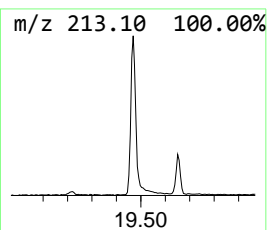
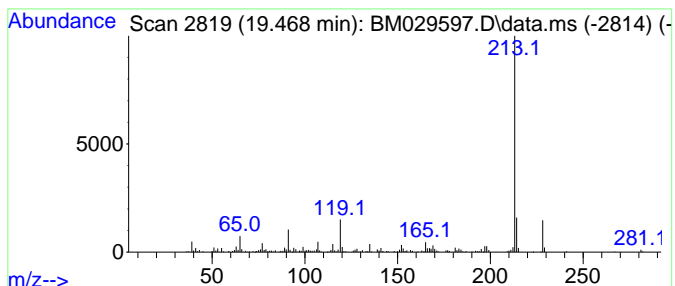
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 Peak Number 4 Phenol, 4,4'-(1-methylethyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.468	4.27 ng	230155	Chrysene-d12	21.203

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	91
2		2,2-Bis-(4-hydroxyphenyl)-butane	242	C16H18O2	000077-40-7	64
3		1,4-Puran, 5,6-dihydro-3-[3-indo...	213	C14H15NO	1000128-72-9	59
4		2-Bromo-7-(methylamino)tropone	213	C8H8BrNO	103539-25-9	59
5		2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	59



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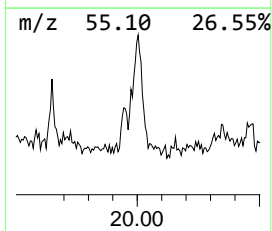
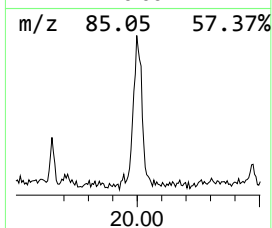
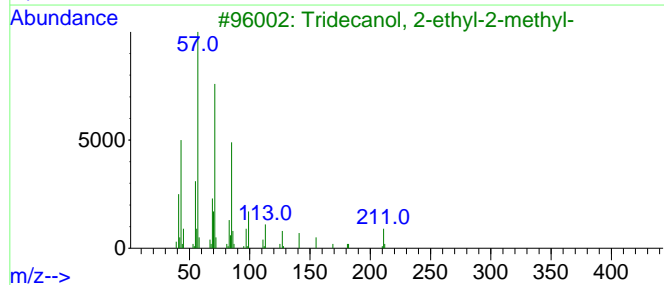
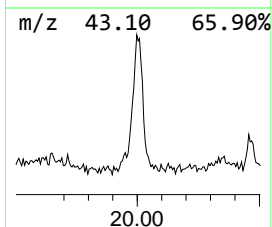
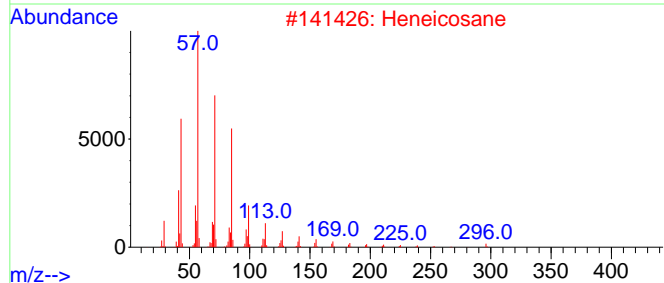
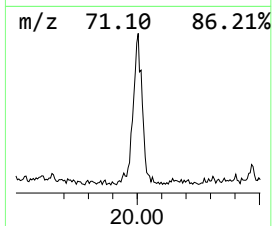
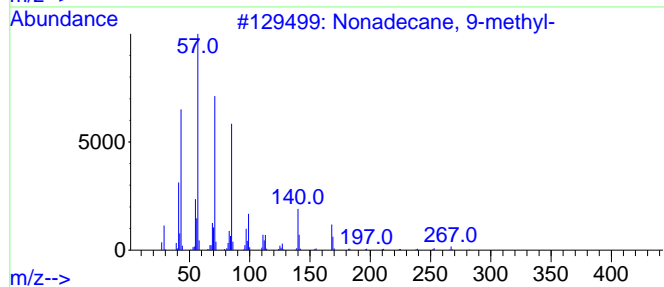
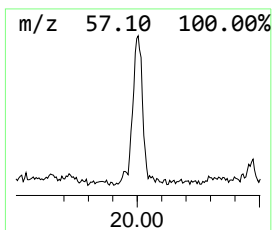
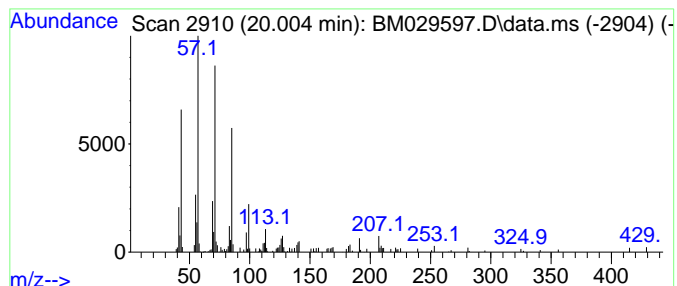
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 Peak Number 5 Nonadecane, 9-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.004	3.69 ng	199131	Chrysene-d12	21.203

