

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042021\
 Data File : BF123656.D
 Acq On : 20 Apr 2021 22:28
 Operator : JU/CG
 Sample : M2076-19
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-19-0-2.0

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_F\METHODS\8270-BF041521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123656.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.057	497	505	510	rBV	47941	66001	1.17%	0.155%
2	5.469	571	575	579	rBV	6244077	5416756	96.21%	12.751%
3	6.481	743	747	759	rVB	5706649	5630392	100.00%	13.253%
4	6.851	806	810	813	rBV	1702171	1498248	26.61%	3.527%
5	7.410	900	905	908	rBV	4345942	3655241	64.92%	8.604%
6	8.133	1024	1028	1031	rBV	2485874	1953938	34.70%	4.599%
7	9.210	1207	1211	1215	rBV	5950659	5618930	99.80%	13.226%
8	9.328	1228	1231	1242	rVB	667756	640689	11.38%	1.508%
9	9.604	1275	1278	1282	rBV	234813	171580	3.05%	0.404%
10	9.892	1323	1327	1330	rBV	2653241	2070165	36.77%	4.873%
11	10.475	1423	1426	1435	rBV	300717	408609	7.26%	0.962%
12	10.680	1457	1461	1464	rBV	4531797	3826717	67.97%	9.008%
13	11.380	1576	1580	1583	rBV	2623616	2090270	37.12%	4.920%
14	11.451	1586	1592	1594	rVB4	51572	61173	1.09%	0.144%
15	11.569	1608	1612	1621	rBV2	45770	82982	1.47%	0.195%
16	11.910	1666	1670	1682	rBV2	235432	254177	4.51%	0.598%
17	12.633	1790	1793	1797	rVB	143674	124633	2.21%	0.293%
18	12.851	1826	1830	1839	rVB2	89001	161990	2.88%	0.381%
19	12.968	1846	1850	1854	rBV	4999580	4892641	86.90%	11.517%
20	13.204	1886	1890	1895	rBV2	61824	89893	1.60%	0.212%
21	13.880	2001	2005	2020	rBV	383947	890683	15.82%	2.097%
22	14.027	2026	2030	2033	rBV	1647109	1434338	25.47%	3.376%
