

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020323\
 Data File : BF132330.D
 Acq On : 03 Feb 2023 19:38
 Operator : CG\JU
 Sample : 01409-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 38414

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-BF013123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132330.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.307	413	420	432	rVB	1184690	1625092	33.61%	4.149%
2	5.684	479	484	487	rBV	3420518	3655225	75.60%	9.332%
3	6.672	646	652	655	rBV	3045286	3741010	77.37%	9.551%
4	7.054	714	717	721	rVB	1471861	1242065	25.69%	3.171%
5	7.619	808	813	816	rBV	2524272	2567484	53.10%	6.555%
6	8.343	932	936	939	rBV	2150653	1687468	34.90%	4.308%
7	9.425	1115	1120	1123	rBV	4963888	4835089	100.00%	12.344%
8	10.107	1232	1236	1239	rBV	2301536	1878951	38.86%	4.797%
9	10.819	1354	1357	1360	rVB	201143	154872	3.20%	0.395%
10	10.901	1366	1371	1374	rBV	3501071	3054406	63.17%	7.798%
11	10.995	1384	1387	1394	rVB	89722	90294	1.87%	0.231%
12	11.607	1487	1491	1493	rBV	1973210	1786298	36.94%	4.560%
13	11.625	1493	1494	1498	rVB	86489	68228	1.41%	0.174%
14	12.113	1573	1577	1583	rBV	660194	630523	13.04%	1.610%
15	12.825	1692	1698	1703	rBV	265165	253403	5.24%	0.647%
16	12.901	1708	1711	1723	rVB	187675	187326	3.87%	0.478%
17	13.060	1731	1738	1743	rBV	163021	209573	4.33%	0.535%
18	13.201	1757	1762	1765	rBV	3711775	3630302	75.08%	9.268%
19	14.083	1909	1912	1926	rVB2	391365	516583	10.68%	1.319%
20	14.225	1933	1936	1938	rBV	56444	56239	1.16%	0.144%
21	14.266	1938	1943	1946	rVV	1193400	1164842	24.09%	2.974%
22	14.289	1946	1947	1953	rVV	132447	100613	2.08%	0.257%
23	14.354	1953	1958	1964	rVV	393256	403207	8.34%	1.029%
24	14.407	1964	1967	1974	rVB	54390	66100	1.37%	0.169%
25	14.730	2017	2022	2030	rBV2	65317	141673	2.93%	0.362%
26	14.901	2046	2051	2055	rBV	3806891	3877293	80.19%	9.898%
27	15.366	2127	2130	2134	rBV	59033	90485	1.87%	0.231%
28	15.430	2138	2141	2144	rVB	48334	51710	1.07%	0.132%
29	15.771	2196	2199	2205	rVB	42764	54668	1.13%	0.140%
30	15.848	2206	2212	2222	rVB	783236	1093957	22.63%	2.793%
31	16.148	2259	2263	2267	rVB2	57874	81081	1.68%	0.207%
32	16.342	2292	2296	2301	rVB2	45345	69772	1.44%	0.178%
33	18.836	2715	2720	2734	rVB3	39653	104968	2.17%	0.268%

