

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081721\
 Data File : BF125079.D
 Acq On : 17 Aug 2021 21:06
 Operator : JU/CG
 Sample : M3428-08
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-03-COMP

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-BF081721.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125079.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	29	rBV	1390178	1749770	45.25%	5.564%
2	5.140	510	519	526	rBV	132449	176894	4.57%	0.562%
3	5.534	580	586	589	rBV	3730950	3707912	95.89%	11.790%
4	6.534	750	756	759	rBV	3567855	3866640	100.00%	12.294%
5	6.739	787	791	796	rVB	42909	43001	1.11%	0.137%
6	6.916	818	821	825	rBV	1221925	1054703	27.28%	3.354%
7	7.481	912	917	920	rBV	2552057	2397881	62.01%	7.624%
8	8.098	1018	1022	1025	rBV	1124122	835497	21.61%	2.657%
9	8.204	1036	1040	1043	rVB	1513120	1386655	35.86%	4.409%
10	9.280	1217	1223	1226	rBV	3782812	3697021	95.61%	11.755%
11	9.957	1334	1338	1341	rBV	1777898	1431726	37.03%	4.552%
12	10.745	1467	1472	1475	rBV	2906877	2561634	66.25%	8.145%
13	11.445	1587	1591	1593	rBV	1716408	1510407	39.06%	4.803%
14	11.463	1593	1594	1597	rVB	81540	62954	1.63%	0.200%
15	11.833	1654	1657	1660	rBV	104420	76763	1.99%	0.244%
16	11.963	1673	1679	1691	rBV3	249861	309631	8.01%	0.985%
17	12.651	1793	1796	1801	rBV	160957	145577	3.76%	0.463%
18	12.745	1809	1812	1818	rBV	85728	101028	2.61%	0.321%
19	12.880	1830	1835	1841	rBV2	148751	189310	4.90%	0.602%
20	13.033	1856	1861	1864	rBV	3747466	3508140	90.73%	11.155%
21	13.827	1985	1996	2003	rBV10	53066	202685	5.24%	0.644%
22	13.921	2008	2012	2024	rVB	331543	372820	9.64%	1.185%
23	14.080	2034	2039	2042	rBV	1149842	1036560	26.81%	3.296%
24	14.557	2117	2120	2124	rBV2	64475	70390	1.82%	0.224%
25	15.133	2213	2218	2221	rBV	42299	71716	1.85%	0.228%
26	15.509	2278	2282	2286	rVB	35769	42370	1.10%	0.135%