23	15.504	2276	2281	2286	rBV	1114711	1442480	25.62%	3.395%

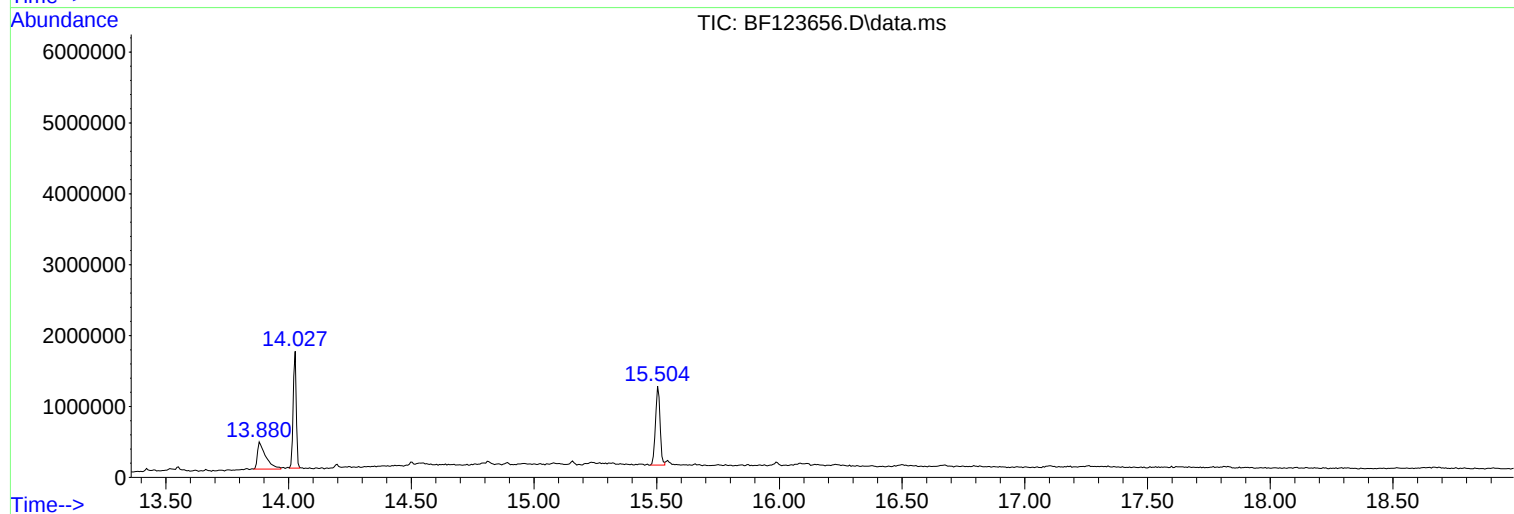
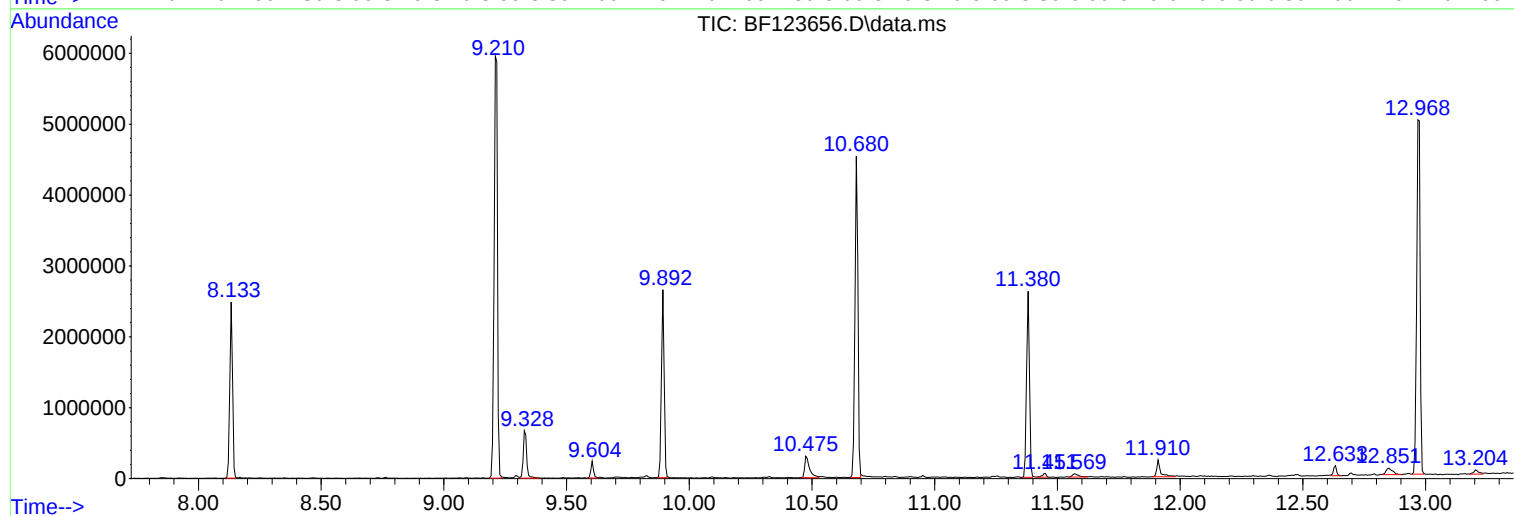
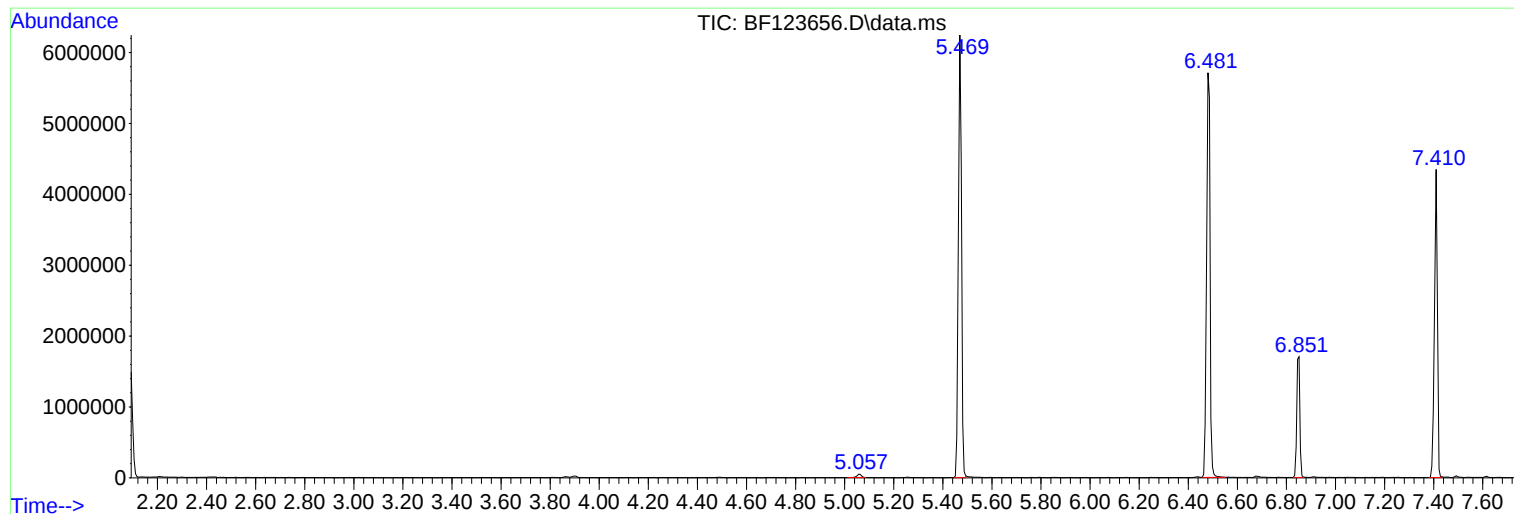
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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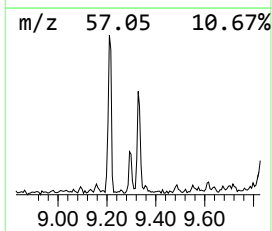
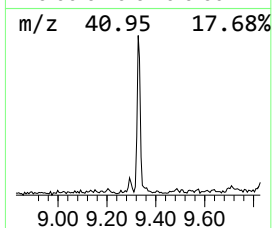
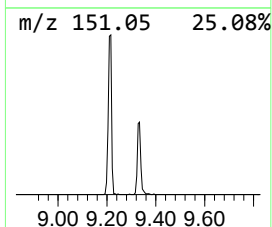
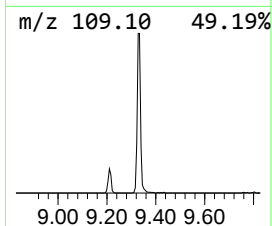
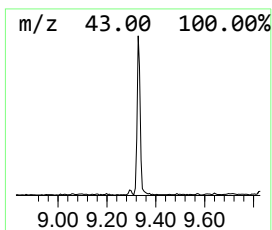
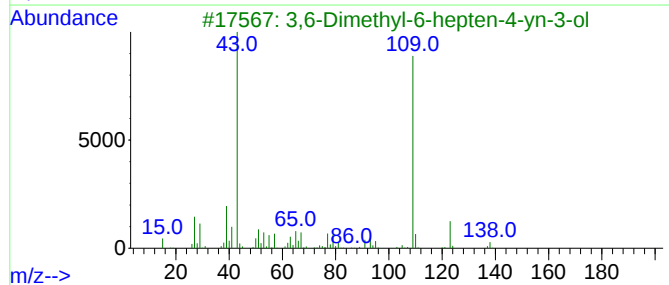
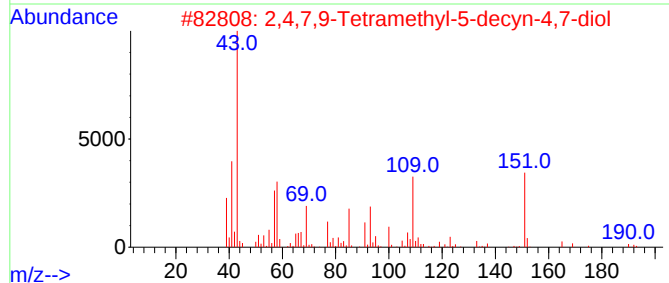
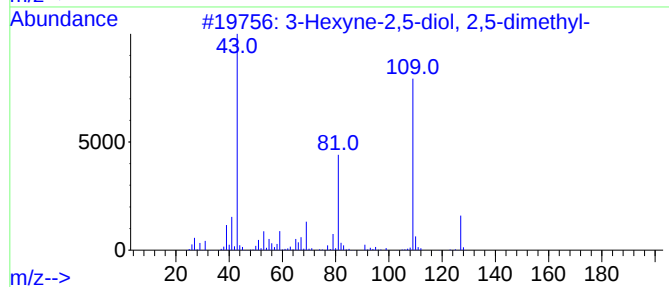
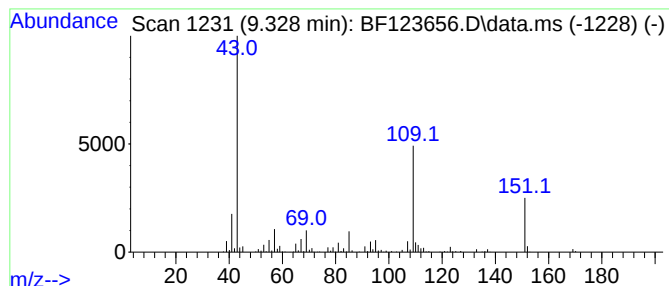
