

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101521\
 Data File : BF125866.D
 Acq On : 15 Oct 2021 16:59
 Operator : JU/CG
 Sample : M4242-10
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 T1-COMP-(1-4)

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-BF100721.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125866.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.051	501	504	511	rVB	89405	104316	2.54%	0.380%
2	5.451	567	572	575	rBV	3260515	3173717	77.15%	11.576%
3	6.463	738	744	747	rBV	3169140	3236833	78.69%	11.806%
4	6.834	803	807	810	rBV	1329041	993961	24.16%	3.625%
5	7.392	897	902	905	rBV	2371374	2128563	51.75%	7.764%
6	8.016	1004	1008	1020	rBV	201603	193208	4.70%	0.705%
7	8.116	1020	1025	1028	rBV	1473150	1340389	32.59%	4.889%
8	9.186	1202	1207	1210	rBV	4546573	4113490	100.00%	15.004%
9	9.863	1318	1322	1326	rBV	1675285	1427823	34.71%	5.208%
10	10.651	1452	1456	1459	rBV	2153830	1925062	46.80%	7.021%
11	10.698	1461	1464	1472	rVB	52249	63246	1.54%	0.231%
12	11.345	1571	1574	1577	rBV	1375482	1219547	29.65%	4.448%
13	11.874	1661	1664	1673	rBV2	228916	255094	6.20%	0.930%