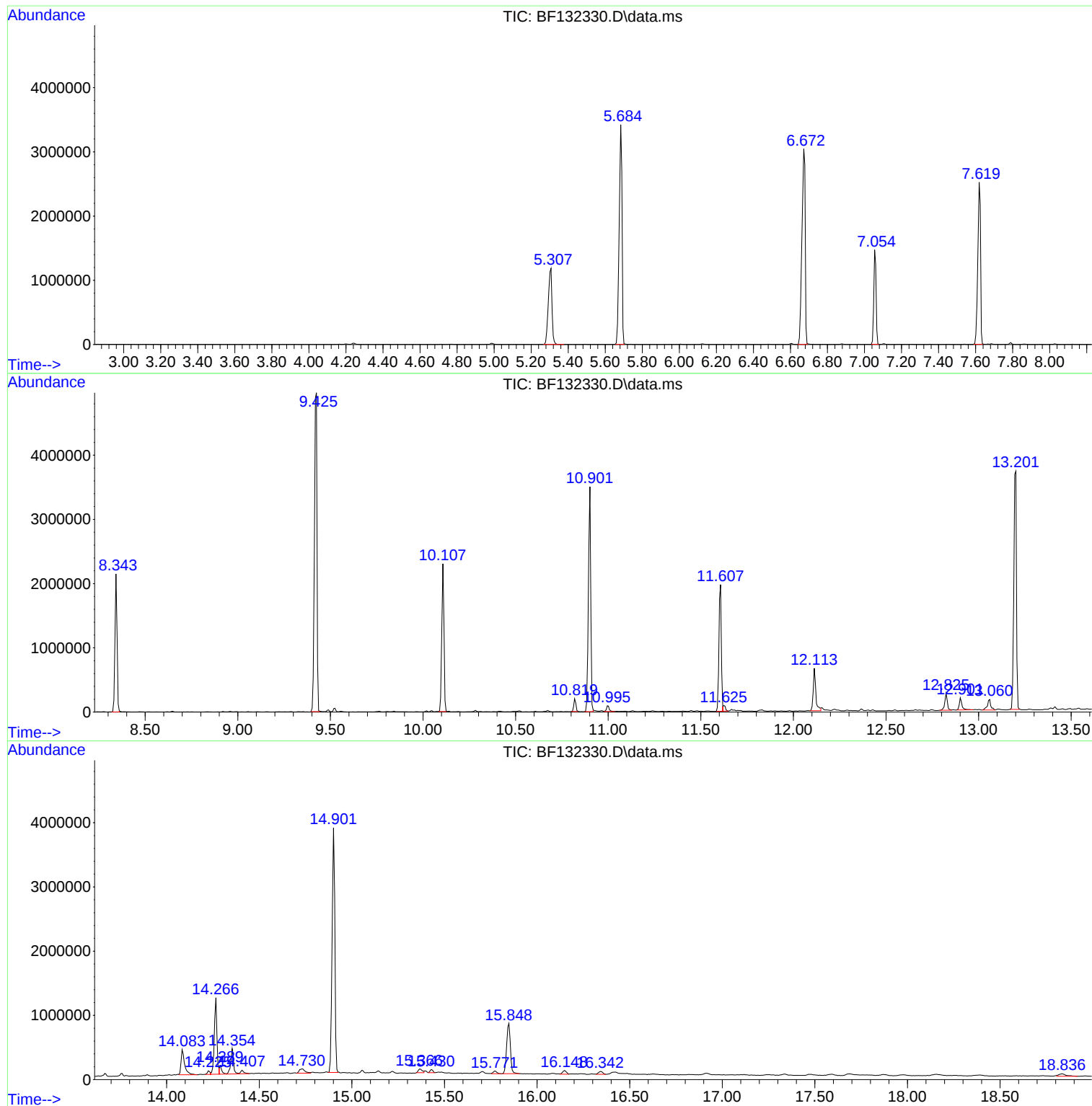
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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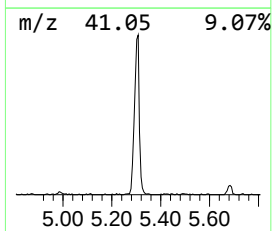
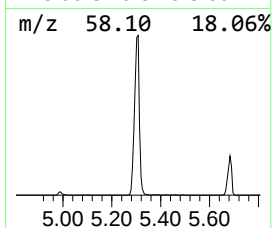
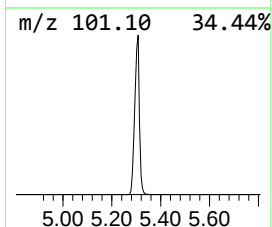
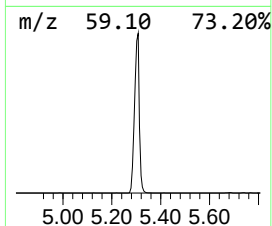
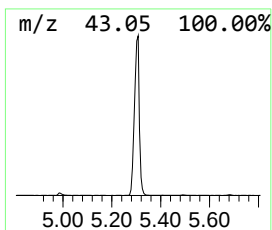
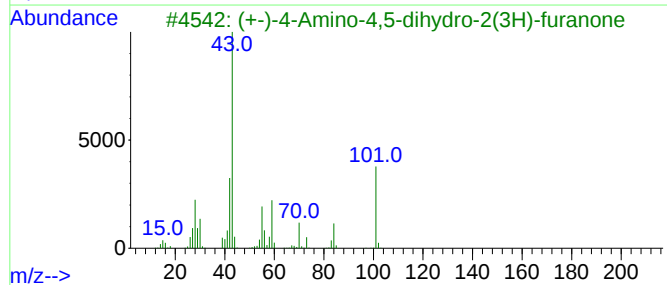
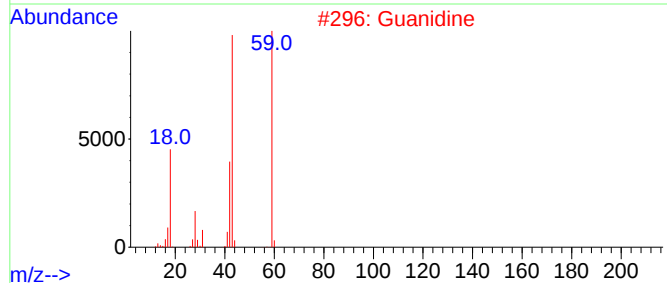
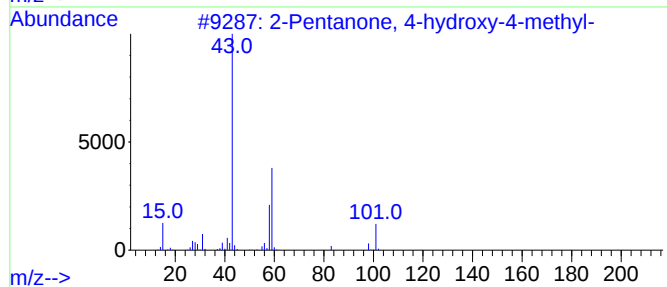
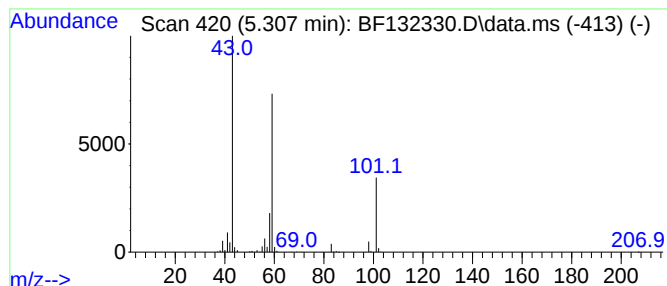
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TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.307	26.17 ng	1625090	1,4-Dichlorobenzene-d4	7.054