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown9.328 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.328	6.19 ng	640689	Acenaphthene-d10	9.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexyne-2,5-diol, 2,5-dimethyl-	142	C8H14O2	000142-30-3	25
2			2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	17
3			3,6-Dimethyl-6-hepten-4-yn-3-ol	138	C9H14O	003601-67-0	17
4			Cyclohexane, 1R-acetamido-2,3-ci...	213	C10H15NO4	1000153-70-8	12
5			5-Oxohexanenitrile	111	C6H9NO	010412-98-3	10



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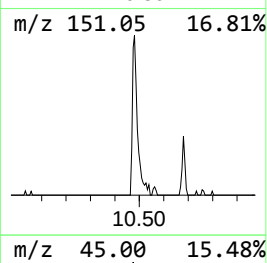
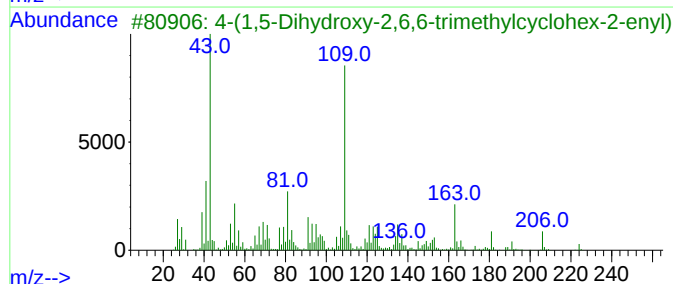
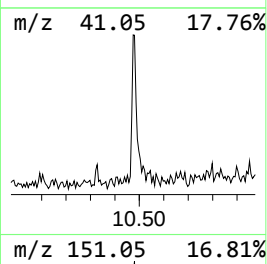
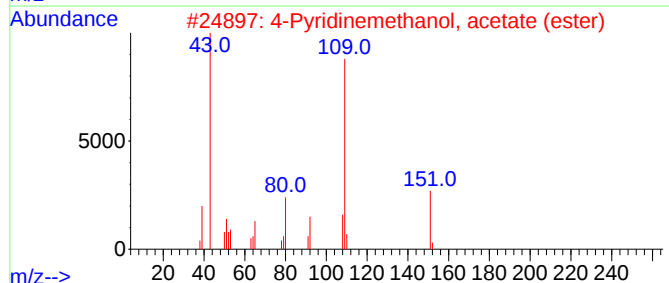
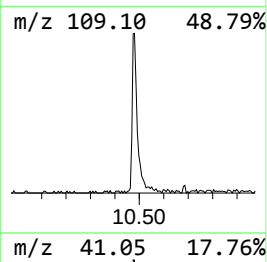
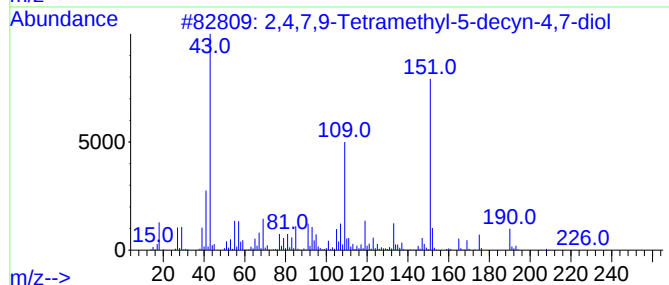
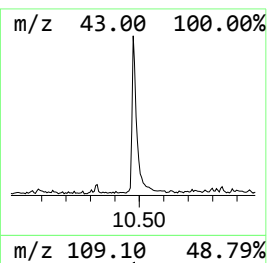
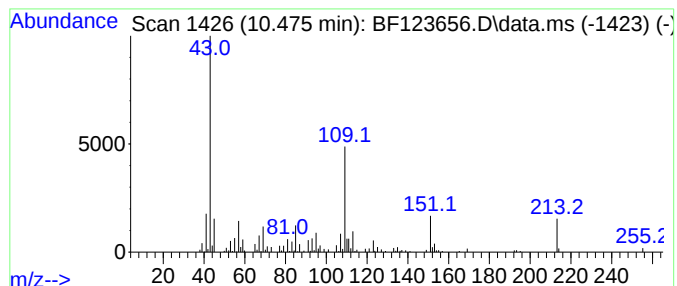
