

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042221\
 Data File : BP005371.D
 Acq On : 22 Apr 2021 12:35
 Operator : CG/JU
 Sample : M2036-05
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 RT-80-W-ROCKAWAY-B-1

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_P\Methods\8270E-BP042121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005371.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.246	359	367	379	rBV	662520	951695	38.20%	8.294%
2	6.834	625	637	651	rBV	608115	1001197	40.19%	8.725%
3	7.640	767	774	781	rBV	136157	214952	8.63%	1.873%
4	8.805	964	972	980	rBV	375237	611053	24.53%	5.325%
5	10.428	1240	1248	1259	rBV	146526	256796	10.31%	2.238%
6	12.916	1664	1671	1682	rBV	808401	1169466	46.94%	10.192%
7	13.769	1810	1816	1826	rBV2	13834	26735	1.07%	0.233%
8	14.304	1900	1907	1915	rBV	226510	337392	13.54%	2.940%
9	15.804	2153	2162	2182	rBV	845534	1245880	50.01%	10.858%
10	16.210	2225	2231	2237	rVB4	15441	28297	1.14%	0.247%
11	16.275	2237	2242	2246	rBV3	14842	26826	1.08%	0.234%
12	16.475	2270	2276	2283	rVB6	16939	31161	1.25%	0.272%
13	17.069	2371	2377	2382	rBV	312291	459131	18.43%	4.001%
