

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011521\
 Data File : BP004594.D
 Acq On : 16 Jan 2021 01:08
 Operator : CG/JU
 Sample : M1141-22
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 ETGI-354

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-BP011221.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP004594.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.399	369	376	393	rBV	2081249	3245178	38.88%	6.905%
2	6.981	634	645	665	rBV	1995949	3363773	40.30%	7.157%
3	7.804	776	785	793	rBV	691165	1114736	13.35%	2.372%
4	8.963	975	982	992	rBV	1240401	2102363	25.19%	4.473%
5	10.598	1249	1260	1273	rBV	914187	1667029	19.97%	3.547%
6	12.269	1540	1544	1551	rVB2	62343	118193	1.42%	0.251%
7	12.486	1575	1581	1584	rBV3	49628	93788	1.12%	0.200%
8	13.069	1673	1680	1690	rBV	3801335	5695146	68.23%	12.118%
9	13.233	1704	1708	1713	rBV	87192	143292	1.72%	0.305%
10	13.875	1813	1817	1820	rBV	112382	168302	2.02%	0.358%
11	13.910	1820	1823	1826	rVB	132565	163525	1.96%	0.348%
12	14.192	1867	1871	1877	rBV5	103589	224091	2.68%	0.477%
13	14.286	1883	1887	1894	rVB4	227573	361667	4.33%	0.770%
14	14.457	1906	1916	1925	rBV2	1516650	2641893	31.65%	5.621%
15	15.245	2046	2050	2056	rBV2	238891	359109	4.30%	0.764%
16	15.957	2165	2171	2179	rBV	2776353	4400955	52.72%	9.364%
17	17.216	2380	2385	2392	rBV	1789167	2611005	31.28%	5.556%
18	18.110	2534	2537	2543	rBV	580148	787350	9.43%	1.675%
19	19.345	2744	2747	2754	rBV	314347	432097	5.18%	0.919%
20	19.780	2816	2821	2830	rVB	6829650	8347478	100.00%	17.761%
21	21.015	3028	3031	3039	rVB2	475475	679695	8.14%	1.446%
22	21.215	3062	3065	3069	rVB	239120	271188	3.25%	0.577%
23	21.309	3076	3081	3087	rVB	2426901	3119728	37.37%	6.638%
24	23.656	3474	3480	3497	rVB2	1666911	3523921	42.22%	7.498%
25	26.009	3875	3880	3892	rVB2	513894	1362497	16.32%	2.899%

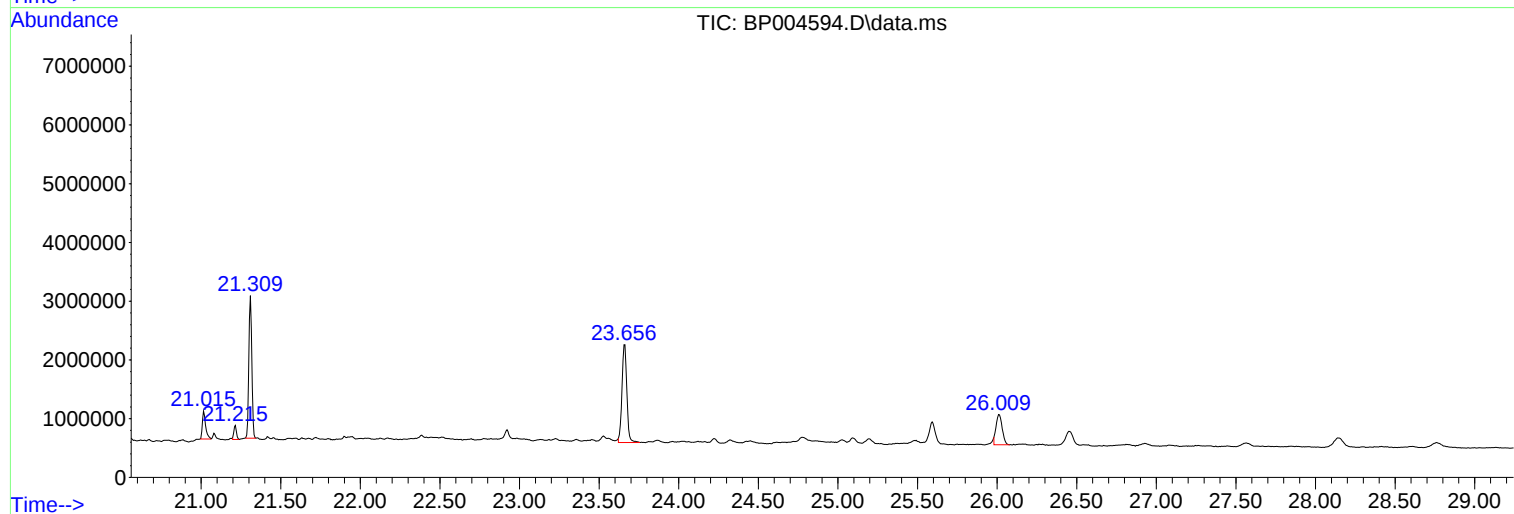
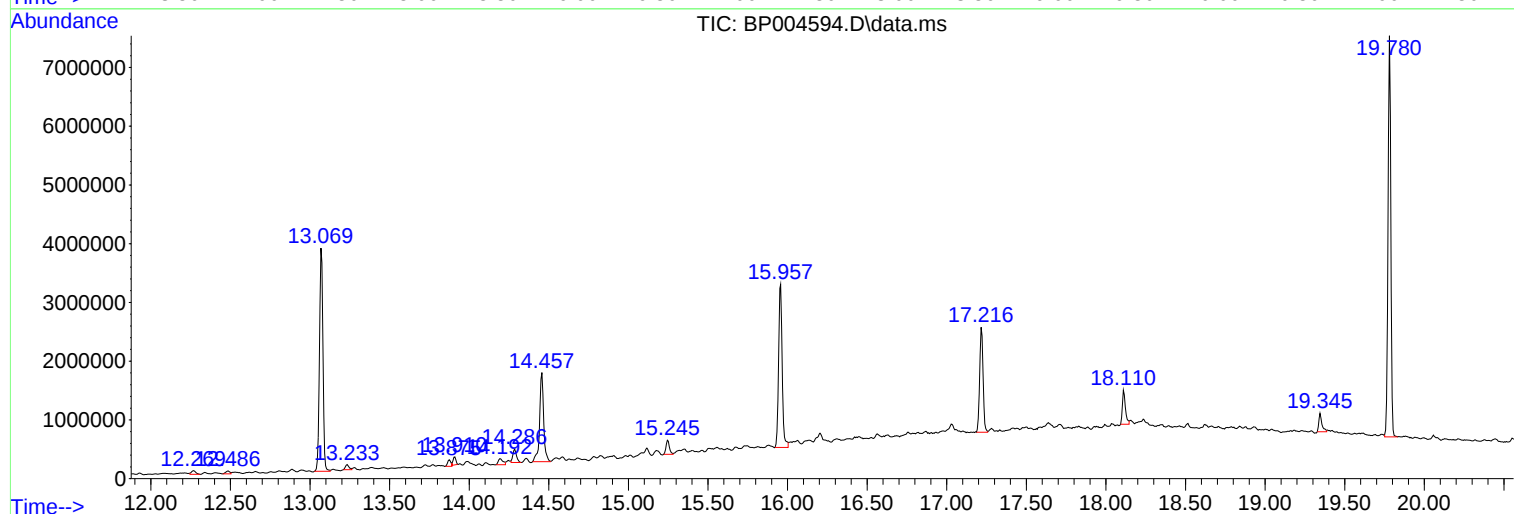
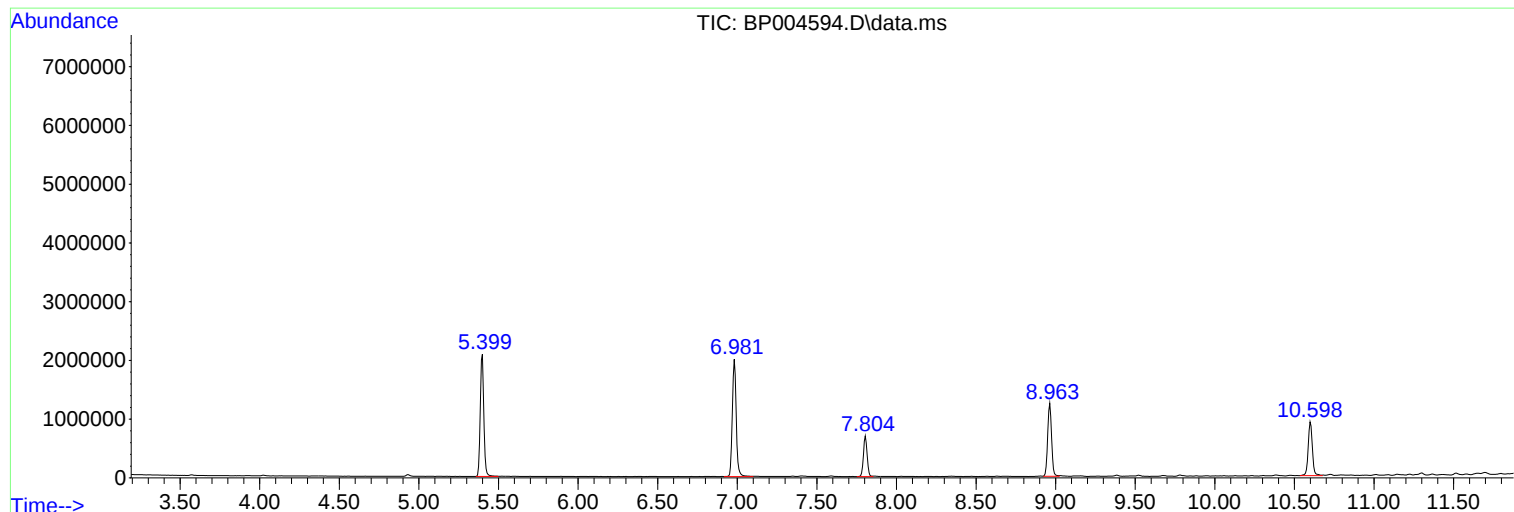