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown10.475 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.475	3.95 ng	408609	Acenaphthene-d10	9.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	38		
2	4-Pyridinemethanol, acetate (ester)	151	C8H9NO2	001007-48-3	32		
3	4-(1,5-Dihydroxy-2,6,6-trimethyl...	224	C13H20O3	1000191-85-2	32		
4	3-Hexyne-2,5-diol, 2,5-dimethyl-	142	C8H14O2	000142-30-3	16		
5	2,4a-Epidioxy-3,4,5,6,7,8-hexahy...	226	C13H22O3	1000212-30-9	12		



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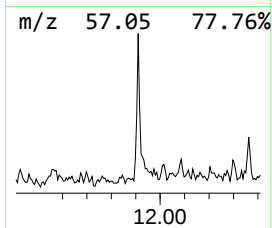
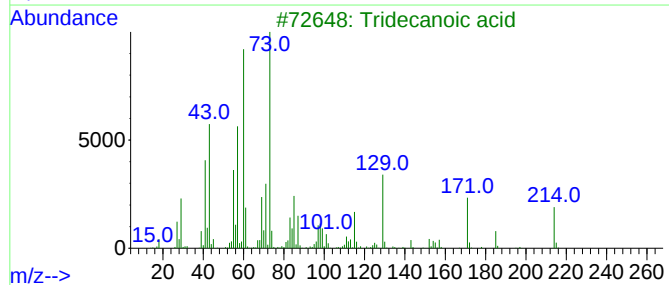
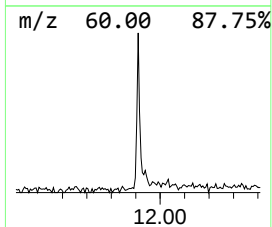
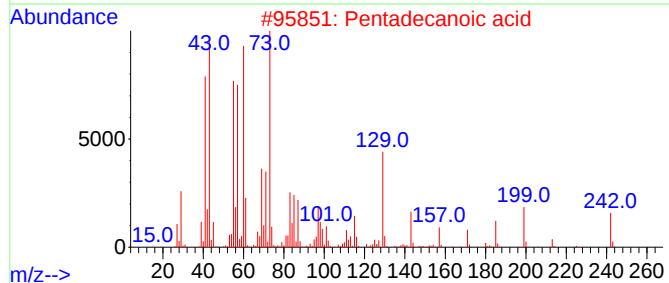
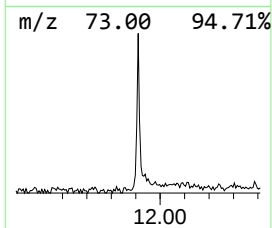
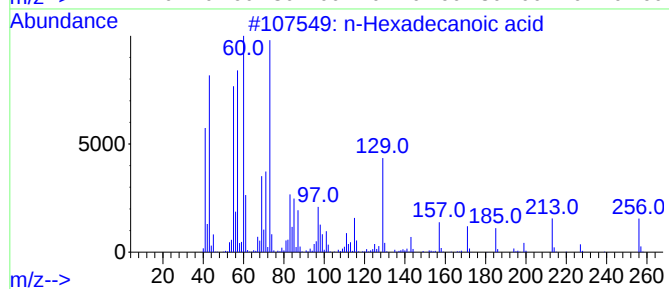
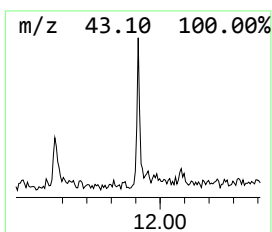