14	17.969	2525	2530	2538	rBV	170831	233635	9.38%	2.036%
15	18.698	2650	2654	2658	rVB	48434	57754	2.32%	0.503%
16	19.092	2717	2721	2729	rVB	55403	76262	3.06%	0.665%
17	19.210	2737	2741	2749	rBV2	71961	101621	4.08%	0.886%
18	19.469	2782	2785	2796	rVB	69885	109874	4.41%	0.958%
19	19.645	2809	2815	2821	rBV	2119976	2491365	100.00%	21.712%
20	20.304	2924	2927	2933	rVB	32542	45455	1.82%	0.396%
21	20.510	2958	2962	2966	rBV	137921	166197	6.67%	1.448%
22	20.551	2967	2969	2972	rVB2	25052	25395	1.02%	0.221%
23	20.886	3021	3026	3035	rBV	222773	341426	13.70%	2.976%
24	21.169	3069	3074	3078	rBV	582804	697545	28.00%	6.079%
25	22.727	3335	3339	3345	rBV5	63254	115219	4.62%	1.004%
26	23.427	3452	3458	3467	rVB2	380267	652087	26.17%	5.683%

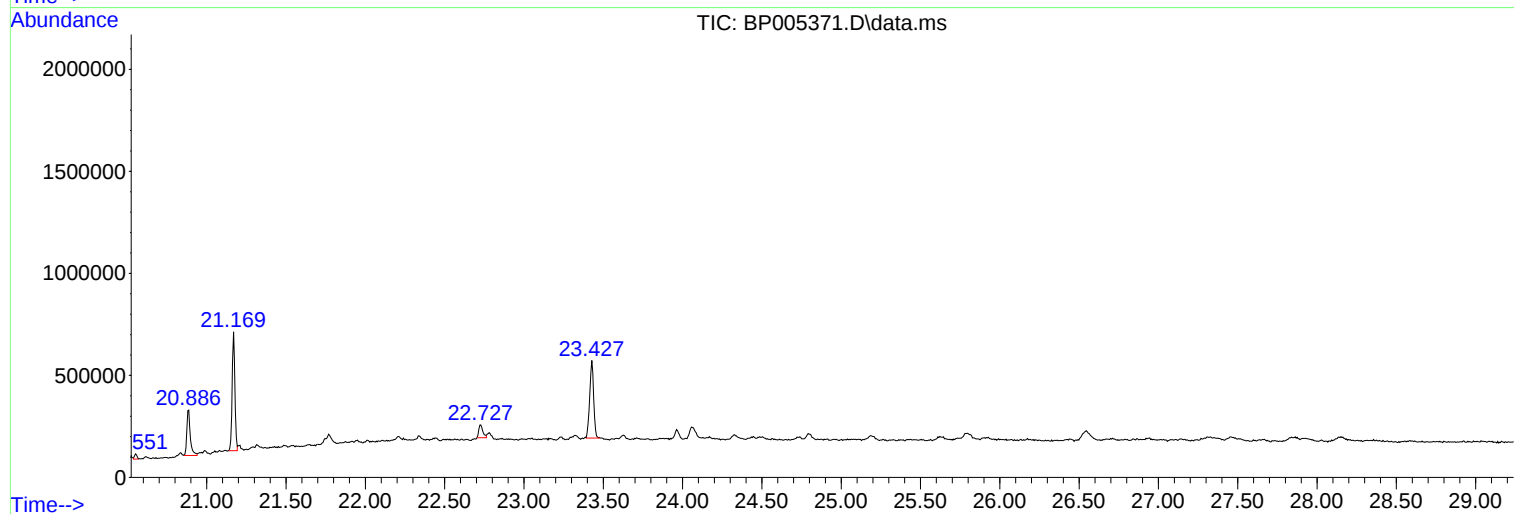
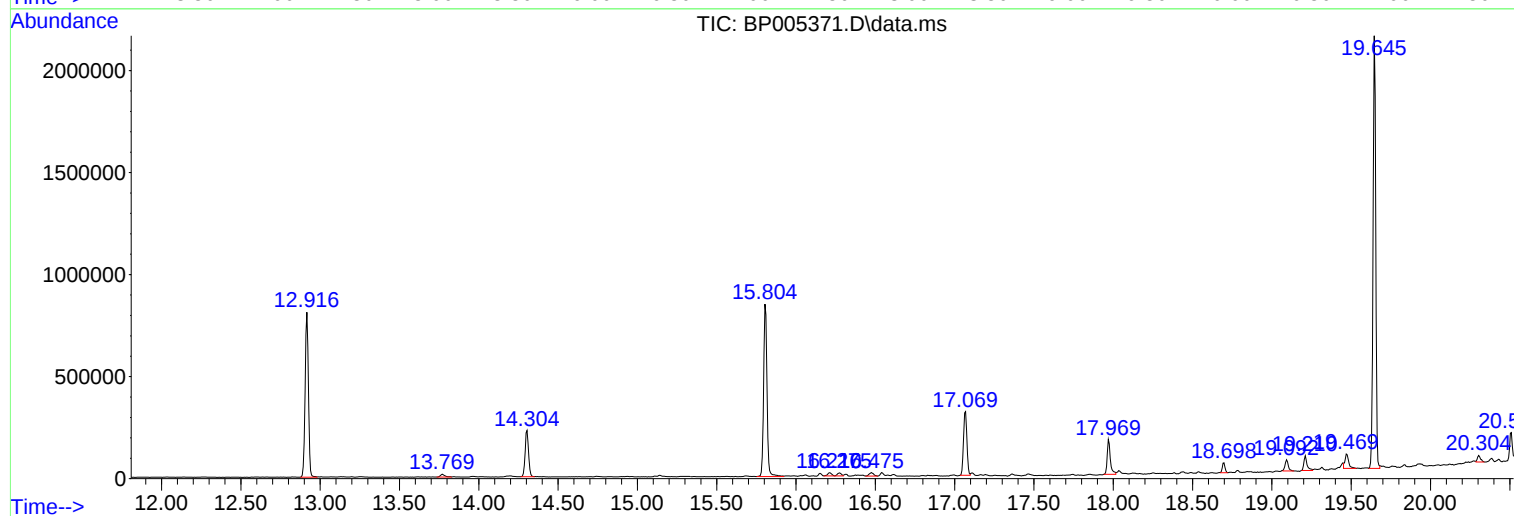
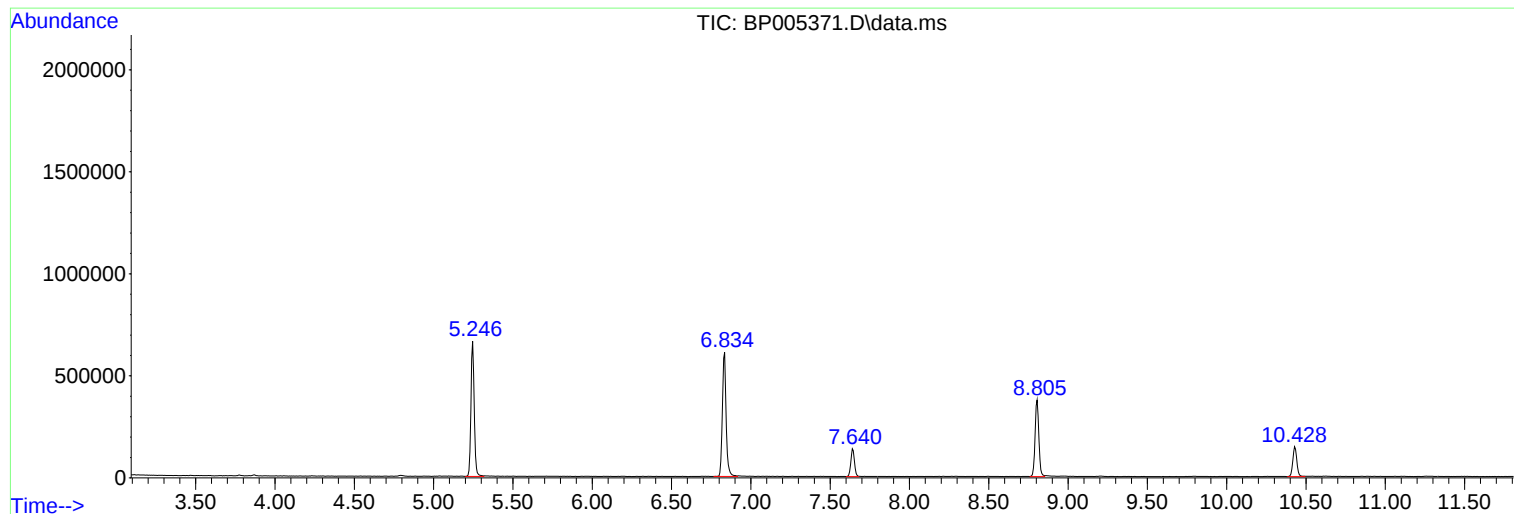
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RT-80-W-ROCKAWAY-B-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.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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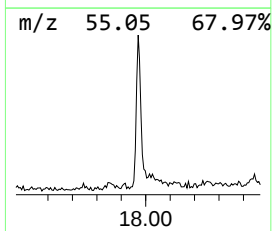
