

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120821\
 Data File : BP008300.D
 Acq On : 09 Dec 2021 03:09
 Operator : CG/JU
 Sample : M4959-07
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 TP-2

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-BP112521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008300.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.905	318	326	338	rBV	26484	44167	1.21%	0.201%
2	5.363	398	404	421	rBV	1392699	2106286	57.90%	9.579%
3	6.957	667	675	694	rBV	1222938	2057676	56.56%	9.358%
4	7.769	804	813	822	rBV	278029	438933	12.07%	1.996%
5	8.934	1004	1011	1026	rBV	790684	1354248	37.23%	6.159%
6	10.369	1247	1255	1270	rBV	169258	427114	11.74%	1.942%
7	10.569	1281	1289	1303	rVB	303650	538930	14.81%	2.451%
8	13.040	1702	1709	1725	rBV	1626863	2447421	67.28%	11.130%
9	14.422	1938	1944	1953	rBV	426935	638044	17.54%	2.902%
10	15.922	2188	2199	2221	rBV	1304903	2103901	57.83%	9.568%
11	17.186	2408	2414	2419	rBV	510116	772185	21.23%	3.512%
12	17.228	2419	2421	2428	rVB	38788	57031	1.57%	0.259%
13	17.322	2433	2437	2445	rVB2	20438	43725	1.20%	0.199%
14	17.869	2526	2530	2534	rBV	39532	47100	1.29%	0.214%
15	18.086	2555	2567	2577	rBV3	94121	219594	6.04%	0.999%
16	19.210	2753	2758	2765	rBV	132074	193081	5.31%	0.878%
17	19.327	2775	2778	2782	rBV5	30854	37566	1.03%	0.171%
18	19.563	2811	2818	2828	rVB	135203	213073	5.86%	0.969%
19	19.763	2846	2852	2857	rBV	3008205	3637927	100.00%	16.544%
20	20.045	2896	2900	2902	rBV4	34856	52297	1.44%	0.238%
21	20.945	3050	3053	3055	rBV2	57327	61756	1.70%	0.281%
22	21.010	3060	3064	3071	rVB2	214865	334572	9.20%	1.522%
23	21.292	3106	3112	3117	rBV	856962	1247187	34.28%	5.672%
24	22.539	3320	3324	3330	rVB	193407	268737	7.39%	1.222%
25	22.645	3338	3342	3348	rBV	297883	428958	11.79%	1.951%
26	22.957	3391	3395	3399	rBV2	196813	331246	9.11%	1.506%
