

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081721\
 Data File : BP006691.D
 Acq On : 16 Aug 2021 19:46
 Operator : CG/JU
 Sample : M3407-02
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 25N

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-BP080321.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP006691.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.858	296	301	308	rBV	268505	389057	4.65%	0.720%
2	5.305	371	377	388	rBV	3535922	5106252	60.98%	9.455%
3	6.893	640	647	661	rVB	3564543	5574164	66.57%	10.321%
4	7.705	779	785	793	rVB	718094	1099602	13.13%	2.036%
5	8.863	975	982	995	rBV	2268614	3623864	43.28%	6.710%
6	10.287	1217	1224	1243	rBV	504668	879941	10.51%	1.629%
7	10.487	1251	1258	1266	rBV	980317	1571890	18.77%	2.911%
8	12.969	1672	1680	1688	rBV	4639777	6584779	78.64%	12.193%
9	14.057	1860	1865	1871	rVB	69252	95752	1.14%	0.177%
10	14.345	1906	1914	1921	rBV	1383050	1962123	23.43%	3.633%
11	15.845	2155	2169	2179	rBV	3914424	5655322	67.54%	10.472%
12	17.104	2376	2383	2387	rBV	1599152	2278540	27.21%	4.219%
13	17.145	2387	2390	2397	rVV	265799	435954	5.21%	0.807%
14	17.234	2397	2405	2411	rVB2	57865	119150	1.42%	0.221%
15	17.798	2496	2501	2507	rVB	118316	136554	1.63%	0.253%
16	18.016	2534	2538	2547	rBV2	313334	415572	4.96%	0.769%
17	19.122	2721	2726	2731	rBV	320723	466490	5.57%	0.864%
18	19.251	2745	2748	2754	rBV	101303	122929	1.47%	0.228%
19	19.475	2782	2786	2789	rVV	246294	274170	3.27%	0.508%
20	19.510	2789	2792	2797	rVB2	81216	105519	1.26%	0.195%
21	19.686	2816	2822	2827	rBV	6679835	8373805	100.00%	15.505%
22	20.939	3031	3035	3045	rBV	888879	1258295	15.03%	2.330%
23	21.204	3074	3080	3085	rBV	1923801	2750848	32.85%	5.094%
24	21.369	3106	3108	3118	rVB2	104180	155273	1.85%	0.288%
25	21.645	3152	3155	3159	rVB	129098	144629	1.73%	0.268%
26	21.845	3182	3189	3198	rBV	736702	1321034	15.78%	2.446%
27	22.892	3364	3367	3380	rVB3	219835	423246	5.05%	0.784%
28	23.521	3467	3474	3489	rVB2	1349066	2680894	32.02%	4.964%