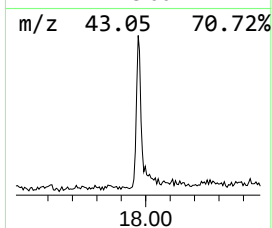
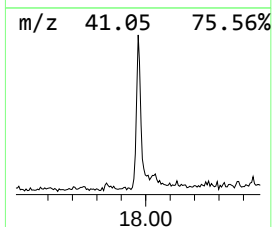
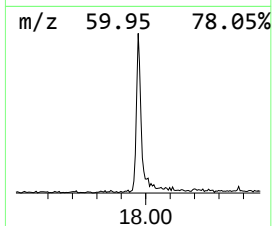
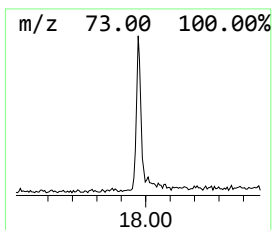
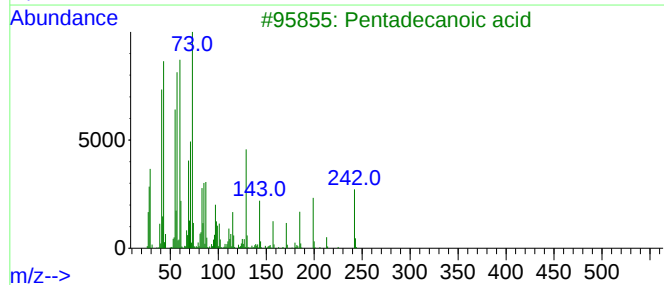
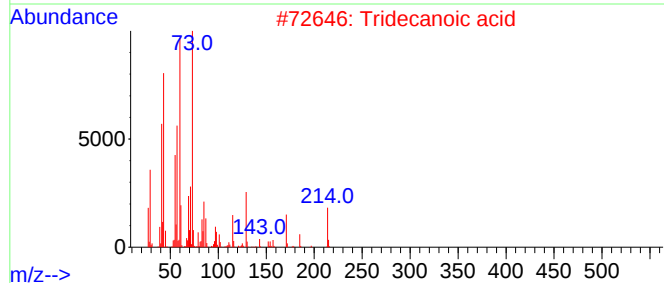
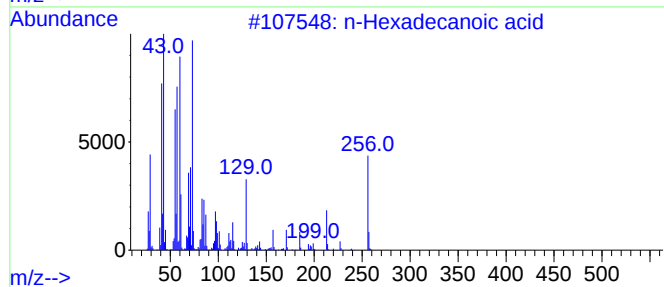
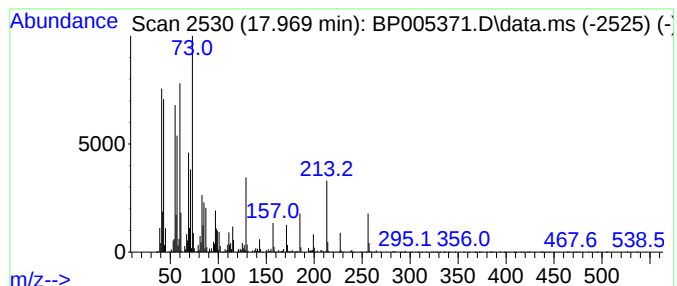
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.969	10.18 ng	233635	Phenanthrene-d10	17.069

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	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Octadecanoic acid	284	C18H36O2	000057-11-4	76
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



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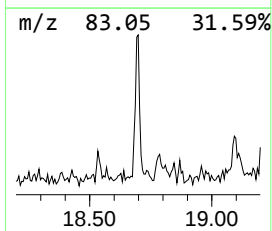
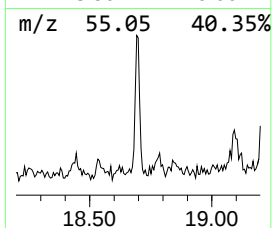
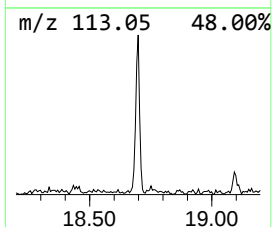
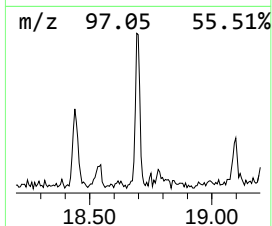
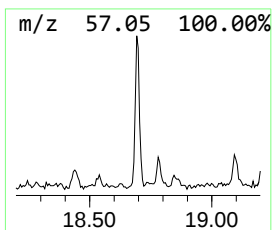
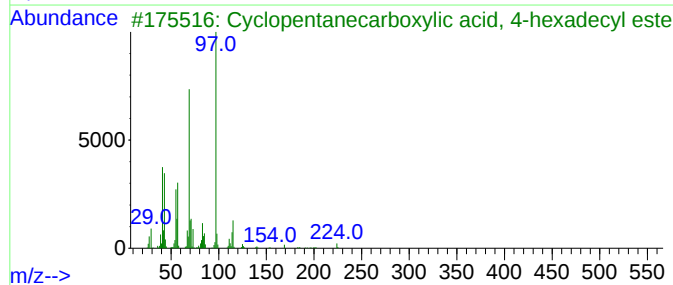
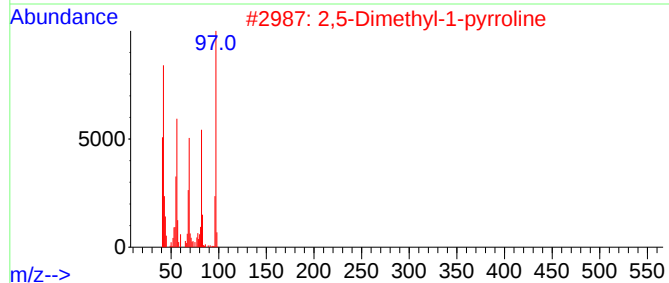
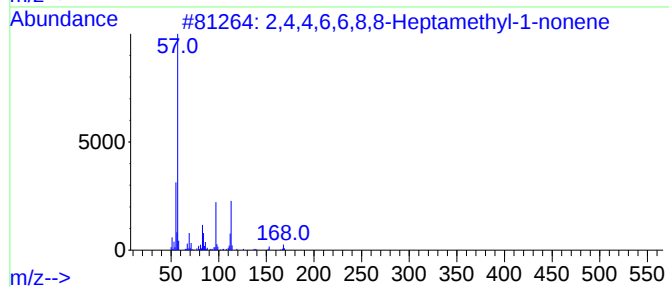
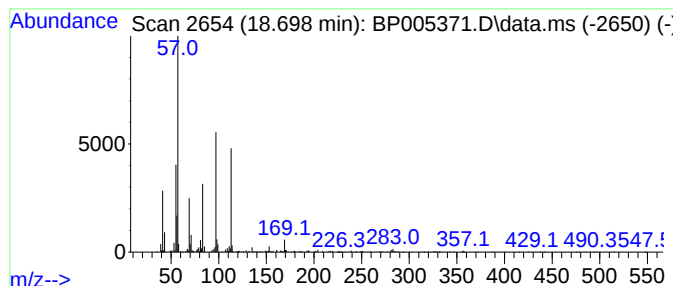