14	12.557	1777	1780	1785	rVB	212666	174091	4.23%	0.635%
15	12.657	1794	1797	1804	rBV3	124219	157685	3.83%	0.575%
16	12.786	1816	1819	1822	rVB	187275	165121	4.01%	0.602%
17	12.933	1839	1844	1847	rBV	3839113	3368013	81.88%	12.284%
18	13.827	1992	1996	1998	rBV2	185560	236902	5.76%	0.864%
19	13.851	1998	2000	2004	rVB	147012	132978	3.23%	0.485%
20	13.980	2017	2022	2025	rBV	1373604	1296261	31.51%	4.728%
21	14.186	2055	2057	2064	rVB3	58844	62858	1.53%	0.229%
22	14.610	2126	2129	2133	rVB	135874	124336	3.02%	0.454%
23	14.833	2164	2167	2174	rVB	106969	126167	3.07%	0.460%
24	15.010	2194	2197	2201	rBV	95945	160519	3.90%	0.585%
25	15.368	2255	2258	2261	rBV	68709	78177	1.90%	0.285%
26	15.433	2264	2269	2273	rBV	889972	1089394	26.48%	3.973%
27	15.898	2345	2348	2352	rVB2	50062	69058	1.68%	0.252%

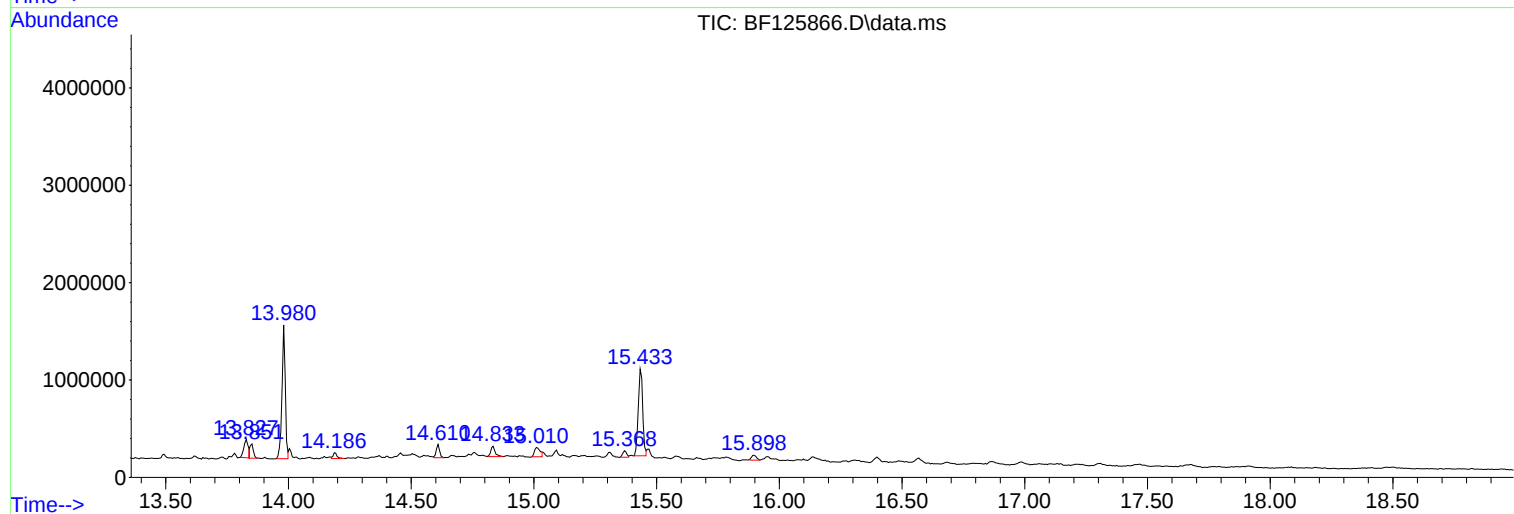
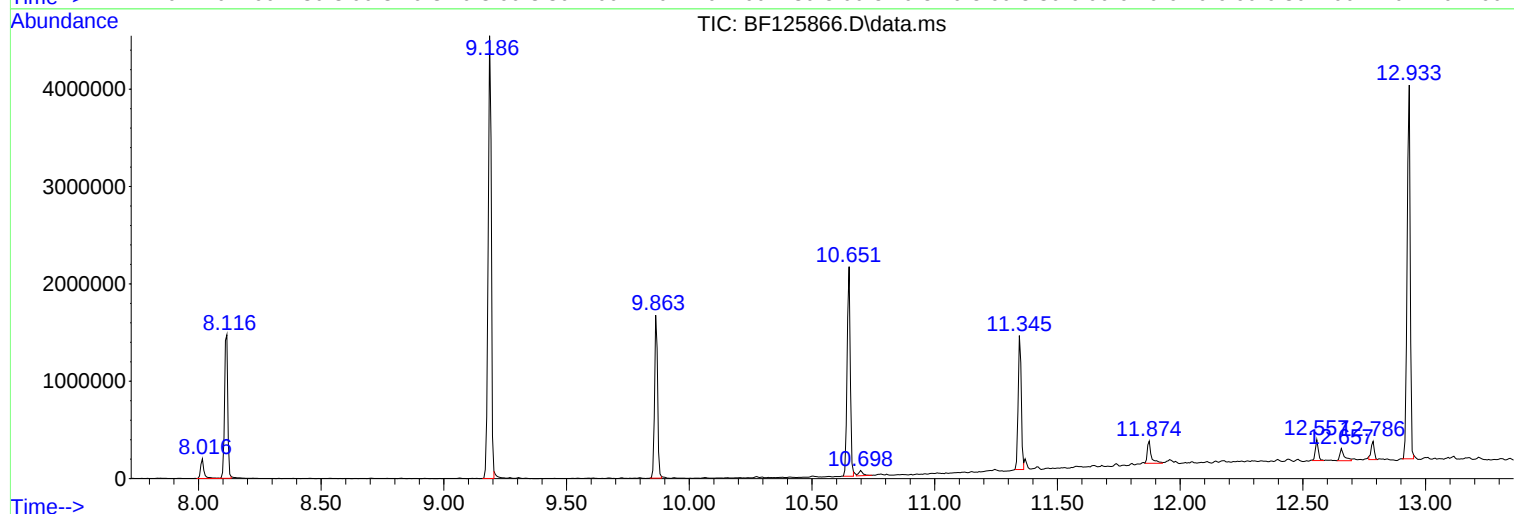
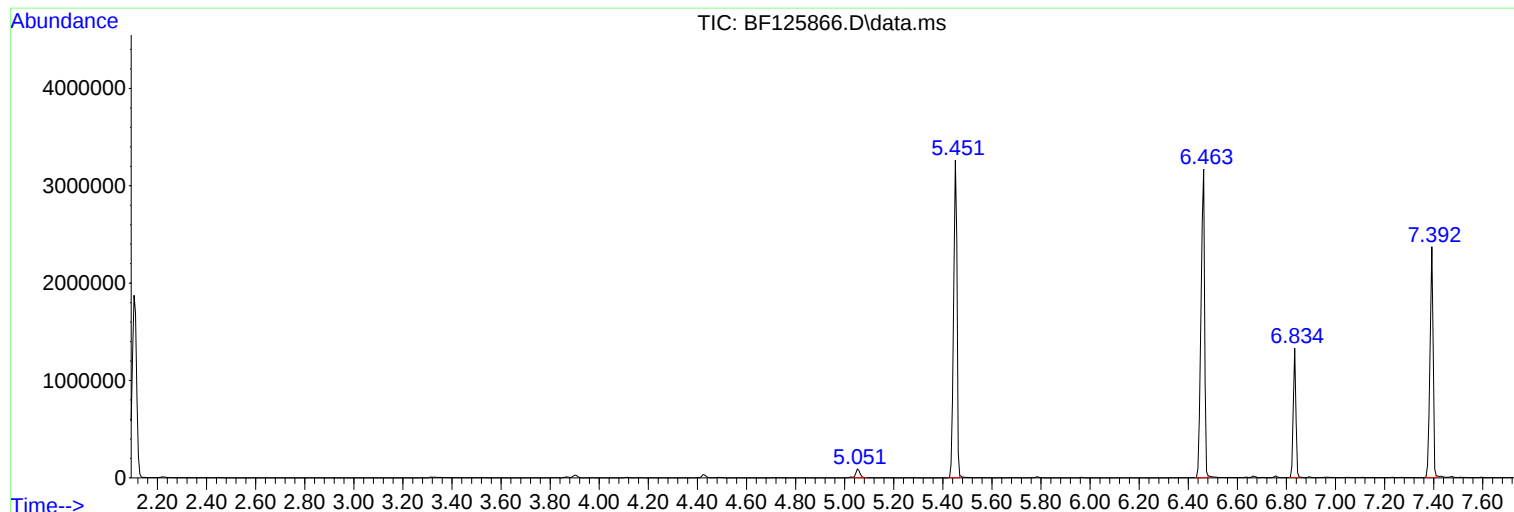
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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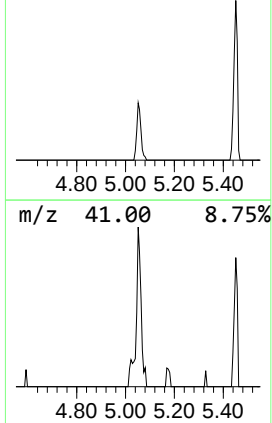
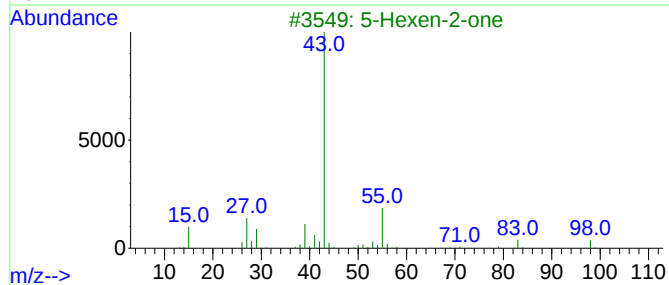