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Guanidine	59	CH5N3	000113-00-8	50
3			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	35
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	28
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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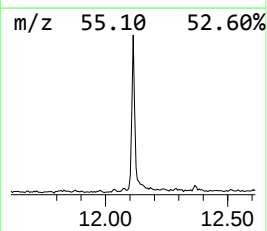
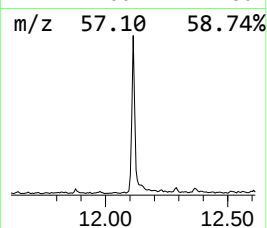
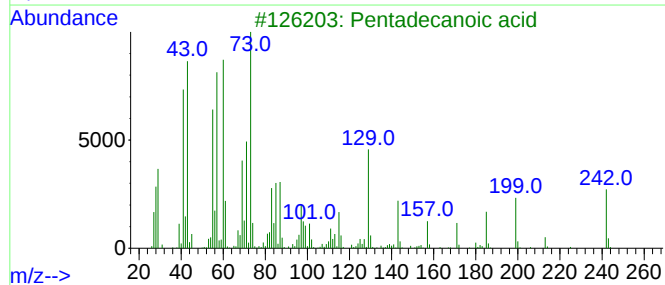
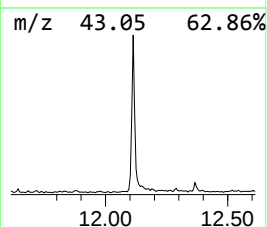
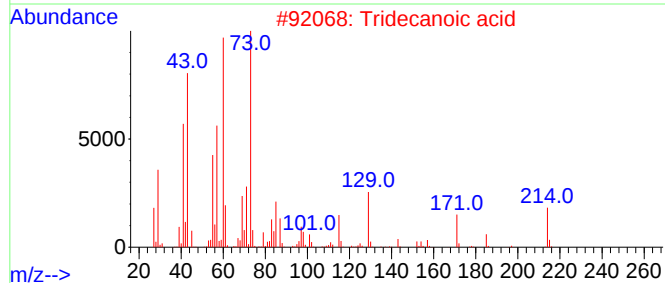
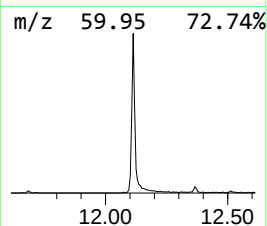
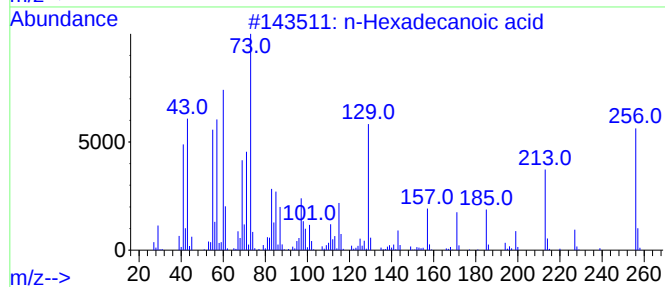
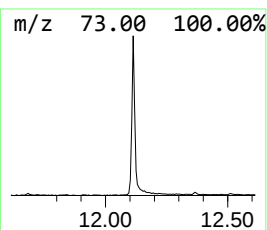
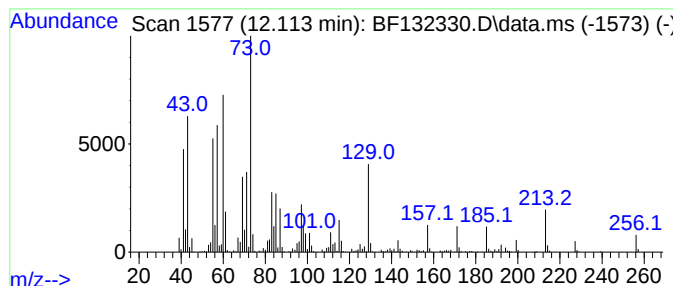
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.113	7.06 ng	630523	Phenanthrene-d10	11.607