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown18.69 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.698	2.52 ng	57754	Phenanthrene-d10	17.069

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	32		
2	2,5-Dimethyl-1-pyrroline	97	C6H11N	000822-64-0	30		
3	Cyclopentanecarboxylic acid, 4-h...	338	C22H42O2	1000282-77-5	22		
4	1H-Pyrazole-1-carboxamide, 4,5-d...	155	C7H13N3O	003786-02-5	16		
5	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	16		



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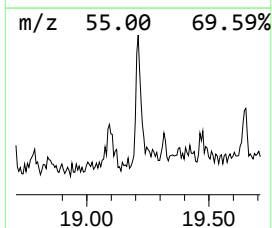
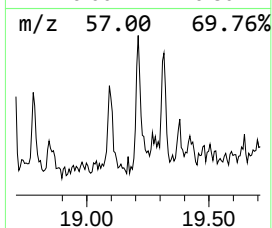
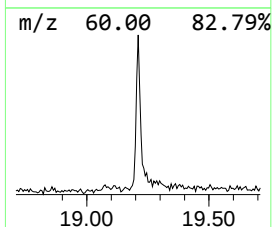
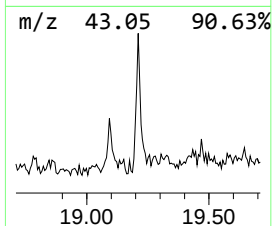
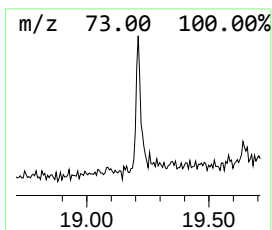
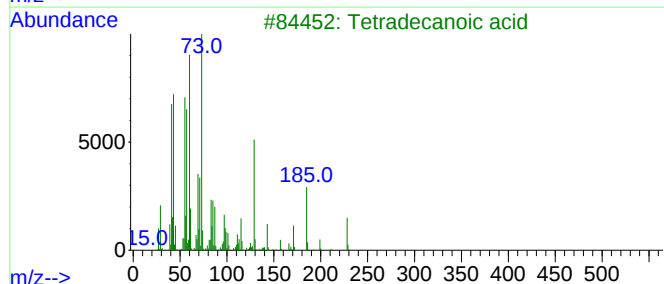
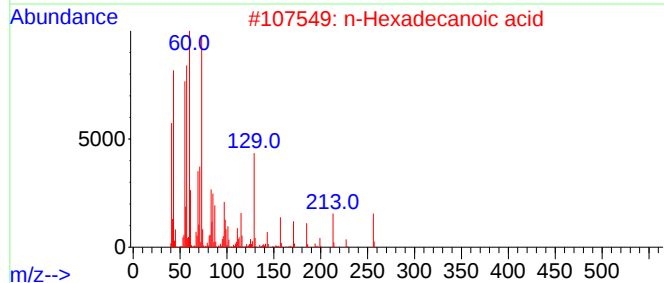
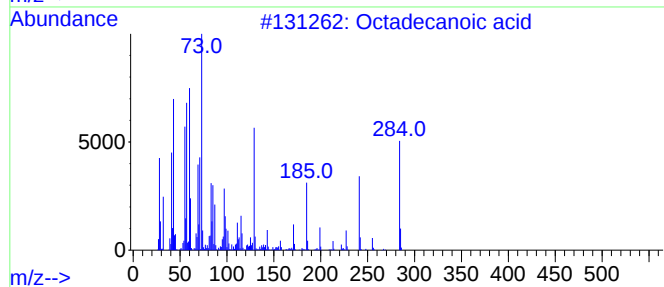
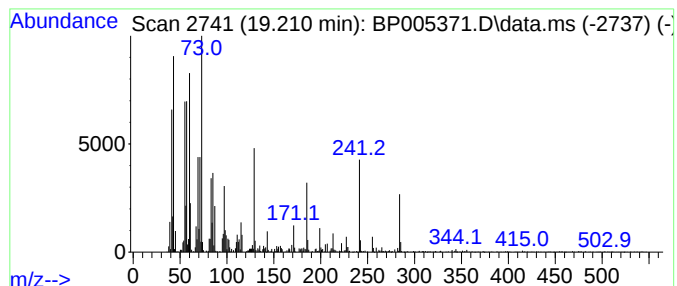
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.210	2.91 ng	101621	Chrysene-d12	21.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	91
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4			n-Decanoic acid	172	C10H20O2	000334-48-5	64