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP011221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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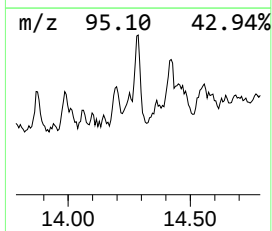
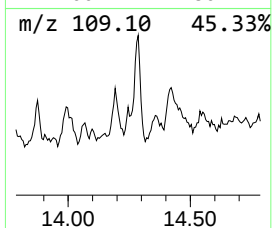
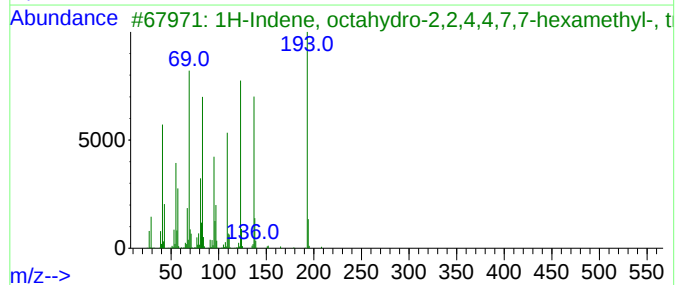
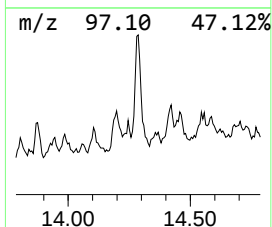
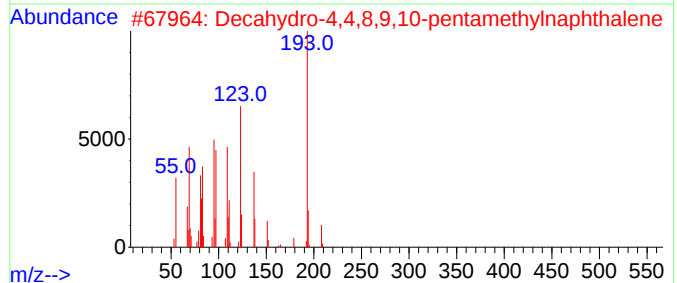
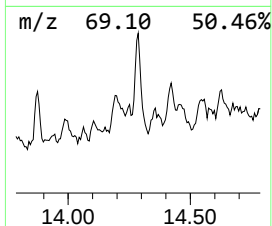
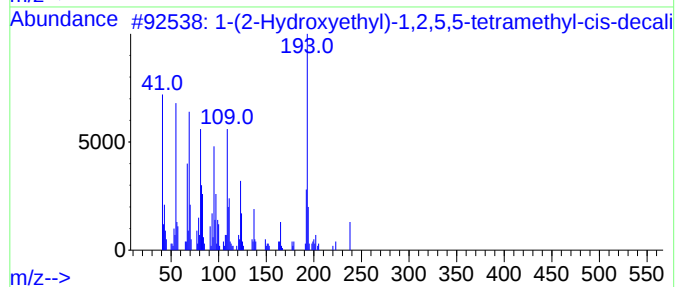
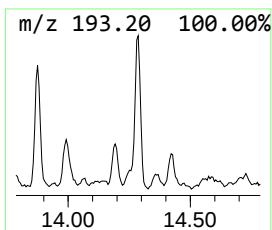
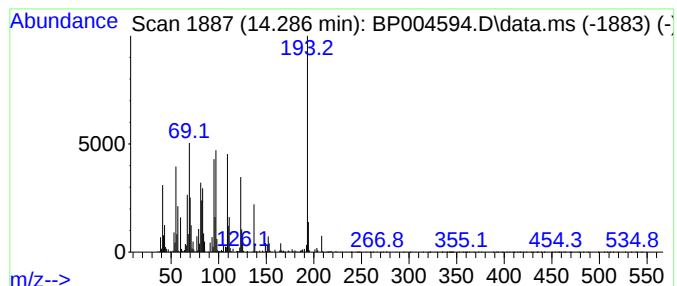
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 1-(2-Hydroxyethyl)-1,2,5,5-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.286	2.74 ng	361667	Acenaphthene-d10	14.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(2-Hydroxyethyl)-1,2,5,5-tetra...	238	C16H30O	1000298-97-4	53		
2	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	49		
3	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	38		
4	2-Diethylamino-4-phenylthiooct-2...	302	C18H26N2S	1000090-57-0	38		