27	23.010	3400	3404	3415	rVB3	378905	800830	22.01%	3.642%
28	23.680	3512	3518	3526	rVB2	527650	1085879	29.85%	4.938%

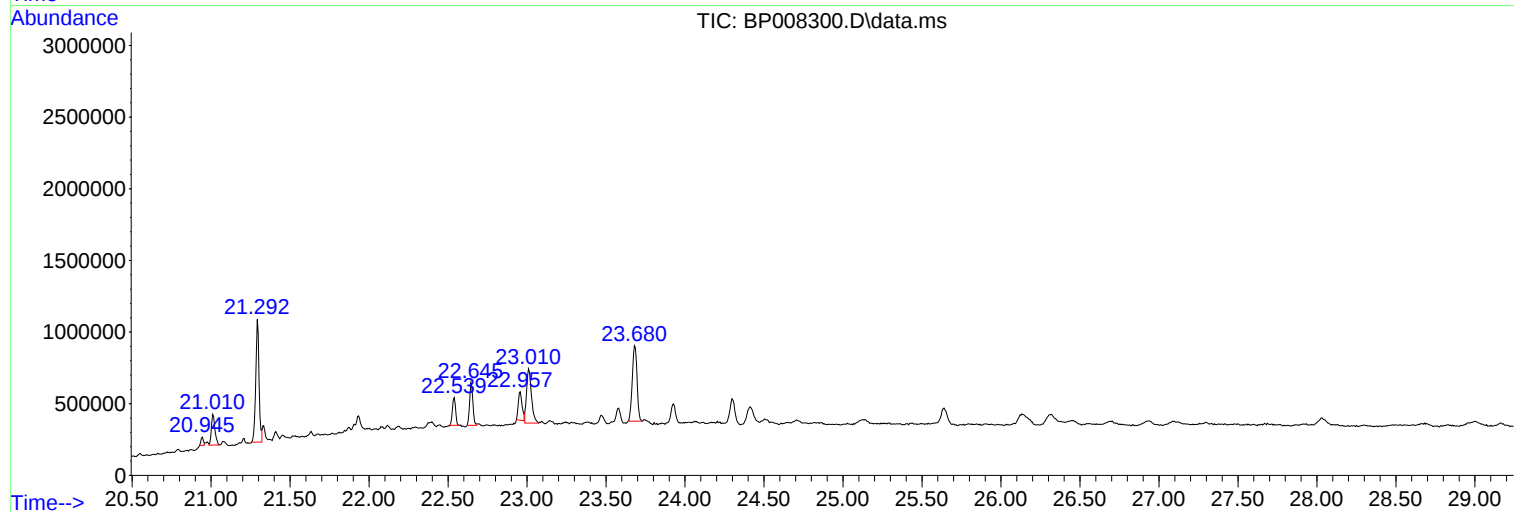
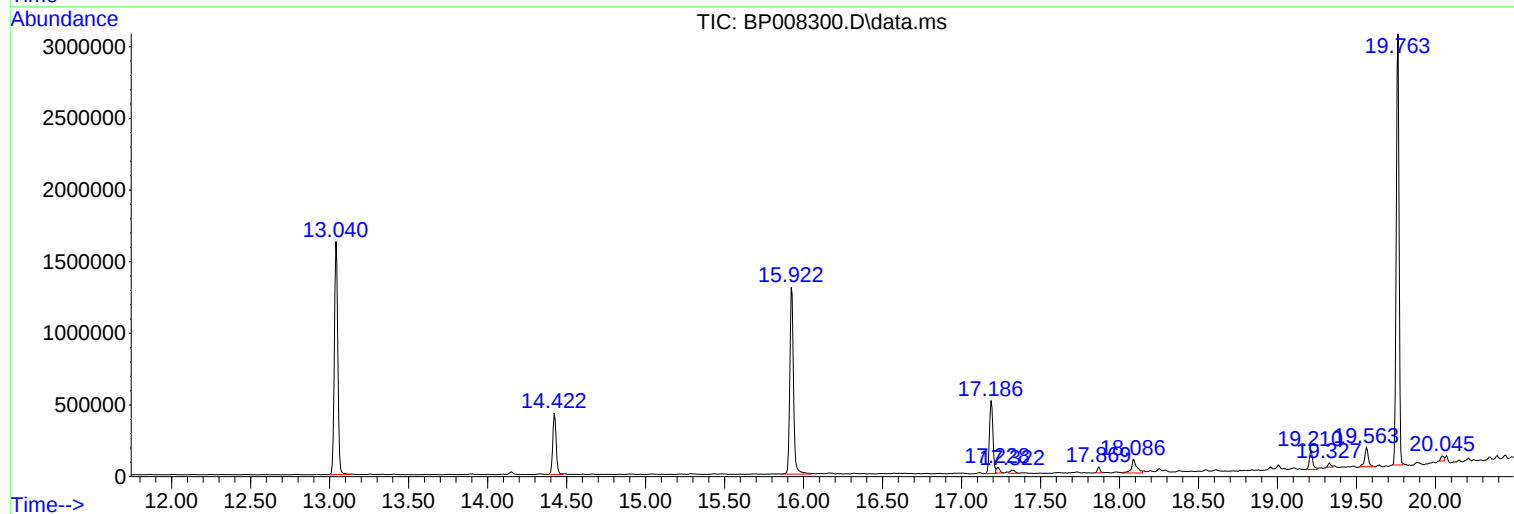
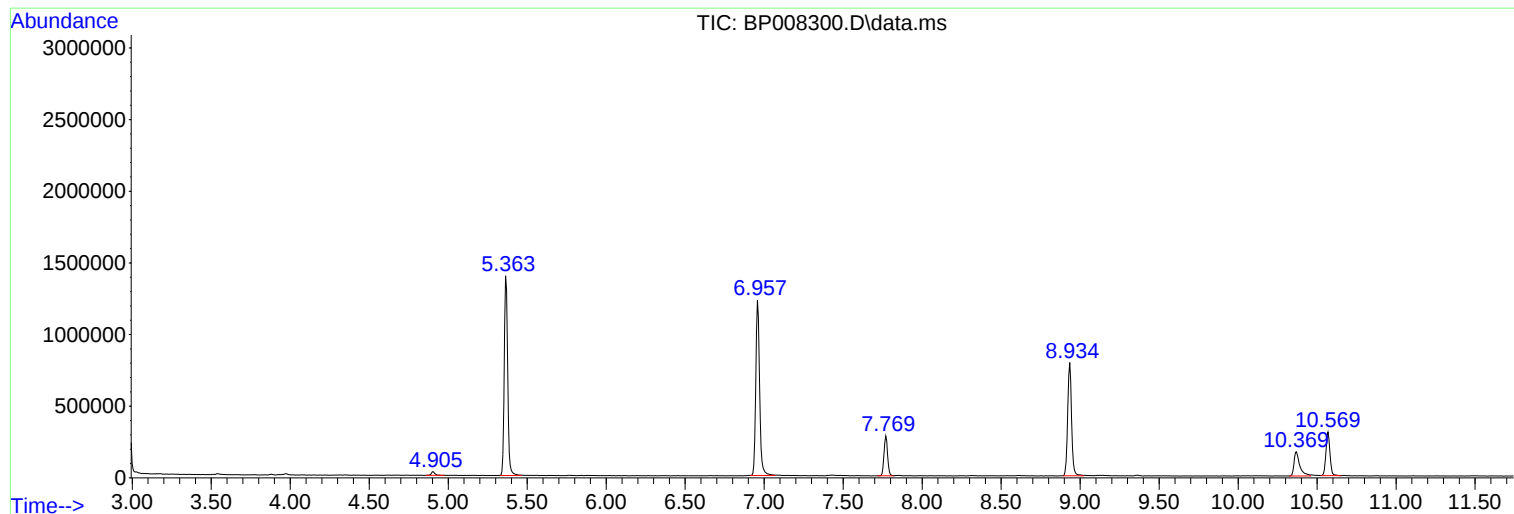
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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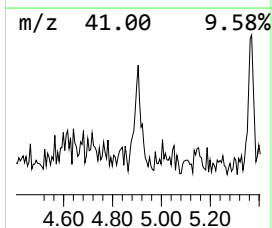
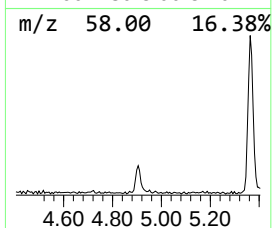
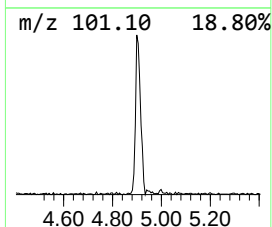
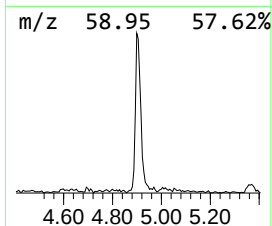
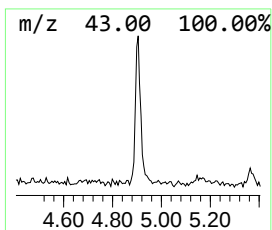
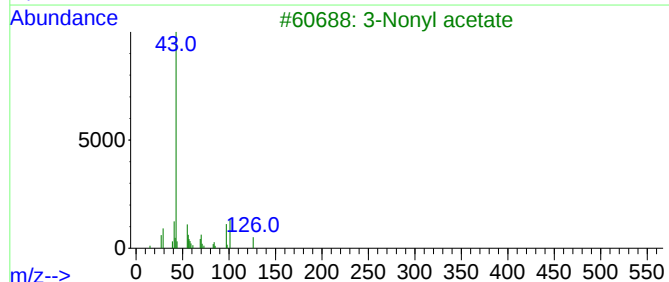
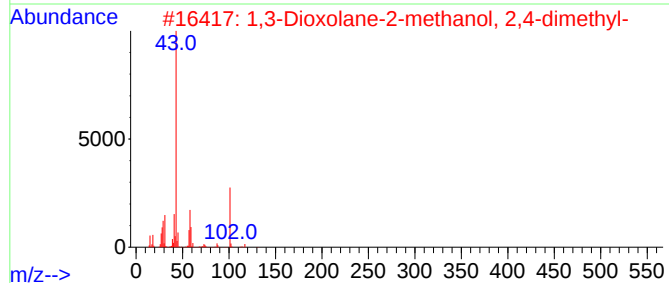
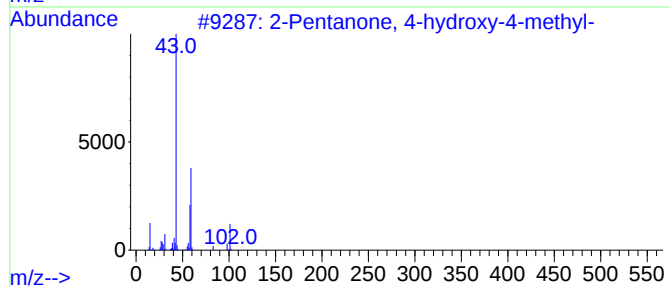
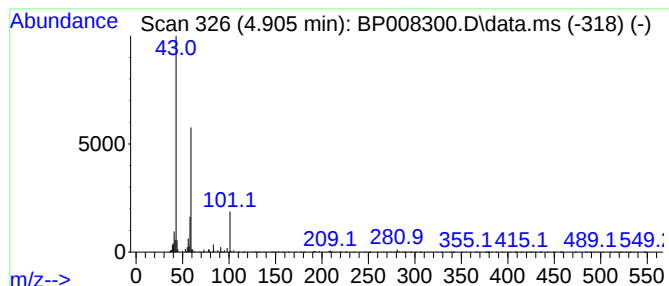
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TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.905	2.01 ng	44167	1,4-Dichlorobenzene-d4	7.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	17		
