

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081921\
 Data File : BF125122.D
 Acq On : 19 Aug 2021 19:25
 Operator : JU/CG
 Sample : M3430-06
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PE-6

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-BF081821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125122.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.222	17	23	31	rVB	1391328	1793256	44.75%	5.664%
2	5.145	513	520	527	rVB	154141	184128	4.60%	0.582%
3	5.534	581	586	589	rBV	3767014	3738437	93.30%	11.809%
4	6.539	751	757	759	rBV	3259130	3747978	93.53%	11.839%
5	6.739	788	791	798	rBV2	36995	43144	1.08%	0.136%
6	6.916	818	821	825	rVB	1252618	1007409	25.14%	3.182%
7	7.480	912	917	920	rBV	2690352	2445167	61.02%	7.724%
8	8.098	1018	1022	1025	rBV	999244	774797	19.34%	2.447%
9	8.198	1035	1039	1043	rBV	1480227	1313881	32.79%	4.150%
10	9.274	1218	1222	1226	rBV	4185358	4007077	100.00%	12.657%
11	9.957	1334	1338	1341	rBV	1823439	1459643	36.43%	4.611%
12	10.745	1467	1472	1475	rBV	2843450	2608467	65.10%	8.240%
13	11.445	1587	1591	1593	rBV	1646497	1460328	36.44%	4.613%
14	11.463	1593	1594	1597	rVB	75791	51472	1.28%	0.163%
15	11.963	1669	1679	1684	rBV2	199689	242197	6.04%	0.765%
16	12.651	1793	1796	1800	rBV	130650	118079	2.95%	0.373%
17	12.745	1809	1812	1817	rBV2	56935	58340	1.46%	0.184%
18	12.880	1830	1835	1841	rVB	107447	118311	2.95%	0.374%
19	13.033	1856	1861	1864	rBV	3743534	3711622	92.63%	11.724%
20	13.927	2009	2013	2031	rBV4	114706	372485	9.30%	1.177%
21	14.080	2033	2039	2042	rVV	1103321	1083125	27.03%	3.421%
22	14.104	2042	2043	2050	rVB	57937	53569	1.34%	0.169%
23	14.592	2121	2126	2134	rVB7	46647	119687	2.99%	0.378%
24	15.133	2214	2218	2222	rBV2	43495	73317	1.83%	0.232%
25	15.509	2278	2282	2286	rVB	32150	42961	1.07%	0.136%
26	15.580	2288	2294	2298	rBV	776126	981065	24.48%	3.099%
27	16.062	2372	2376	2381	rVB3	29984	47995	1.20%	0.152%

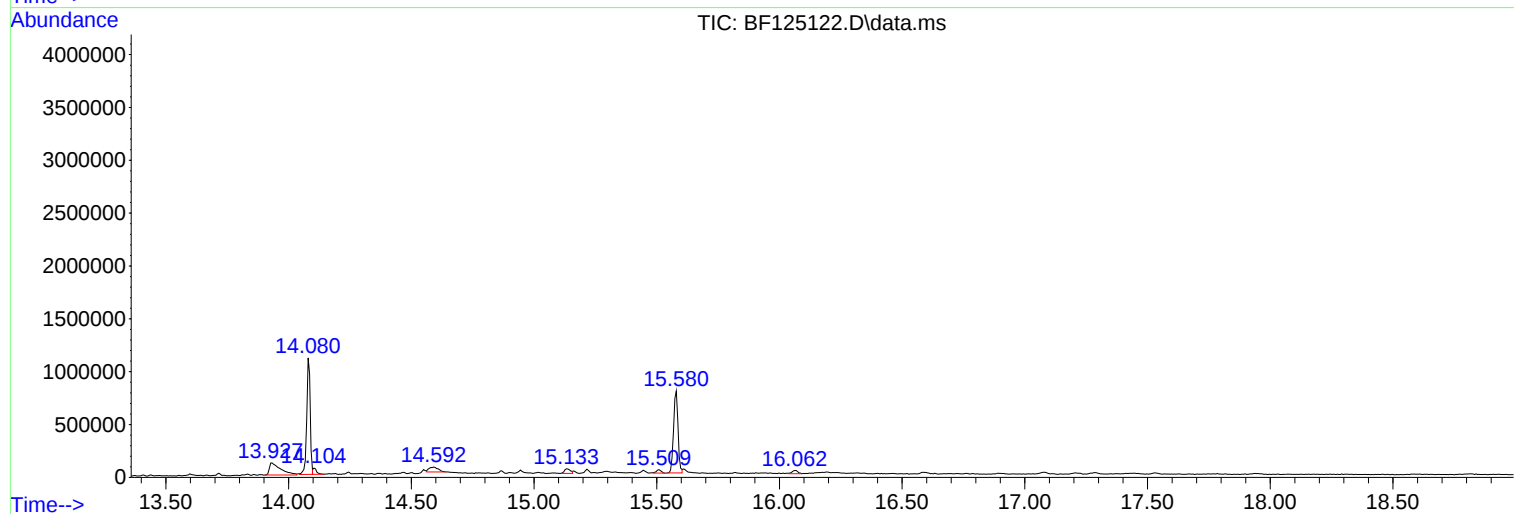
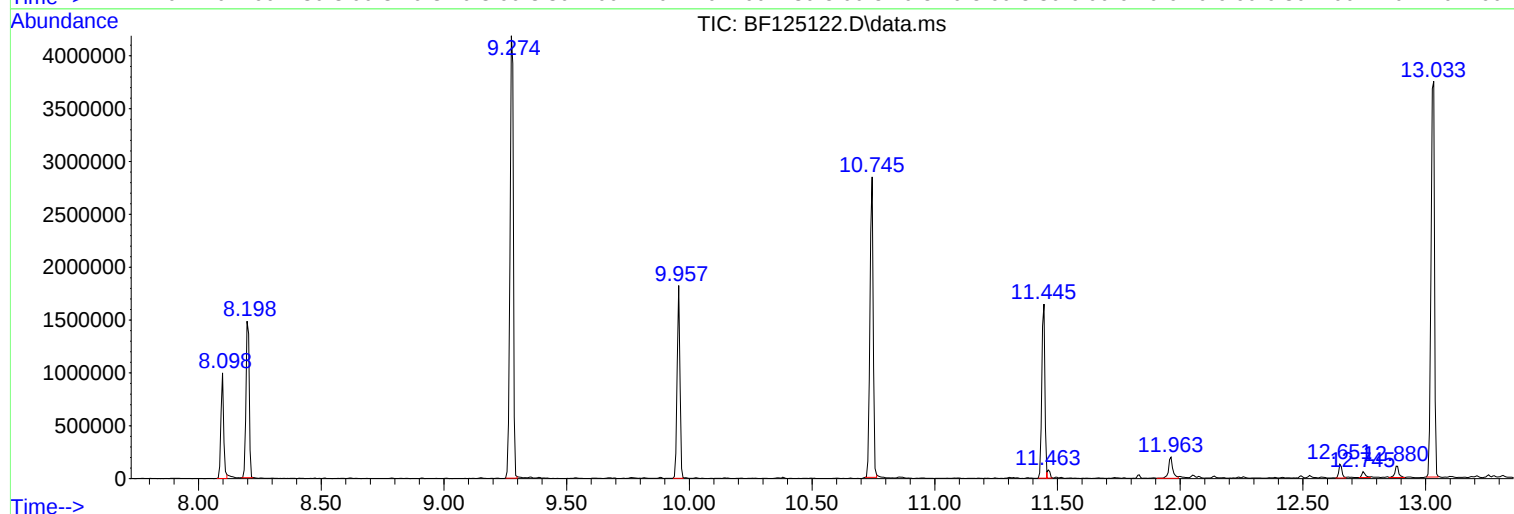
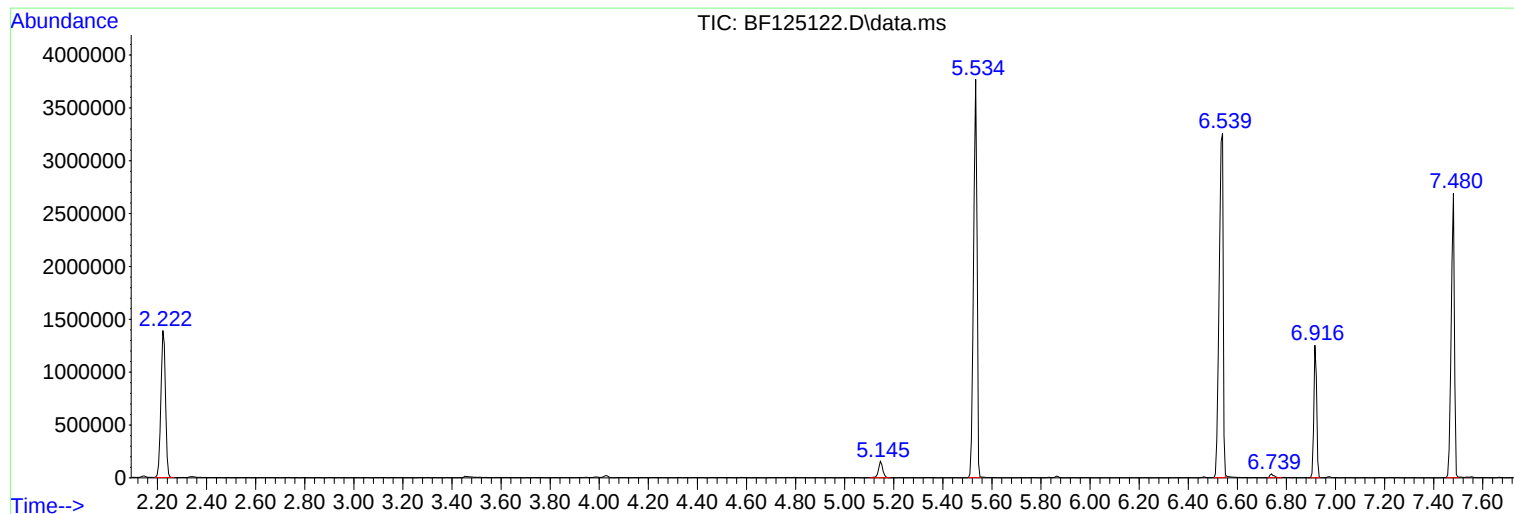