5	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	38		



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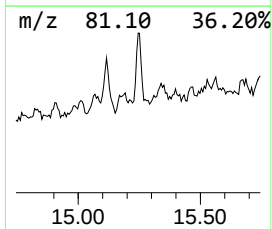
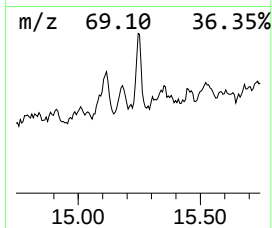
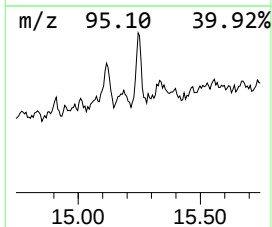
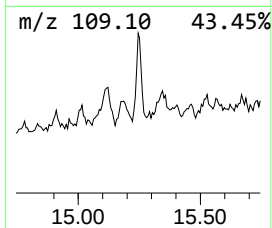
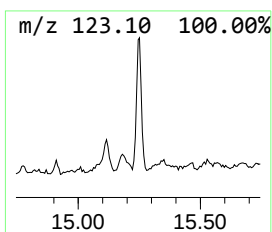
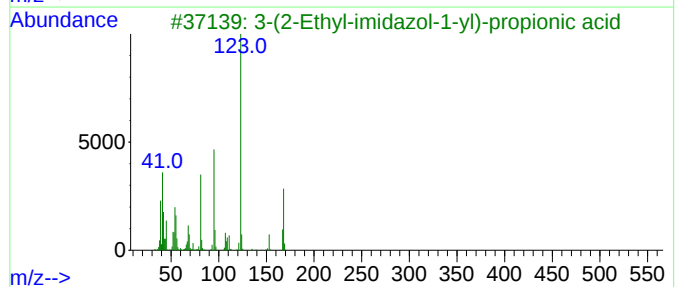
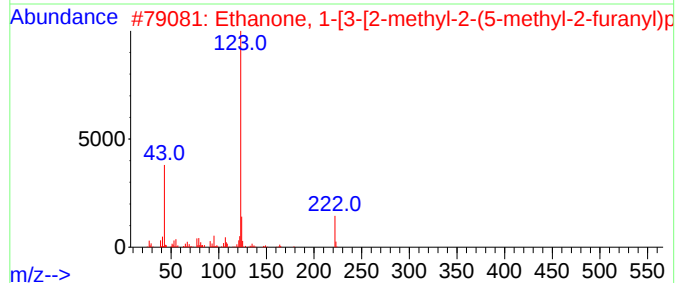
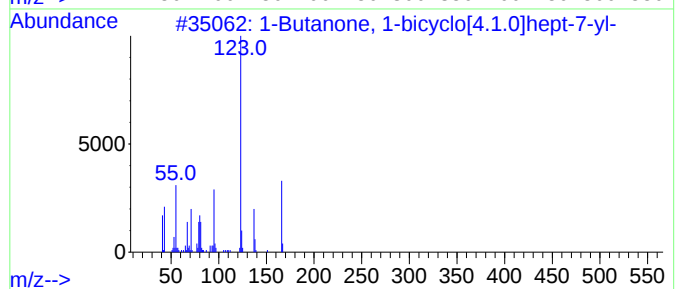
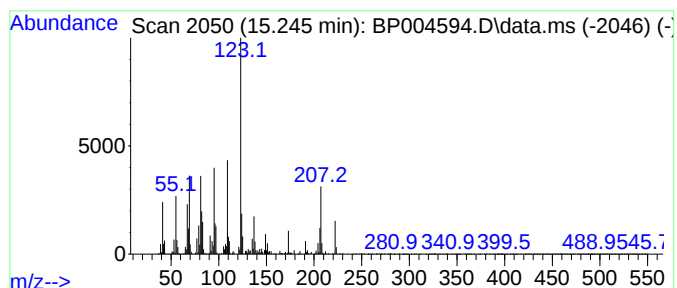
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Peak Number 2 unknown15.245 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.245	2.72 ng	359109	Acenaphthene-d10	14.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanone, 1-bicyclo[4.1.0]hept...	166	C11H18O	054764-62-4	43
2			Ethanone, 1-[3-[2-methyl-2-(5-me...	222	C13H18O3	080114-28-9	42
3			3-(2-Ethyl-imidazol-1-yl)-propio...	168	C8H12N2O2	1000277-78-0	38
4			Magnesium, bis(acetylacetonate)	222	C10H14MgO4	068488-07-3	38