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	89
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4		n-Decanoic acid	172	C10H20O2	000334-48-5	60
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	59



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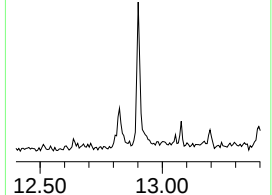
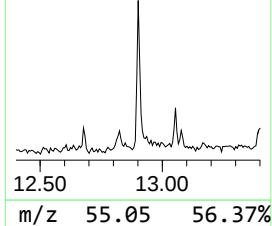
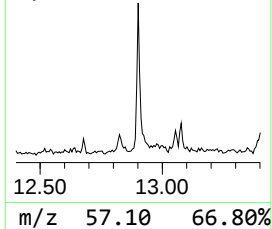
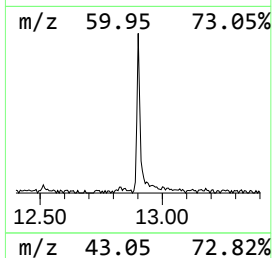
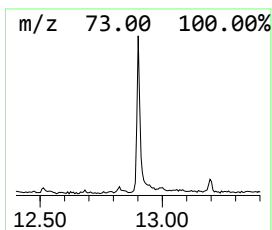
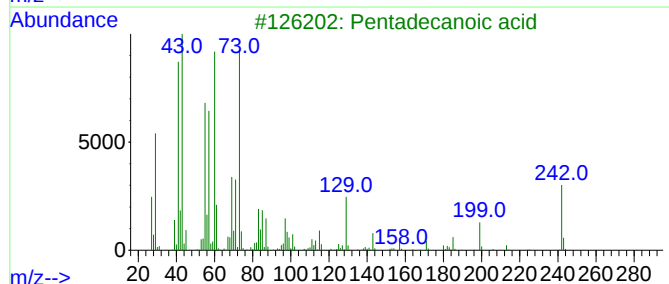
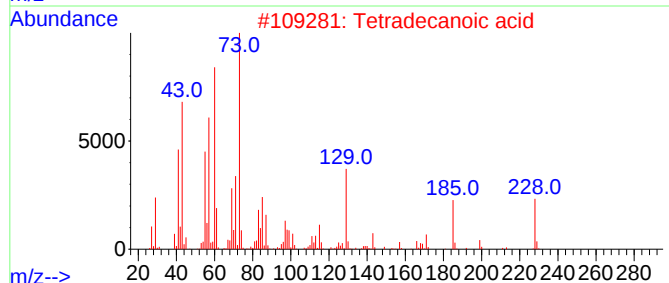
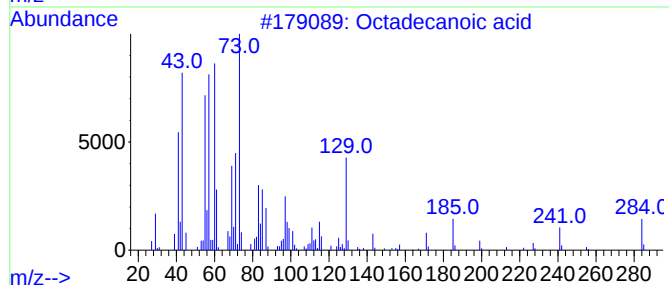
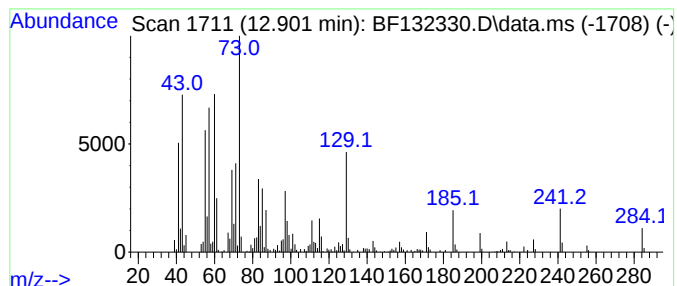
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.901	2.10 ng	187326	Phenanthrene-d10	11.607