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Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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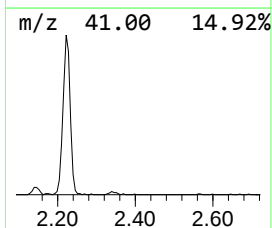
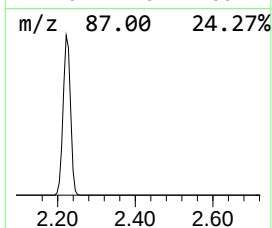
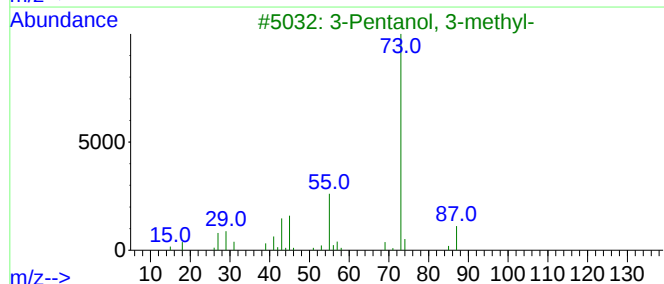
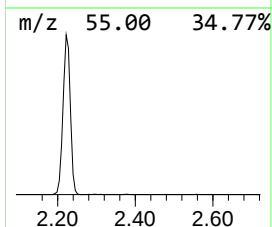
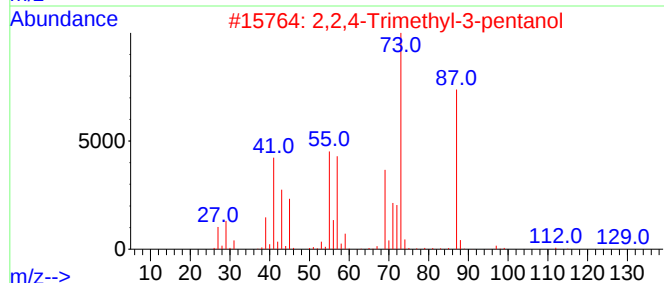
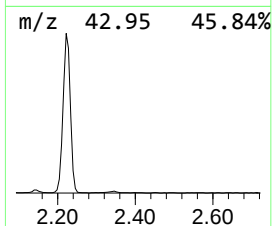
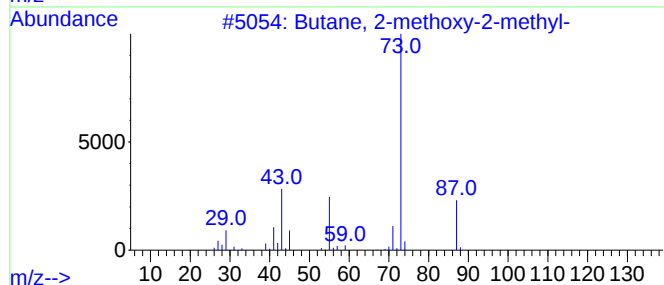
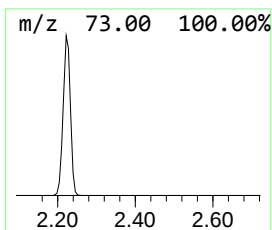
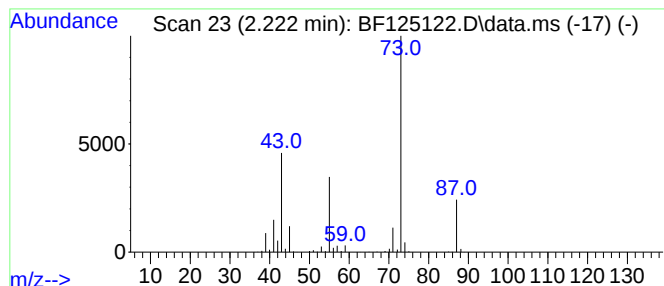
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.222	35.60 ng	1793260	1,4-Dichlorobenzene-d4	6.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	25
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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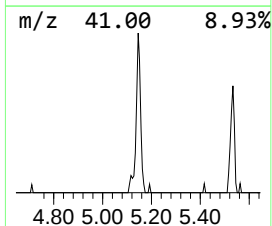
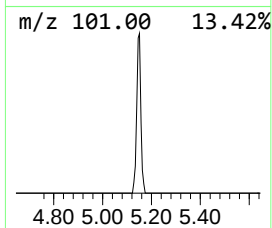
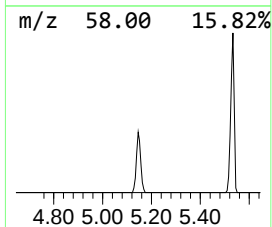
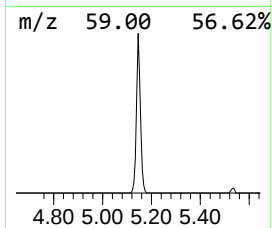
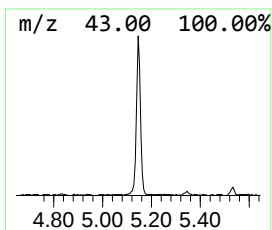
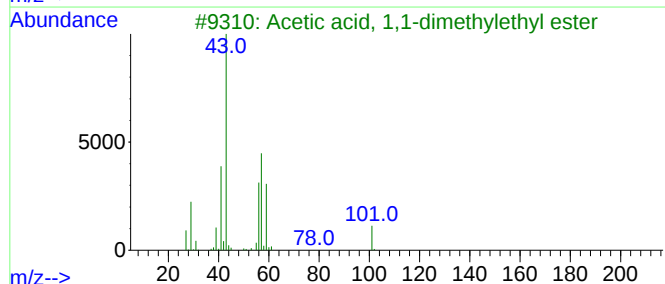