5			3-Fluorobenzoic acid, 2-ethylcyc...	250	C15H19FO2	1000279-04-9	38



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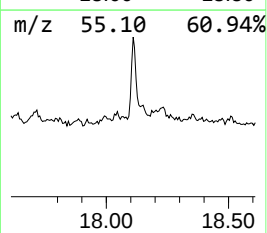
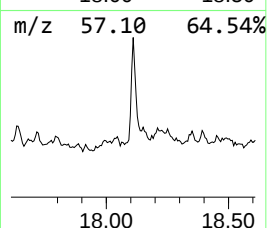
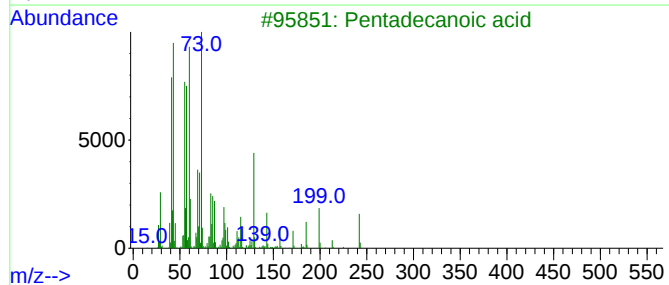
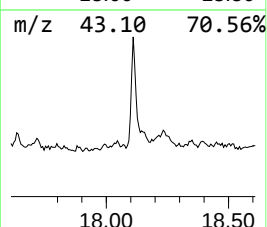
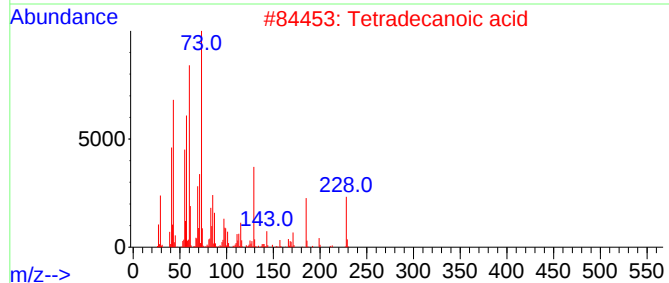
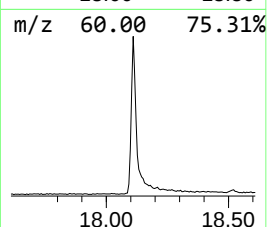
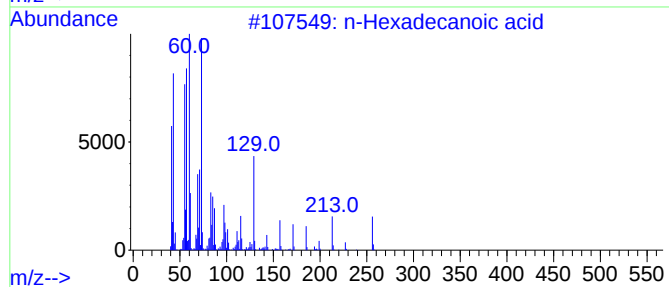
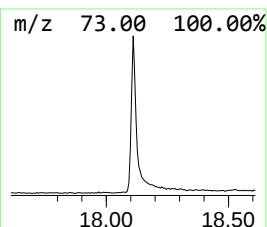
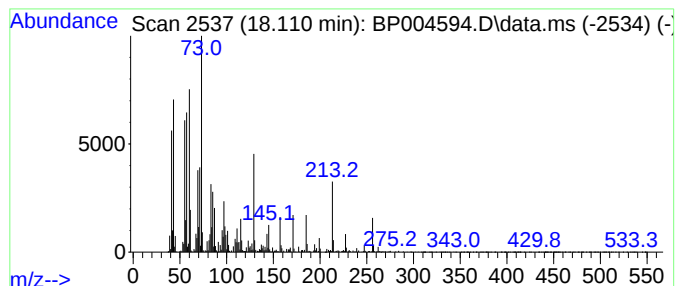
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.110	6.03 ng	787350	Phenanthrene-d10	17.216

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	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Octadecanoic acid	284	C18H36O2	000057-11-4	87
5			Undecanoic acid	186	C11H22O2	000112-37-8	83



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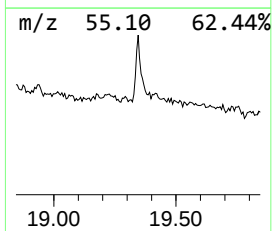
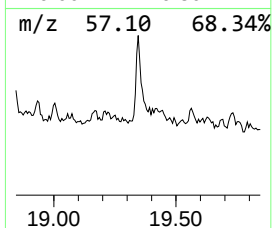
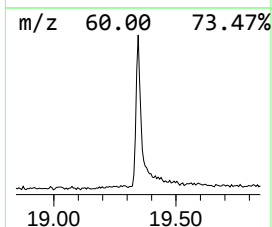
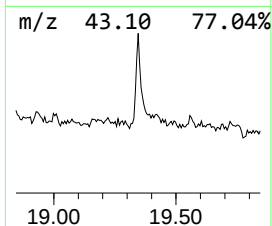