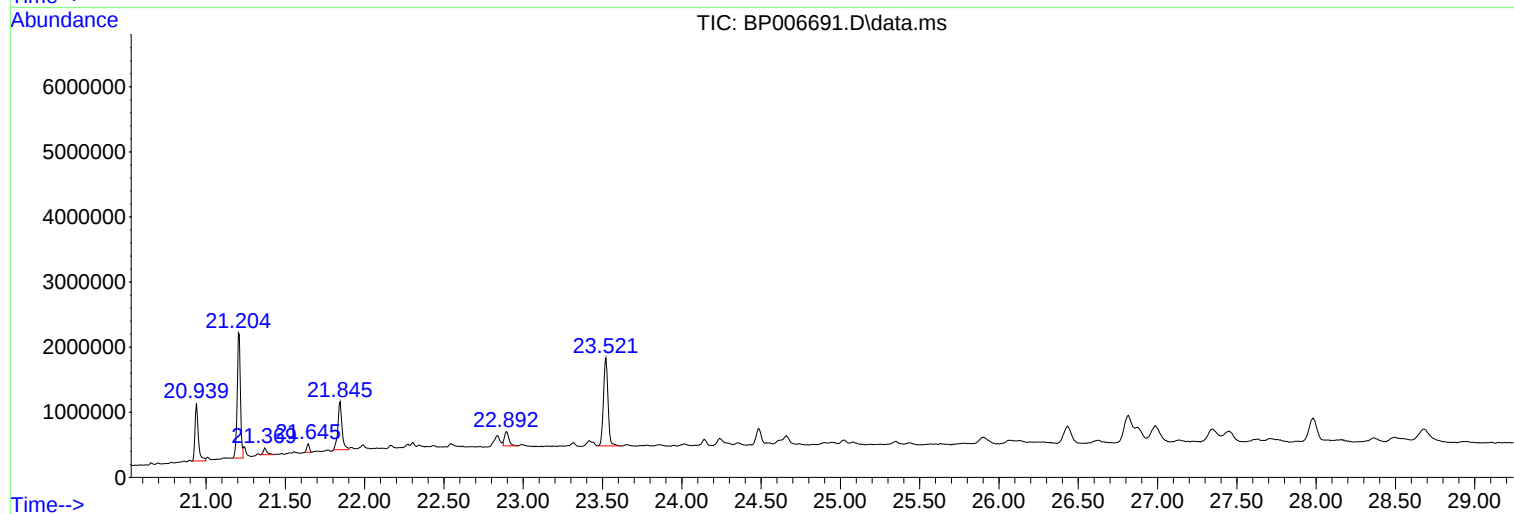
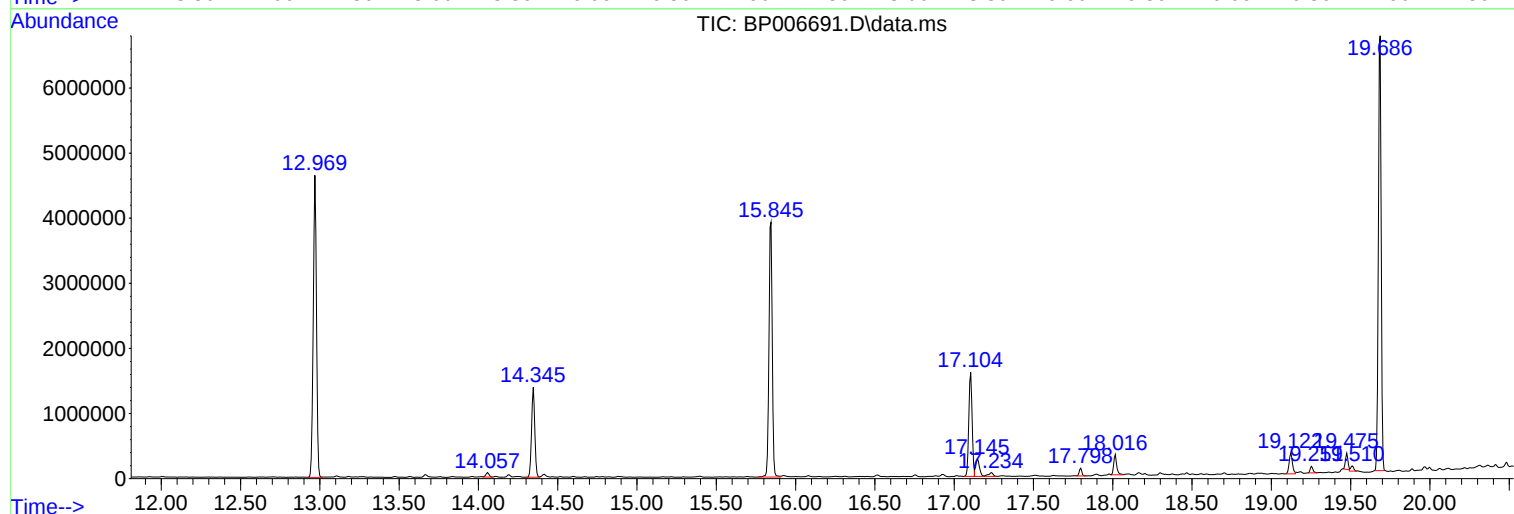
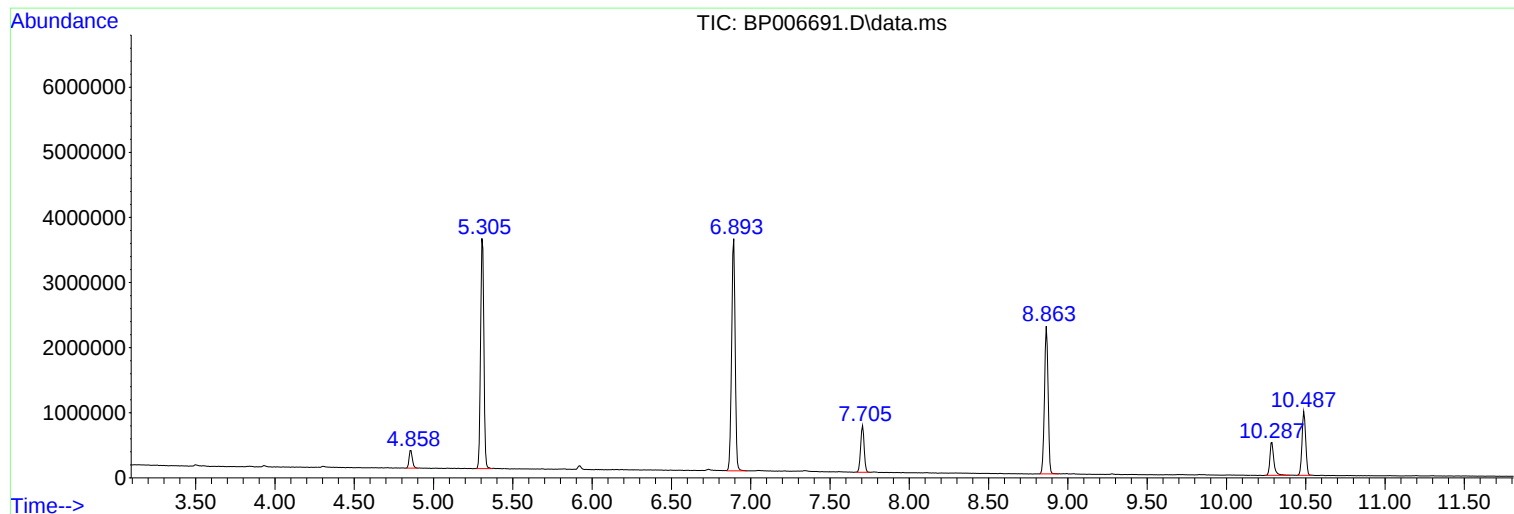
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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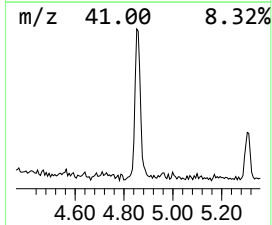
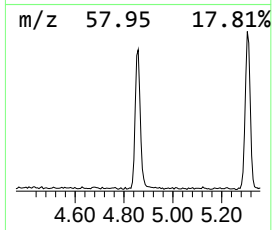
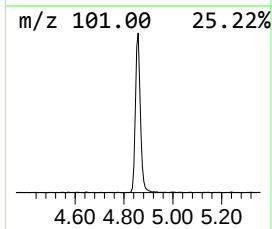