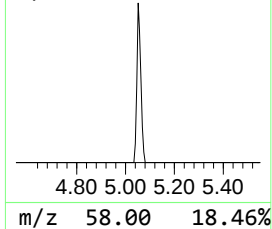
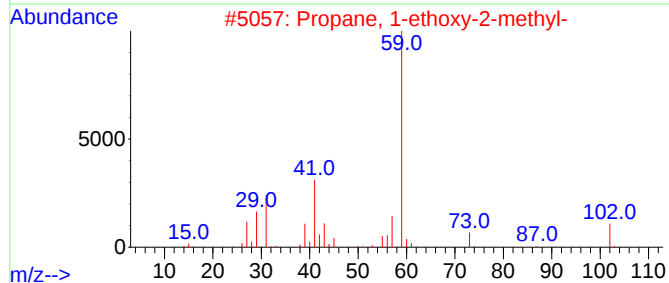
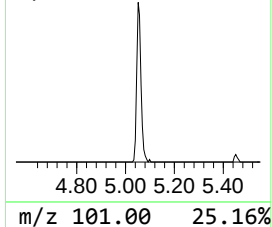
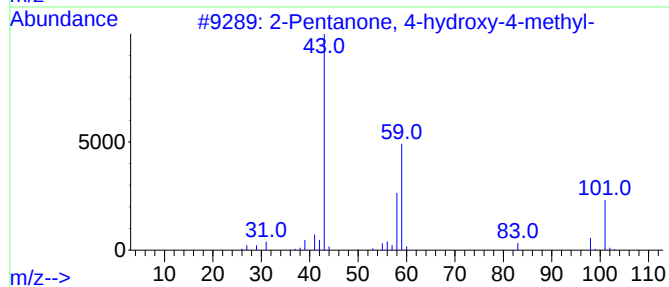
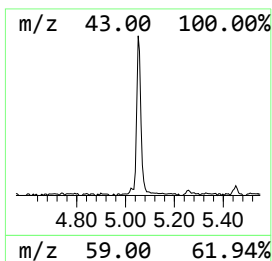
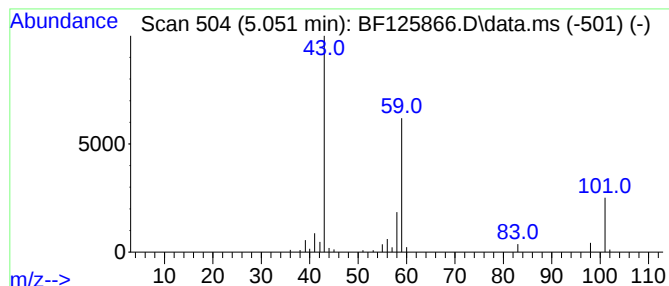
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.051	2.10 ng	104316	1,4-Dichlorobenzene-d4	6.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53		
2	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	17		
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9		
4	Acetone	58	C3H6O	000067-64-1	9		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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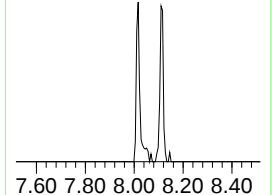
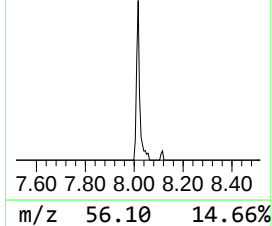
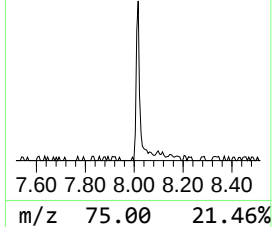
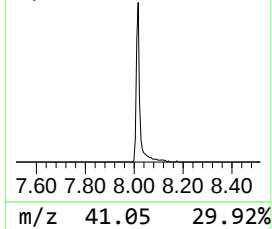
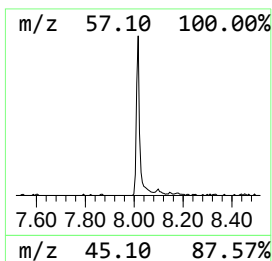
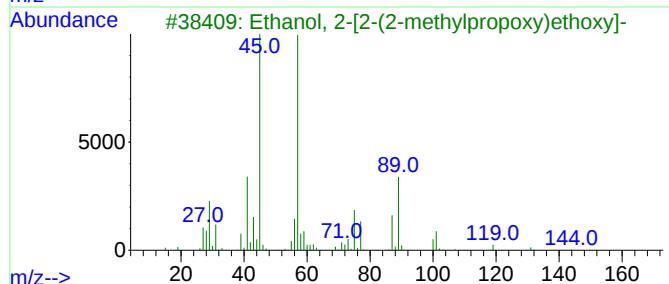
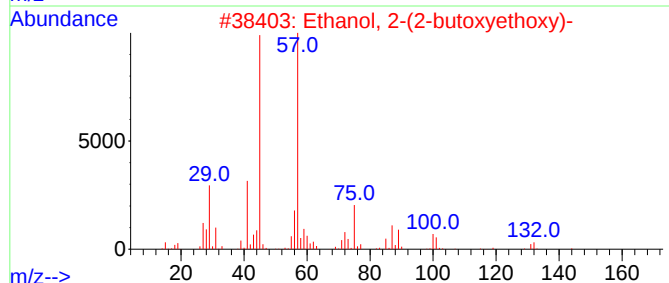
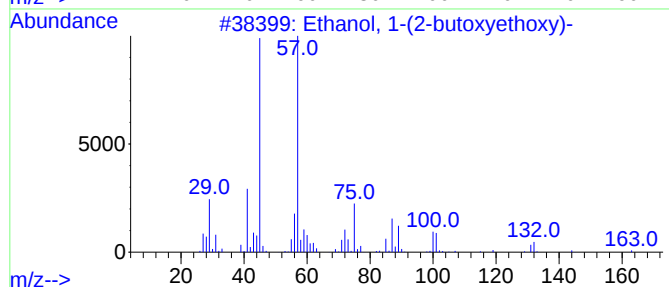
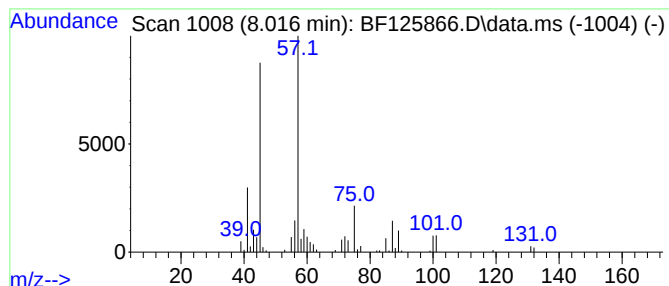
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Peak Number 2 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.016	2.88 ng	193208	Naphthalene-d8	8.116