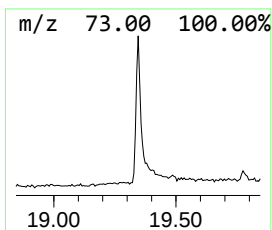
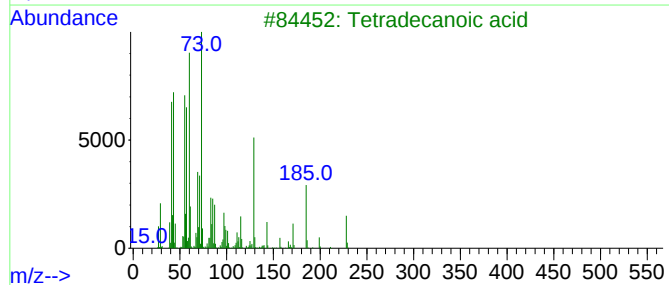
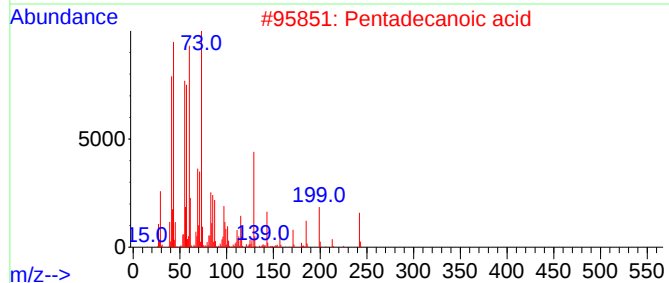
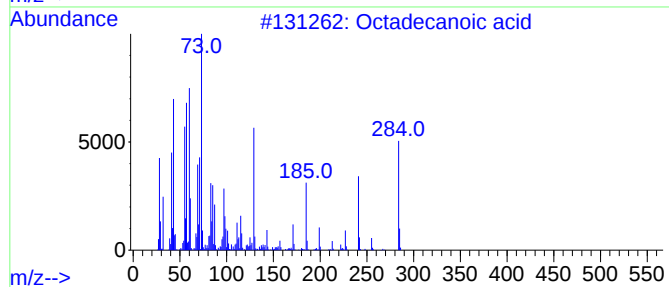
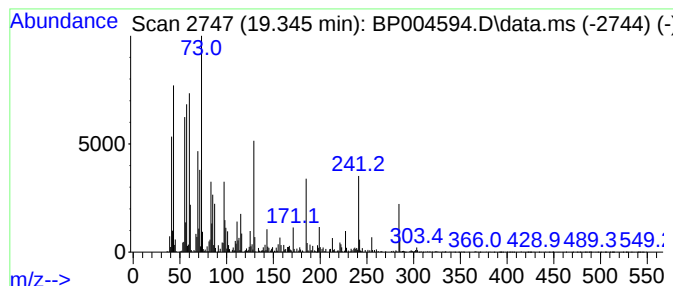
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.345	2.77 ng	432097	Chrysene-d12	21.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	81
4			Tridecanoic acid	214	C13H26O2	000638-53-9	70
5			Dodecanoic acid	200	C12H24O2	000143-07-7	53



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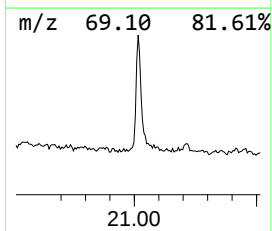
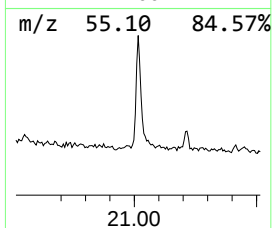
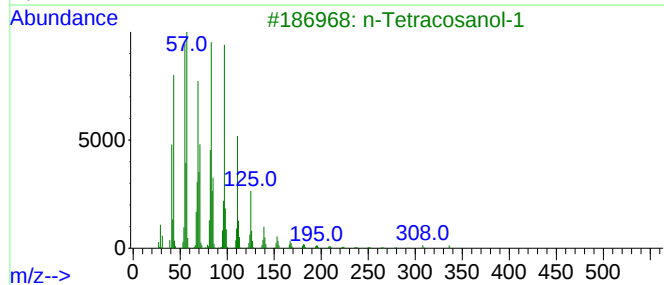
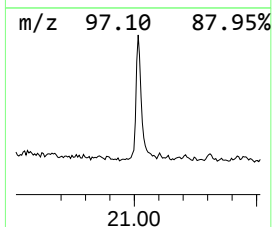
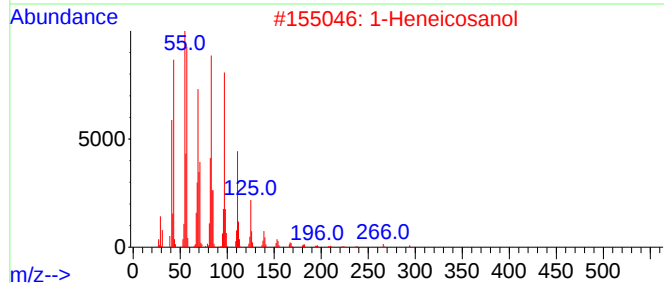
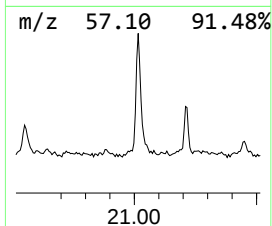
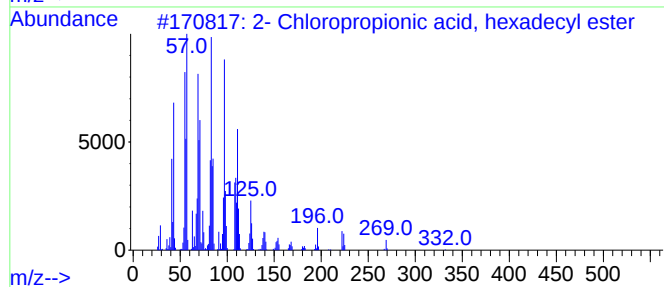
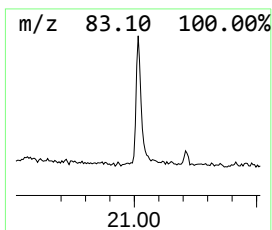
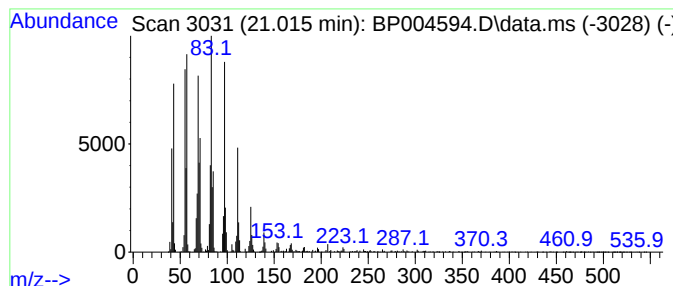