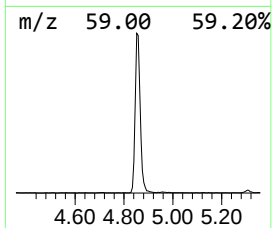
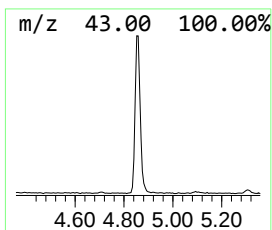
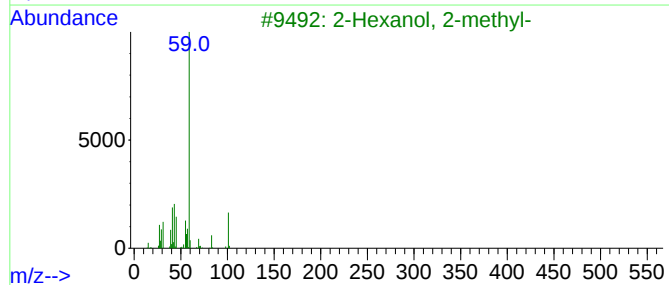
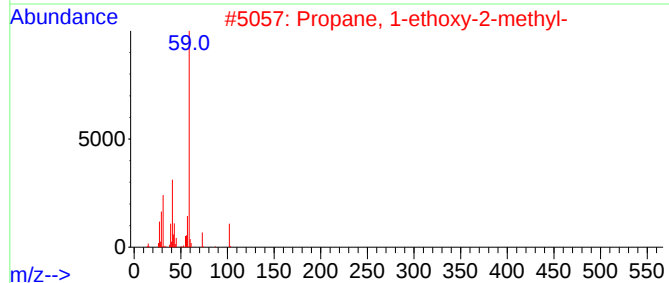
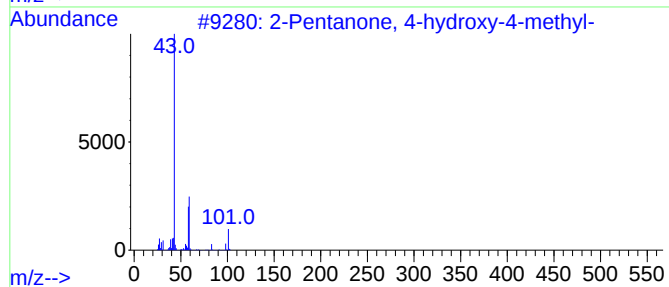
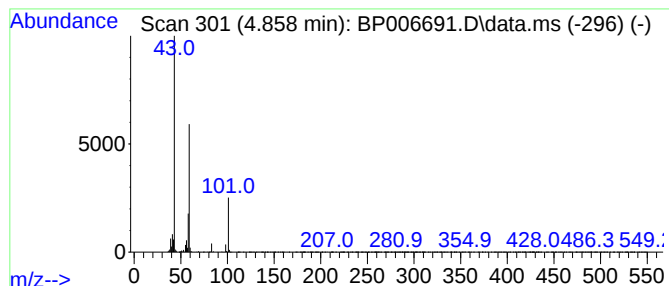
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.858	7.08 ng	389057	1,4-Dichlorobenzene-d4	7.705