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)e...	162	C8H18O3	018912-80-6	72
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
5			Di-sec-Butyl ether	130	C8H18O	006863-58-7	50



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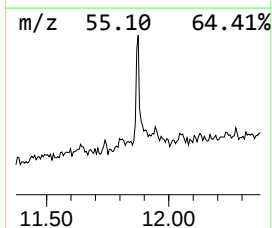
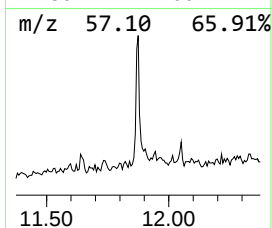
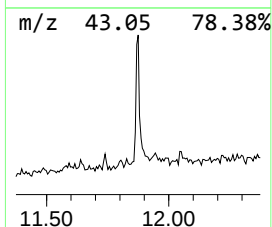
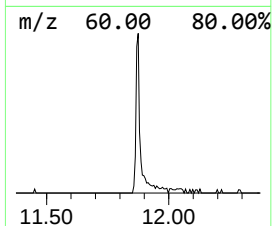
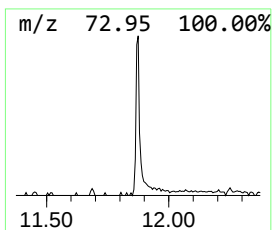
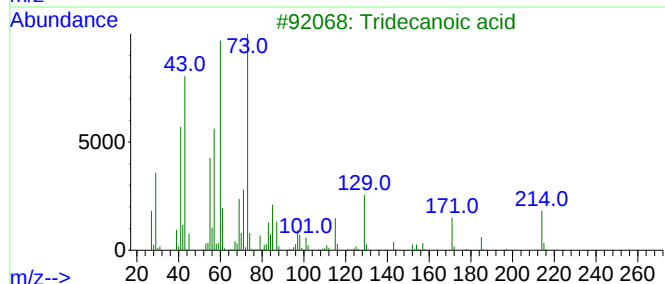
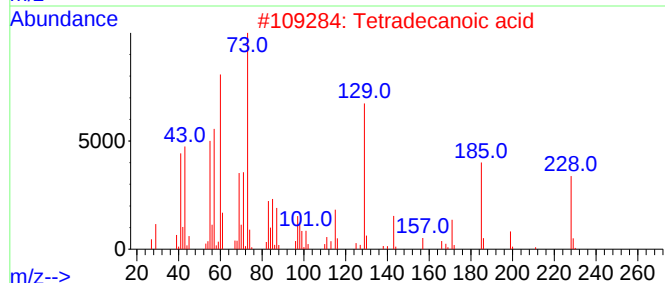
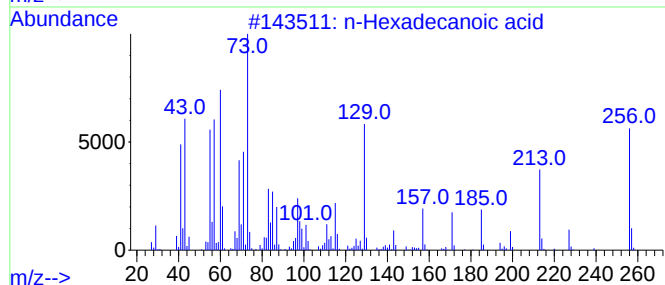
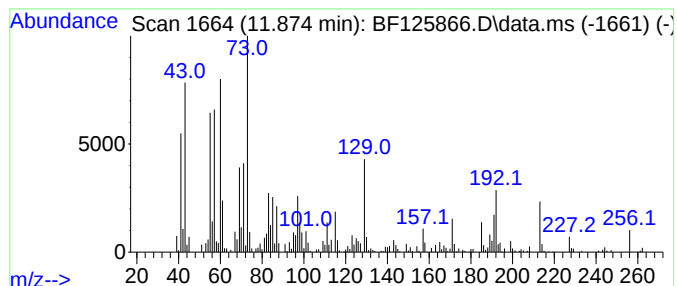
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BNA_F
ClientSampleId :
T1-COMP-(1-4)

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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.874	4.18 ng	255094	Phenanthrene-d10		11.345	
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	Tridecanoic acid		214	C13H26O2	000638-53-9	86
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	81
5	n-Decanoic acid		172	C10H20O2	000334-48-5	62