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4			Tridecanoic acid	214	C13H26O2	000638-53-9	62
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



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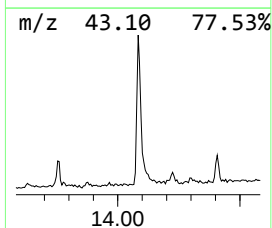
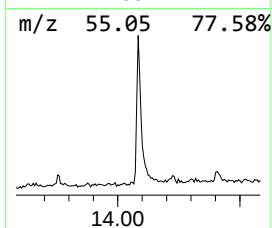
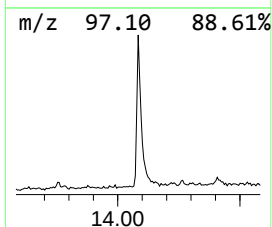
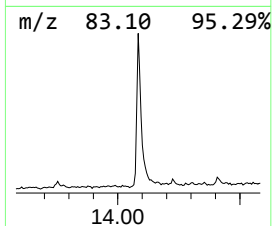
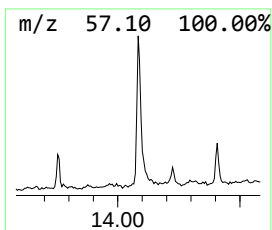
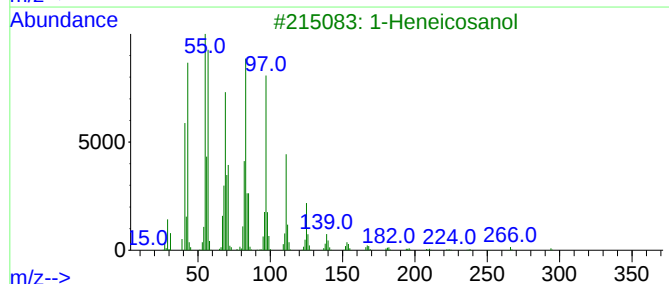
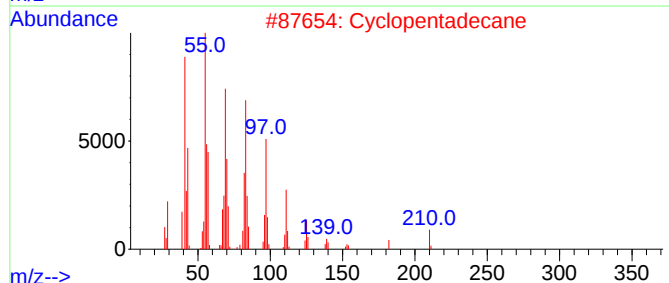
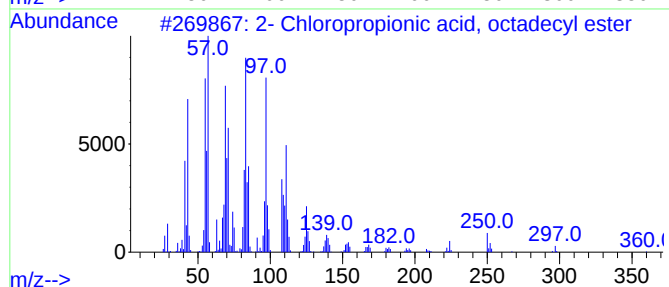
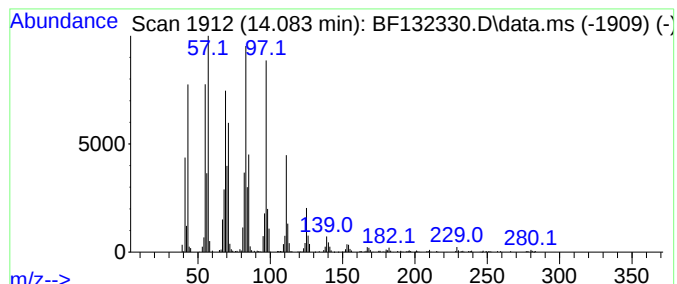
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Peak Number 4 2- Chloropropionic acid, oc... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.083	8.87 ng	516583	Chrysene-d12	14.266

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-	Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94	
2	Cyclopentadecane		210	C15H30	000295-48-7	93	
3	1-Heneicosanol		312	C21H44O	015594-90-8	93	
4	2-	Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	91	
5	Dichloroacetic acid, heptadecyl ...		366	C19H36Cl2O2	1000282-98-2	91	