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	64



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ALS Vial : 7 Sample Multiplier: 1

Instrument :
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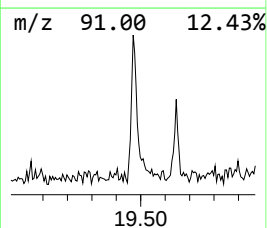
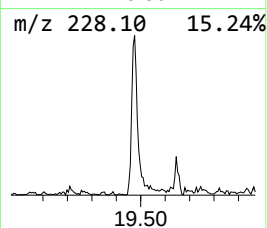
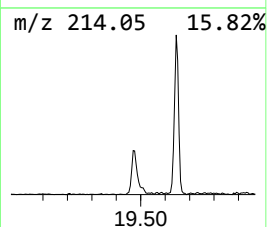
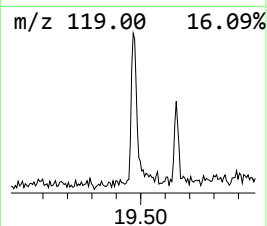
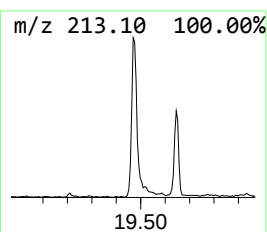
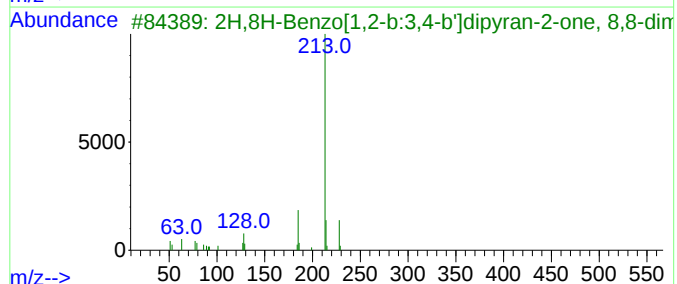
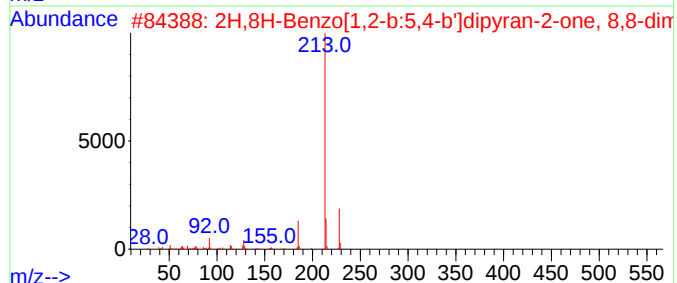
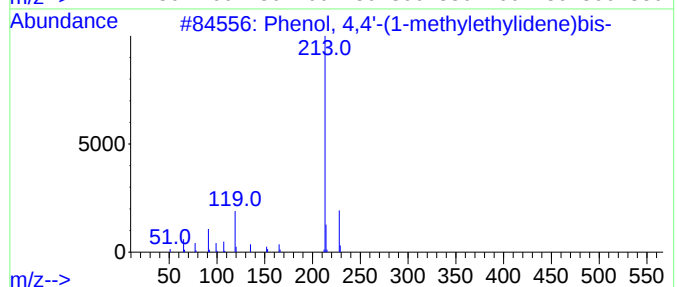
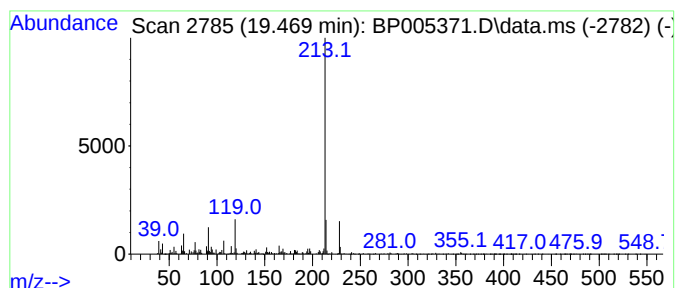
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Peak Number 5 Phenol, 4,4'-(1-methylethyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.469	3.15 ng	109874	Chrysene-d12	21.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	93
2			2H,8H-Benzo[1,2-b:5,4-b']dipyr...	228	C14H12O3	000553-19-5	72
3			2H,8H-Benzo[1,2-b:3,4-b']dipyr...	228	C14H12O3	000523-59-1	64
4			Pyridine, 3-(5-trifluoromethyl-3...	213	C9H6F3N3	003974-70-7	59
5			Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	58