27	15.574	2288	2293	2298	rBV	666118	840682	21.74%	2.673%

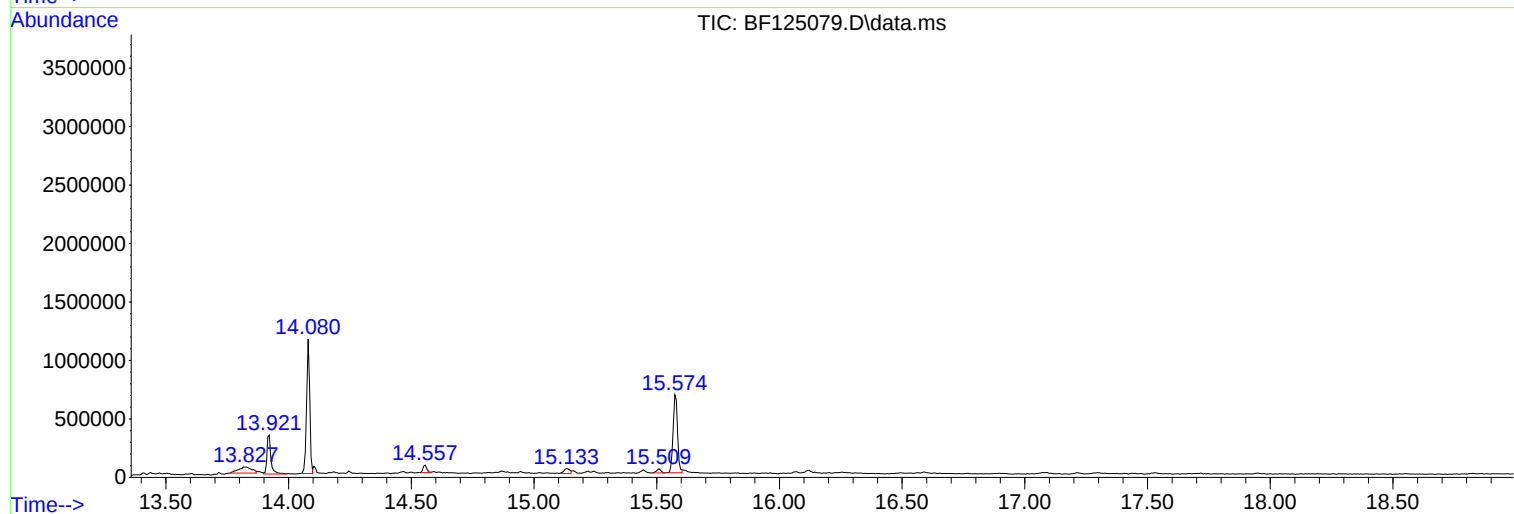
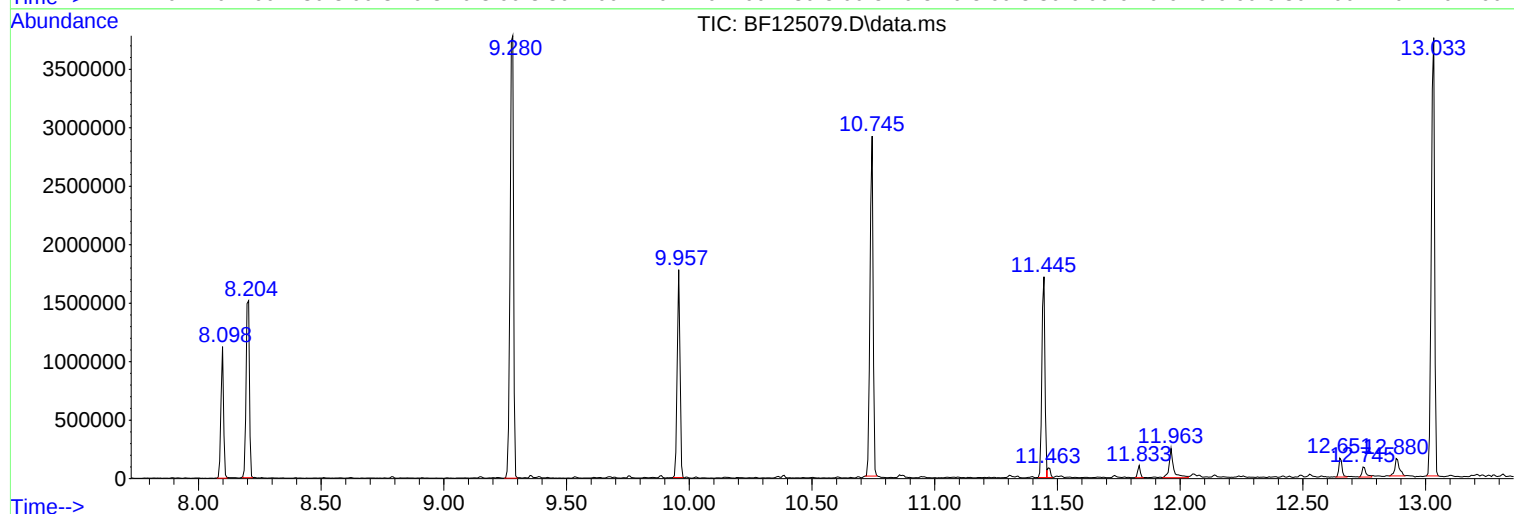
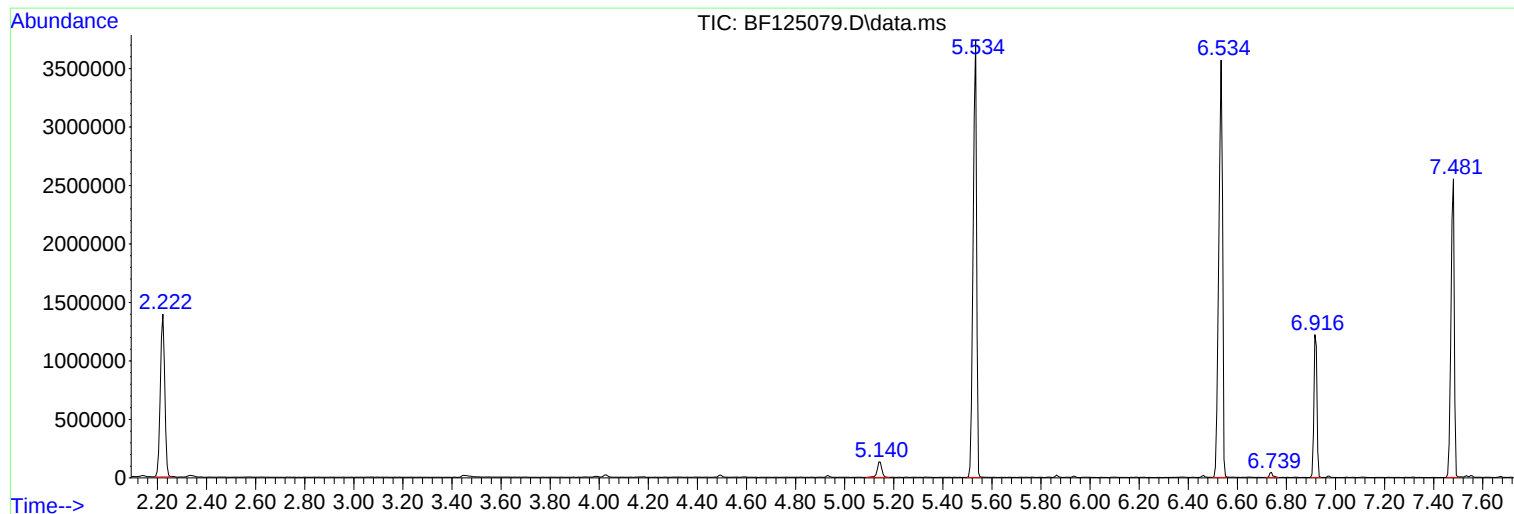
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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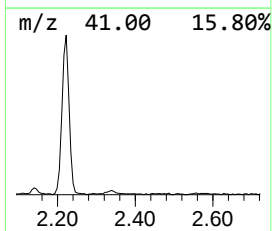
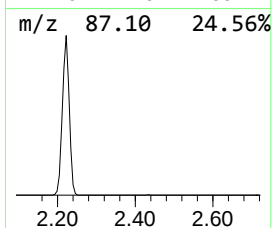
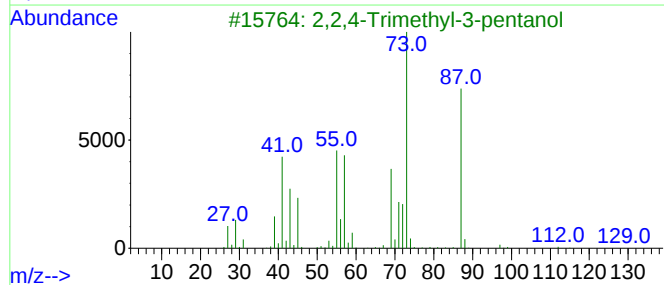
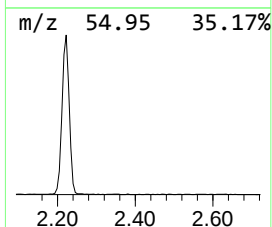
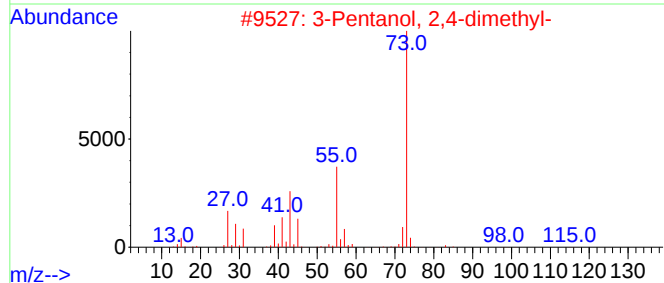
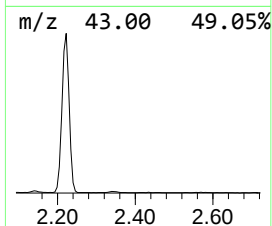
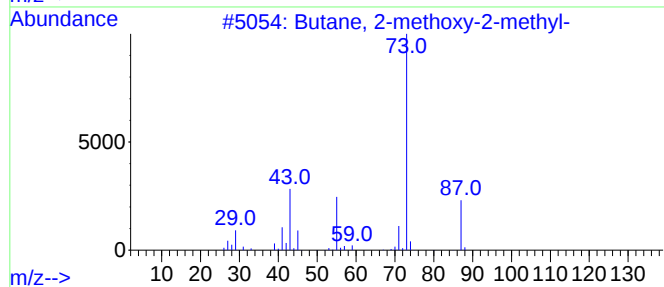
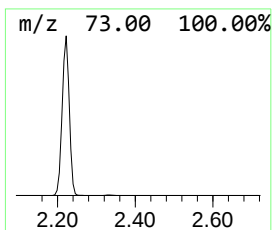
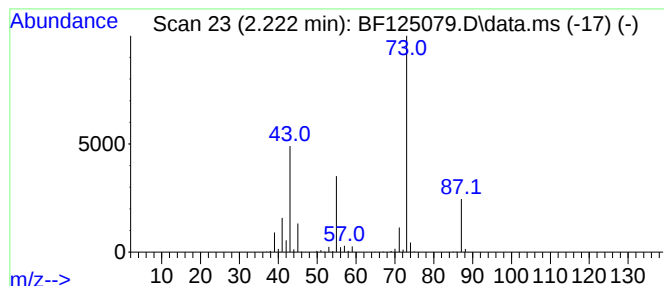
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	33.18 ng	1749770	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			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25



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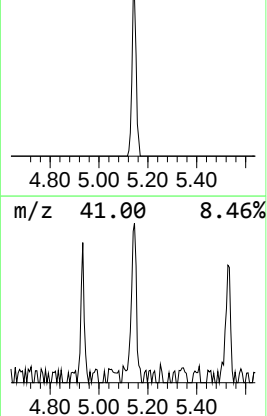