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25		
4	4-Pentene-2-ol, 2-methyl	100	C6H12O	000624-97-5	12		
5	Propanenitrile, 3-ethoxy-	99	C5H9NO	002141-62-0	9		



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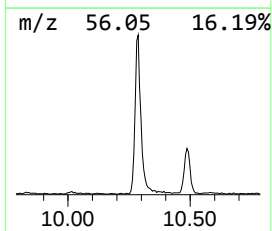
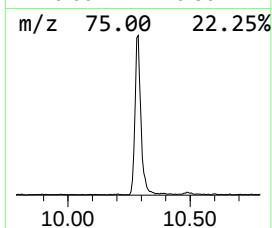
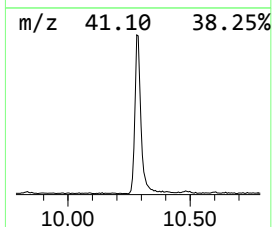
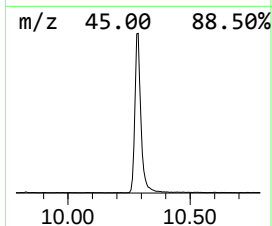
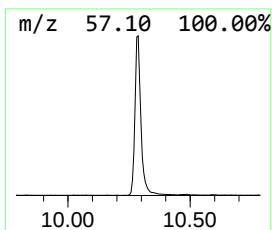
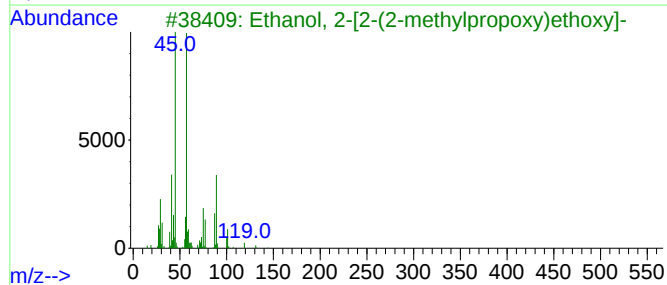
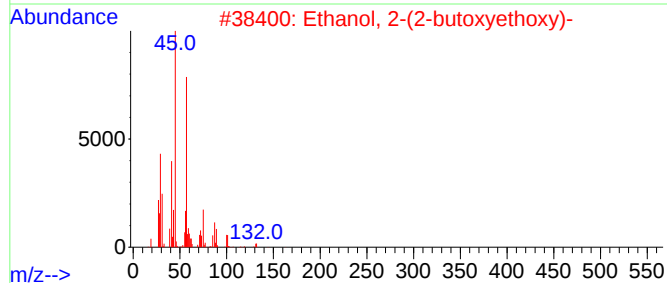
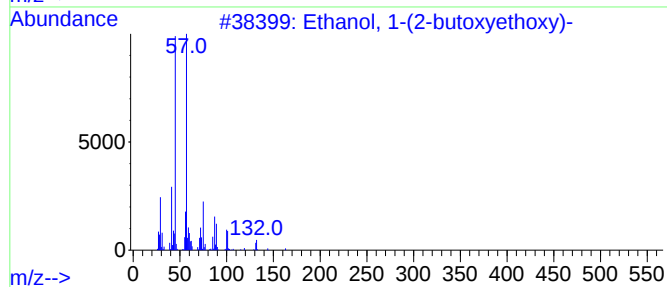
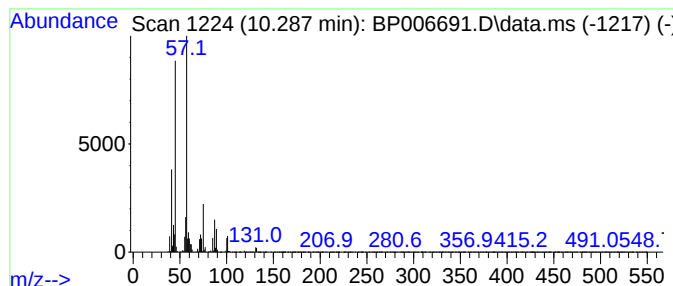
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Peak Number 2 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.287	11.20 ng	879941	Naphthalene-d8	10.487