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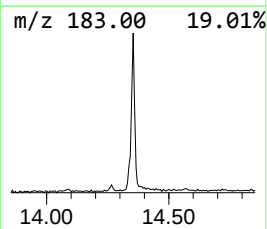
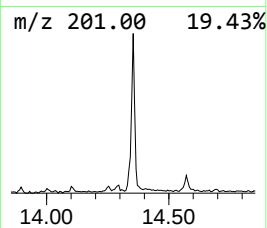
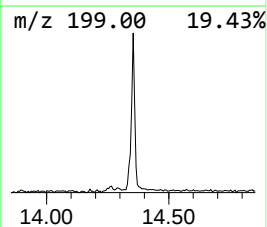
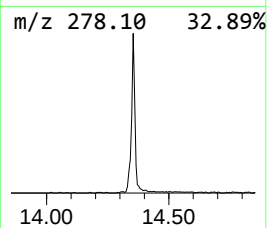
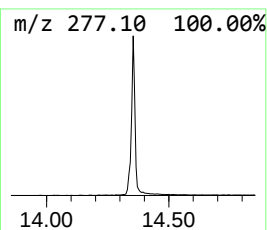
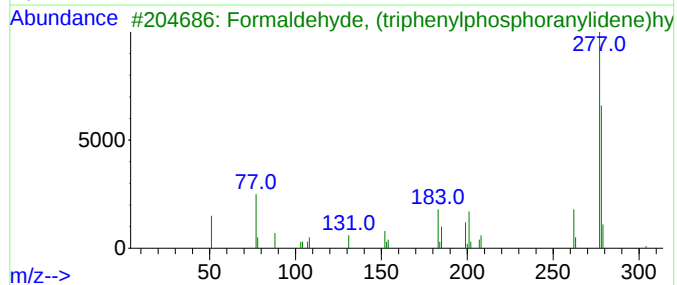
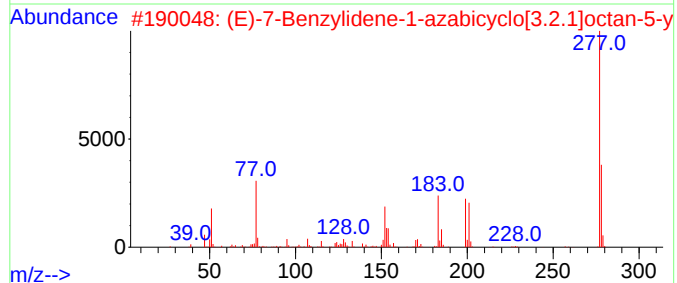
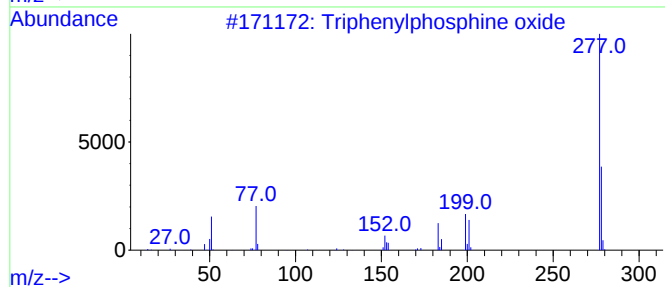
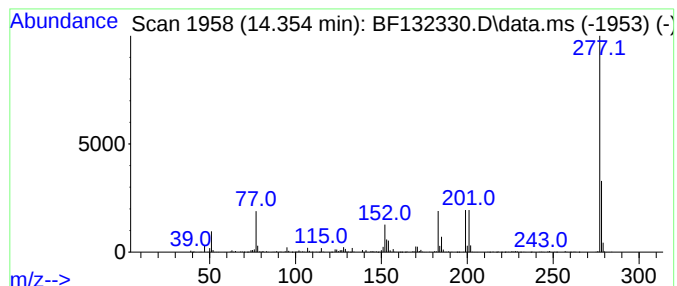
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.354	6.92 ng	403207	Chrysene-d12	14.266

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	45
4			Vanadium, cycloheptatrienyl-(pen...]	277	C17H22V	1000155-20-5	33
5			5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	25