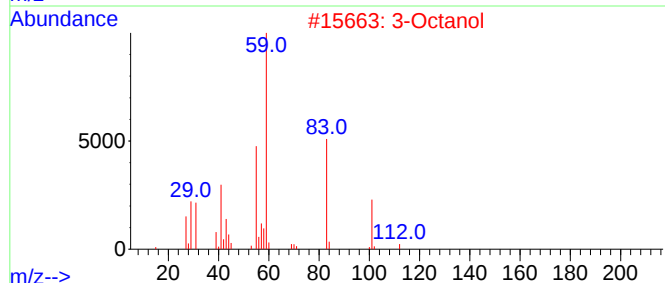
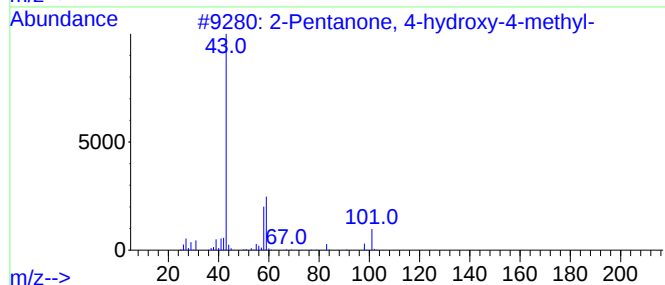
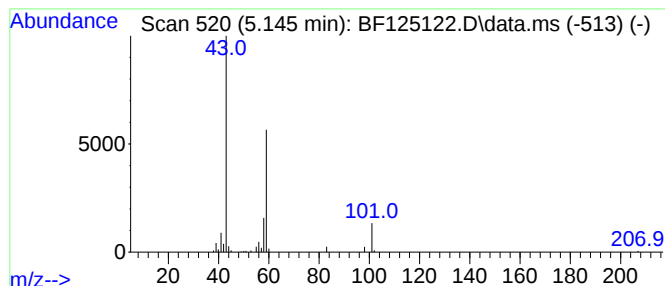
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.145	3.66 ng	184128	1,4-Dichlorobenzene-d4	6.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	3-Octanol	130	C8H18O	000589-98-0	33		
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28		
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9		



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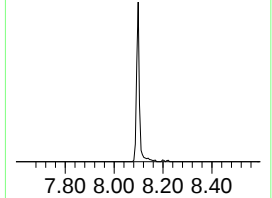
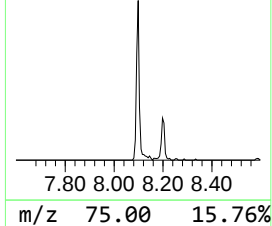
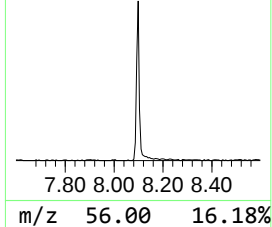
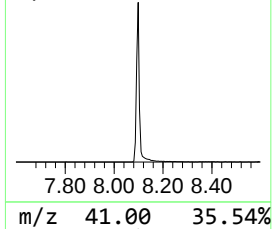
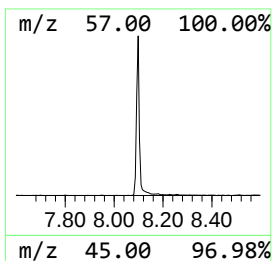
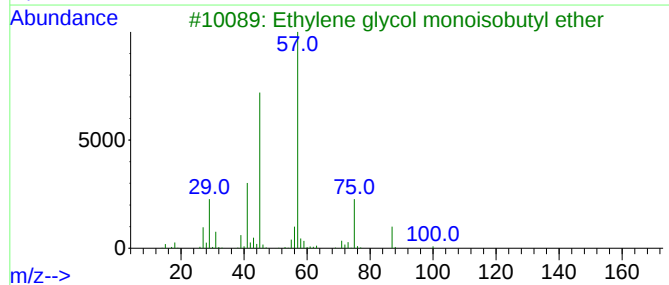
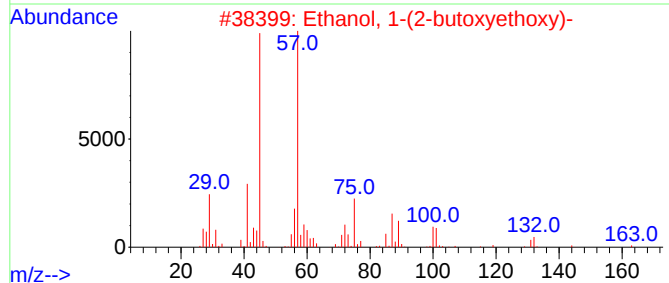
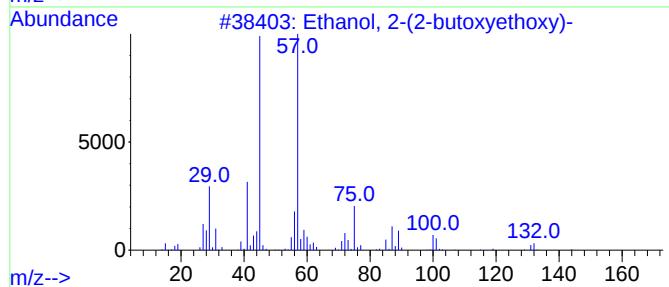
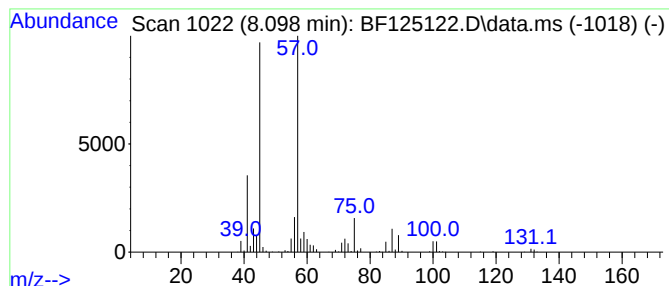
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.098	11.79 ng	774797	Naphthalene-d8	8.198

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	78