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Nonadecane, 9-methyl-	282	C20H42	013287-24-6	94
2		Heneicosane	296	C21H44	000629-94-7	91
3		Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	90
4		Heptadecane	240	C17H36	000629-78-7	90
5		Octacosane	394	C28H58	000630-02-4	87



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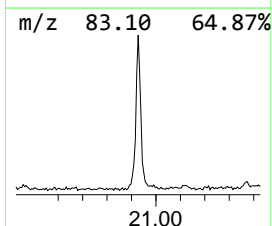
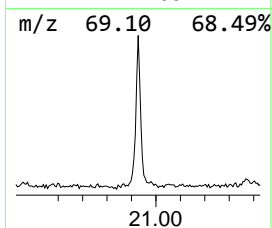
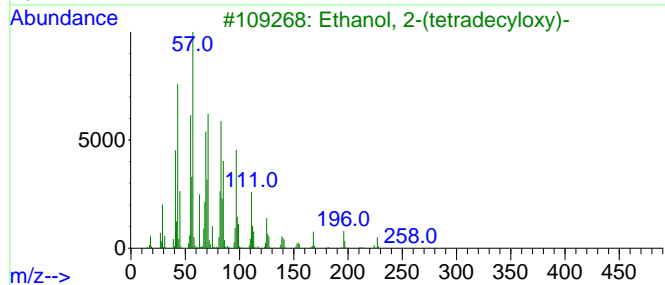
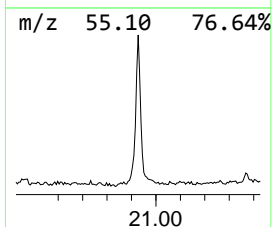
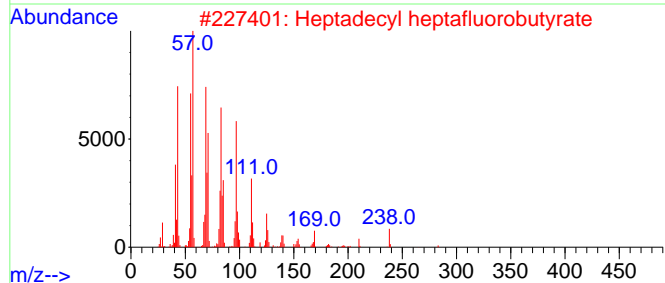
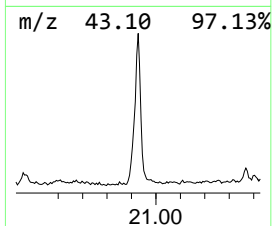
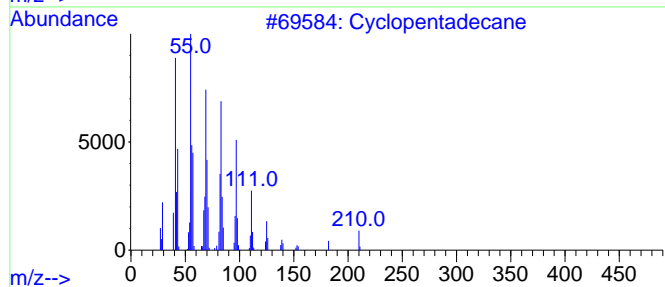
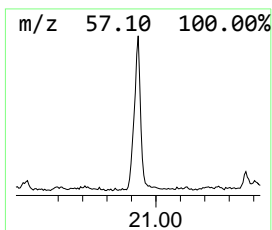
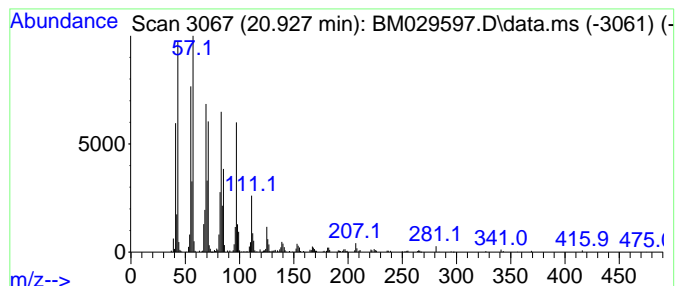
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 6 Cyclopentadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.927	8.49 ng	457958	Chrysene-d12	21.203

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	95
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
3			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
4			Nonadecyl heptafluorobutyrate	480	C23H39F7O2	1000351-83-9	91
5			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042221\
 Data File : BM029597.D
 Acq On : 22 Apr 2021 17:05
 Operator : CG/JU
 Sample : M2106-06
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