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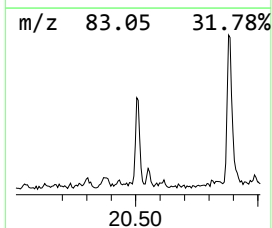
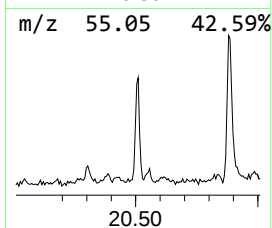
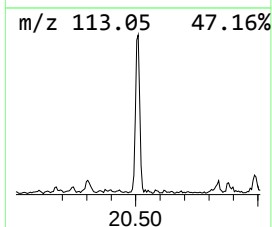
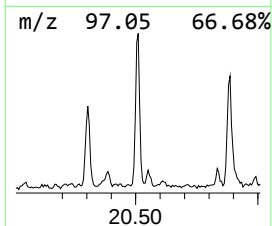
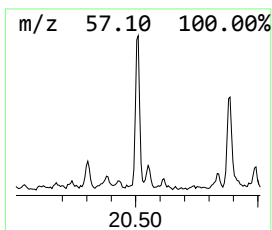
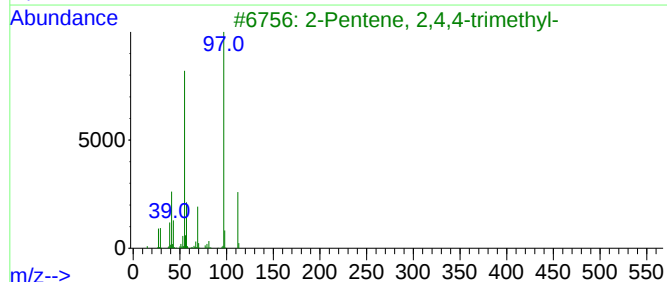
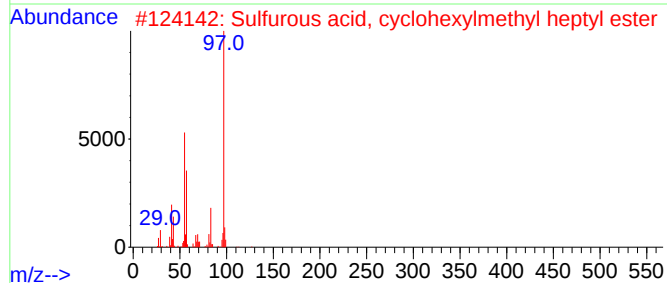
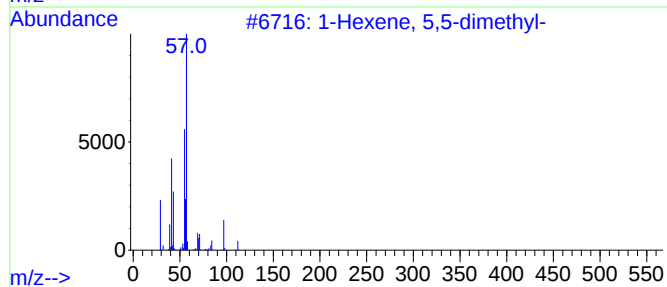
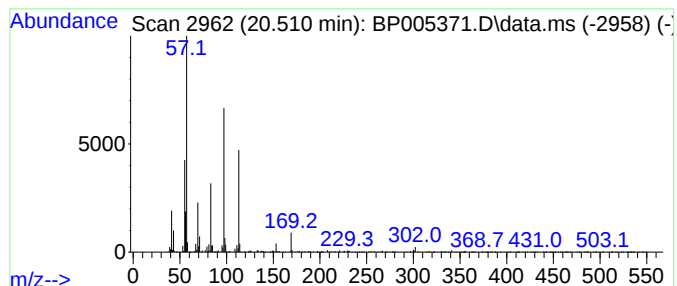
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 unknown20.51 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.510	4.77 ng	166197	Chrysene-d12	21.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexene, 5,5-dimethyl-	112	C8H16	007116-86-1	35
2			Sulfurous acid, cyclohexylmethyl...	276	C14H28O3S	1000309-21-7	35
3			2-Pentene, 2,4,4-trimethyl-	112	C8H16	000107-40-4	22
4			Sulfurous acid, cyclohexylmethyl...	332	C18H36O3S	1000309-21-9	16
5			3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	14



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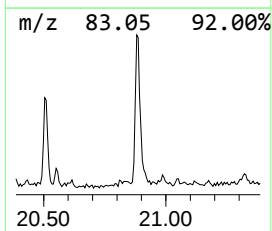
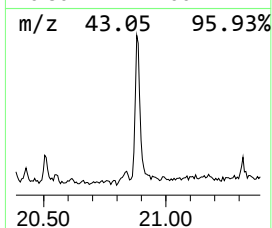
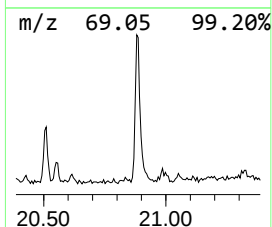
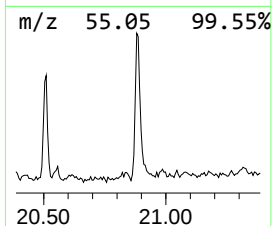