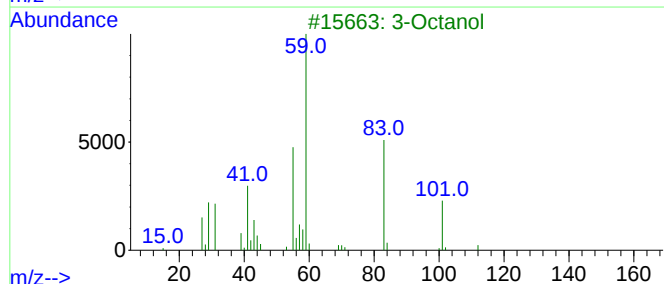
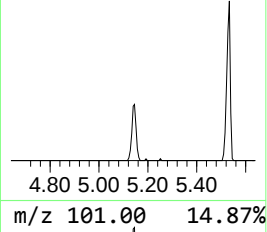
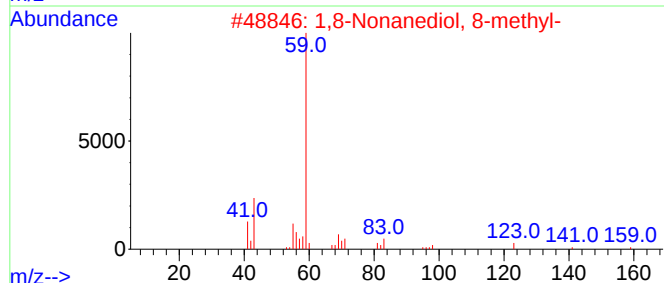
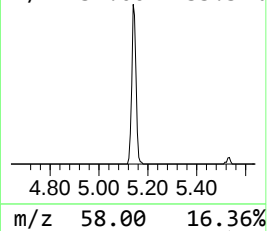
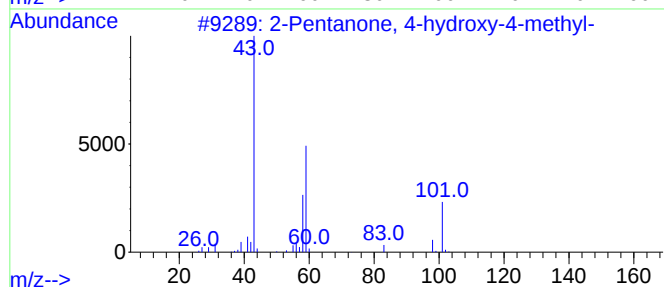
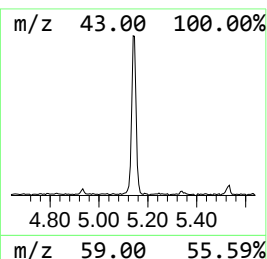
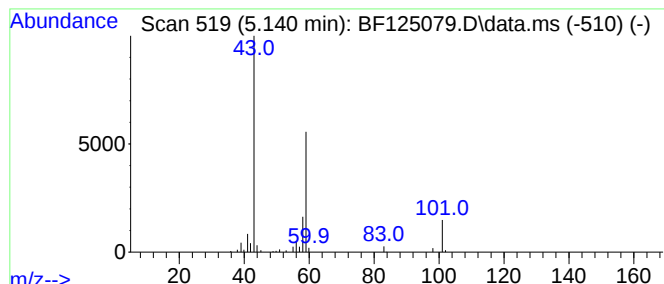
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.140	3.35 ng	176894	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	56
2		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	37
3		3-Octanol	130	C8H18O	000589-98-0	36
4		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33



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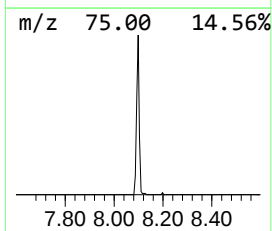
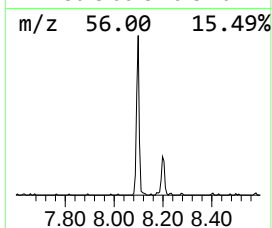
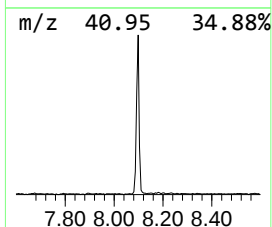
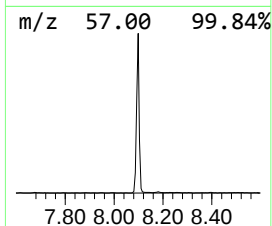
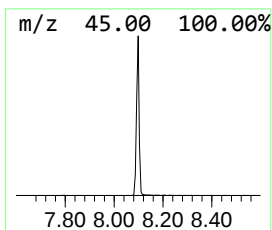
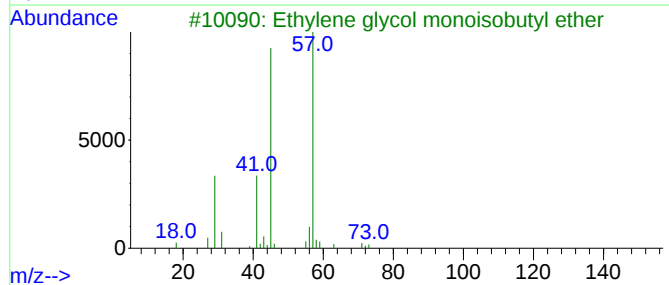