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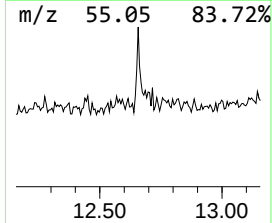
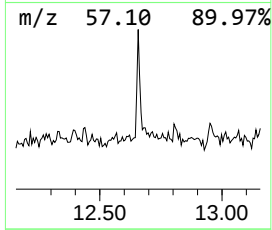
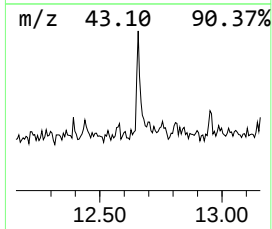
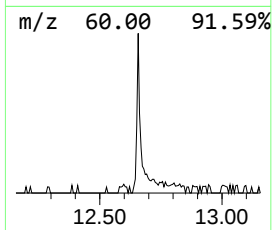
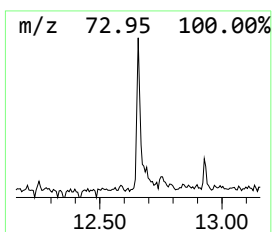
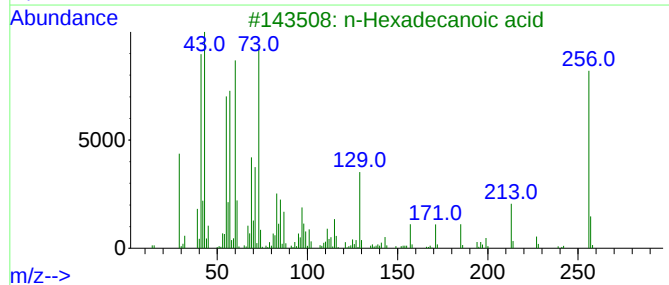
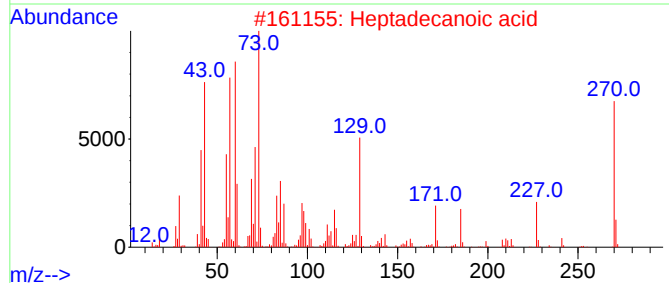
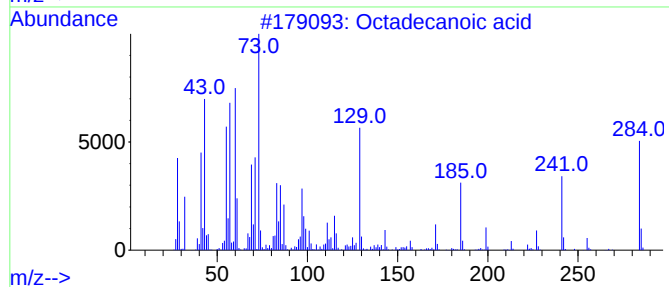
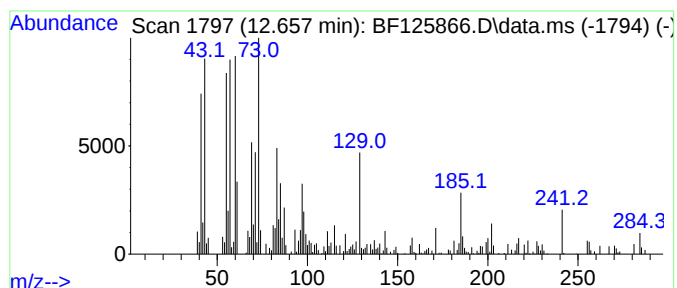
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.657	2.59 ng	157685	Phenanthrene-d10	11.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	97
2			Heptadecanoic acid	270	C17H34O2	000506-12-7	93
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	58



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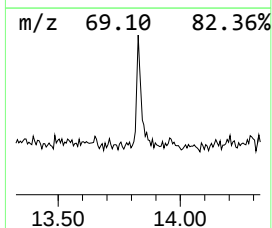
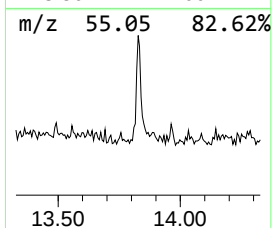
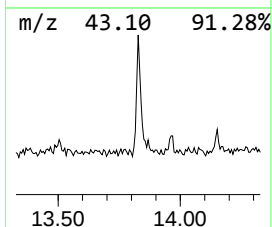
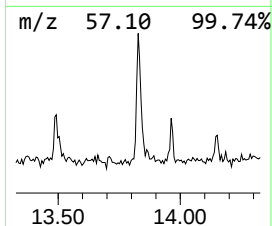
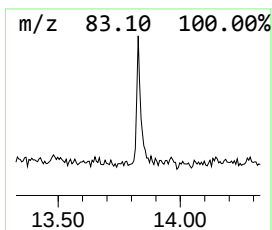
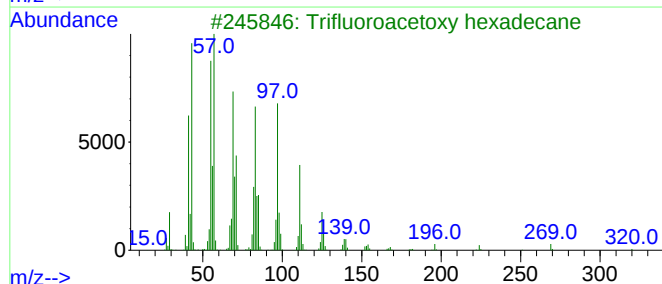
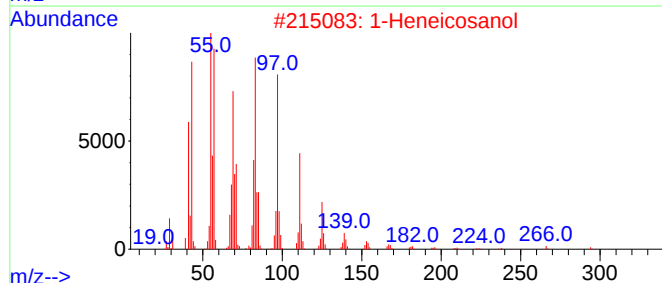
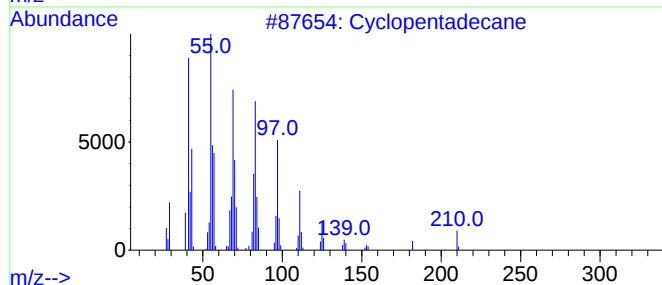
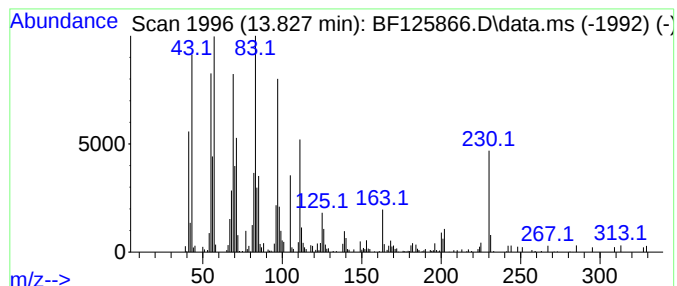