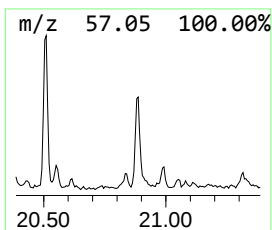
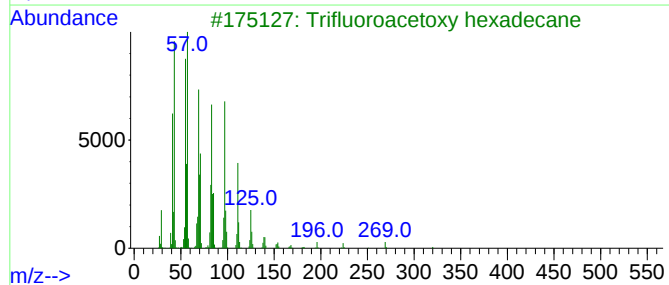
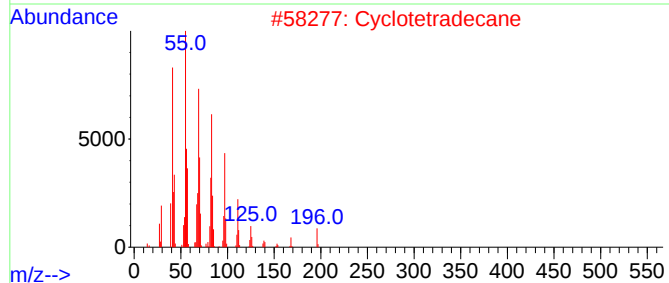
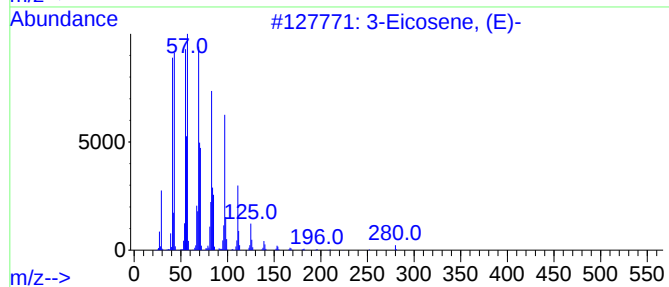
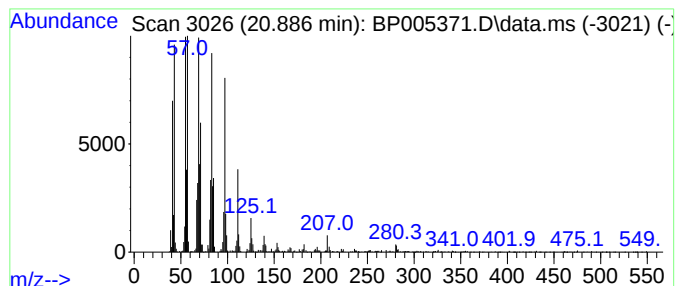
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 3-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.886	9.79 ng	341426	Chrysene-d12	21.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Eicosene, (E)-	280	C20H40	074685-33-9	94
2			Cyclotetradecane	196	C14H28	000295-17-0	93
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4			1-Heptacosanol	396	C27H56O	002004-39-9	91
5			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042221\
Data File : BP005371.D
Acq On : 22 Apr 2021 12:35
Operator : CG/JU
Sample : M2036-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RT-80-W-ROCKAWAY-B-1

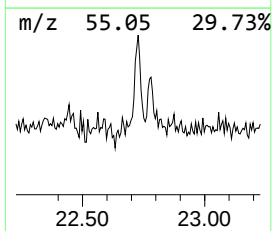
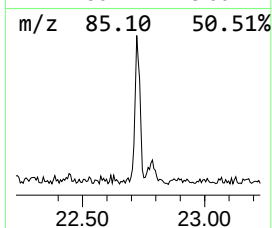
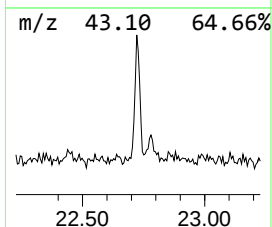
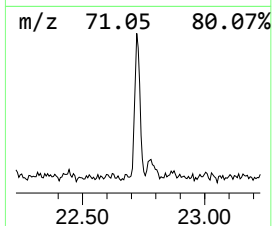
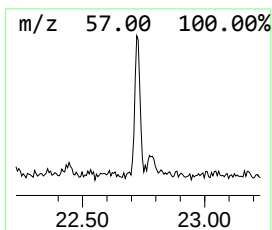
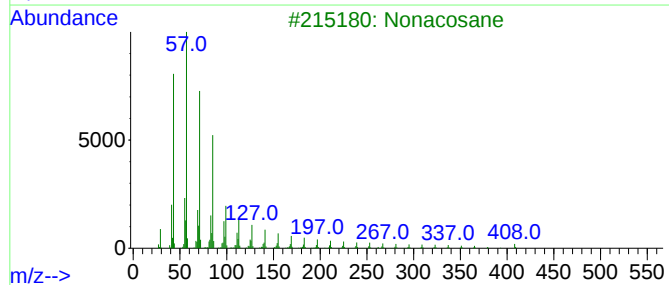
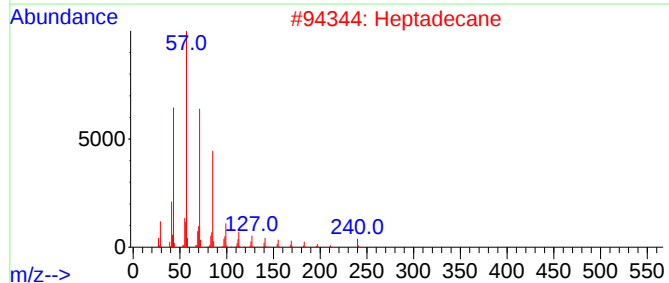
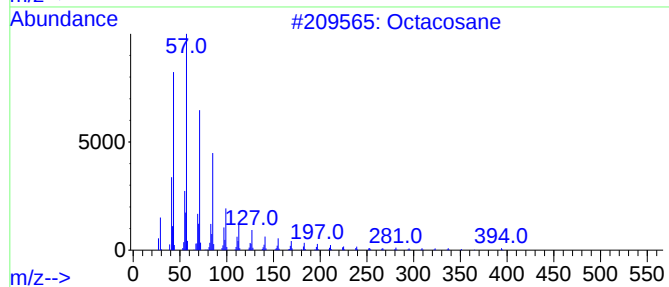