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
2			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
3			Ethanol, 2-[2-(2-methylpropoxy)ethoxy]-	162	C8H18O3	018912-80-6	72
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
5			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50



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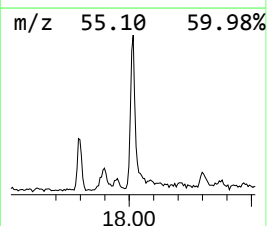
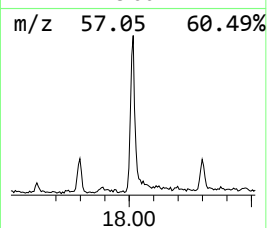
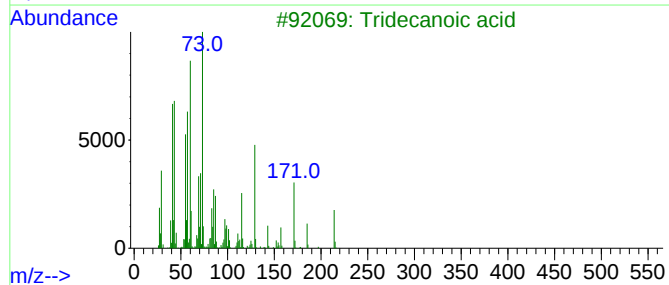
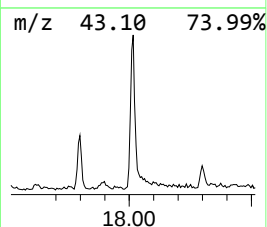
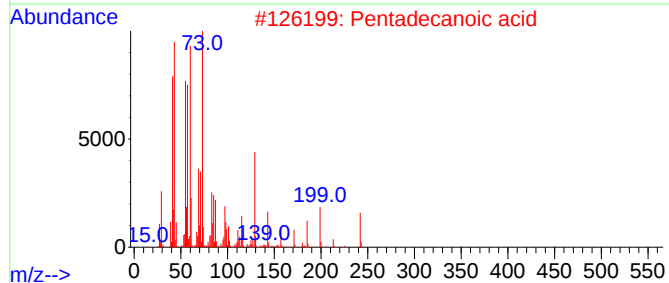
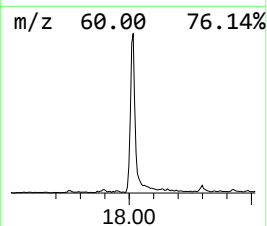
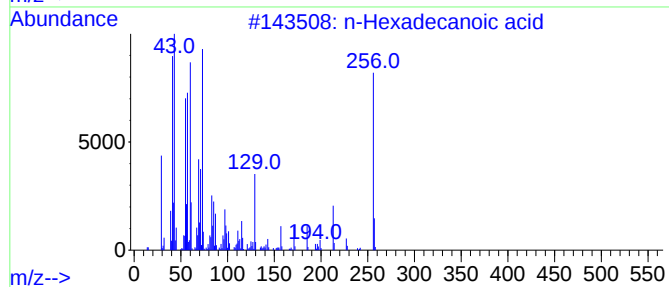
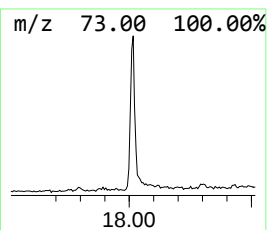
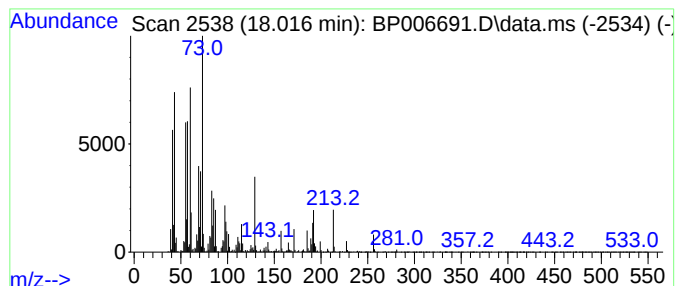
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.016	3.65 ng	415572	Phenanthrene-d10	17.104