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TIC Library : C:\Database\NIST20.L
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Peak Number 6 Cyclopentadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	3.66 ng	236902	Chrysene-d12	13.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	97
2			1-Heneicosanol	312	C21H44O	015594-90-8	93
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
4			Cetene	224	C16H32	000629-73-2	91
5			2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91



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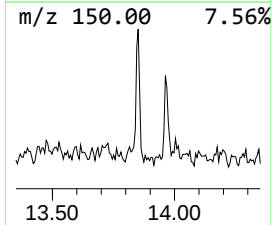
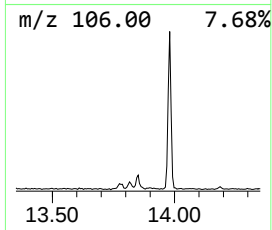
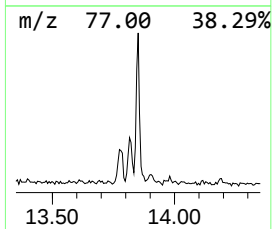
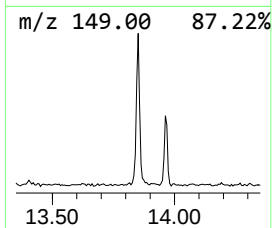
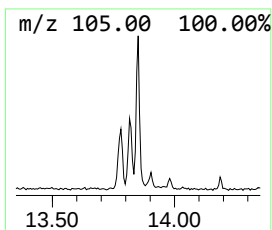
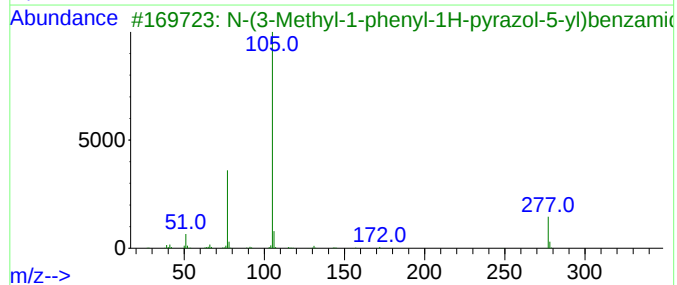
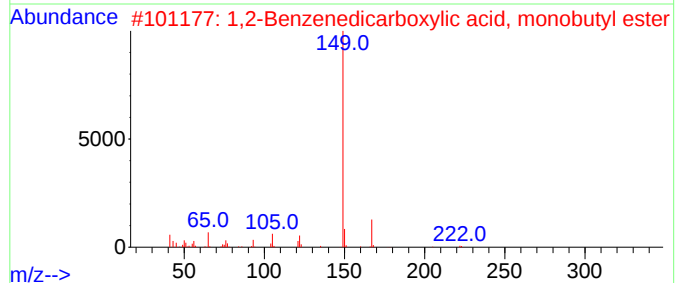
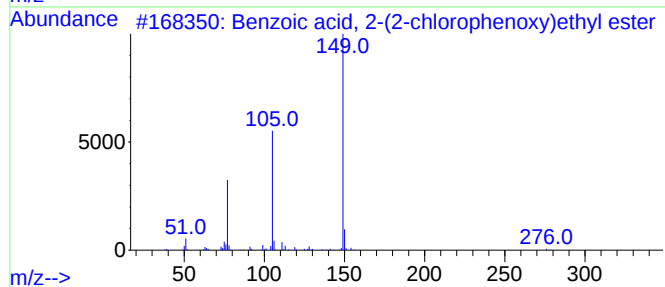
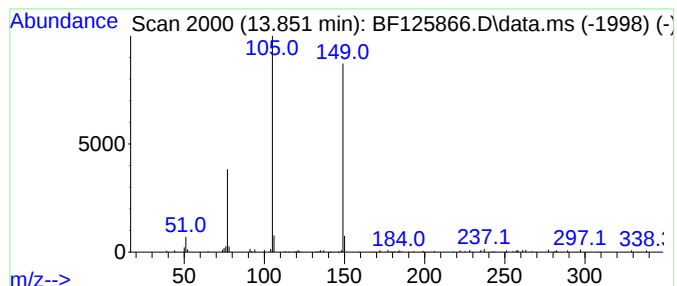
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzoic acid, 2-(2-chloroph... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.851	2.05 ng	132978	Chrysene-d12	13.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2-(2-chlorophenoxy...	276	C15H13ClO3	1000368-25-9	72