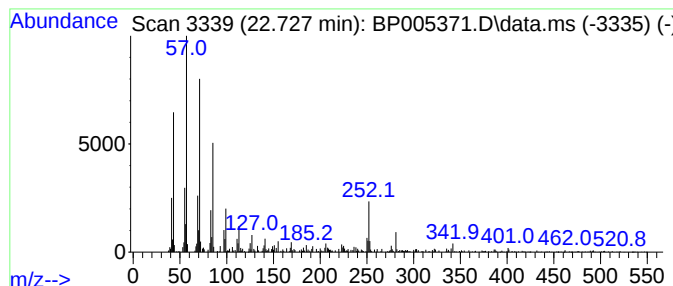
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.727	3.53 ng	115219	Perylene-d12	23.427

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane	394	C28H58	000630-02-4	95
2		Heptadecane	240	C17H36	000629-78-7	93
3		Nonacosane	408	C29H60	000630-03-5	89
4		Hexadecane	226	C16H34	000544-76-3	89
5		Pentacosane	352	C25H52	000629-99-2	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042221\
Data File : BP005371.D
Acq On : 22 Apr 2021 12:35
Operator : CG/JU
Sample : M2036-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RT-80-W-ROCKAWAY-B-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.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
n-Hexadecanoic ...	17.969	10.2	ng	233635	4	17.069	459131	20.0
unknown18.69	18.698	2.5	ng	57754	4	17.069	459131	20.0
Octadecanoic acid	19.210	2.9	ng	101621	5	21.169	697545	20.0
Phenol, 4,4'-(1...	19.469	3.1	ng	109874	5	21.169	697545	20.0
unknown20.51	20.510	4.8	ng	166197	5	21.169	697545	20.0
3-Eicosene, (E)-	20.886	9.8	ng	341426	5	21.169	697545	20.0
Octacosane	22.727	3.5	ng	115219	6	23.427	652087	20.0