3	3-Nonyl acetate	186	C11H22O2	1010429-16-2	16		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
5	TATP	222	C9H18O6	017088-37-8	9		



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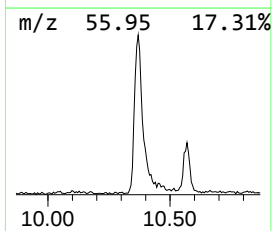
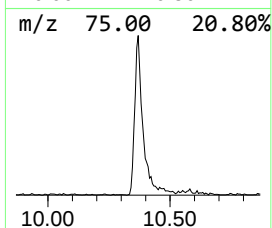
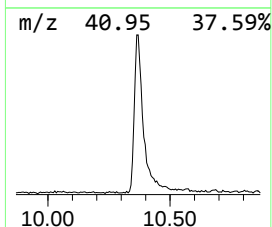
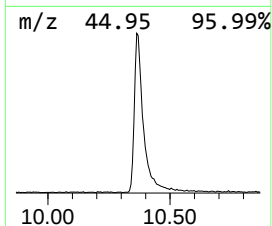
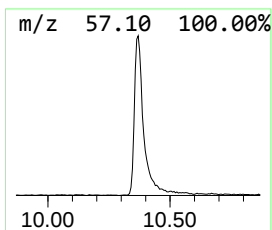
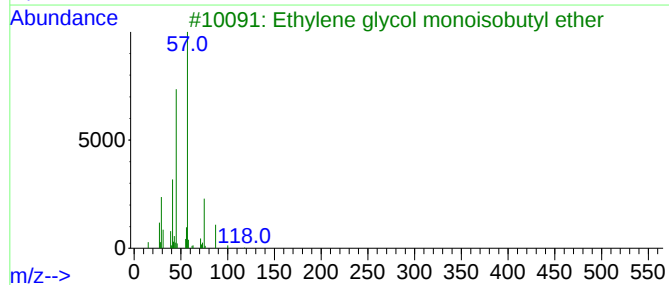
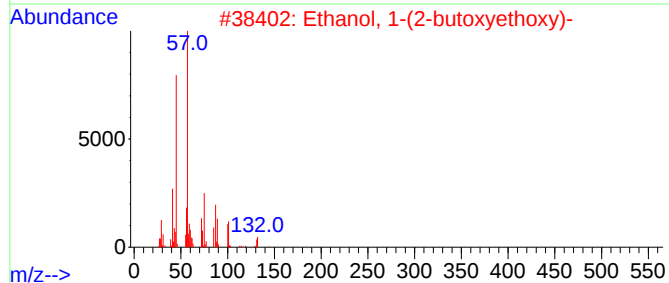
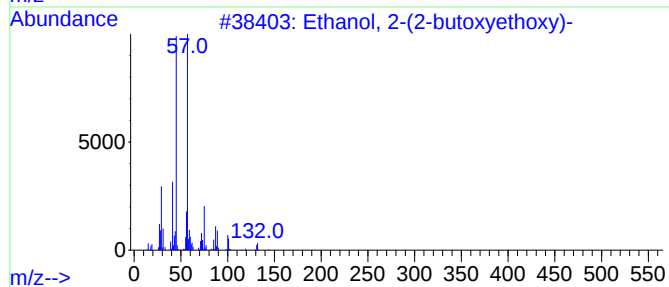
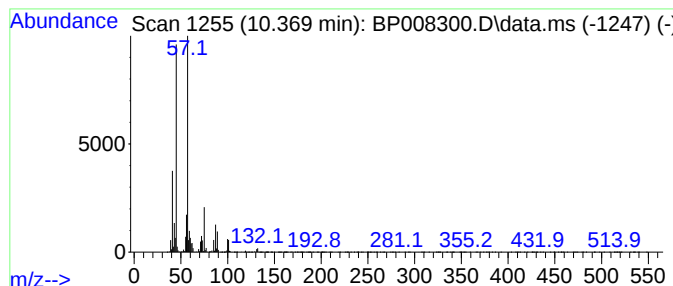
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.369	15.85 ng	427114	Naphthalene-d8	10.569

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5			Di-sec-Butyl ether	130	C8H18O	006863-58-7	50



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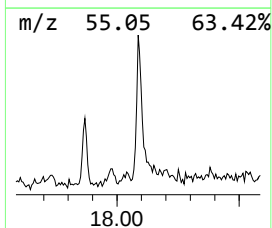
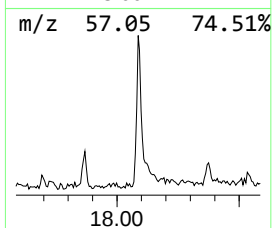
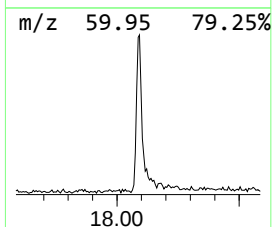