2			1,2-Benzenedicarboxylic acid, mo...	222	C12H14O4	000131-70-4	43
3			N-(3-Methyl-1-phenyl-1H-pyrazol-...	277	C17H15N3O	064664-15-9	30
4			Ethanone, 2-bromo-1,2-diphenyl-	274	C14H11BrO	001484-50-0	27
5			4-Nitrophenyl benzoate	243	C13H9NO4	000959-22-8	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101521\
Data File : BF125866.D
Acq On : 15 Oct 2021 16:59
Operator : JU/CG
Sample : M4242-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T1-COMP-(1-4)

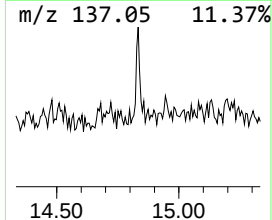
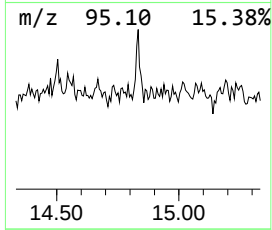
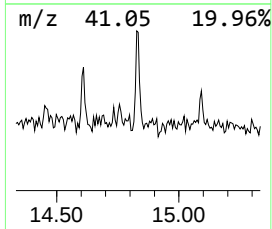
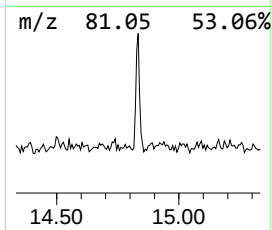
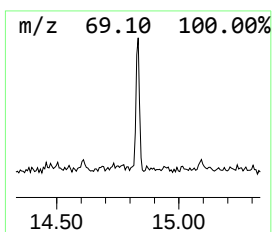
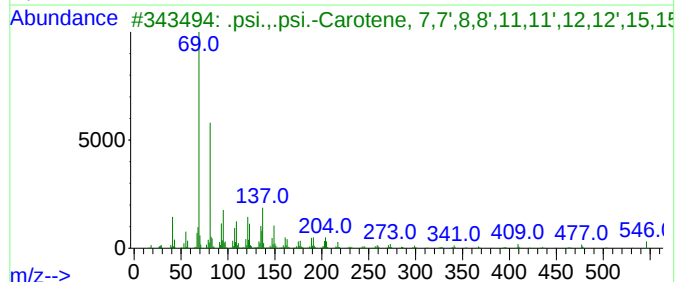
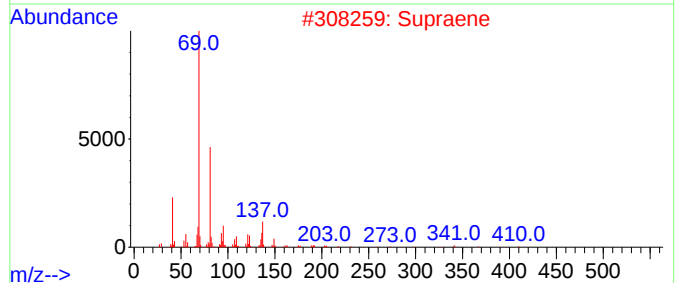
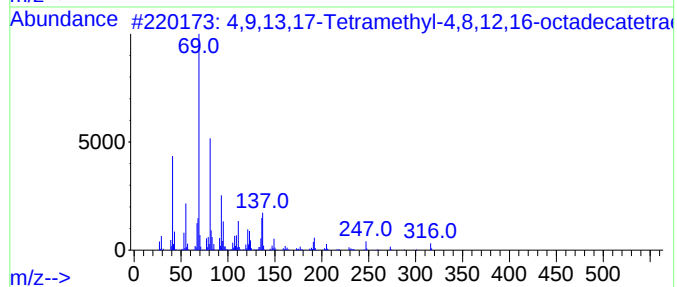
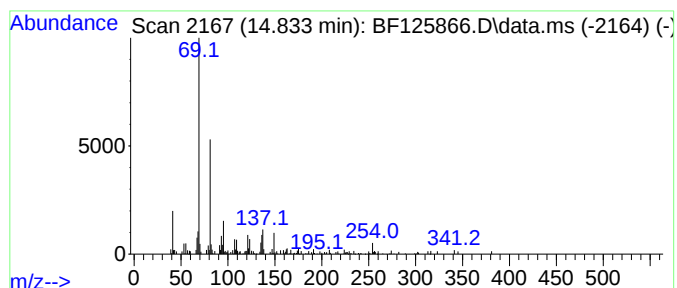
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 4,9,13,17-Tetramethyl-4,8,11,15-octadecatetraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.833	2.32 ng	126167	Perylene-d12	15.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,9,13,17-Tetramethyl-4,8,12,16-octadecatetraene	316	C22H36O	056882-09-8	81		