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
5			Butyl lactate	146	C7H14O3	000138-22-7	47



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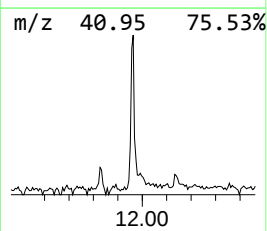
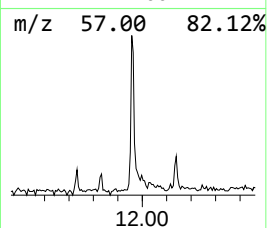
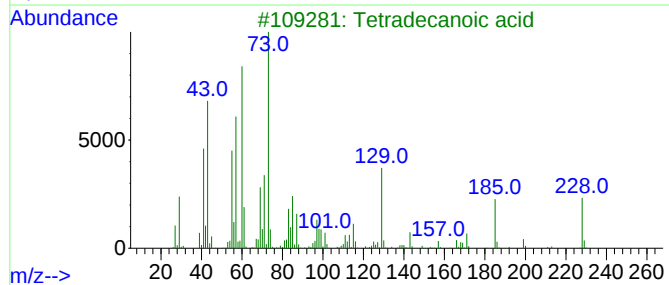
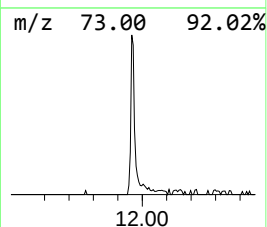
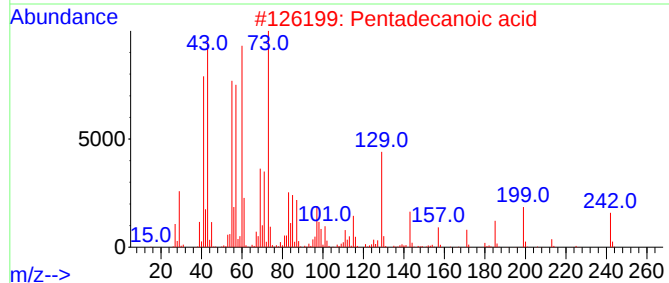
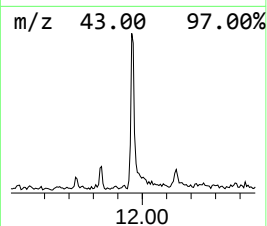
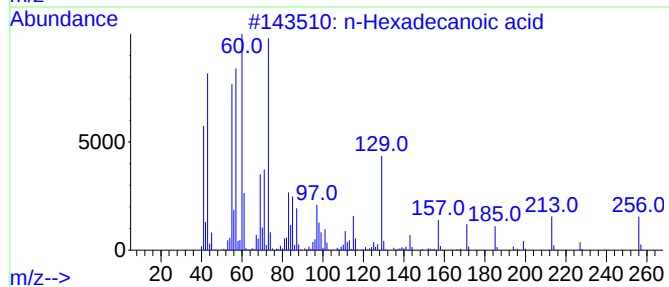
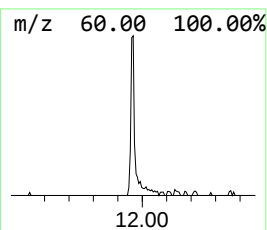
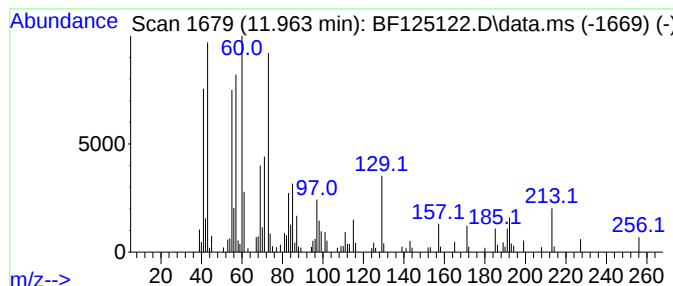
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.963	3.32 ng	242197	Phenanthrene-d10	11.445	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	55



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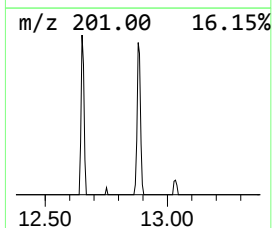
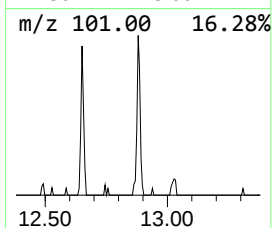
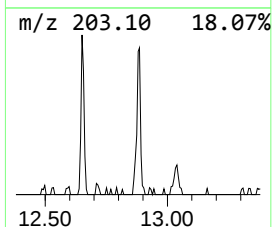
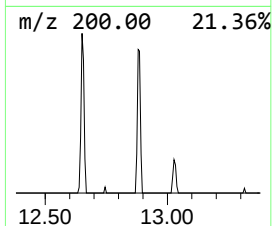
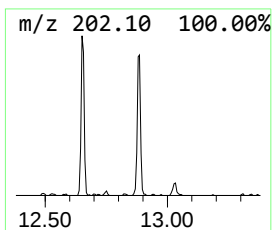
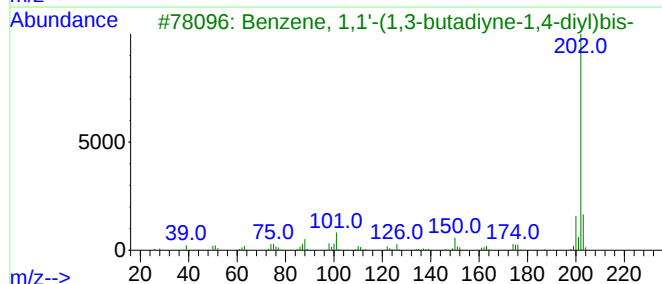
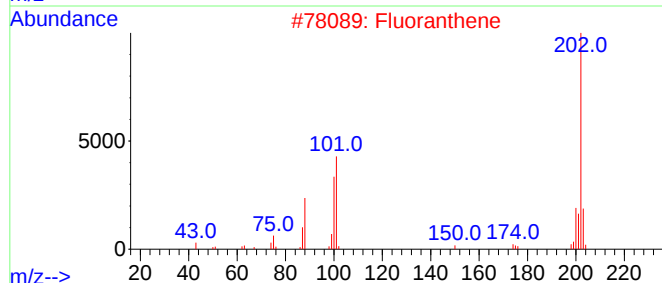