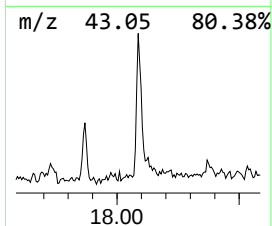
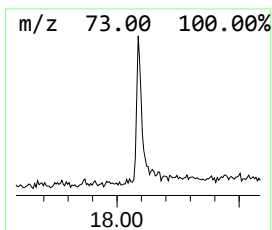
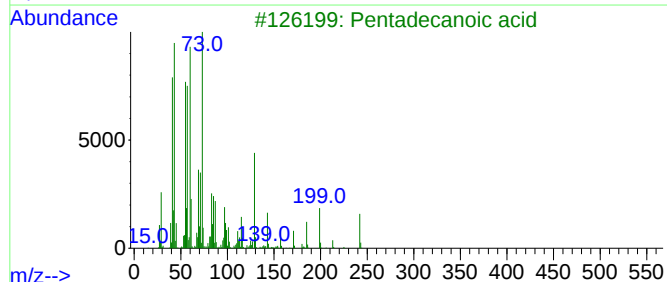
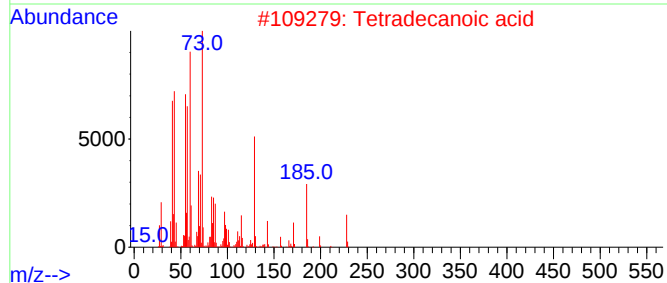
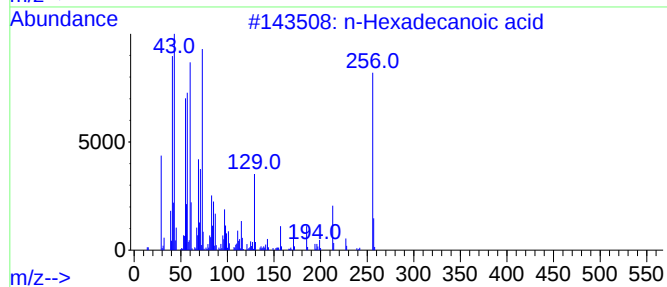
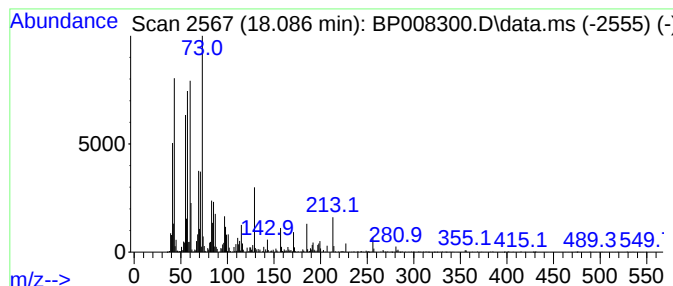
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.086	5.69 ng	219594	Phenanthrene-d10	17.186

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	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Octadecanoic acid	284	C18H36O2	000057-11-4	87
5			Tridecanoic acid	214	C13H26O2	000638-53-9	83



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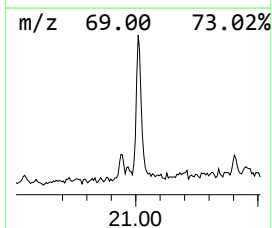
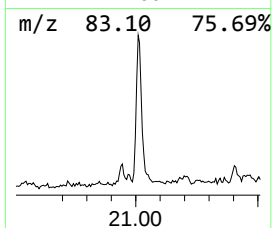
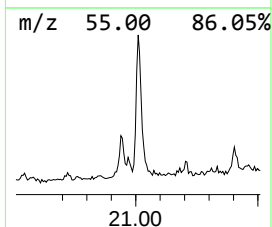
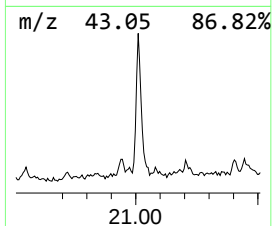
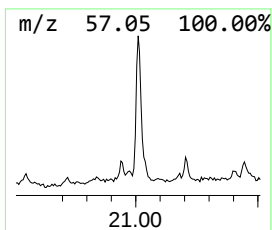
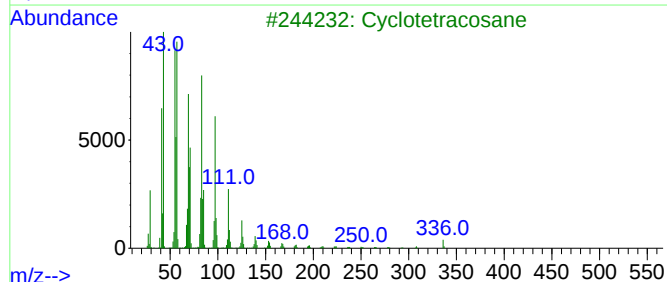
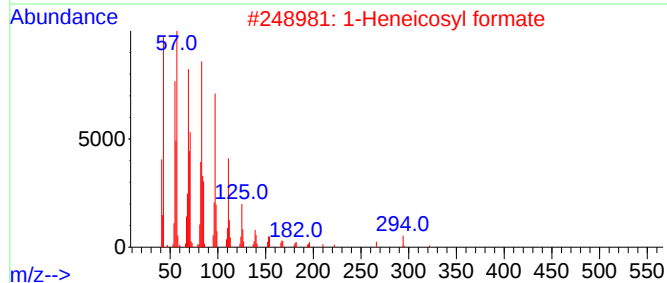