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	81
3			Tridecanoic acid	214	C13H26O2	000638-53-9	64
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	55



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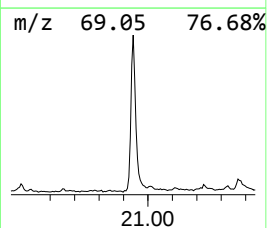
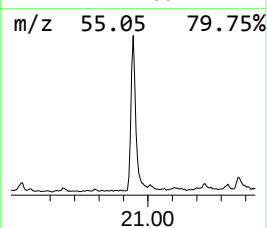
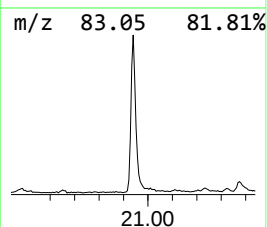
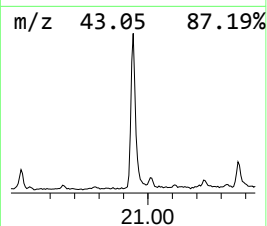
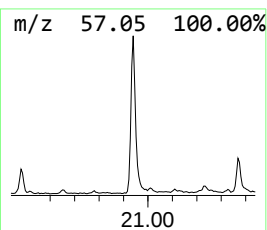
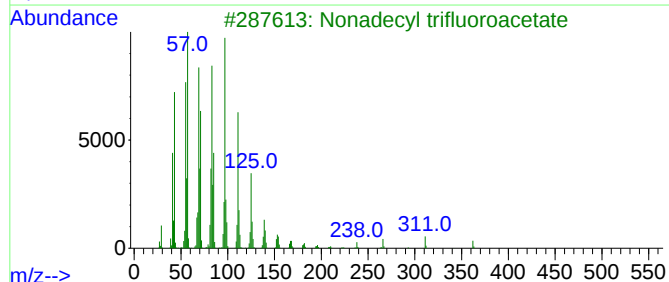
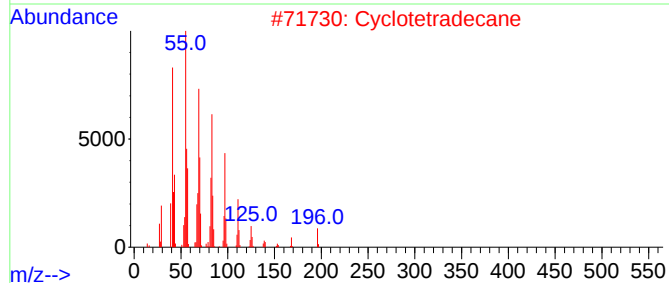
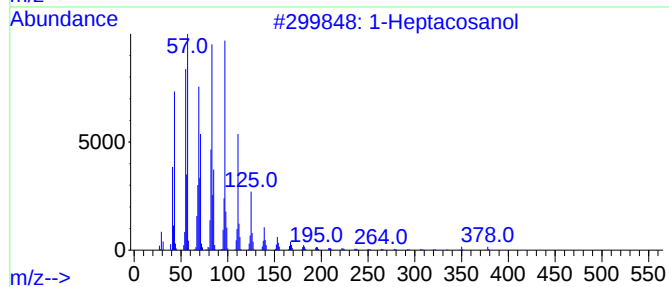
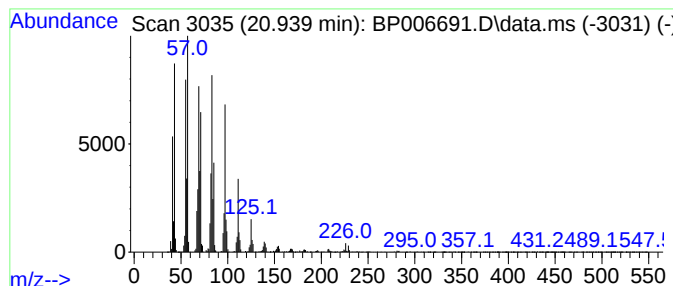
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Peak Number 4 1-Heptacosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.939	9.15 ng	1258300	Chrysene-d12	21.210

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptacosanol	396	C27H56O	002004-39-9	94
2			Cyclotetradecane	196	C14H28	000295-17-0	93
3			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
4			Octacosanol	410	C28H58O	000557-61-9	91
5			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91