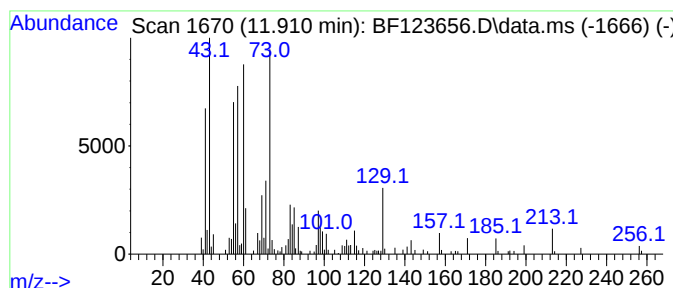
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	2.43 ng	254177	Phenanthrene-d10	11.380

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3			Tridecanoic acid	214	C13H26O2	000638-53-9	74
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



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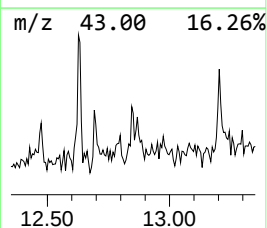
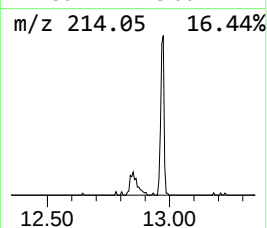
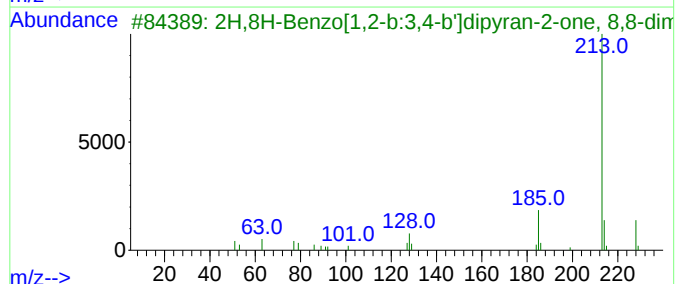
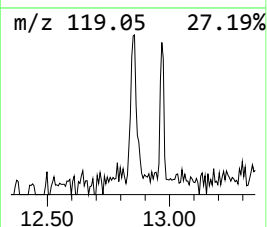
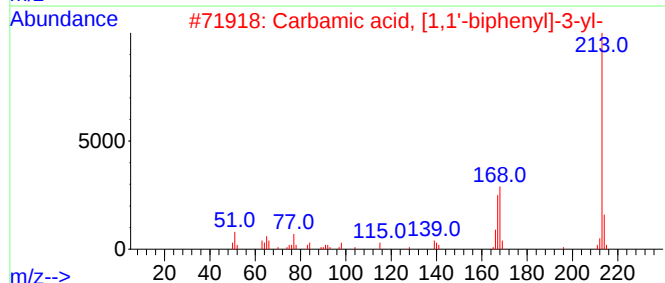
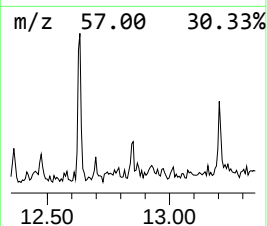
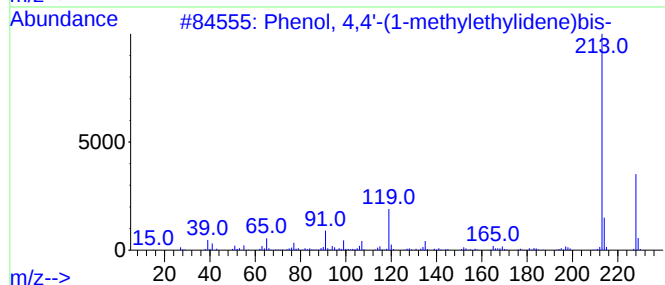
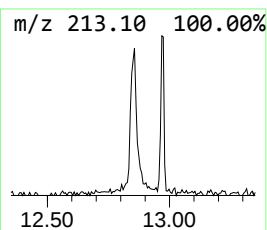
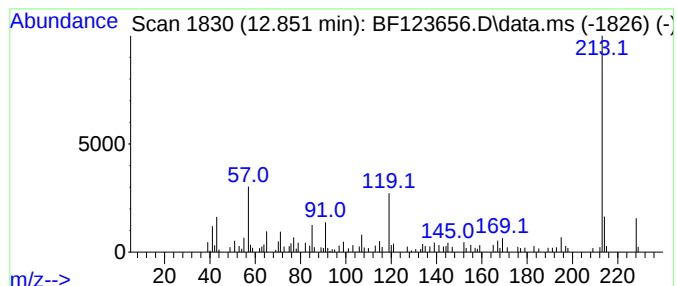