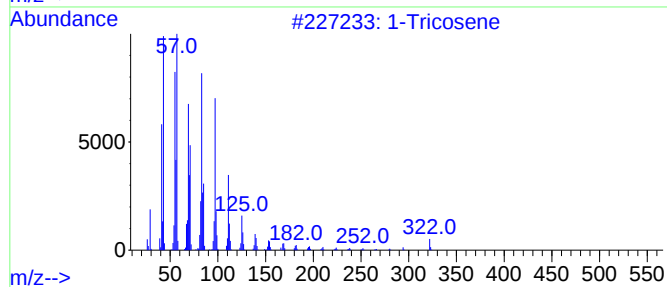
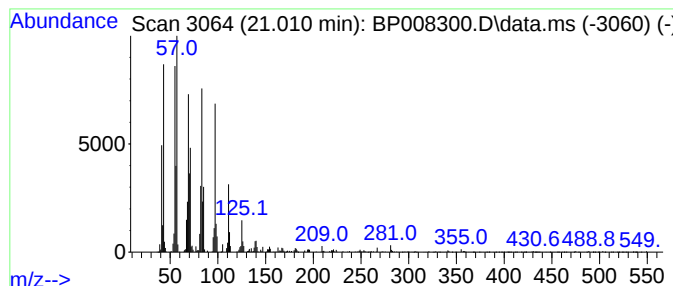
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Peak Number 5 1-Tricosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.010	5.37 ng	334572	Chrysene-d12	21.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene			322	C23H46	018835-32-0	96
2	1-Heneicosyl formate			340	C22H44O2	077899-03-7	96
3	Cyclotetracosane			336	C24H48	000297-03-0	95
4	Trichloroacetic acid, hexadecyl ...			386	C18H33Cl3O2	074339-54-1	94
5	1-Heptacosanol			396	C27H56O	002004-39-9	91



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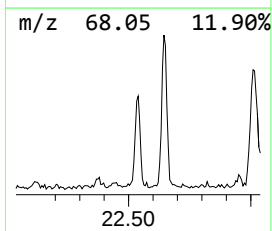
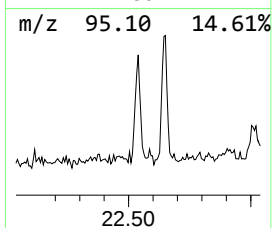
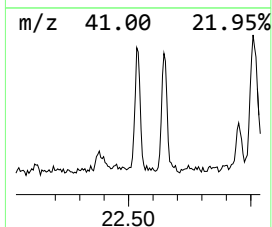
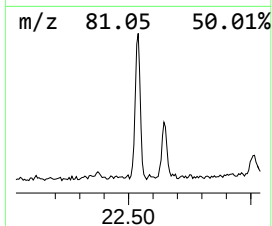
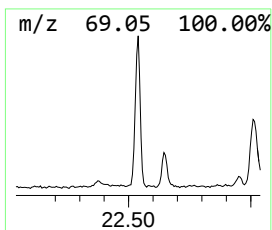
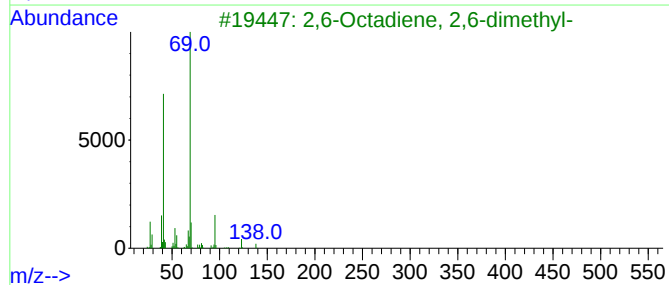
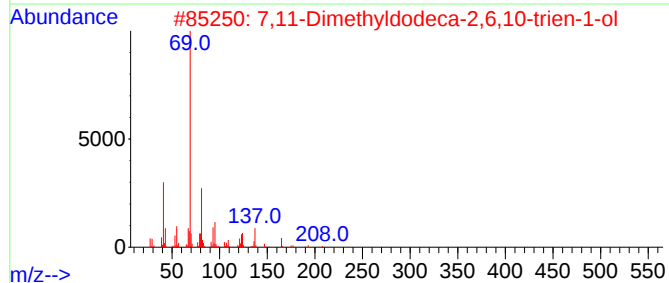
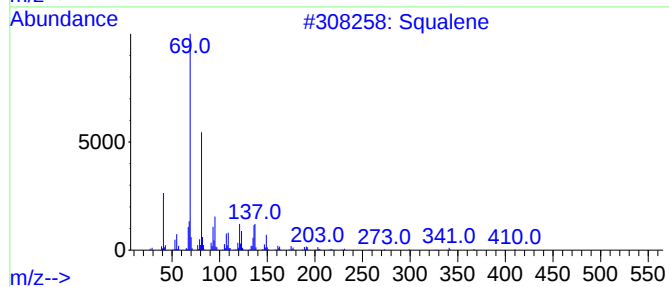