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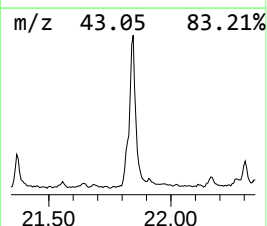
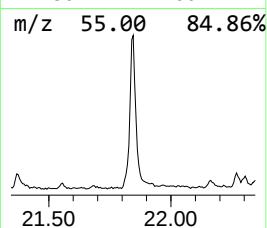
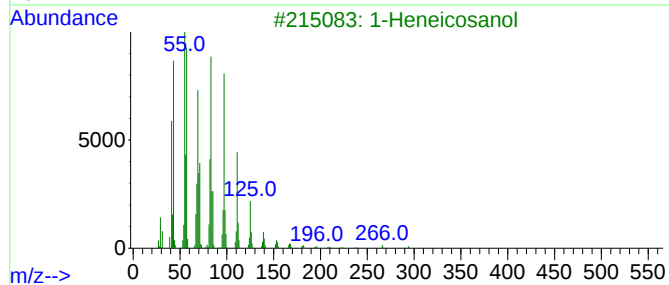
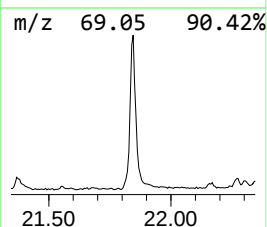
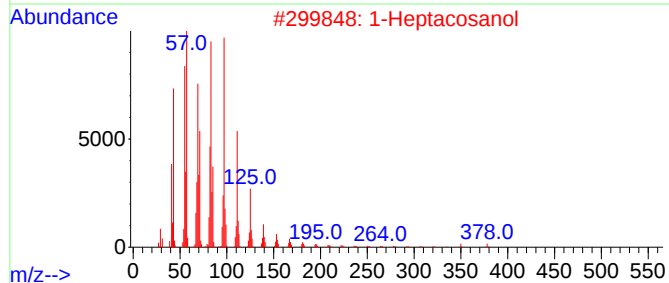
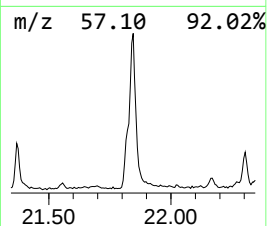
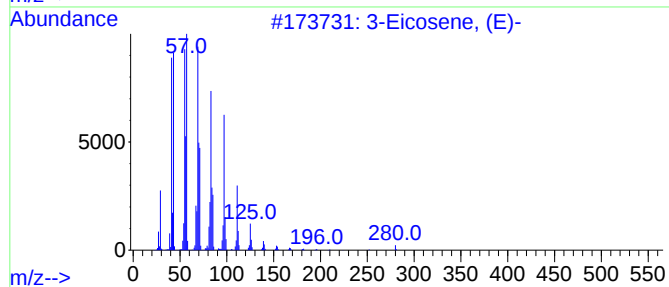
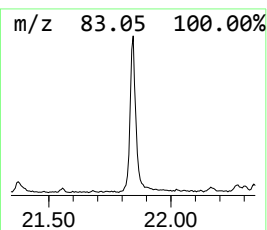
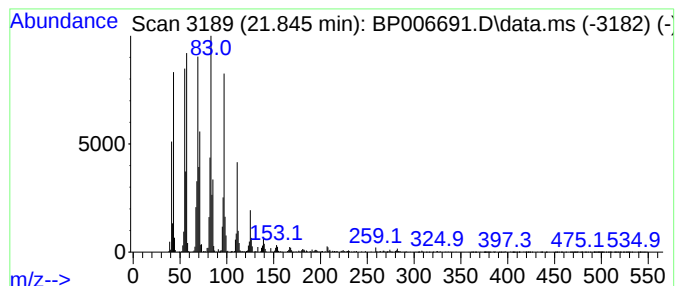
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Peak Number 5 3-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.845	9.60 ng	1321030	Chrysene-d12	21.210

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-		280	C20H40	074685-33-9	99
2	1-Heptacosanol		396	C27H56O	002004-39-9	94
3	1-Heneicosanol		312	C21H44O	015594-90-8	93
4	Octacosanol		410	C28H58O	000557-61-9	91
5	n-Tetracosanol-1		354	C24H50O	000506-51-4	91