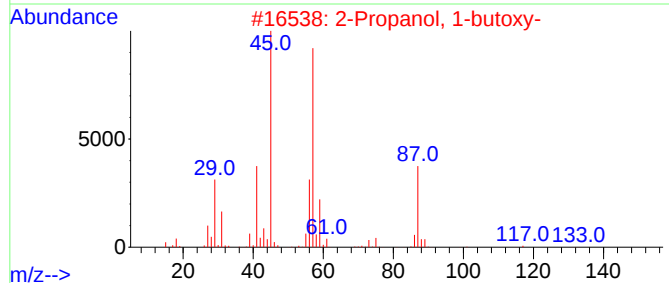
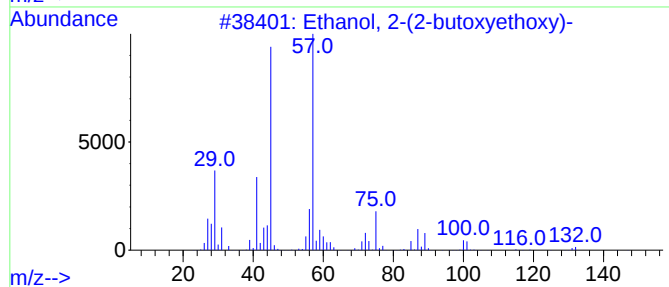
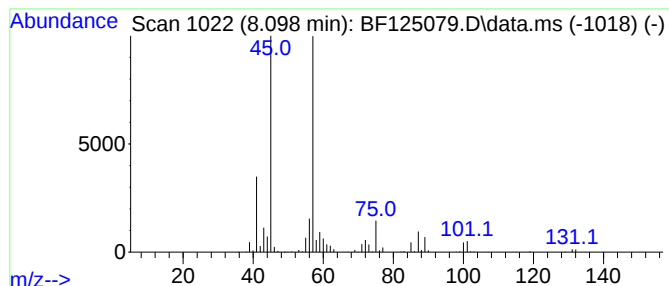
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Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.098	12.05 ng	835497	Naphthalene-d8	8.204

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	64
2			2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	59
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	53
4			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
5			Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	50



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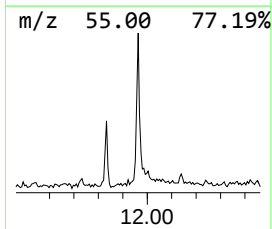
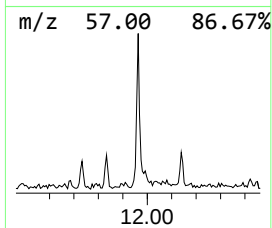
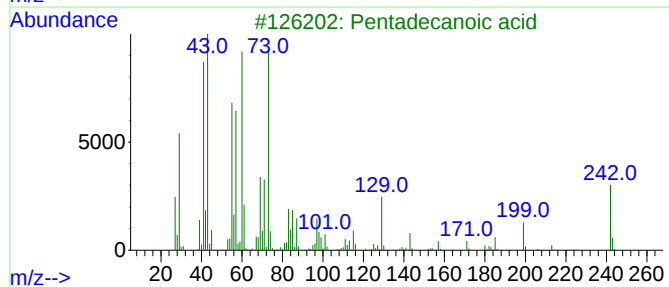
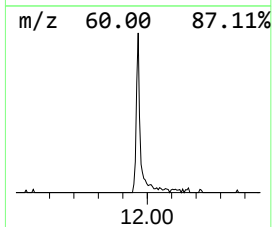
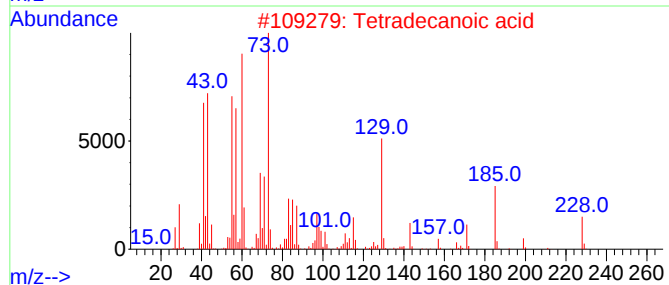
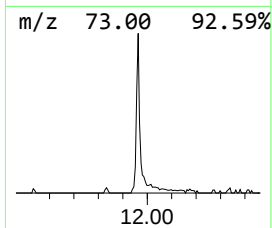
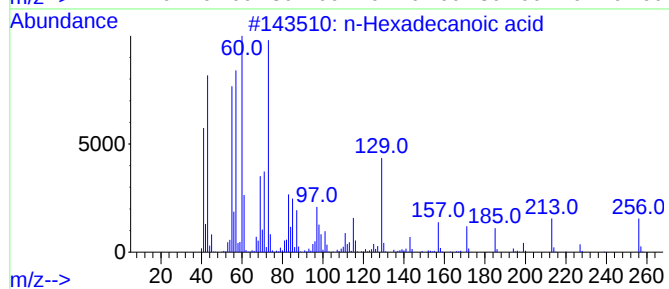