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Peak Number 4 Phenol, 4,4'-(1-methylethyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.851	2.26 ng	161990	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	91
2			Carbamic acid, [1,1'-biphenyl]-3...	213	C13H11NO2	055030-29-0	53
3			2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	52
4			2,5-bis(Trimethylsilyl)thiophene	228	C10H20SSi2	017906-71-7	50
5			Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	49



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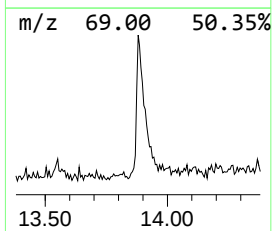
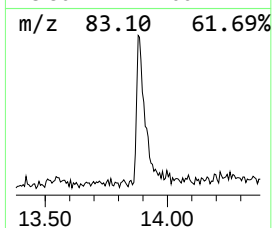
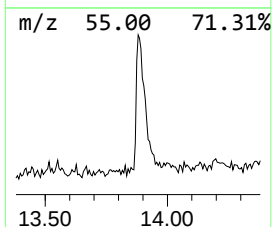
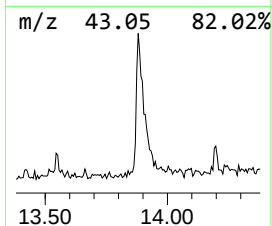
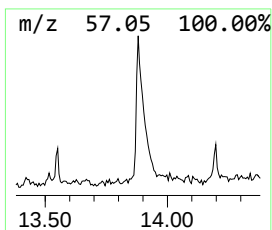
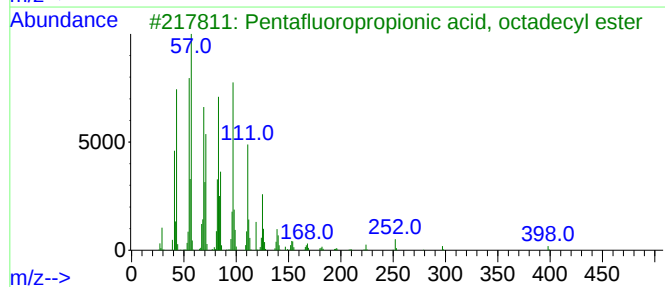
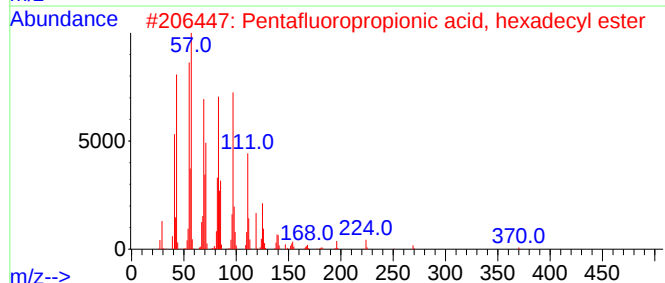
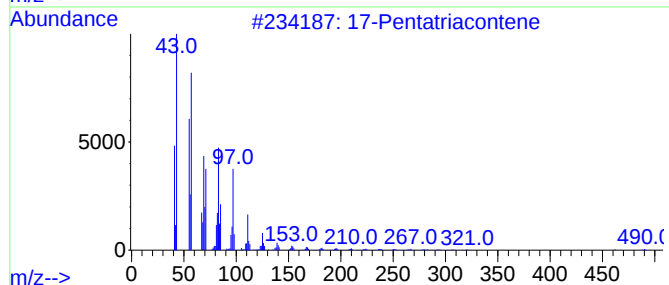
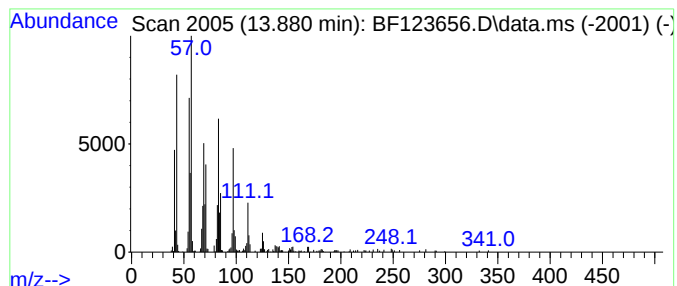
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 17-Pentatriacontene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	12.42 ng	890683	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17-Pentatriacontene	491	C35H70	006971-40-0	91
2			Pentafluoropropionic acid, hexadecyl ester	388	C19H33F5O2	006222-07-7	90
3			Pentafluoropropionic acid, octadecyl ester	416	C21H37F5O2	959261-25-7	90
4			Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	87
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown9.328	9.328	6.2	ng	640689	3	9.892	2070170	20.0
unknown10.475	10.475	4.0	ng	408609	3	9.892	2070170	20.0
n-Hexadecanoic ...	11.910	2.4	ng	254177	4	11.380	2090270	20.0
Phenol, 4,4'-(1...	12.851	2.3	ng	161990	5	14.027	1434340	20.0
17-Pentatriacon...	13.880	12.4	ng	890683	5	14.027	1434340	20.0