2	Supraene	410	C30H50	007683-64-9	74		
3	.psi.,.psi.-Carotene, 7,7',8,8',11,11',12,12',15,15'-hexamethyl-2,6-dimethyldodeca-2,6,10-triene	547	C40H66	000502-62-5	64		
4	1,6,10,14,18,22-Tetracosahexaene	426	C30H50O	097232-74-1	59		
5	7,11-Dimethyldodeca-2,6,10-triene	208	C14H24O	125529-10-4	59		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101521\
Data File : BF125866.D
Acq On : 15 Oct 2021 16:59
Operator : JU/CG
Sample : M4242-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T1-COMP-(1-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.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-...	5.051	2.1	ng	104316	1	6.834	993961	20.0
Ethanol, 1-(2-b...	8.016	2.9	ng	193208	2	8.116	1340390	20.0
n-Hexadecanoic ...	11.874	4.2	ng	255094	4	11.345	1219550	20.0
Octadecanoic acid	12.657	2.6	ng	157685	4	11.345	1219550	20.0
Cyclopentadecane	13.827	3.7	ng	236902	5	13.980	1296260	20.0
Benzoic acid, 2...	13.851	2.0	ng	132978	5	13.980	1296260	20.0
4,9,13,17-Tetra...	14.833	2.3	ng	126167	6	15.433	1089390	20.0