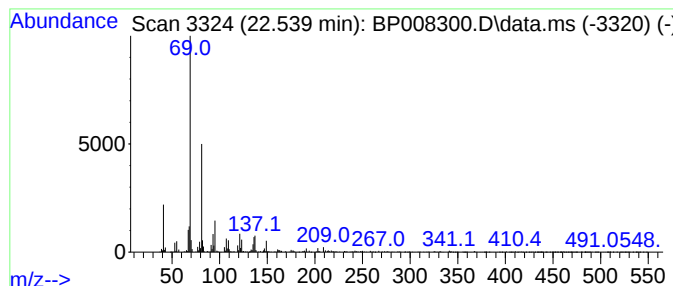
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Peak Number 6 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.539	4.95 ng	268737	Perylene-d12	23.680

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	97
2			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
3			2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	59
4			3,7,11-Tridecatrienitrile, 4,8...	231	C16H25N	006006-01-5	56
5			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	53



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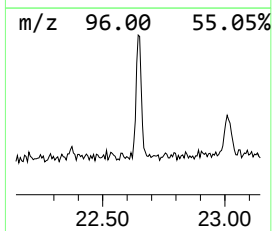
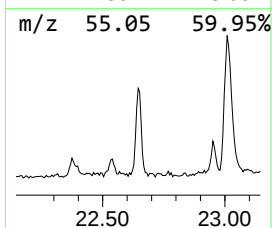
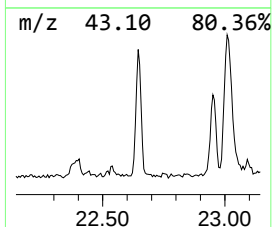
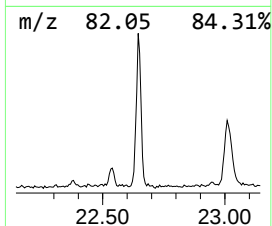
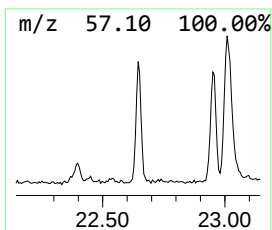
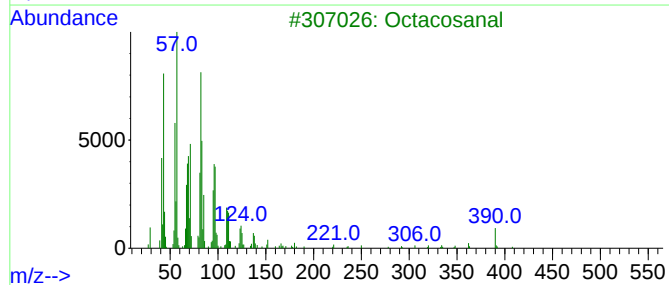
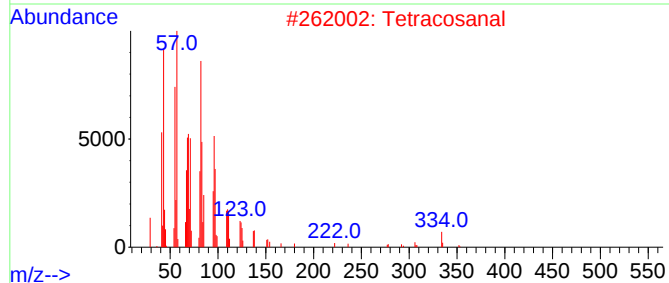
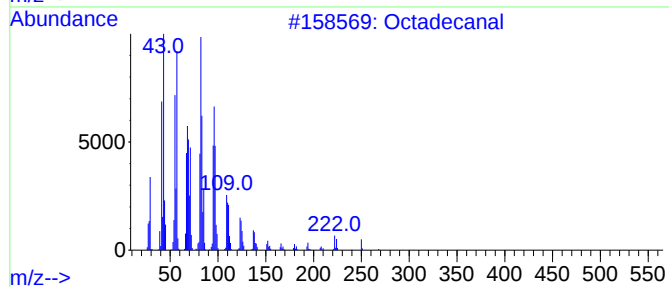
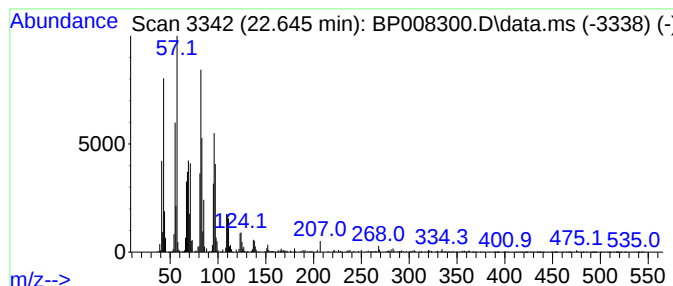
Instrument :
BNA_P
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.645	7.90 ng	428958	Perylene-d12	23.680	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	91
2	Tetracosanal	352	C24H48O	057866-08-7	91
3	Octacosanal	408	C28H56O	022725-64-0	90
4	1,19-Eicosadiene	278	C20H38	014811-95-1	90
5	Eicosanal-	296	C20H40O	002400-66-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120821\
Data File : BP008300.D
Acq On : 09 Dec 2021 03:09
Operator : CG/JU
Sample : M4959-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.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-...	4.905	2.0	ng	44167	1	7.769	438933	20.0
Ethanol, 2-(2-b...	10.369	15.9	ng	427114	2	10.569	538930	20.0
n-Hexadecanoic ...	18.086	5.7	ng	219594	4	17.186	772185	20.0
1-Tricosene	21.010	5.4	ng	334572	5	21.292	1247190	20.0
Squalene	22.539	5.0	ng	268737	6	23.680	1085880	20.0
Octadecanal	22.645	7.9	ng	428958	6	23.680	1085880	20.0