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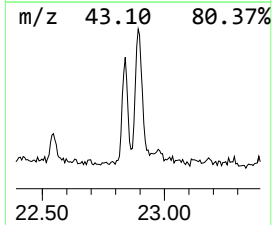
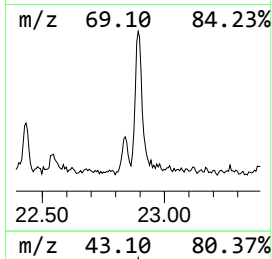
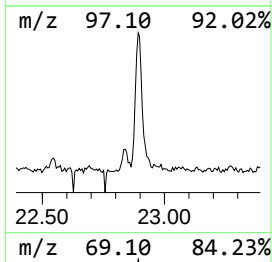
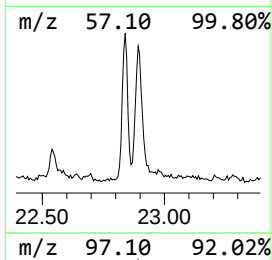
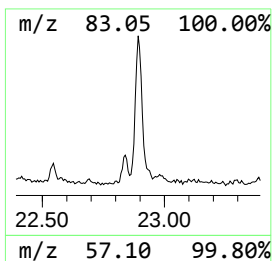
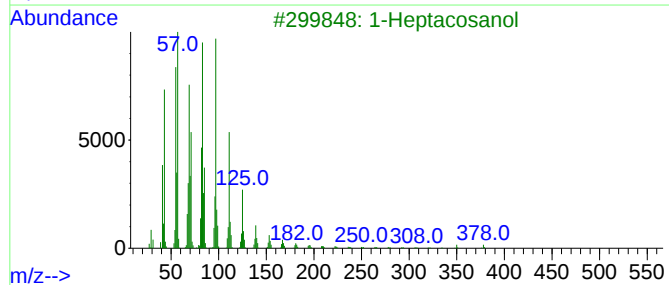
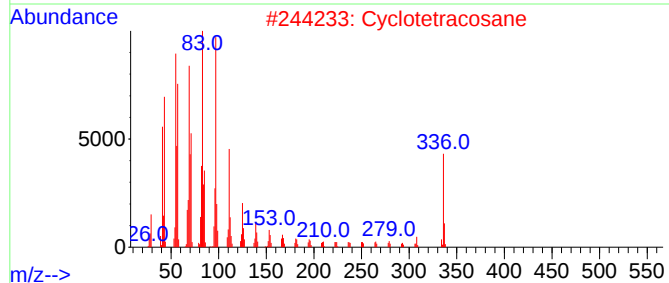
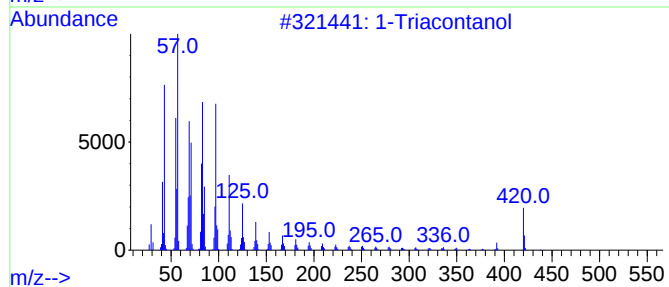
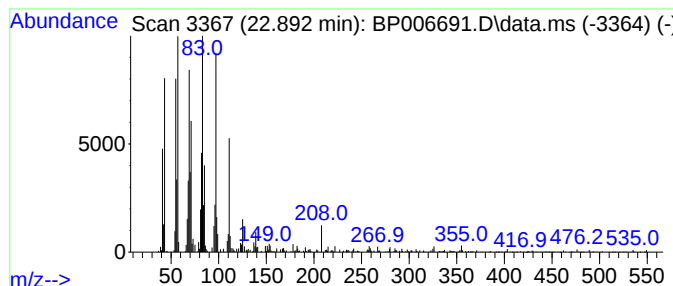
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Triacontanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.892	3.16 ng	423246	Perylene-d12	23.522

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Triacontanol	438	C30H62O	000593-50-0	94
2		Cyclotetracosane	336	C24H48	000297-03-0	91
3		1-Heptacosanol	396	C27H56O	002004-39-9	91
4		Tetracosan-10-yl acetate	396	C26H52O2	1000466-24-3	87
5		Behenic alcohol	326	C22H46O	000661-19-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081721\
Data File : BP006691.D
Acq On : 16 Aug 2021 19:46
Operator : CG/JU
Sample : M3407-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
25N

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.858	7.1	ng	389057	1	7.705	1099600	20.0
Ethanol, 1-(2-b...	10.287	11.2	ng	879941	2	10.487	1571890	20.0
n-Hexadecanoic ...	18.016	3.6	ng	415572	4	17.104	2278540	20.0
1-Heptacosanol	20.939	9.2	ng	1258300	5	21.210	2750850	20.0
3-Eicosene, (E)-	21.845	9.6	ng	1321030	5	21.210	2750850	20.0
1-Triacontanol	22.892	3.2	ng	423246	6	23.522	2680890	20.0