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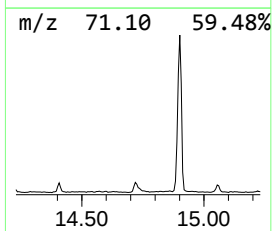
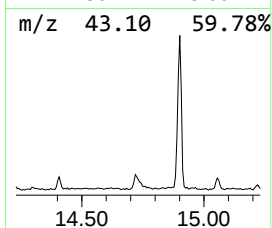
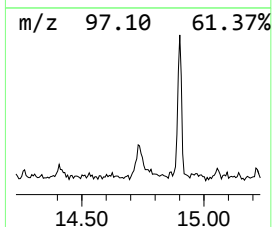
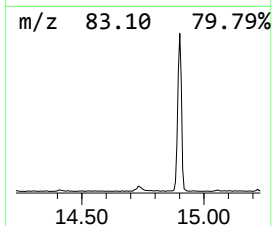
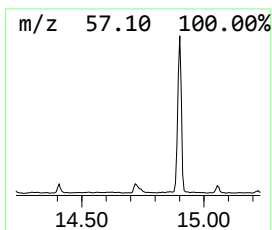
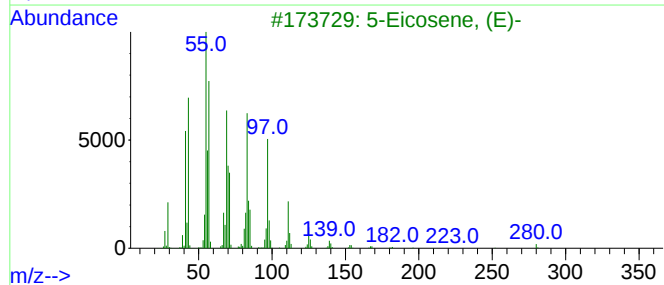
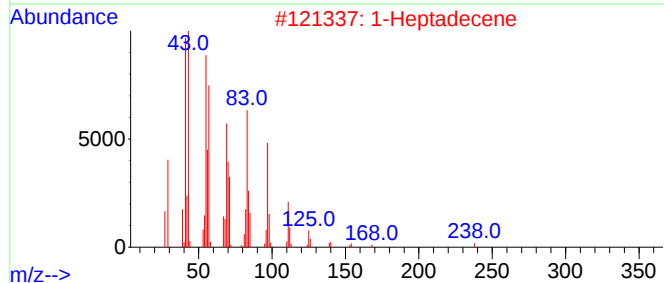
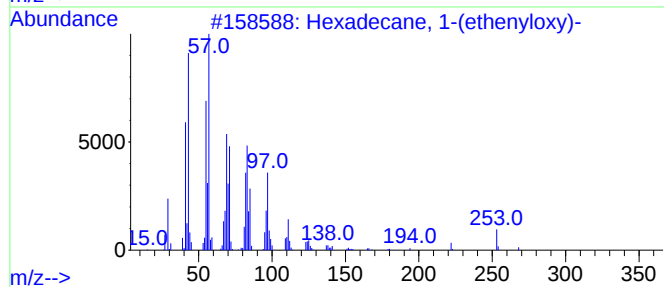
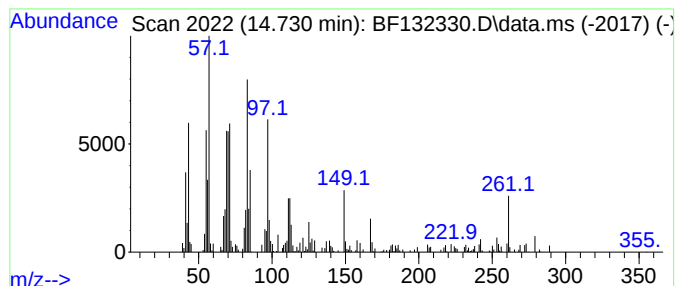
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecane, 1-(ethenyloxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.730	2.43 ng	141673	Chrysene-d12	14.266

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane, 1-(ethenyloxy)-	268	C18H36O	000822-28-6	76
2			1-Heptadecene	238	C17H34	006765-39-5	58
3			5-Eicosene, (E)-	280	C20H40	074685-30-6	52
4			1-Tridecene	182	C13H26	002437-56-1	52
5			2-Ethyl-1-dodecanol	214	C14H30O	019780-33-7	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020323\
Data File : BF132330.D
Acq On : 03 Feb 2023 19:38
Operator : CG\JU
Sample : 01409-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
38414