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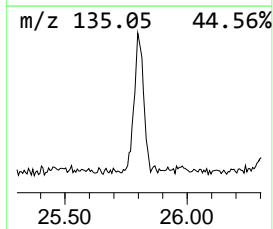
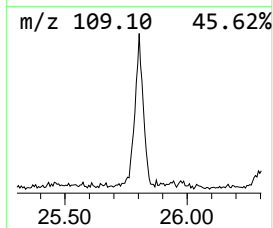
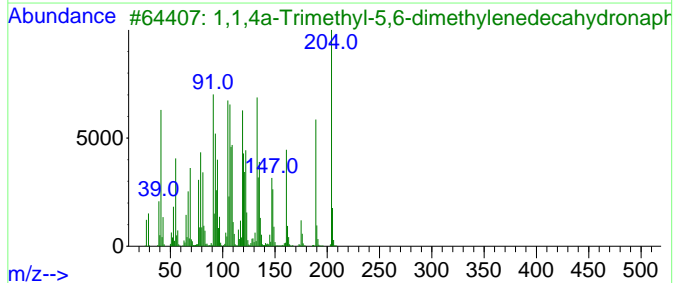
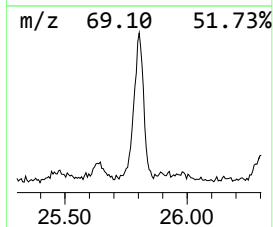
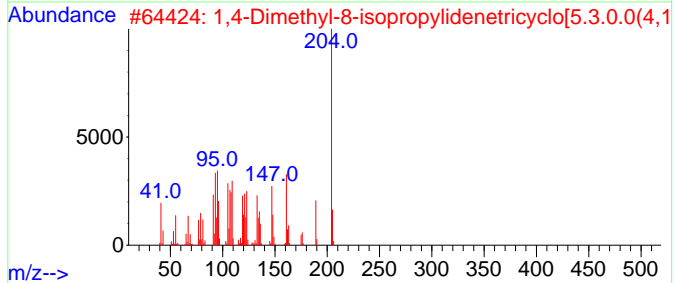
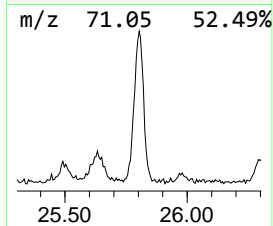
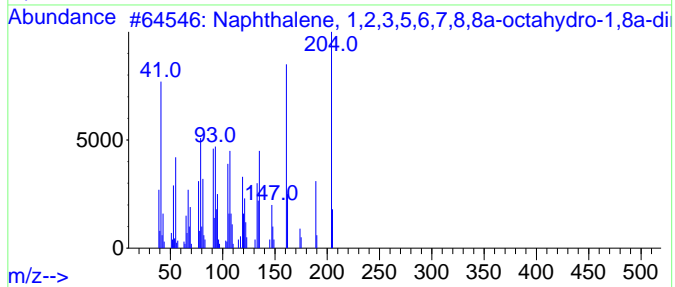
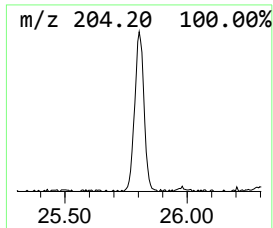
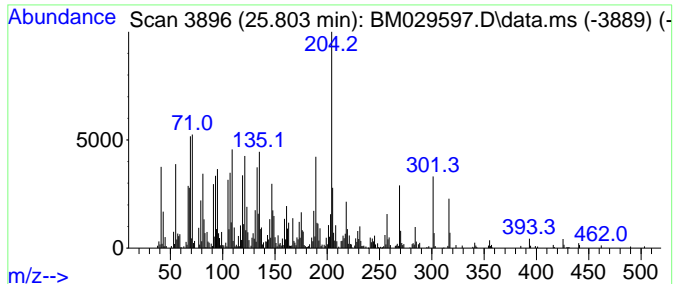
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 7 unknown25.80 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.803	19.65 ng	1125220	Perylene-d12	23.392

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	45
2		1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	38
3		1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	38
4		5-Methyl-4-(0-tolyl)-2-thiazolamine	204	C11H12N2S	016942-68-0	27
5		Pyridine-3-carbonitrile, 5-allyl...	204	C11H12N2S	186337-14-4	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042221\
 Data File : BM029597.D
 Acq On : 22 Apr 2021 17:05
 Operator : CG/JU
 Sample : M2106-06
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SB-23-14.5-15.0

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
Hexathiane	14.828	5.1	ng	171123	3	14.275	675231	20.0
n-Hexadecanoic ...	17.933	28.3	ng	1172540	4	17.021	829111	20.0
Octadecanoic acid	19.215	11.4	ng	613053	5	21.203	1078460	20.0
Phenol, 4,4'-(1...	19.468	4.3	ng	230155	5	21.203	1078460	20.0
Nonadecane, 9-m...	20.004	3.7	ng	199131	5	21.203	1078460	20.0
Cyclopentadecane	20.927	8.5	ng	457958	5	21.203	1078460	20.0
unknown25.80	25.803	19.6	ng	1125220	6	23.392	1145520	20.0