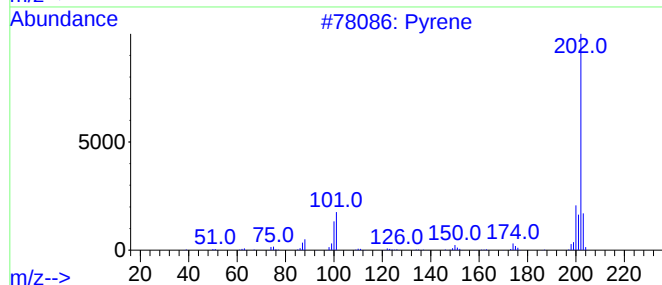
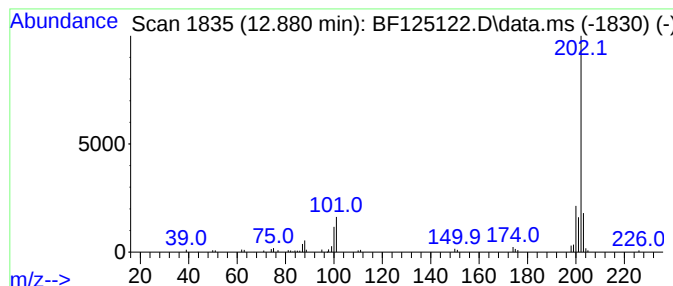
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Peak Number 5 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.880	2.18 ng	118311	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrene	202	C16H10	000129-00-0	95
2			Fluoranthene	202	C16H10	000206-44-0	93
3			Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	53
4			4-Methoxy-naphthalene-1-carboxyl...	202	C12H10O3	1000317-85-4	38
5			Succinic acid, di(4-cyanophenyl)...	320	C18H12N2O4	1000360-71-2	37



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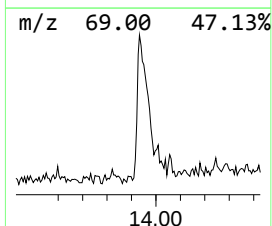
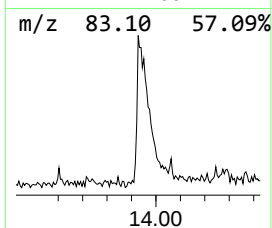
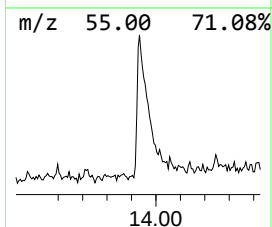
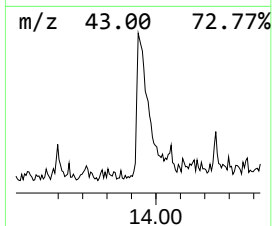
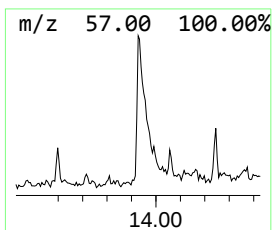
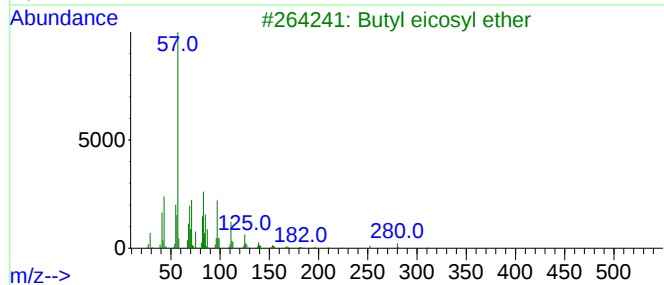
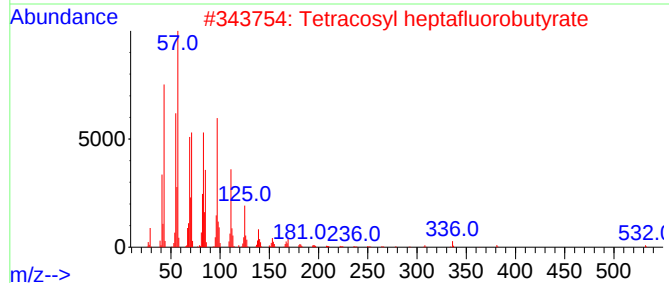
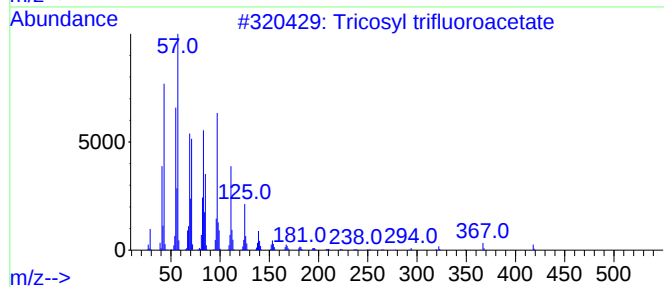
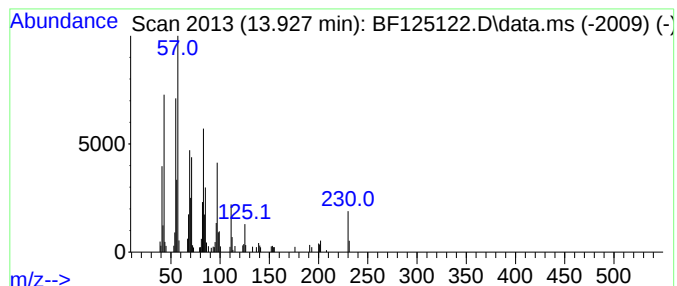