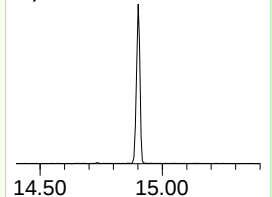
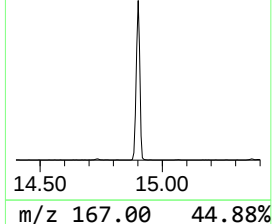
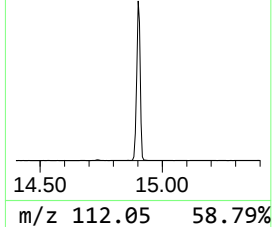
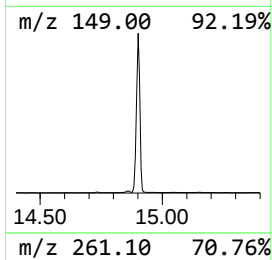
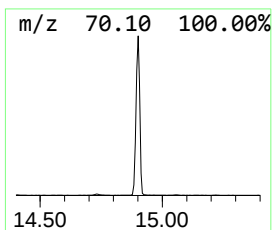
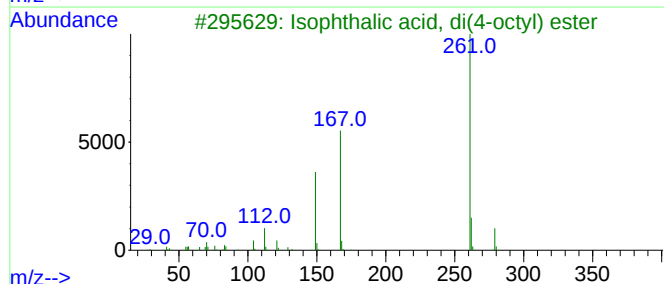
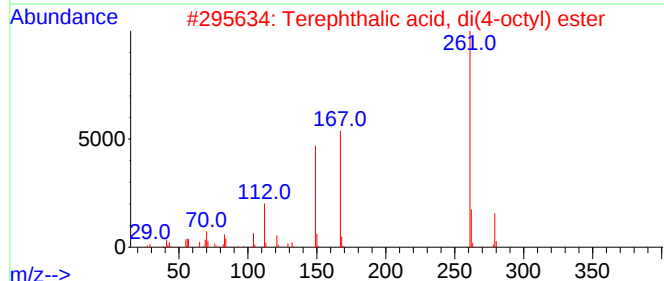
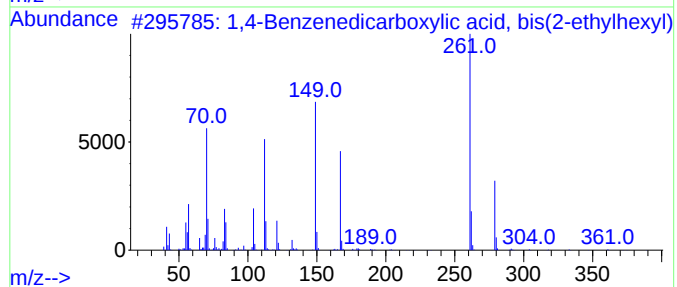
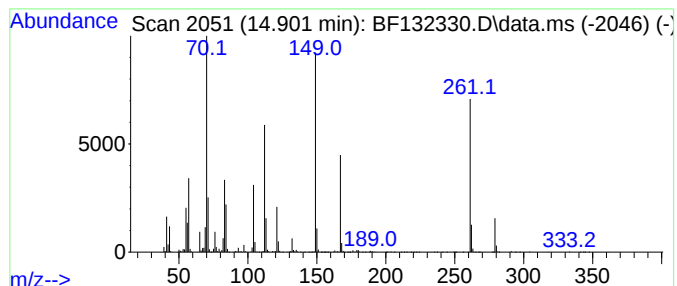
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1,4-Benzenedicarboxylic aci... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.901	66.57 ng	3877290	Chrysene-d12	14.266

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H3804	006422-86-2	94
2			Terephthalic acid, di(4-octyl) e...	390	C24H3804	1000323-74-2	81
3			Isophthalic acid, di(4-octyl) ester	390	C24H3804	1000344-04-3	80
4			Terephthalic acid, 4-octyl octyl...	390	C24H3804	1000323-73-7	68
5			Terephthalic acid, 3-methylbut-2...	348	C21H3204	1000356-27-6	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020323\
Data File : BF132330.D
Acq On : 03 Feb 2023 19:38
Operator : CG\JU
Sample : 01409-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
38414

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.307	26.2	ng	1625090	1	7.054	1242070	20.0
n-Hexadecanoic ...	12.113	7.1	ng	630523	4	11.607	1786300	20.0
Octadecanoic acid	12.901	2.1	ng	187326	4	11.607	1786300	20.0
2- Chloropropio...	14.083	8.9	ng	516583	5	14.266	1164840	20.0
Triphenylphosph...	14.354	6.9	ng	403207	5	14.266	1164840	20.0
Hexadecane, 1-(...	14.730	2.4	ng	141673	5	14.266	1164840	20.0
1,4-Benzenedica...	14.901	66.6	ng	3877290	5	14.266	1164840	20.0