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Peak Number 5 2- Chloropropionic acid, he... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.015	4.36 ng	679695	Chrysene-d12	21.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	97
2			1-Heneicosanol	312	C21H44O	015594-90-8	95
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4			Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	94
5			Behenic alcohol	326	C22H46O	000661-19-8	94



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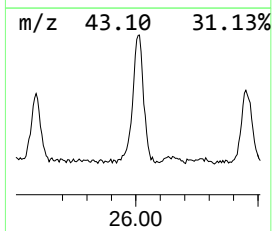
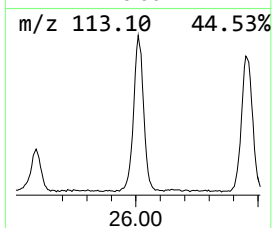
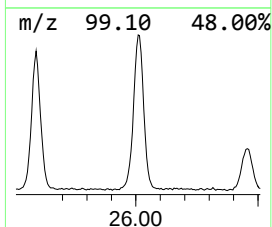
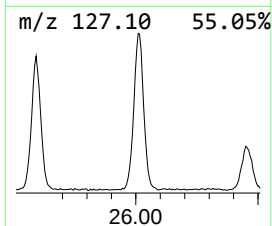
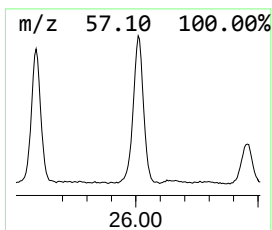
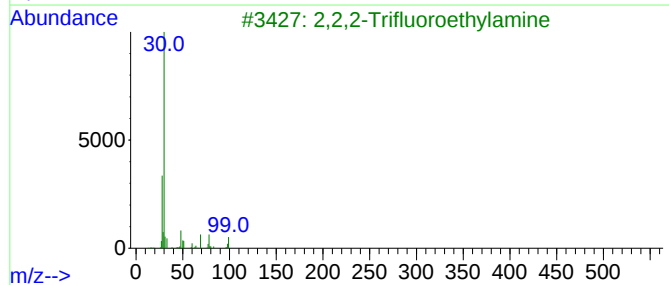
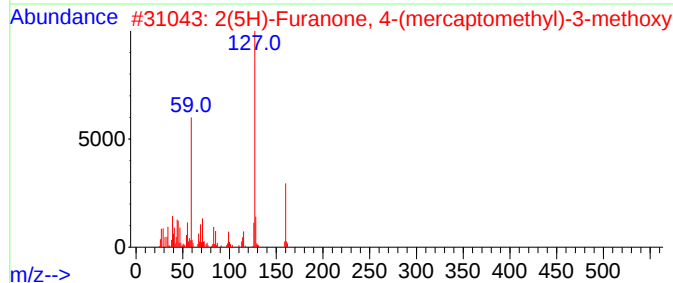
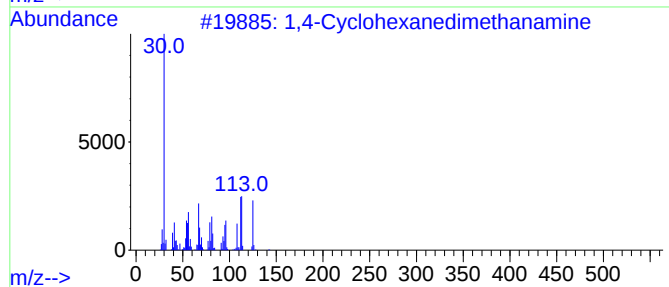
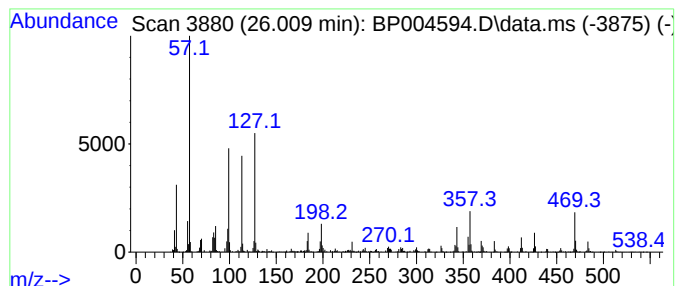
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown26.009 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.009	7.73 ng	1362500	Perylene-d12	23.656

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Cyclohexanedimethanamine	142	C8H18N2	002549-93-1	4
2			2(5H)-Furanone, 4-(mercaptomethy...	160	C6H8O3S	010478-17-8	4
3			2,2,2-Trifluoroethylamine	99	C2H4F3N	000753-90-2	1
4			2,2,3,4,4,4-Hexafluorobutanol-1	182	C4H4F6O	000382-31-0	1
5			1-Azacyclononan-2-one	141	C8H15NO	000935-30-8	1



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011521\
Data File : BP004594.D
Acq On : 16 Jan 2021 01:08
Operator : CG/JU
Sample : M1141-22
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
ETGI-354

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP011221.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
1-(2-Hydroxyeth...	14.286	2.7	ng	361667	3	14.457	2641890	20.0
unknown15.245	15.245	2.7	ng	359109	3	14.457	2641890	20.0
n-Hexadecanoic ...	18.110	6.0	ng	787350	4	17.216	2611010	20.0
Octadecanoic acid	19.345	2.8	ng	432097	5	21.310	3119730	20.0
2- Chloropropio...	21.015	4.4	ng	679695	5	21.310	3119730	20.0
unknown26.009	26.009	7.7	ng	1362500	6	23.656	3523920	20.0