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tricosyl trifluoroacetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.927	6.88 ng	372485	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
2			Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	91
3			Butyl eicosyl ether	354	C24H50O	1000406-40-7	91
4			Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	91
5			Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081921\
Data File : BF125122.D
Acq On : 19 Aug 2021 19:25
Operator : JU/CG
Sample : M3430-06
Misc :
ALS Vial : 19 Sample Multiplier: 1

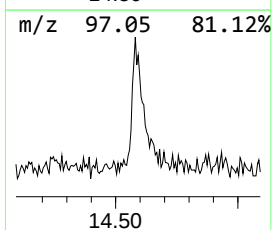
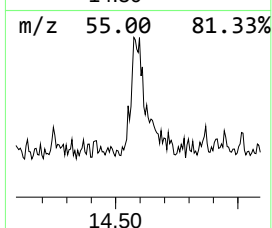
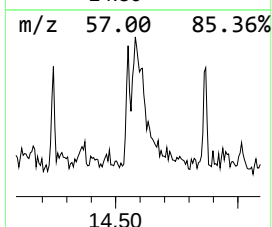
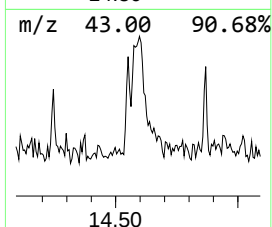
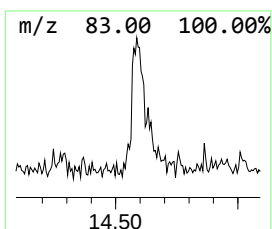
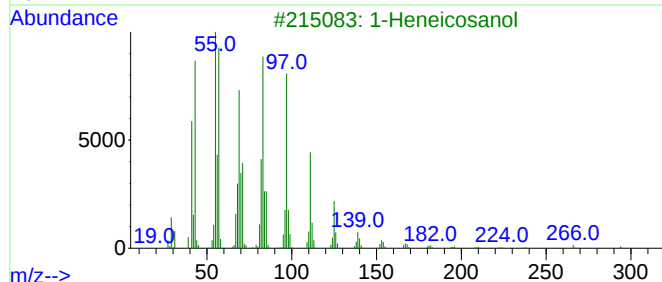
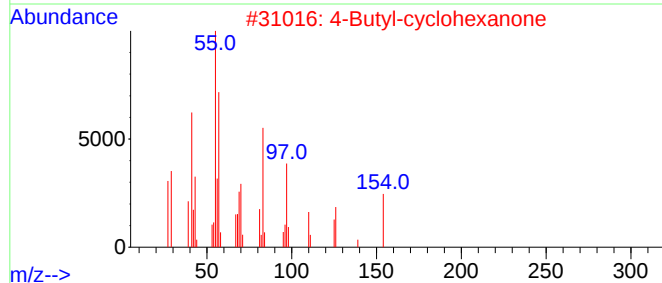
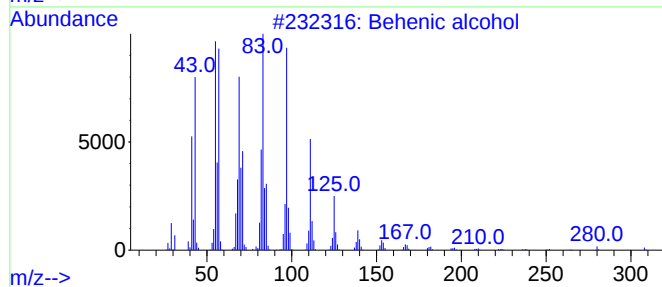
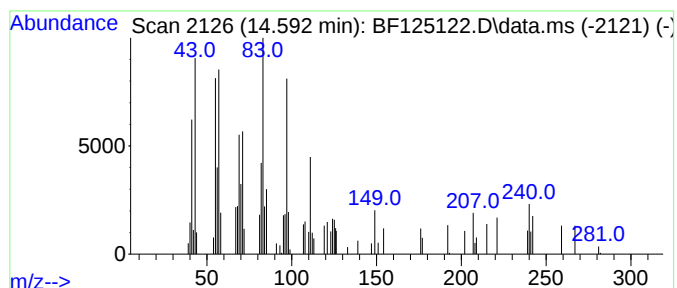
Instrument :
BNA_F
ClientSampleId :
PE-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Behenic alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.592	2.21 ng	119687	Chrysene-d12	14.080	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	70
2	4-Butyl-cyclohexanone	154	C10H18O	061203-82-5	60
3	1-Heneicosanol	312	C21H44O	015594-90-8	55
4	1-Docosene	308	C22H44	001599-67-3	53
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081921\
Data File : BF125122.D
Acq On : 19 Aug 2021 19:25
Operator : JU/CG
Sample : M3430-06
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PE-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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
Butane, 2-metho...	2.222	35.6	ng	1793260	1	6.916	1007410	20.0
2-Pentanone, 4-...	5.145	3.7	ng	184128	1	6.916	1007410	20.0
Ethanol, 2-(2-b...	8.098	11.8	ng	774797	2	8.198	1313880	20.0
n-Hexadecanoic ...	11.963	3.3	ng	242197	4	11.445	1460330	20.0
Benzene, 1,1'-(...	12.880	2.2	ng	118311	5	14.080	1083130	20.0
Tricosyl triflu...	13.927	6.9	ng	372485	5	14.080	1083130	20.0
Behenic alcohol	14.592	2.2	ng	119687	5	14.080	1083130	20.0