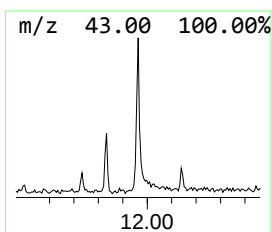
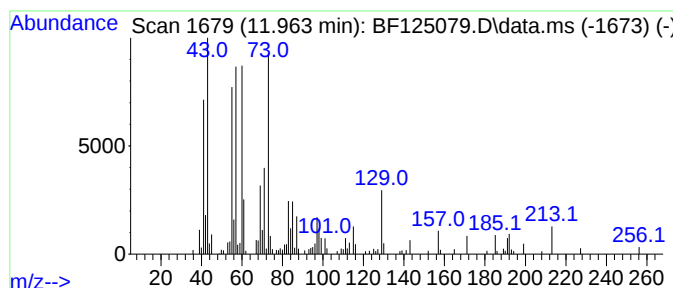
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.963	4.10 ng	309631	Phenanthrene-d10	11.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4			Tridecanoic acid	214	C13H26O2	000638-53-9	64
5			Nonanoic acid	158	C9H18O2	000112-05-0	55



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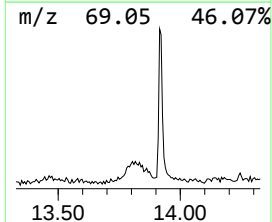
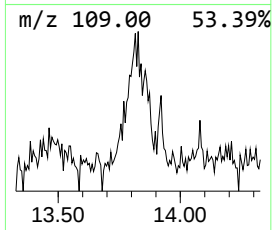
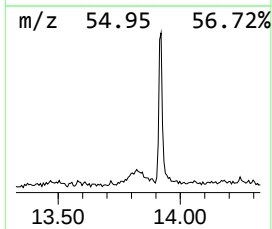
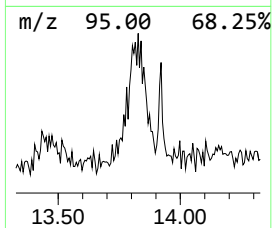
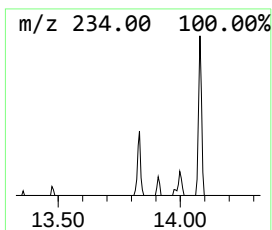
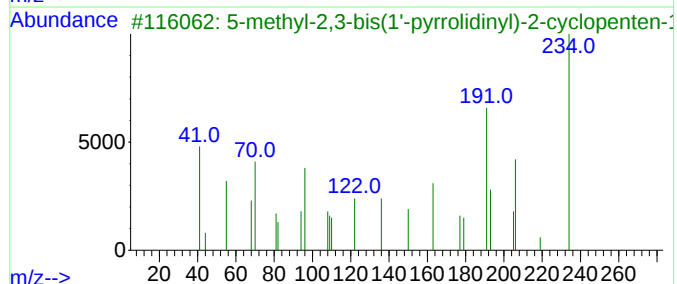
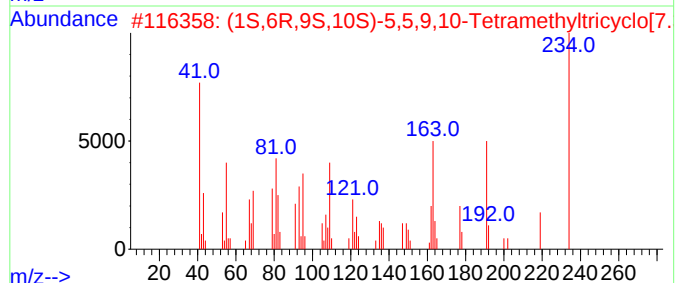
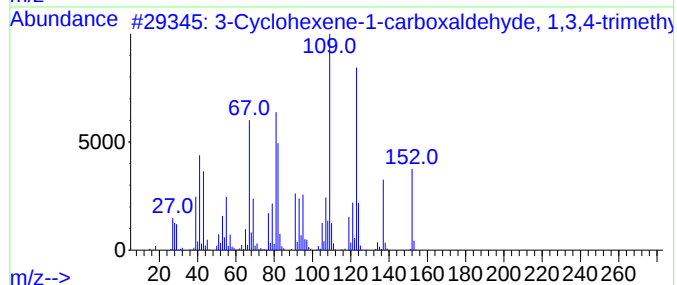
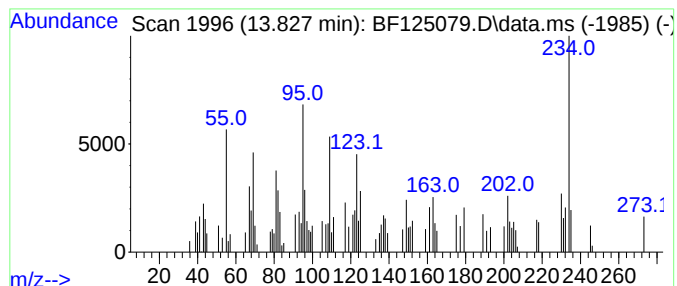
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Peak Number 6 3-Cyclohexene-1-carboxalde... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.827	3.91 ng	202685	Chrysene-d12	14.080	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Cyclohexene-1-carboxaldehyde, ...	152	C10H16O	040702-26-9	66
2	(1S,6R,9S,10S)-5,5,9,10-Tetramet...	234	C16H26O	1000298-98-1	49
3	5-methyl-2,3-bis(1'-pyrrolidinyl...	234	C14H22N2O	1000366-03-5	35
4	Pyreno[4,5-b:9,10-b']bisoxirene,...	234	C16H10O2	055400-88-9	30
5	Phenanthrene, 2,4,5,7-tetramethyl-	234	C18H18	007396-38-5	25



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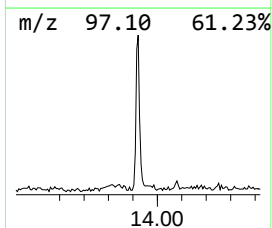
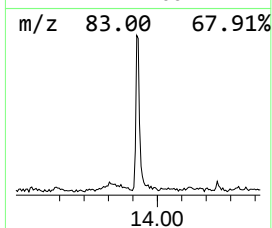
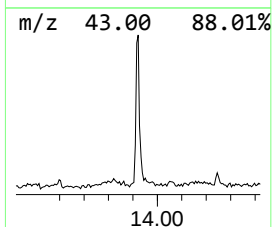
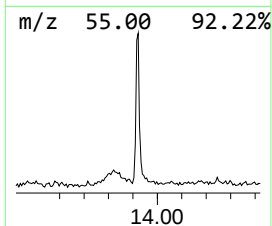
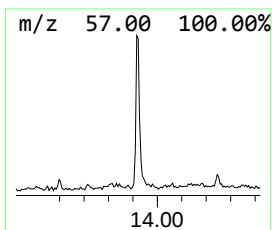
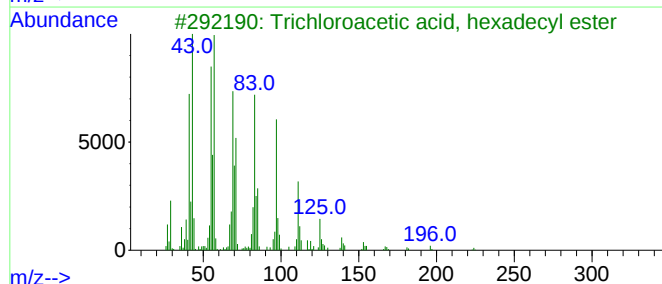
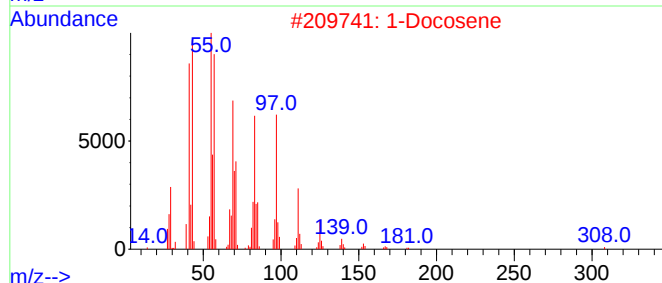
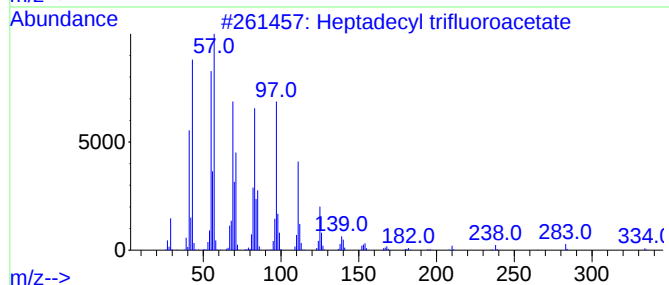
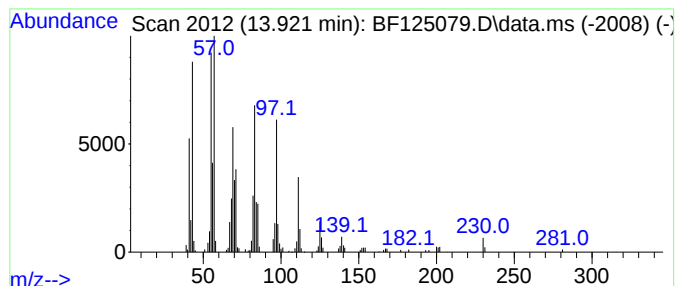
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecyl trifluoroacetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.921	7.19 ng	372820	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
2			1-Docosene	308	C22H44	001599-67-3	94
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
5			n-Nonadecanol-1	284	C19H40O	001454-84-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081721\
Data File : BF125079.D
Acq On : 17 Aug 2021 21:06
Operator : JU/CG
Sample : M3428-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081721.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
Butane, 2-metho...	2.222	33.2	ng	1749770	1	6.916	1054700	20.0
2-Pentanone, 4-...	5.140	3.4	ng	176894	1	6.916	1054700	20.0
Ethanol, 2-(2-b...	8.098	12.1	ng	835497	2	8.204	1386660	20.0
n-Hexadecanoic ...	11.963	4.1	ng	309631	4	11.445	1510410	20.0
3-Cyclohexene-1...	13.827	3.9	ng	202685	5	14.080	1036560	20.0
Heptadecyl trif...	13.921	7.2	ng	372820	5	14.080	1036560	20.0